



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 02:56 PM EDT

PDB ID : 2AXT / pdb_00002axt
Title : Crystal Structure of Photosystem II from Thermosynechococcus elongatus
Authors : Loll, B.; Kern, J.; Saenger, W.; Zouni, A.; Biesiadka, J.
Deposited on : 2005-09-06
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

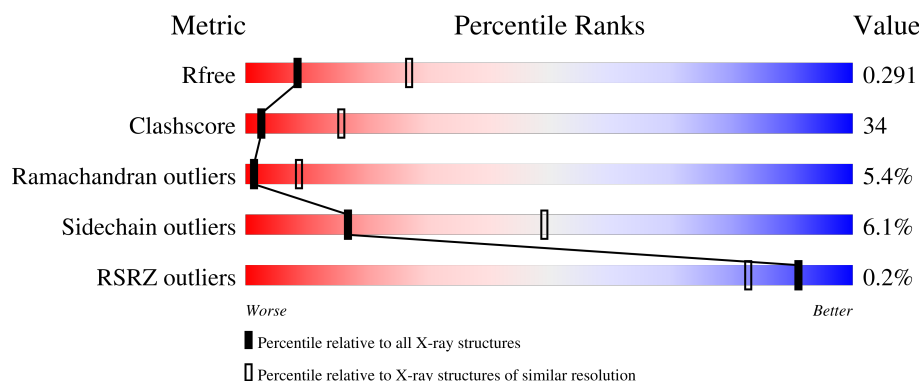
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



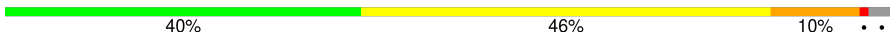
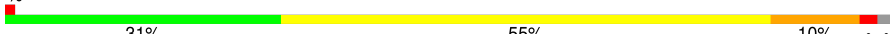
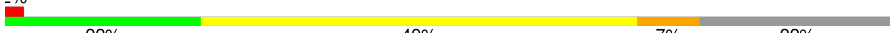
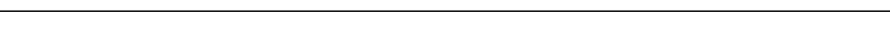
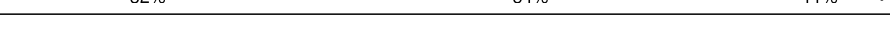
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	344	
1	a	344	
2	B	510	
2	b	510	
3	C	473	

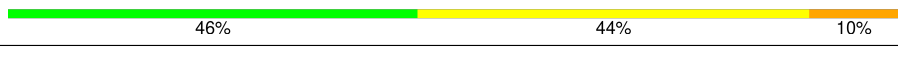
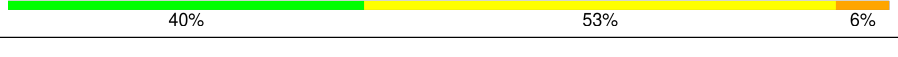
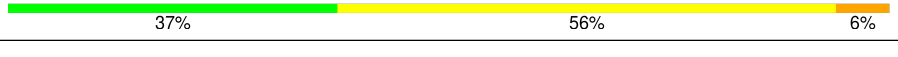
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Mol	Chain	Length	Quality of chain
3	c	473	
4	D	352	
4	d	352	
5	E	84	
5	e	84	
6	F	45	
6	f	45	
7	H	66	
7	h	66	
8	I	38	
8	i	38	
9	J	40	
9	j	40	
10	K	37	
10	k	37	
11	L	37	
11	l	37	
12	M	36	
12	m	36	
13	O	247	
13	o	247	
14	T	32	
14	t	32	
15	U	104	
15	u	104	

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Mol	Chain	Length	Quality of chain
16	V	137	
16	v	137	
17	X	129	
17	x	129	
18	Z	62	
18	z	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	DGD	C	507	X	-	-	-
30	DGD	C	508	X	-	-	-
30	DGD	C	509	X	-	-	-
30	DGD	H	208	X	-	-	-
30	DGD	c	5507	X	-	-	-
30	DGD	c	5508	X	-	-	-
30	DGD	c	5509	X	-	-	-
30	DGD	h	5208	X	-	-	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 48254 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem Q(B) protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2623	1718	432	458	15			
1	a	335	Total	C	N	O	S	0	0	0
			2623	1718	432	458	15			

- Molecule 2 is a protein called CP47 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	488	Total	C	N	O	S	0	0	0
			3800	2498	632	657	13			
2	b	488	Total	C	N	O	S	0	0	0
			3800	2498	632	657	13			

- Molecule 3 is a protein called photosystem II CP43 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	447	Total	C	N	O	S	0	0	0
			3421	2244	571	593	13			
3	c	447	Total	C	N	O	S	0	0	0
			3421	2244	571	593	13			

- Molecule 4 is a protein called photosystem II reaction center D2 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	340	Total	C	N	O	S	0	0	0
			2696	1789	436	459	12			
4	d	340	Total	C	N	O	S	0	0	0
			2696	1789	436	459	12			

- Molecule 5 is a protein called Cytochrome b559 alpha subunit.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			646	424	101	121			
5	e	82	Total	C	N	O	0	0	0
			646	424	101	121			

- Molecule 6 is a protein called Cytochrome b559 beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			278	189	46	42	1			
6	f	35	Total	C	N	O	S	0	0	0
			278	189	46	42	1			

- Molecule 7 is a protein called Photosystem II reaction center H protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	64	Total	C	N	O	S	0	0	0
			492	330	77	83	2			
7	h	64	Total	C	N	O	S	0	0	0
			492	330	77	83	2			

- Molecule 8 is a protein called Photosystem II reaction center I protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			
8	i	35	Total	C	N	O	S	0	0	0
			286	195	45	45	1			

- Molecule 9 is a protein called Photosystem II reaction center J protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	34	Total	C	N	O	S	0	0	0
			240	164	35	40	1			
9	j	34	Total	C	N	O	S	0	0	0
			240	164	35	40	1			

- Molecule 10 is a protein called Photosystem II reaction center protein K.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	K	37	Total	C	N	O	0	0	0
			289	201	42	46			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	k	37	Total	C	N	O	0	0	0
			289	201	42	46			

- Molecule 11 is a protein called Photosystem II reaction center L protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	L	37	Total	C	N	O	0	0	0
			301	200	48	53			
11	l	37	Total	C	N	O	0	0	0
			301	200	48	53			

- Molecule 12 is a protein called Photosystem II reaction center M protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	M	36	Total	C	N	O	S	0	0	0
			276	181	41	53	1			
12	m	36	Total	C	N	O	S	0	0	0
			276	181	41	53	1			

- Molecule 13 is a protein called Photosystem II manganese-stabilizing polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	O	242	Total	C	N	O	S	0	0	0
			1772	1113	295	360	4			
13	o	242	Total	C	N	O	S	0	0	0
			1772	1113	295	360	4			

- Molecule 14 is a protein called Photosystem II reaction center T protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	T	30	Total	C	N	O	S	0	0	0
			254	179	36	37	2			
14	t	30	Total	C	N	O	S	0	0	0
			254	179	36	37	2			

- Molecule 15 is a protein called Photosystem II 12 kDa extrinsic protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
15	U	98	Total	C	N	O	0	0	0
			775	492	130	153			
15	u	98	Total	C	N	O	0	0	0
			775	492	130	153			

- Molecule 16 is a protein called Cytochrome c-550.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	V	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			
16	v	137	Total	C	N	O	S	0	0	0
			1064	675	177	208	4			

- Molecule 17 is a protein called Unassigned subunits.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
17	X	104	Total	C	N	Ne	O	S	0	0	0
			687	442	111	2	131	1			
17	x	104	Total	C	N	Ne	O	S	0	0	0
			687	442	111	2	131	1			

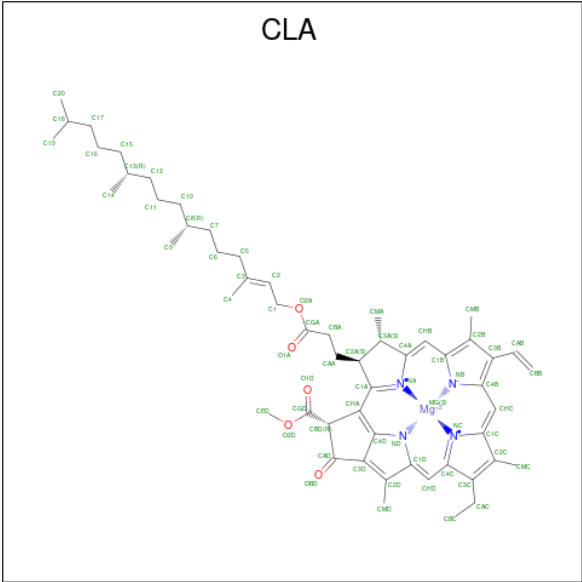
- Molecule 18 is a protein called Photosystem II reaction center Z protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	Z	62	Total	C	N	O	S	0	0	0
			442	306	65	69	2			
18	z	62	Total	C	N	O	S	0	0	0
			442	306	65	69	2			

- Molecule 19 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	Fe	0	0
			1	1		
19	a	1	Total	Fe	0	0
			1	1		

- Molecule 20 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	A	1	Total	C	Mg	N	O	0	0
			55	45	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			41	33	1	4	3		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			56	46	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	C	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	D	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	D	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

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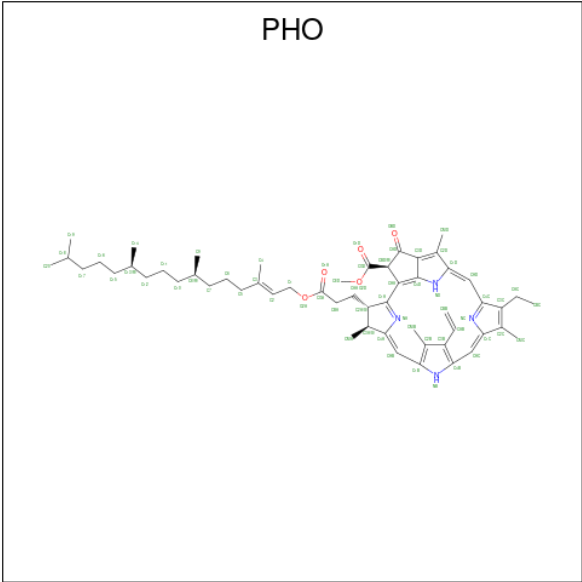
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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20	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	a	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	a	1	Total 55	C 45	Mg 1	N 4	O 5	0	0
20	b	1	Total 41	C 33	Mg 1	N 4	O 3	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 56	C 46	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	b	1	Total 65	C 55	Mg 1	N 4	O 5	0	0
20	c	1	Total 65	C 55	Mg 1	N 4	O 5	0	0

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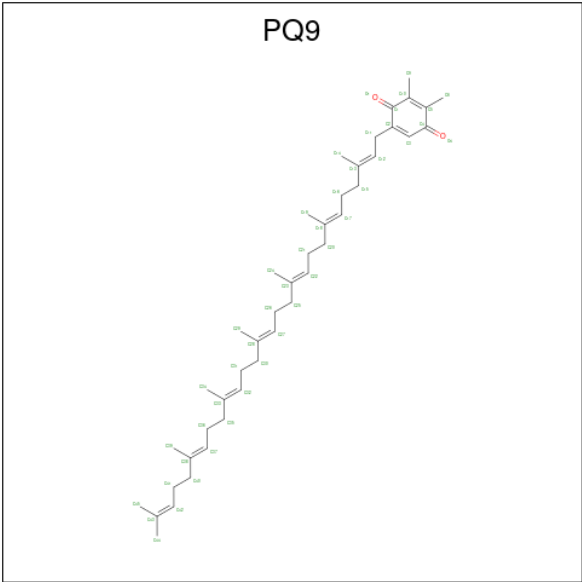
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
20	c	1	Total	C	Mg	N	O	0	0
			60	50	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			46	36	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			47	37	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			51	41	1	4	5		
20	c	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
20	d	1	Total	C	Mg	N	O	0	0
			50	40	1	4	5		

- Molecule 21 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



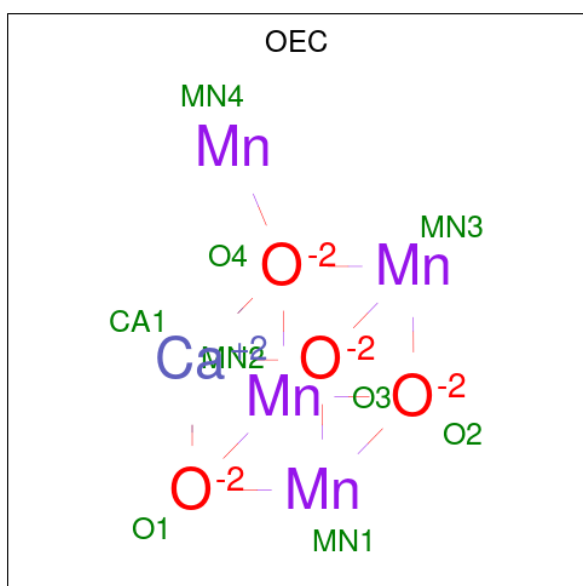
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
21	A	1	Total	C	N	O	0	0
			64	55	4	5		
21	A	1	Total	C	N	O	0	0
			64	55	4	5		
21	a	1	Total	C	N	O	0	0
			64	55	4	5		
21	a	1	Total	C	N	O	0	0
			64	55	4	5		

- Molecule 22 is 5-[(2E,6E,10E,14E,18E,22E)-3,7,11,15,19,23,27-HEPTAMETHYLOCTACO SA-2,6,10,14,18,22,26-HEPTAENYL]-2,3-DIMETHYLBENZO-1,4-QUINONE (CCD ID: PQ9) (formula: C₄₃H₆₄O₂).



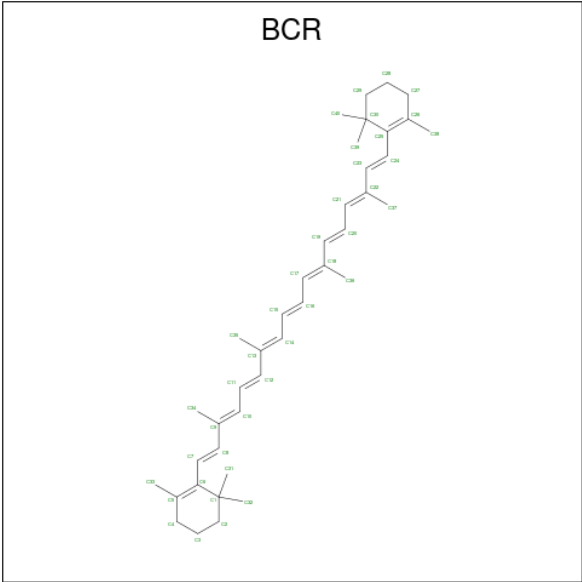
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	A	1	Total	C	O	0	0
			30	28	2		
22	D	1	Total	C	O	0	0
			30	28	2		
22	a	1	Total	C	O	0	0
			30	28	2		
22	d	1	Total	C	O	0	0
			30	28	2		

- Molecule 23 is OXYGEN EVOLVING SYSTEM (CCD ID: OEC) (formula: CaMn_4O_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	A	1	Total	Ca	Mn	0	0
			5	1	4		
23	a	1	Total	Ca	Mn	0	0
			5	1	4		

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $\text{C}_{40}\text{H}_{56}$).



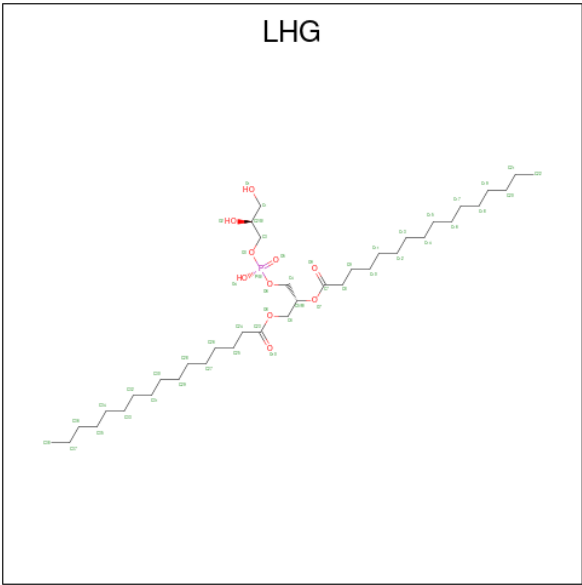
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	A	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	B	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	C	1	Total C 40 40	0	0
24	D	1	Total C 40 40	0	0
24	H	1	Total C 40 40	0	0
24	T	1	Total C 40 40	0	0
24	X	1	Total C 40 40	0	0
24	a	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0
24	b	1	Total C 40 40	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	b	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	c	1	Total C 40 40	0	0
24	d	1	Total C 40 40	0	0
24	h	1	Total C 40 40	0	0
24	t	1	Total C 40 40	0	0
24	x	1	Total C 40 40	0	0

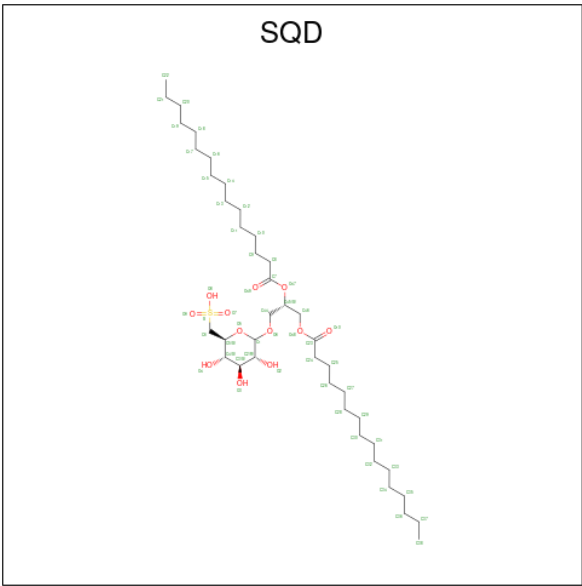
- Molecule 25 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	A	1	Total C O P 39 28 10 1	0	0
25	a	1	Total C O P 39 28 10 1	0	0

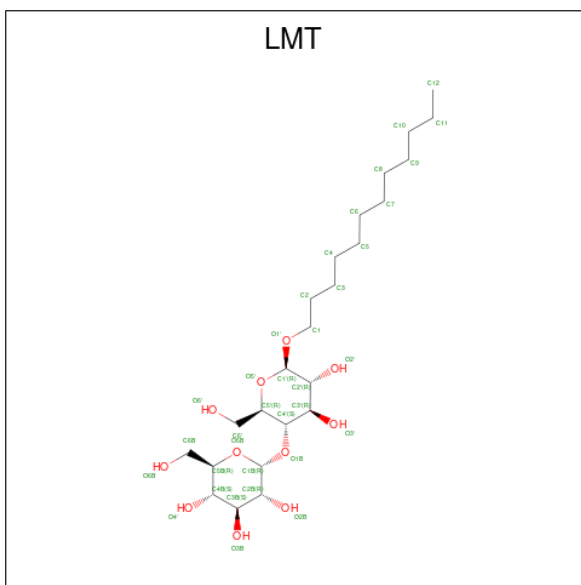
- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSY

L]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



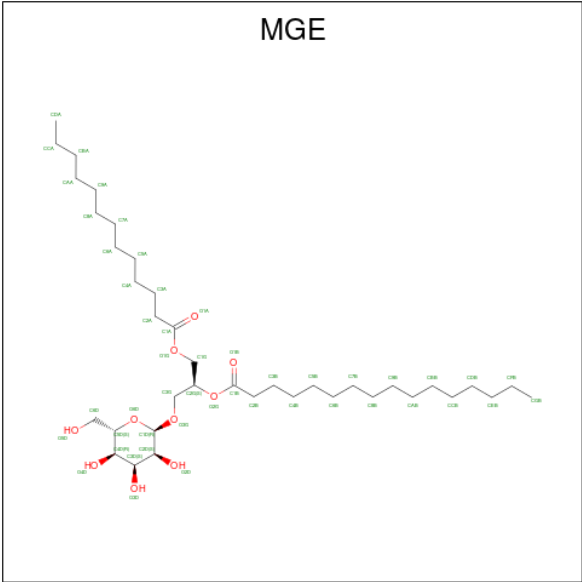
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	O	S	0	0
			54	41	12	1		
26	A	1	Total	C	O	S	0	0
			26	13	12	1		
26	L	1	Total	C	O	S	0	0
			47	34	12	1		
26	a	1	Total	C	O	S	0	0
			26	13	12	1		
26	d	1	Total	C	O	S	0	0
			54	41	12	1		
26	t	1	Total	C	O	S	0	0
			47	34	12	1		

- Molecule 27 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	A	1	Total 35	C 24	O 11	0	0
27	M	1	Total 35	C 24	O 11	0	0
27	T	1	Total 35	C 24	O 11	0	0
27	a	1	Total 35	C 24	O 11	0	0
27	m	1	Total 35	C 24	O 11	0	0
27	t	1	Total 35	C 24	O 11	0	0

- Molecule 28 is (1S)-2-(ALPHA-L-ALLOPYRANOSYLOXY)-1-[(TRIDECANOYLOXY)METHYL]ETHYL PALMITATE (CCD ID: MGE) (formula: $C_{38}H_{72}O_{10}$).

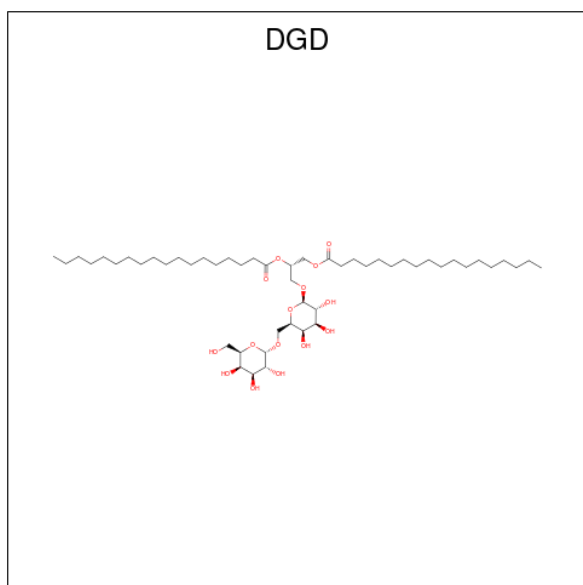


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
28	B	1	Total	C	O	0	0
			48	38	10		
28	D	1	Total	C	O	0	0
			47	37	10		
28	D	1	Total	C	O	0	0
			41	31	10		
28	D	1	Total	C	O	0	0
			48	38	10		
28	I	1	Total	C	O	0	0
			48	38	10		
28	L	1	Total	C	O	0	0
			48	38	10		
28	b	1	Total	C	O	0	0
			48	38	10		
28	d	1	Total	C	O	0	0
			47	37	10		
28	d	1	Total	C	O	0	0
			41	31	10		
28	d	1	Total	C	O	0	0
			48	38	10		
28	i	1	Total	C	O	0	0
			48	38	10		
28	l	1	Total	C	O	0	0
			48	38	10		

- Molecule 29 is UNKNOWN LIGAND (CCD ID: UNL) (formula:).

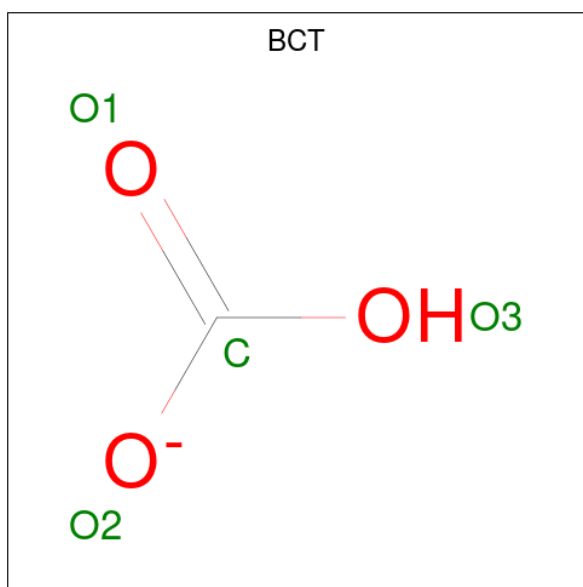
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	C	17	Total	C	0	0
			152	152		
29	c	17	Total	C	0	0
			152	152		

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



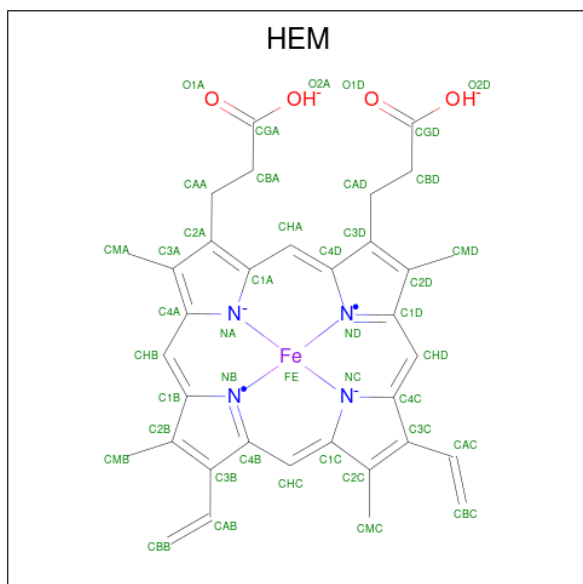
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
30	C	1	Total	C	O	0	0
			53	38	15		
30	C	1	Total	C	O	0	0
			47	32	15		
30	C	1	Total	C	O	0	0
			57	42	15		
30	H	1	Total	C	O	0	0
			54	39	15		
30	c	1	Total	C	O	0	0
			53	38	15		
30	c	1	Total	C	O	0	0
			47	32	15		
30	c	1	Total	C	O	0	0
			57	42	15		
30	h	1	Total	C	O	0	0
			54	39	15		

- Molecule 31 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
31	D	1	Total	C	O	0	0
			4	1	3		
31	d	1	Total	C	O	0	0
			4	1	3		

- Molecule 32 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

Continued on next page...

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
32	V	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
32	f	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
32	v	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

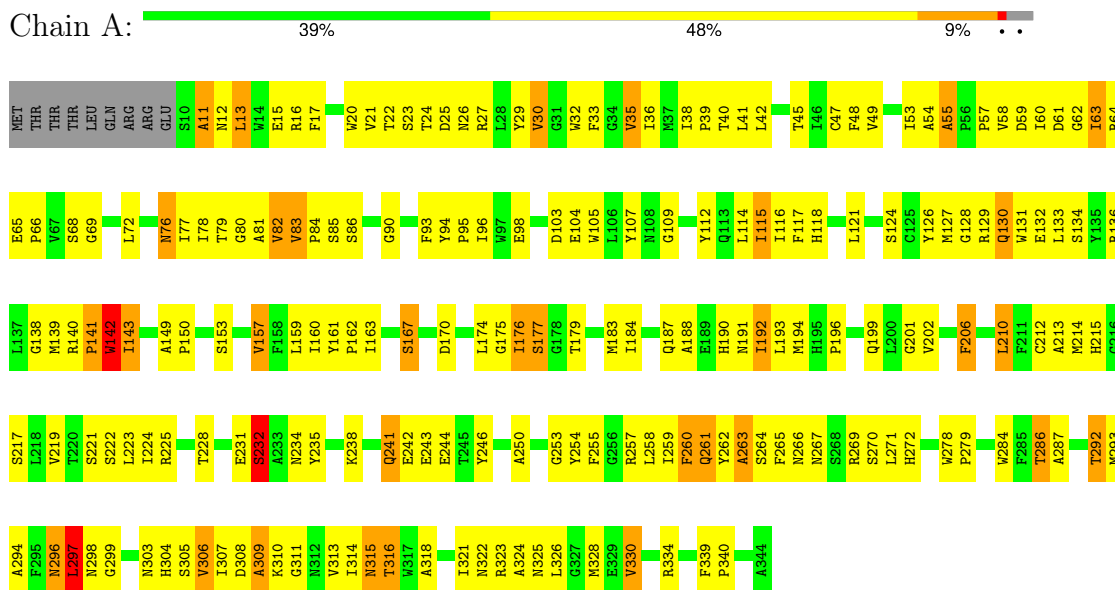
- Molecule 33 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	K	1	Total	Ca	0	0
			1	1		
33	k	1	Total	Ca	0	0
			1	1		

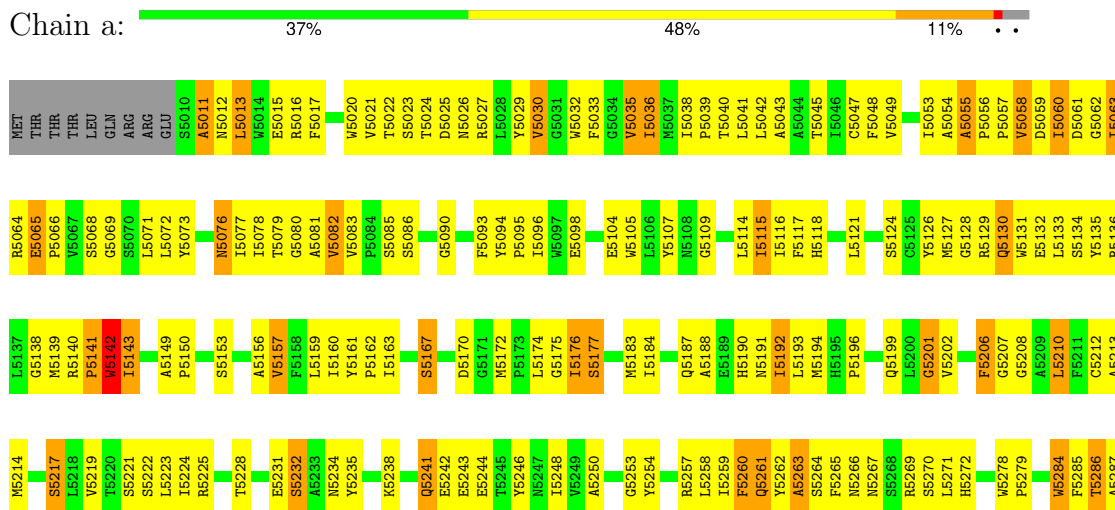
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem Q(B) protein

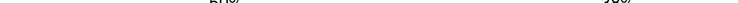


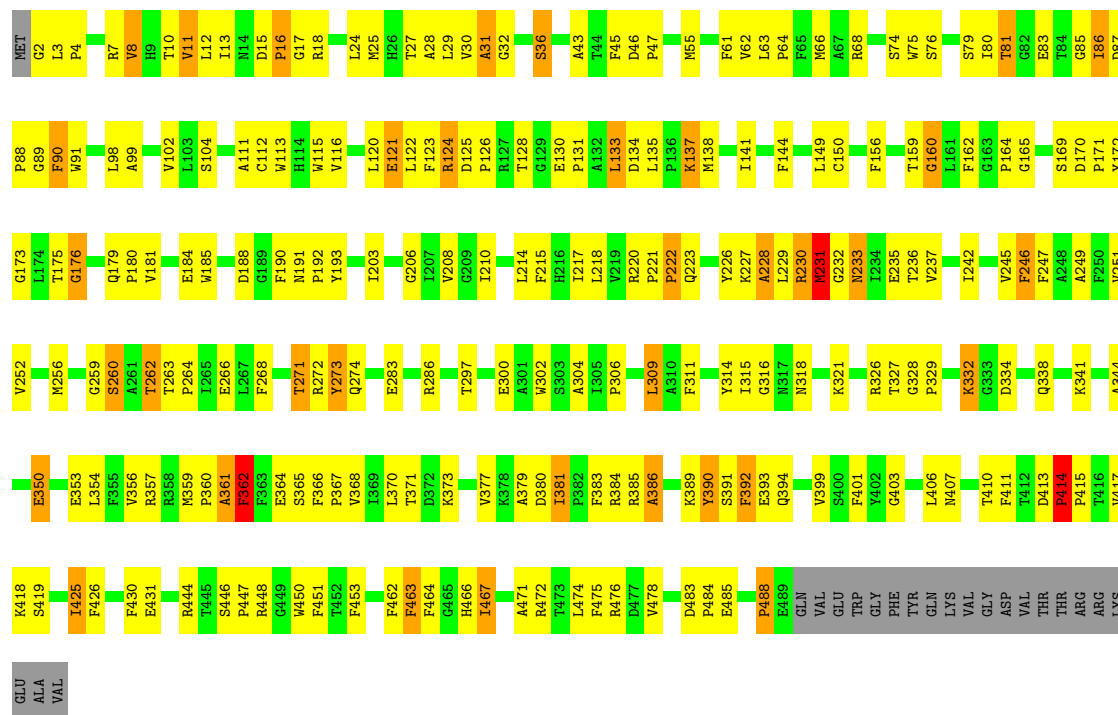
- Molecule 1: Photosystem Q(B) protein





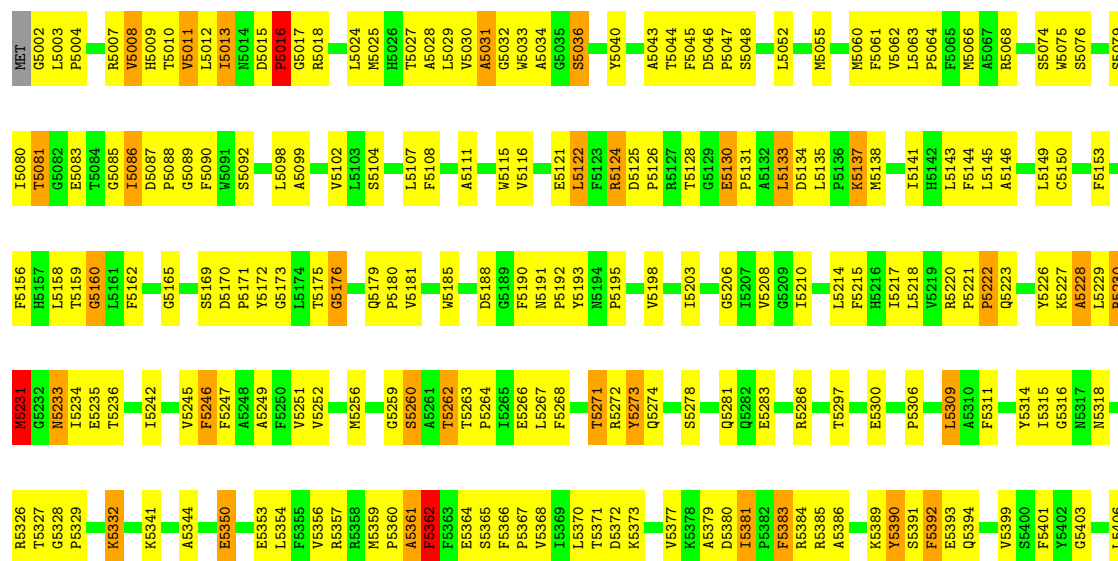
- Molecule 2: CP47 protein

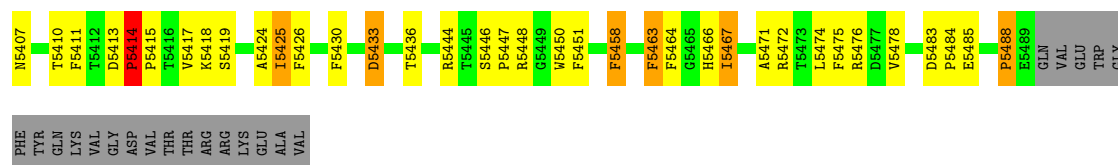
Chain B:  50% 38% 7% . .



- Molecule 2: CP47 protein

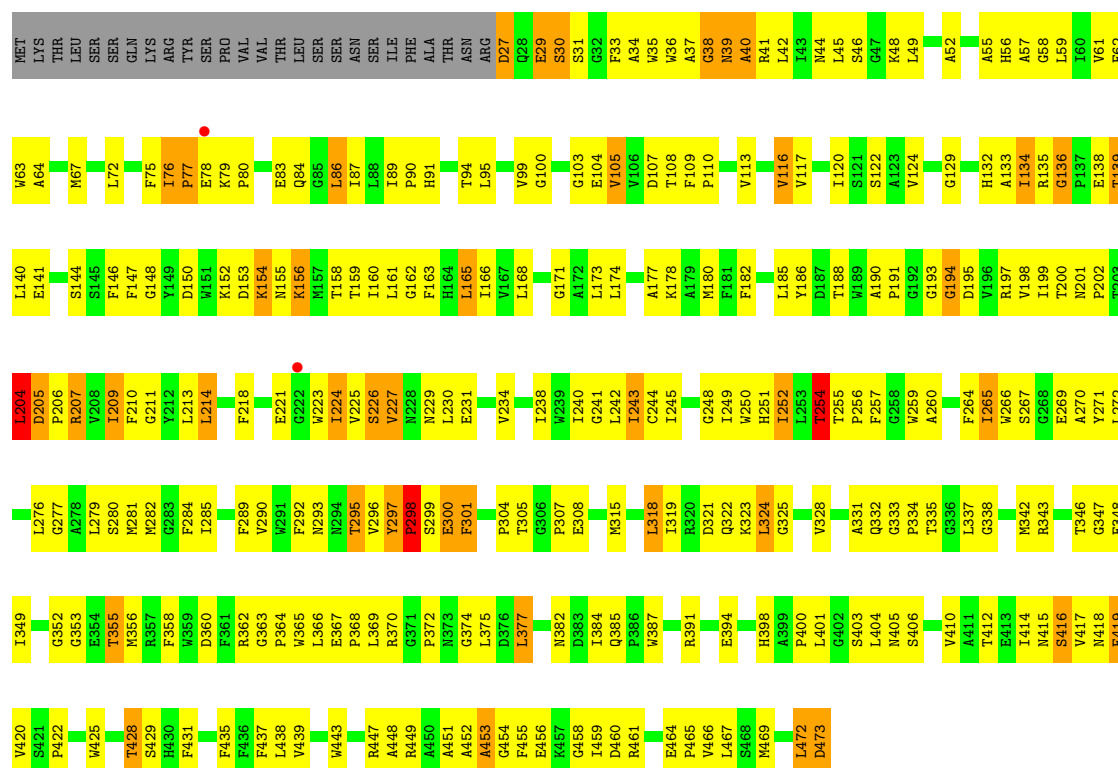
Chain b: 48% 40% 7% ..





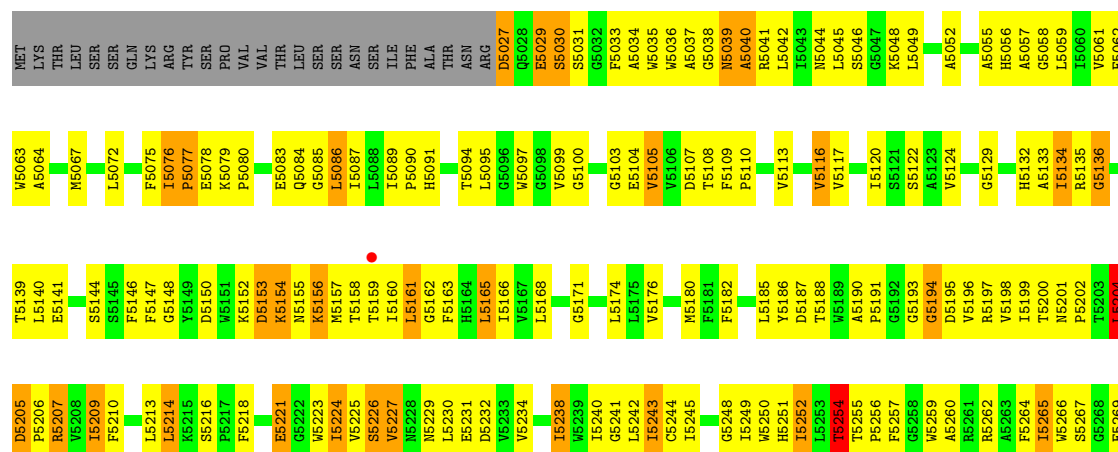
• Molecule 3: photosystem II CP43 protein

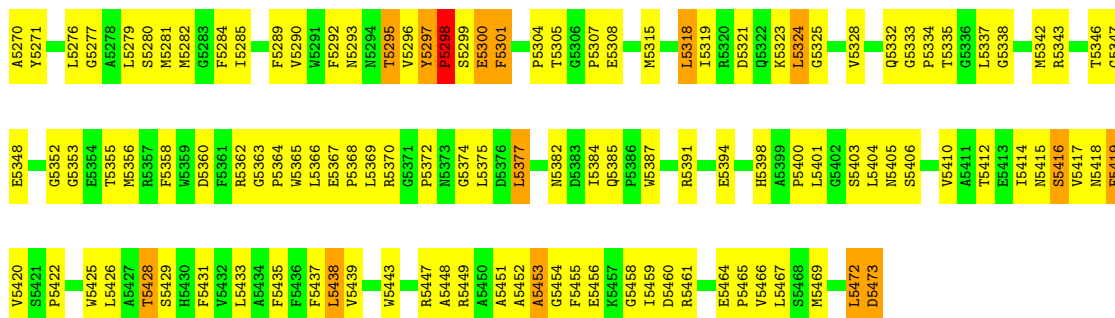
Chain C: 37% 48% 9% 5%



• Molecule 3: photosystem II CP43 protein

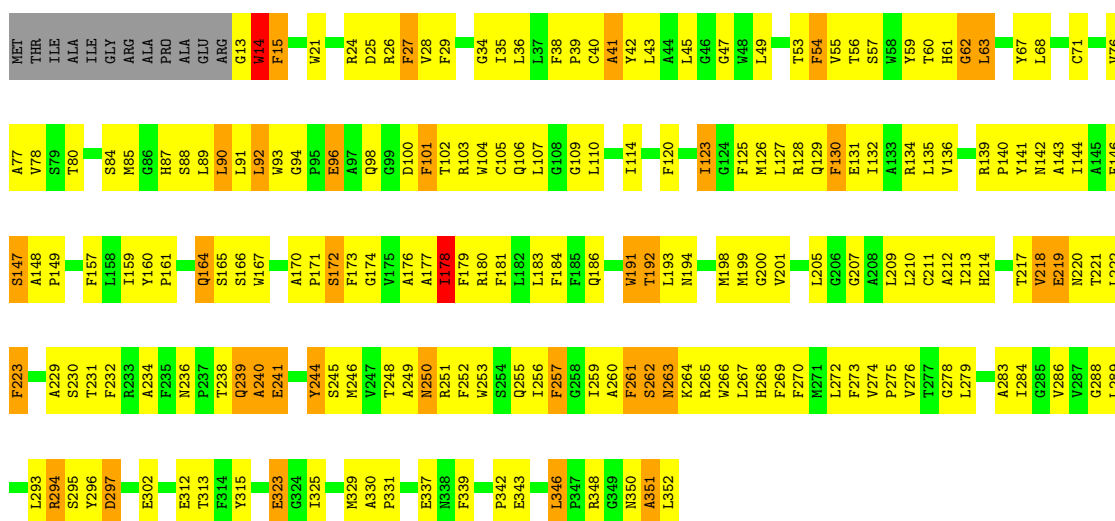
Chain c: 36% 48% 9% 5%





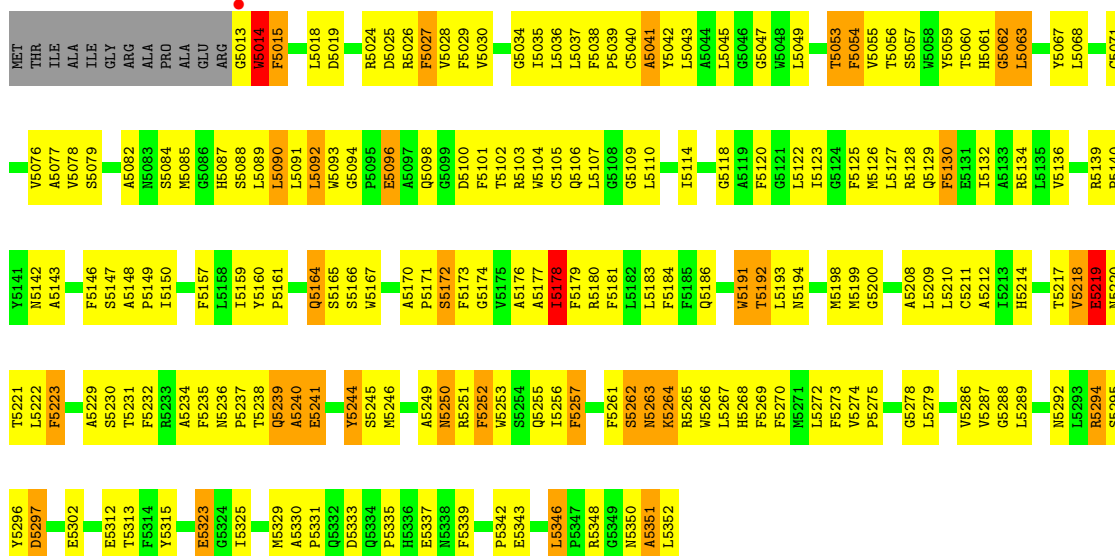
• Molecule 4: photosystem II reaction center D2 protein

Chain D: 40% 46% 10% ..

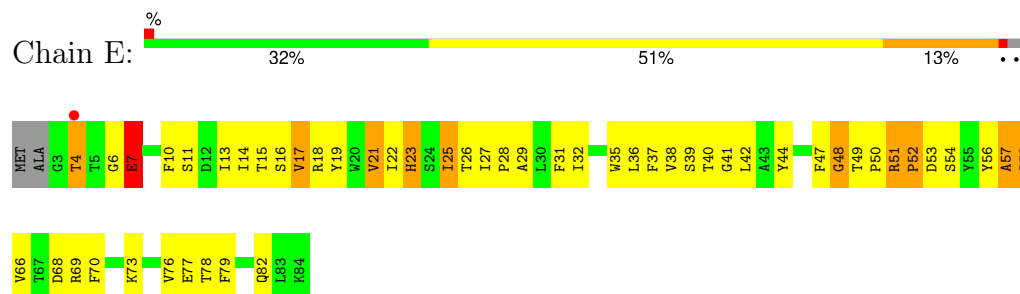


• Molecule 4: photosystem II reaction center D2 protein

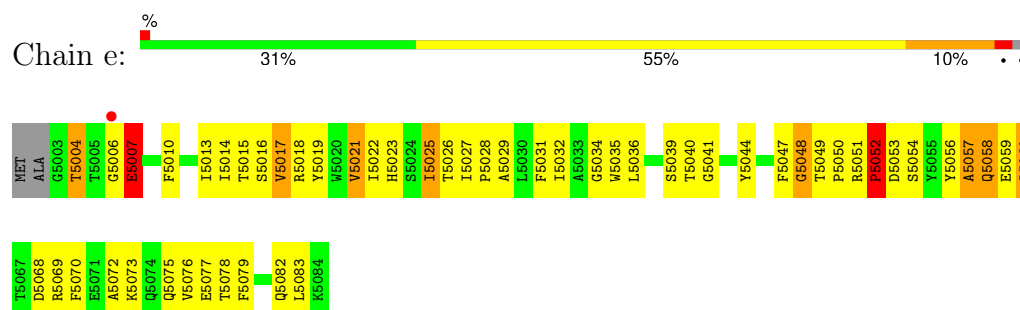
Chain d: 40% 46% 9% ..



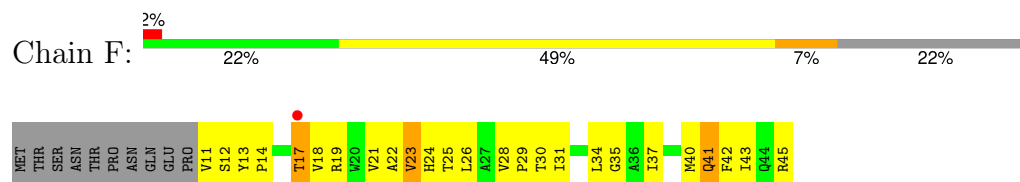
- Molecule 5: Cytochrome b559 alpha subunit



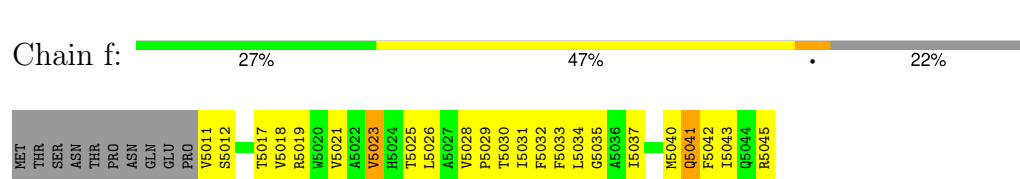
- Molecule 5: Cytochrome b559 alpha subunit



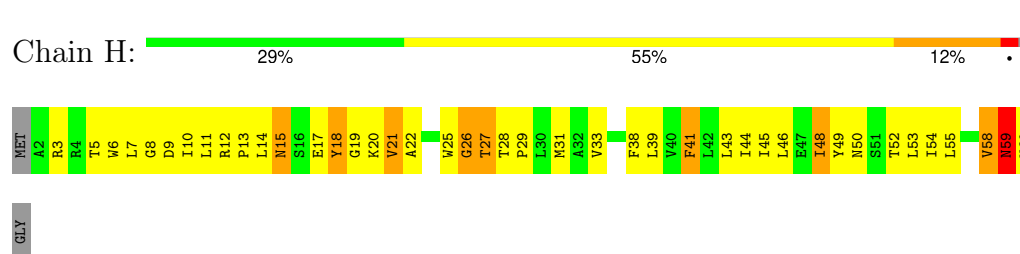
- Molecule 6: Cytochrome b559 beta subunit



- Molecule 6: Cytochrome b559 beta subunit



- Molecule 7: Photosystem II reaction center H protein



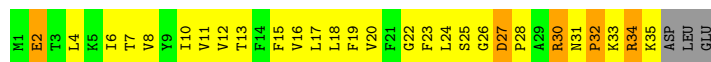
- Molecule 7: Photosystem II reaction center H protein





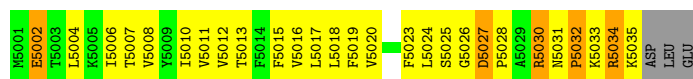
• Molecule 8: Photosystem II reaction center I protein

Chain I: 18% 61% 13% 8%



• Molecule 8: Photosystem II reaction center I protein

Chain i: 21% 58% 13% 8%



• Molecule 9: Photosystem II reaction center J protein

Chain J: 25% 50% 10% 15%



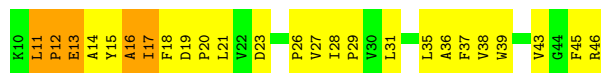
• Molecule 9: Photosystem II reaction center J protein

Chain j: 22% 52% 10% 15%



• Molecule 10: Photosystem II reaction center protein K

Chain K: 32% 54% 14%



• Molecule 10: Photosystem II reaction center protein K

Chain k: 32% 54% 11%



• Molecule 11: Photosystem II reaction center L protein

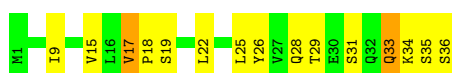
Chain L: 57% 30% 14%



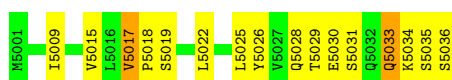
- Molecule 11: Photosystem II reaction center L protein



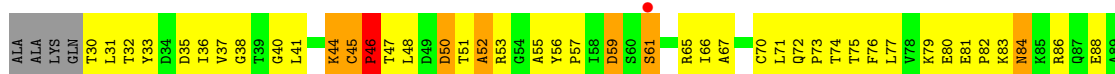
- Molecule 12: Photosystem II reaction center M protein



- Molecule 12: Photosystem II reaction center M protein

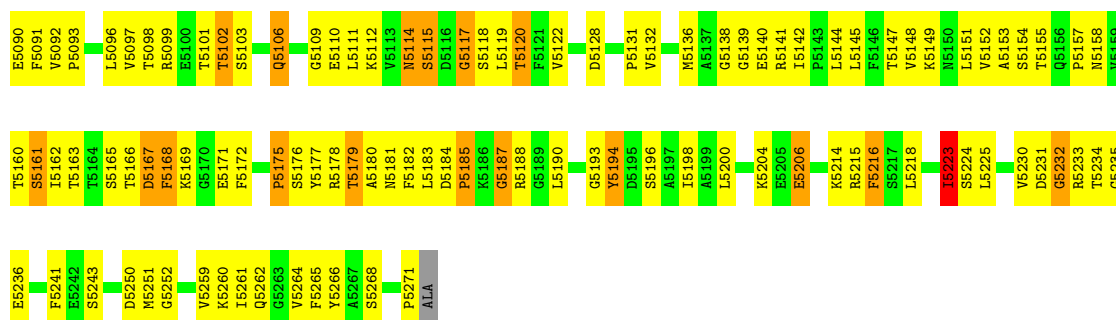


- Molecule 13: Photosystem II manganese-stabilizing polypeptide



- Molecule 13: Photosystem II manganese-stabilizing polypeptide





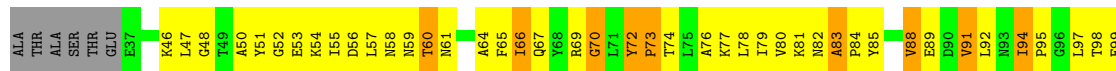
• Molecule 14: Photosystem II reaction center T protein



• Molecule 14: Photosystem II reaction center T protein



• Molecule 15: Photosystem II 12 kDa extrinsic protein

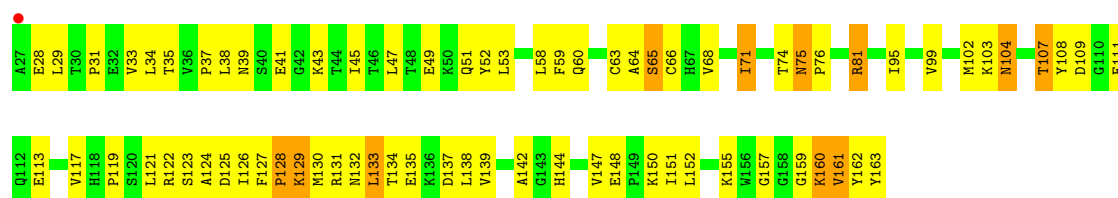


• Molecule 15: Photosystem II 12 kDa extrinsic protein



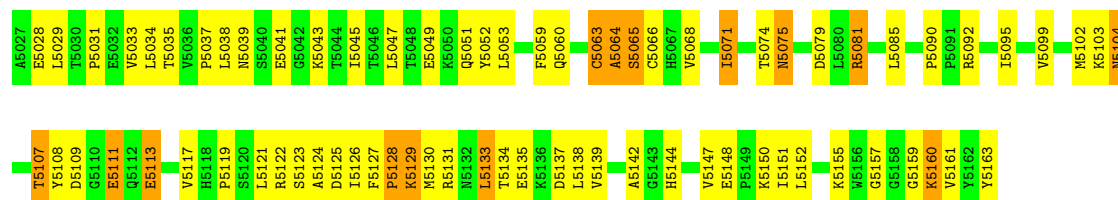
• Molecule 16: Cytochrome c-550





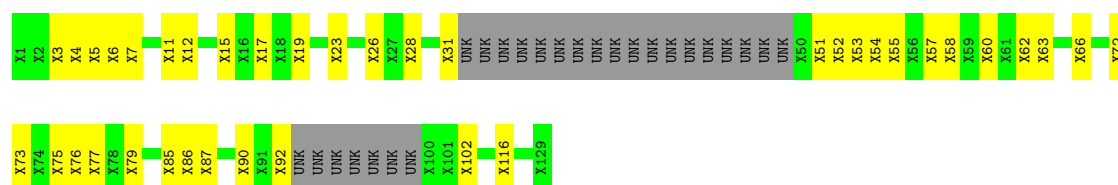
• Molecule 16: Cytochrome c-550

Chain v: 46% 44% 10%



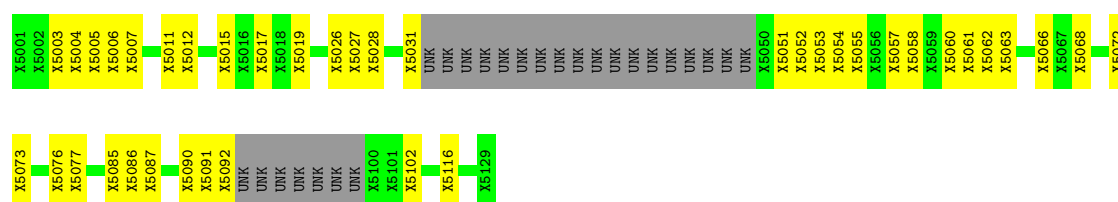
• Molecule 17: Unassigned subunits

Chain X: 51% 29% 19%



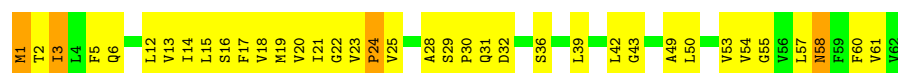
• Molecule 17: Unassigned subunits

Chain x: 50% 30% 19%



• Molecule 18: Photosystem II reaction center Z protein

Chain Z: 40% 53% 6%



• Molecule 18: Photosystem II reaction center Z protein

Chain z: 37% 56% 6%

M5001	T5002	L5003	L5004	F5005	Q5006	L5012	V5013	L5014	L5015	S5016	F5017	V5018	M5019	V5020	L5021	G5022	V5023	F5024	V5025	A5026	Y5027	A5028	S5029	F5030	Q5031	D5032	S5036	L5039	L5042	G5043	Y5047	L5048	A5049	L5050	V5053	V5054	G5055	V5056	L5057	N5058	F5059	F5060	V5061	V5062
-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------	-------

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.69Å 225.40Å 306.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.00 10.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	75.6 (10.00-3.00) 79.0 (10.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 2.98Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.234 , 0.286 0.241 , 0.291	Depositor DCC
R_{free} test set	1908 reflections (1.23%)	wwPDB-VP
Wilson B-factor (Å ²)	78.2	Xtriage
Anisotropy	0.468	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 59.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	48254	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: LMT, CLA, LHG, UNL, BCT, SQD, FE2, PQ9, PHO, DGD, OEC, HEM, BCR, MGE, CA

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.80	0/2708	1.15	24/3694 (0.6%)
1	a	0.76	0/2708	1.16	29/3694 (0.8%)
2	B	0.74	0/3935	1.06	21/5366 (0.4%)
2	b	0.74	0/3935	1.07	23/5366 (0.4%)
3	C	0.66	0/3533	1.11	26/4815 (0.5%)
3	c	0.67	0/3533	1.13	27/4815 (0.6%)
4	D	0.81	1/2791 (0.0%)	1.08	19/3806 (0.5%)
4	d	0.75	1/2791 (0.0%)	1.08	15/3806 (0.4%)
5	E	0.75	0/665	1.24	7/911 (0.8%)
5	e	0.73	0/665	1.21	4/911 (0.4%)
6	F	0.77	0/287	0.98	0/392
6	f	0.75	0/287	0.93	0/392
7	H	0.72	0/505	1.07	3/692 (0.4%)
7	h	0.69	0/505	1.07	3/692 (0.4%)
8	I	0.77	0/293	1.06	1/395 (0.3%)
8	i	0.70	0/293	1.08	1/395 (0.3%)
9	J	0.75	0/246	1.22	4/335 (1.2%)
9	j	0.69	0/246	1.24	4/335 (1.2%)
10	K	0.78	0/299	1.11	1/412 (0.2%)
10	k	0.88	0/299	1.08	2/412 (0.5%)
11	L	0.78	0/308	1.07	1/419 (0.2%)
11	l	0.85	0/308	1.05	2/419 (0.5%)
12	M	0.90	0/279	1.04	0/379
12	m	0.92	0/279	1.06	0/379
13	O	0.78	1/1803 (0.1%)	1.10	13/2461 (0.5%)
13	o	0.76	1/1803 (0.1%)	1.10	14/2461 (0.6%)
14	T	0.93	0/263	1.08	2/356 (0.6%)
14	t	0.90	0/263	1.07	2/356 (0.6%)
15	U	0.79	0/786	1.13	7/1066 (0.7%)
15	u	0.74	0/786	1.12	5/1066 (0.5%)
16	V	0.74	0/1085	1.03	3/1473 (0.2%)
16	v	0.71	0/1085	1.00	4/1473 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
18	Z	0.82	1/451 (0.2%)	1.08	0/620
18	z	0.90	1/451 (0.2%)	1.11	0/620
All	All	0.75	6/40474 (0.0%)	1.10	267/55184 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
2	b	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	z	5001	MET	SD-CE	6.21	1.95	1.79
18	Z	1	MET	SD-CE	5.99	1.94	1.79
4	d	5013	GLY	N-CA	5.40	1.54	1.45
13	O	213	VAL	CA-CB	-5.32	1.47	1.53
4	D	13	GLY	N-CA	5.12	1.53	1.45
13	o	5136	MET	SD-CE	5.02	1.92	1.79

All (267) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	5090	PHE	N-CA-C	-9.53	100.42	112.90
4	D	143	ALA	N-CA-C	-9.33	102.03	113.50
4	d	5143	ALA	N-CA-C	-8.99	102.44	113.41
8	i	5002	GLU	N-CA-C	-8.92	101.97	113.12
4	D	14	TRP	N-CA-C	-8.88	102.60	113.97
3	c	5297	TYR	CA-C-N	8.71	130.72	119.84
3	c	5297	TYR	C-N-CA	8.71	130.72	119.84
13	O	196	SER	N-CA-C	8.62	120.12	108.23
2	B	90	PHE	N-CA-C	-8.60	100.50	112.45
2	b	5003	LEU	N-CA-C	-8.60	97.34	110.32
4	d	5014	TRP	N-CA-C	-8.57	103.00	113.97
2	B	392	PHE	N-CA-C	-8.48	99.39	110.33
1	A	263	ALA	N-CA-C	-8.43	104.04	112.97
2	b	5392	PHE	N-CA-C	-8.32	99.60	110.33
2	B	3	LEU	N-CA-C	-8.23	97.89	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	o	5196	SER	N-CA-C	8.15	119.48	108.23
1	a	5263	ALA	N-CA-C	-8.13	104.35	112.97
1	a	5296	ASN	N-CA-C	8.12	122.63	112.24
3	C	297	TYR	CA-C-N	8.11	129.98	119.84
3	C	297	TYR	C-N-CA	8.11	129.98	119.84
3	c	5451	ALA	N-CA-C	-8.01	102.14	112.23
13	o	5045	CYS	CA-C-N	7.94	129.76	119.84
13	o	5045	CYS	C-N-CA	7.94	129.76	119.84
3	c	5318	LEU	N-CA-C	-7.88	102.67	111.82
13	O	45	CYS	CA-C-N	7.80	129.59	119.84
13	O	45	CYS	C-N-CA	7.80	129.59	119.84
10	K	17	ILE	N-CA-C	-7.73	105.02	112.29
5	e	5057	ALA	N-CA-C	-7.58	99.81	110.50
1	A	296	ASN	N-CA-C	7.50	121.73	112.58
1	A	30	VAL	N-CA-C	-7.39	100.05	109.58
3	C	318	LEU	N-CA-C	-7.32	103.33	111.82
5	E	57	ALA	N-CA-C	-7.25	100.28	110.50
3	C	451	ALA	N-CA-C	-7.23	103.12	112.23
4	d	5223	PHE	N-CA-C	-7.21	101.22	110.53
3	C	300	GLU	N-CA-C	-7.21	103.46	112.90
1	a	5176	ILE	N-CA-C	7.20	117.33	110.42
13	O	102	THR	N-CA-C	7.14	122.12	113.41
2	B	268	PHE	N-CA-C	-7.09	99.71	110.14
2	B	463	PHE	N-CA-C	-7.07	103.65	111.36
2	B	31	ALA	N-CA-C	-7.06	102.78	111.40
13	o	5059	ASP	N-CA-C	7.05	118.97	111.28
4	D	172	SER	N-CA-C	7.04	121.97	112.88
15	u	5074	THR	N-CA-C	7.03	119.97	111.40
15	U	74	THR	N-CA-C	7.02	120.32	111.69
8	I	2	GLU	N-CA-C	-7.01	102.71	112.45
3	c	5204	LEU	N-CA-C	-6.97	99.05	109.86
13	O	103	SER	N-CA-C	6.94	120.29	110.23
7	H	52	THR	N-CA-C	-6.92	104.83	112.72
4	d	5172	SER	N-CA-C	6.92	121.80	112.88
3	C	422	PRO	N-CA-C	-6.91	103.93	113.53
3	c	5300	GLU	N-CA-C	-6.91	103.85	112.90
4	D	15	PHE	N-CA-C	-6.90	102.83	111.11
4	D	223	PHE	N-CA-C	-6.89	101.64	110.53
13	O	59	ASP	N-CA-C	6.89	118.79	111.28
3	c	5040	ALA	N-CA-C	-6.89	104.69	113.23
4	d	5015	PHE	N-CA-C	-6.83	102.91	111.11
2	B	236	THR	N-CA-C	-6.83	104.98	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	5339	PHE	CA-C-N	6.81	128.35	119.84
1	a	5339	PHE	C-N-CA	6.81	128.35	119.84
14	t	5002	GLU	N-CA-C	-6.81	102.24	112.04
15	u	5051	TYR	N-CA-C	-6.78	99.99	110.10
10	k	5017	ILE	N-CA-C	-6.77	105.92	112.29
3	C	204	LEU	N-CA-C	-6.75	99.39	109.86
14	T	25	GLU	N-CA-C	-6.74	98.79	109.04
1	a	5032	TRP	N-CA-C	-6.73	103.42	111.69
1	a	5142	TRP	N-CA-C	6.71	125.09	110.80
2	b	5236	THR	N-CA-C	-6.70	105.01	113.72
13	o	5103	SER	N-CA-C	6.69	120.18	110.28
15	U	94	ILE	CA-C-N	6.69	126.72	119.90
15	U	94	ILE	C-N-CA	6.69	126.72	119.90
1	A	330	VAL	N-CA-C	6.68	116.69	110.42
3	c	5439	VAL	N-CA-C	-6.65	104.04	110.42
1	a	5297	LEU	N-CA-C	-6.64	95.40	107.75
3	c	5422	PRO	N-CA-C	-6.63	104.31	113.53
3	C	40	ALA	N-CA-C	-6.62	105.02	113.23
13	o	5102	THR	N-CA-C	6.61	121.47	113.41
14	t	5025	GLU	N-CA-C	-6.61	99.00	109.04
3	c	5076	ILE	CA-C-N	6.59	128.08	119.84
3	c	5076	ILE	C-N-CA	6.59	128.08	119.84
9	j	5033	TYR	N-CA-C	-6.56	99.61	110.17
15	u	5094	ILE	CA-C-N	6.54	126.58	119.90
15	u	5094	ILE	C-N-CA	6.54	126.58	119.90
15	U	51	TYR	N-CA-C	-6.52	100.24	109.96
11	l	5036	PHE	N-CA-C	-6.52	104.26	111.82
3	c	5453	ALA	N-CA-C	-6.49	103.91	112.34
9	j	5036	LEU	N-CA-C	-6.47	104.07	112.23
13	o	5187	GLY	N-CA-C	6.47	122.78	115.08
1	A	65	GLU	CA-C-N	6.46	126.85	119.93
1	A	65	GLU	C-N-CA	6.46	126.85	119.93
1	A	115	ILE	N-CA-C	6.45	117.23	110.72
2	B	160	GLY	N-CA-C	-6.45	106.79	115.36
11	L	36	PHE	N-CA-C	-6.41	104.38	111.82
4	D	219	GLU	N-CA-C	6.41	119.08	111.71
3	c	5254	THR	N-CA-C	6.39	117.01	108.38
9	j	5013	VAL	N-CA-C	-6.38	104.05	111.00
1	A	192	ILE	N-CA-C	6.36	116.52	110.42
1	A	339	PHE	CA-C-N	6.35	127.78	119.84
1	A	339	PHE	C-N-CA	6.35	127.78	119.84
4	D	297	ASP	N-CA-C	6.32	119.02	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	c	5224	ILE	N-CA-C	-6.31	102.98	111.44
16	V	104	ASN	CA-C-N	6.30	126.22	119.85
16	V	104	ASN	C-N-CA	6.30	126.22	119.85
2	b	5160	GLY	N-CA-C	-6.29	106.99	115.36
2	B	137	LYS	N-CA-C	-6.28	104.32	112.23
2	b	5268	PHE	N-CA-C	-6.28	100.91	110.14
1	A	170	ASP	N-CA-C	-6.27	101.50	110.59
9	J	36	LEU	N-CA-C	-6.27	104.33	112.23
1	a	5030	VAL	N-CA-C	-6.24	101.50	109.30
5	e	5007	GLU	N-CA-C	6.23	124.08	110.80
1	A	142	TRP	N-CA-C	6.22	124.05	110.80
2	B	332	LYS	N-CA-C	-6.19	105.22	112.89
1	a	5330	VAL	N-CA-C	6.16	116.21	110.42
5	e	5041	GLY	N-CA-C	-6.15	106.76	115.43
13	o	5223	ILE	CB-CA-C	-6.14	101.21	111.29
13	O	271	PRO	CA-C-O	6.13	137.40	119.00
4	D	54	PHE	N-CA-C	6.11	121.06	112.93
1	a	5065	GLU	CA-C-N	6.11	126.47	119.93
1	a	5065	GLU	C-N-CA	6.11	126.47	119.93
4	d	5054	PHE	N-CA-C	6.11	121.06	112.93
3	C	295	THR	N-CA-C	6.09	117.79	111.03
5	E	7	GLU	N-CA-C	6.08	123.76	110.80
1	a	5167	SER	N-CA-C	6.08	118.40	108.55
2	B	81	THR	N-CA-C	-6.07	105.91	113.38
1	a	5170	ASP	N-CA-C	-6.06	101.80	110.59
3	c	5333	GLY	CA-C-N	6.05	127.41	119.84
3	c	5333	GLY	C-N-CA	6.05	127.41	119.84
3	c	5295	THR	N-CA-C	6.05	117.74	111.03
3	c	5116	VAL	N-CA-C	6.03	116.21	110.42
3	c	5156	LYS	N-CA-C	-6.03	105.02	112.38
1	a	5086	SER	N-CA-C	6.02	118.32	110.43
2	B	75	TRP	N-CA-C	-6.02	105.65	112.87
14	T	2	GLU	N-CA-C	-6.00	103.40	112.04
2	b	5031	ALA	N-CA-C	-6.00	104.09	111.40
3	C	224	ILE	N-CA-C	-5.99	103.42	111.44
1	a	5115	ILE	N-CA-C	5.99	116.77	110.72
3	C	76	ILE	CA-C-N	5.98	127.32	119.84
3	C	76	ILE	C-N-CA	5.98	127.32	119.84
1	A	297	LEU	N-CA-C	-5.96	96.00	107.57
2	b	5414	PRO	N-CA-C	5.96	117.98	110.70
13	O	223	ILE	CB-CA-C	-5.94	101.55	111.29
13	o	5061	SER	N-CA-C	-5.92	105.71	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	453	ALA	N-CA-C	-5.91	104.66	112.34
1	a	5083	VAL	CA-C-N	5.89	125.83	119.76
1	a	5083	VAL	C-N-CA	5.89	125.83	119.76
2	b	5328	GLY	CA-C-N	5.88	126.07	120.31
2	b	5328	GLY	C-N-CA	5.88	126.07	120.31
13	o	5194	TYR	N-CA-C	5.87	118.12	110.43
2	b	5137	LYS	N-CA-C	-5.86	104.85	112.23
4	D	295	SER	N-CA-C	-5.84	100.81	109.11
2	b	5463	PHE	N-CA-C	-5.83	105.01	111.36
3	c	5347	GLY	N-CA-C	5.82	121.62	114.69
7	h	5052	THR	N-CA-C	-5.80	106.10	112.72
4	d	5219	GLU	N-CA-C	5.79	118.37	111.71
3	C	347	GLY	N-CA-C	5.78	121.56	114.69
9	J	13	VAL	N-CA-C	-5.77	104.71	111.00
15	U	52	GLY	N-CA-C	-5.75	107.06	115.63
3	c	5252	ILE	N-CA-C	-5.75	105.53	113.00
3	c	5238	ILE	N-CA-C	-5.75	104.76	110.62
4	D	165	SER	N-CA-C	5.74	118.75	111.69
5	E	41	GLY	N-CA-C	-5.72	107.36	115.43
3	C	333	GLY	CA-C-N	5.71	126.98	119.84
3	C	333	GLY	C-N-CA	5.71	126.98	119.84
1	A	179	THR	N-CA-C	-5.71	104.67	111.69
3	C	439	VAL	N-CA-C	-5.71	104.94	110.42
2	b	5332	LYS	N-CA-C	-5.69	105.83	112.89
1	A	250	ALA	N-CA-C	-5.68	105.08	112.23
2	b	5075	TRP	N-CA-C	-5.66	106.08	112.87
13	O	194	TYR	N-CA-C	5.66	117.84	110.43
3	C	238	ILE	N-CA-C	-5.66	104.99	110.42
1	A	167	SER	N-CA-C	5.64	117.68	108.55
2	b	5458	PHE	N-CA-C	-5.63	105.22	111.36
3	C	218	PHE	N-CA-C	5.62	117.78	110.53
16	v	5113	GLU	N-CA-C	-5.62	100.13	109.46
3	C	254	THR	N-CA-C	5.57	115.90	108.38
9	J	33	TYR	N-CA-C	-5.56	101.22	110.17
3	c	5161	LEU	N-CA-C	-5.55	104.92	110.97
1	A	157	VAL	N-CA-C	5.54	117.97	111.05
3	C	41	ARG	N-CA-C	-5.53	106.37	113.01
4	D	244	TYR	N-CA-C	-5.53	101.73	109.69
4	d	5165	SER	N-CA-C	5.53	117.39	111.36
1	a	5250	ALA	N-CA-C	-5.52	105.27	112.23
2	b	5267	LEU	N-CA-C	-5.52	106.22	113.12
15	u	5052	GLY	N-CA-C	-5.52	107.58	115.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	207	GLY	N-CA-C	-5.52	105.58	113.86
1	a	5201	GLY	N-CA-C	-5.51	105.83	112.49
7	H	15	ASN	N-CA-C	-5.48	103.74	110.65
1	a	5036	ILE	N-CA-C	-5.48	106.84	111.56
1	a	5192	ILE	N-CA-C	5.48	116.11	110.36
2	B	381	ILE	CA-C-N	5.47	125.47	120.21
2	B	381	ILE	C-N-CA	5.47	125.47	120.21
5	E	38	VAL	N-CA-C	-5.47	106.36	111.45
4	D	27	PHE	N-CA-C	-5.47	104.96	111.03
4	D	147	SER	N-CA-C	-5.47	105.48	111.82
9	j	5030	TYR	N-CA-C	-5.47	104.96	111.69
5	e	5021	VAL	N-CA-C	-5.47	105.17	110.42
3	C	301	PHE	N-CA-C	-5.46	106.29	113.12
1	a	5082	VAL	N-CA-C	-5.46	100.01	107.99
4	d	5297	ASP	N-CA-C	5.46	117.70	109.41
2	B	414	PRO	N-CA-C	5.45	117.35	110.70
1	A	82	VAL	N-CA-C	-5.45	100.04	107.99
16	V	60	GLN	OE1-CD-NE2	-5.45	117.15	122.60
2	b	5081	THR	N-CA-C	-5.45	106.68	113.38
1	a	5157	VAL	N-CA-C	5.44	117.84	111.05
3	c	5301	PHE	N-CA-C	-5.41	106.36	113.12
1	A	309	ALA	N-CA-C	5.41	117.18	111.28
1	a	5305	SER	N-CA-C	-5.38	99.33	110.80
3	C	116	VAL	N-CA-C	5.37	115.58	110.53
1	A	83	VAL	CA-C-N	5.37	125.29	119.76
1	A	83	VAL	C-N-CA	5.37	125.29	119.76
3	C	252	ILE	N-CA-C	-5.37	106.02	113.00
11	l	5031	PHE	N-CA-C	5.37	119.55	112.89
3	c	5041	ARG	N-CA-C	-5.36	106.57	113.01
2	b	5381	ILE	CA-C-N	5.35	125.35	120.21
2	b	5381	ILE	C-N-CA	5.35	125.35	120.21
4	D	144	ILE	N-CA-C	-5.34	105.64	110.82
2	B	328	GLY	CA-C-N	5.34	125.55	120.31
2	B	328	GLY	C-N-CA	5.34	125.55	120.31
4	d	5295	SER	N-CA-C	-5.34	101.01	108.54
10	k	5027	VAL	N-CA-C	5.33	117.75	111.09
4	d	5027	PHE	N-CA-C	-5.31	105.14	111.03
1	A	176	ILE	N-CA-C	5.29	115.92	110.36
2	B	383	PHE	N-CA-C	-5.28	105.97	112.72
4	D	293	LEU	N-CA-C	-5.28	103.35	110.68
1	a	5284	TRP	N-CA-C	-5.27	105.22	110.97
2	B	237	VAL	N-CA-C	-5.24	105.29	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	d	5208	ALA	N-CA-C	-5.24	105.48	111.14
13	o	5271	PRO	N-CA-C	-5.23	99.02	112.10
1	A	86	SER	N-CA-C	5.22	117.27	110.43
5	E	23	HIS	N-CA-C	5.22	119.36	112.89
5	E	51	ARG	N-CA-C	-5.21	103.47	109.93
7	h	5030	LEU	N-CA-C	-5.21	105.69	111.36
7	h	5048	ILE	N-CA-C	-5.20	106.07	111.58
9	J	30	TYR	N-CA-C	-5.20	105.30	111.69
1	a	5316	THR	N-CA-C	-5.20	102.20	109.69
2	B	321	LYS	N-CA-C	-5.19	103.75	110.19
1	a	5024	THR	N-CA-C	-5.18	106.96	113.28
7	H	48	ILE	N-CA-C	-5.18	106.09	111.58
13	O	61	SER	N-CA-C	-5.17	106.75	113.16
13	o	5044	LYS	N-CA-C	-5.17	103.21	110.50
2	B	389	LYS	N-CA-C	-5.17	107.63	114.04
5	E	21	VAL	N-CA-C	-5.16	105.46	110.42
1	A	316	THR	N-CA-C	-5.16	102.27	109.69
3	c	5325	GLY	N-CA-C	5.15	119.09	113.58
3	C	325	GLY	N-CA-C	5.15	119.09	113.58
13	O	44	LYS	N-CA-C	-5.15	102.66	110.28
2	b	5092	SER	N-CA-C	-5.14	102.58	110.14
2	b	5389	LYS	N-CA-C	-5.14	107.67	114.04
3	c	5438	LEU	N-CA-C	-5.14	105.68	111.28
13	o	5200	LEU	CA-C-N	5.14	126.26	119.84
13	o	5200	LEU	C-N-CA	5.14	126.26	119.84
4	d	5244	TYR	N-CA-C	-5.13	102.31	109.69
2	b	5383	PHE	N-CA-C	-5.12	106.16	112.72
16	v	5104	ASN	CA-C-N	5.12	125.02	119.85
16	v	5104	ASN	C-N-CA	5.12	125.02	119.85
3	C	156	LYS	N-CA-C	-5.11	106.14	112.38
4	D	101	PHE	N-CA-C	5.11	117.24	111.11
4	D	178	ILE	N-CA-C	-5.07	107.20	111.56
4	D	123	ILE	N-CA-C	-5.06	105.78	110.53
13	O	200	LEU	CA-C-N	5.04	126.14	119.84
13	O	200	LEU	C-N-CA	5.04	126.14	119.84
4	d	5178	ILE	N-CA-C	-5.03	107.23	111.56
16	v	5060	GLN	OE1-CD-NE2	-5.03	117.57	122.60
4	d	5079	SER	N-CA-C	5.01	117.70	110.28
15	U	91	VAL	CB-CA-C	-5.01	105.56	111.97
1	a	5058	VAL	N-CA-C	5.01	115.06	107.80
2	b	5048	SER	N-CA-C	5.01	118.85	112.34
15	U	47	LEU	N-CA-C	-5.01	107.32	112.93

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	273	TYR	Sidechain
2	b	5273	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2623	0	2517	233	0
1	a	2623	0	2517	251	0
2	B	3800	0	3637	285	0
2	b	3800	0	3637	288	0
3	C	3421	0	3326	310	0
3	c	3421	0	3326	320	0
4	D	2696	0	2591	251	0
4	d	2696	0	2591	257	0
5	E	646	0	616	56	0
5	e	646	0	616	63	0
6	F	278	0	279	31	0
6	f	278	0	279	30	0
7	H	492	0	495	56	0
7	h	492	0	495	51	0
8	I	286	0	308	33	0
8	i	286	0	305	31	0
9	J	240	0	242	27	0
9	j	240	0	242	29	0
10	K	289	0	294	51	0
10	k	289	0	294	47	0
11	L	301	0	309	25	0
11	l	301	0	306	25	0
12	M	276	0	288	23	0
12	m	276	0	285	21	0
13	O	1772	0	1664	166	0
13	o	1772	0	1664	162	0
14	T	254	0	257	27	0
14	t	254	0	254	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	U	775	0	771	61	0
15	u	775	0	771	64	0
16	V	1064	0	1072	73	0
16	v	1064	0	1072	76	0
17	X	687	0	268	44	0
17	x	687	0	268	45	0
18	Z	442	0	460	40	0
18	z	442	0	457	44	0
19	A	1	0	0	0	0
19	a	1	0	0	0	0
20	A	250	0	265	13	0
20	B	1007	0	1088	62	0
20	C	774	0	783	44	0
20	D	115	0	111	9	0
20	a	250	0	265	15	0
20	b	1007	0	1088	61	0
20	c	774	0	783	42	0
20	d	115	0	111	10	0
21	A	128	0	148	12	0
21	a	128	0	148	12	0
22	A	30	0	37	1	0
22	D	30	0	37	5	0
22	a	30	0	37	0	0
22	d	30	0	37	5	0
23	A	5	0	0	0	0
23	a	5	0	0	0	0
24	A	40	0	56	1	0
24	B	120	0	168	7	0
24	C	120	0	168	19	0
24	D	40	0	56	4	0
24	H	40	0	56	2	0
24	T	40	0	56	8	0
24	X	40	0	56	9	0
24	a	40	0	56	3	0
24	b	120	0	168	6	0
24	c	120	0	168	21	0
24	d	40	0	56	6	0
24	h	40	0	56	3	0
24	t	40	0	56	9	0
24	x	40	0	56	10	0
25	A	39	0	51	4	0
25	a	39	0	51	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	A	80	0	92	0	0
26	L	47	0	60	1	0
26	a	26	0	15	0	0
26	d	54	0	77	0	0
26	t	47	0	60	1	0
27	A	35	0	46	3	0
27	M	35	0	46	0	0
27	T	35	0	46	6	0
27	a	35	0	46	1	0
27	m	35	0	46	0	0
27	t	35	0	46	5	0
28	B	48	0	72	1	0
28	D	136	0	194	10	0
28	I	48	0	72	1	0
28	L	48	0	72	2	0
28	b	48	0	72	1	0
28	d	136	0	194	11	0
28	i	48	0	72	2	0
28	l	48	0	72	4	0
29	C	152	0	0	1	0
29	c	152	0	0	1	0
30	C	157	0	188	18	0
30	H	54	0	66	3	0
30	c	157	0	188	18	0
30	h	54	0	66	3	0
31	D	4	0	0	0	0
31	d	4	0	0	0	0
32	F	43	0	30	3	0
32	V	43	0	30	2	0
32	f	43	0	30	3	0
32	v	43	0	30	1	0
33	K	1	0	0	0	0
33	k	1	0	0	0	0
All	All	48254	0	47073	3260	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 34.

All (3260) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:6:UNK:NE2	17:X:6:UNK:CD	1.33	1.42
17:X:26:UNK:NE2	17:X:26:UNK:CD	1.33	1.41
17:x:5026:UNK:NE2	17:x:5026:UNK:CD	1.34	1.41
17:x:5006:UNK:NE2	17:x:5006:UNK:CD	1.33	1.40
1:A:76:ASN:HD21	1:A:79:THR:HG23	1.13	1.14
13:O:223:ILE:HG23	13:O:243:SER:HB3	1.31	1.12
2:B:36:SER:HB3	24:t:104:BCR:H401	1.31	1.10
13:o:5223:ILE:HG23	13:o:5243:SER:HB3	1.34	1.09
24:T:5104:BCR:H401	2:b:5036:SER:HB3	1.34	1.09
15:U:113:THR:HG22	15:U:114:VAL:H	1.15	1.07
15:u:5113:THR:HG22	15:u:5114:VAL:H	1.15	1.06
3:C:473:ASP:HB3	14:T:26:PRO:HB3	1.33	1.05
3:c:5473:ASP:HB3	14:t:5026:PRO:HB3	1.33	1.05
13:o:5098:THR:HG22	13:o:5099:ARG:H	1.17	1.04
2:b:5068:ARG:HH22	20:b:5514:CLA:HED1	1.23	1.03
1:a:5076:ASN:HD21	1:a:5079:THR:HG23	1.21	1.03
1:A:322:ASN:HD21	3:C:412:THR:HA	1.24	1.01
4:d:5160:TYR:HB3	4:d:5161:PRO:HD3	1.43	1.01
4:D:160:TYR:HB3	4:D:161:PRO:HD3	1.40	1.01
13:O:98:THR:HG22	13:O:99:ARG:H	1.21	1.01
2:B:329:PRO:HB3	20:B:517:CLA:HED1	1.43	1.00
3:c:5305:THR:HG22	3:c:5307:PRO:HD2	1.42	1.00
1:a:5190:HIS:HA	1:a:5298:ASN:HD22	1.24	1.00
16:v:5038:LEU:HB2	16:v:5045:ILE:HG13	1.43	0.99
2:b:5263:THR:HG21	2:b:5448:ARG:HH12	1.27	0.99
3:C:466:VAL:HA	3:C:469:MET:HE3	1.45	0.99
16:V:38:LEU:HB2	16:V:45:ILE:HG13	1.45	0.99
2:B:68:ARG:HH22	20:B:514:CLA:HED1	1.28	0.98
2:B:263:THR:HG21	2:B:448:ARG:HH12	1.28	0.98
10:k:5039:TRP:HE1	17:x:5031:UNK:HG3	1.29	0.98
3:C:305:THR:HG22	3:C:307:PRO:HD2	1.45	0.98
1:A:310:LYS:HB2	16:V:28:GLU:HB3	1.45	0.98
3:c:5466:VAL:HA	3:c:5469:MET:HE3	1.43	0.97
1:A:190:HIS:HA	1:A:298:ASN:HD22	1.26	0.97
1:a:5322:ASN:HD21	3:c:5412:THR:HA	1.24	0.97
2:b:5329:PRO:HB3	20:b:5517:CLA:HED1	1.46	0.97
2:B:36:SER:HB3	24:t:104:BCR:C40	1.95	0.97
3:C:204:LEU:HD23	3:C:204:LEU:H	1.28	0.96
1:A:212:CYS:HB2	4:D:211:CYS:HB2	1.44	0.96
3:c:5269:GLU:HG2	3:c:5448:ALA:HB2	1.48	0.96
13:o:5179:THR:HG22	13:o:5181:ASN:H	1.26	0.96
3:c:5150:ASP:HB3	3:c:5153:ASP:HB2	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:LEU:HG	20:B:513:CLA:HBC1	1.46	0.96
13:O:45:CYS:HB2	13:O:46:PRO:HD2	1.47	0.96
2:b:5149:LEU:HG	20:b:5513:CLA:HBC1	1.45	0.95
13:O:179:THR:HG22	13:O:181:ASN:H	1.30	0.95
8:i:5034:ARG:HE	8:i:5034:ARG:H	0.97	0.95
1:a:5310:LYS:HB2	16:v:5028:GLU:HB3	1.46	0.94
16:v:5038:LEU:HD13	16:v:5045:ILE:HD11	1.46	0.94
1:a:5060:ILE:HG23	1:a:5061:ASP:H	1.33	0.93
3:c:5204:LEU:HD23	3:c:5204:LEU:H	1.33	0.93
1:a:5225:ARG:HH12	2:b:5483:ASP:HA	1.31	0.93
3:C:269:GLU:HG2	3:C:448:ALA:HB2	1.50	0.93
24:T:5104:BCR:C40	2:b:5036:SER:HB3	1.98	0.92
3:C:150:ASP:HB3	3:C:153:ASP:HB2	1.49	0.92
8:I:34:ARG:H	8:I:34:ARG:NE	1.67	0.92
18:z:5036:SER:HA	18:z:5039:LEU:HD12	1.51	0.92
4:D:148:ALA:HB3	4:D:149:PRO:HD3	1.52	0.92
24:d:5357:BCR:H403	9:j:5025:VAL:HG21	1.52	0.91
13:o:5045:CYS:HB2	13:o:5046:PRO:HD2	1.51	0.91
1:A:149:ALA:HB3	1:A:150:PRO:HD3	1.52	0.91
8:I:33:LYS:HA	8:I:34:ARG:HH21	1.34	0.91
10:K:39:TRP:HE1	17:X:31:UNK:HG3	1.33	0.91
1:a:5212:CYS:HB2	4:d:5211:CYS:HB2	1.49	0.91
2:b:5368:VAL:HG11	2:b:5381:ILE:HD12	1.52	0.91
2:b:5414:PRO:HB2	2:b:5415:PRO:HD3	1.53	0.90
17:x:5012:UNK:HG3	18:z:5017:PHE:CE1	2.06	0.90
2:b:5271:THR:H	2:b:5274:GLN:HE21	1.16	0.90
13:o:5145:LEU:HD23	13:o:5175:PRO:HG2	1.52	0.89
24:D:357:BCR:H403	9:J:25:VAL:HG21	1.52	0.89
17:X:86:UNK:O	17:X:87:UNK:HB2	1.73	0.89
2:b:5327:THR:HG22	20:b:5517:CLA:H12	1.55	0.89
4:D:186:GLN:HB2	20:D:354:CLA:HBC1	1.52	0.89
18:Z:36:SER:HA	18:Z:39:LEU:HD12	1.53	0.89
1:A:225:ARG:HH12	2:B:483:ASP:HA	1.35	0.89
8:I:34:ARG:H	8:I:34:ARG:HE	0.92	0.89
15:U:50:ALA:CB	15:U:113:THR:HG21	2.04	0.89
15:u:5113:THR:HG22	15:u:5114:VAL:N	1.84	0.88
18:z:5005:PHE:HA	18:z:5057:LEU:HD13	1.53	0.88
2:B:414:PRO:HB2	2:B:415:PRO:HD3	1.54	0.88
8:i:5033:LYS:HA	8:i:5034:ARG:HH21	1.36	0.88
4:d:5148:ALA:HB3	4:d:5149:PRO:HD3	1.52	0.88
13:o:5145:LEU:CD2	13:o:5175:PRO:HG2	2.04	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:x:5006:UNK:NE2	17:x:5006:UNK:CG	2.41	0.88
28:d:5361:MGE:H6D2	11:l:5015:THR:HG21	1.55	0.87
17:X:12:UNK:HG3	18:Z:17:PHE:CE1	2.10	0.87
3:C:254:THR:HG22	3:C:255:THR:H	1.40	0.87
3:C:473:ASP:HB3	14:T:26:PRO:CB	2.04	0.87
1:a:5192:ILE:HG13	1:a:5293:MET:HE1	1.56	0.87
15:u:5050:ALA:CB	15:u:5113:THR:HG21	2.04	0.87
17:X:6:UNK:NE2	17:X:6:UNK:CG	2.43	0.87
1:a:5149:ALA:HB3	1:a:5150:PRO:HD3	1.56	0.87
5:e:5018:ARG:HG2	5:e:5022:ILE:HD11	1.57	0.87
20:B:518:CLA:HAB	4:D:123:ILE:HG23	1.55	0.86
10:K:28:ILE:HA	10:K:31:LEU:HD12	1.57	0.86
2:B:271:THR:H	2:B:274:GLN:HE21	1.17	0.86
28:D:360:MGE:H6D2	11:L:15:THR:HG21	1.57	0.86
13:O:92:VAL:CG1	13:O:93:PRO:HD2	2.04	0.86
8:i:5034:ARG:H	8:i:5034:ARG:NE	1.72	0.86
2:B:327:THR:HG22	20:B:517:CLA:H12	1.58	0.86
13:O:145:LEU:HD23	13:O:175:PRO:HG2	1.57	0.86
16:V:159:GLY:O	16:V:161:VAL:N	2.08	0.86
17:x:5086:UNK:O	17:x:5087:UNK:HB2	1.74	0.86
15:U:113:THR:HG22	15:U:114:VAL:N	1.84	0.86
3:c:5473:ASP:HB3	14:t:5026:PRO:CB	2.05	0.86
24:c:5504:BCR:H353	24:x:5130:BCR:H321	1.57	0.86
10:k:5028:ILE:HA	10:k:5031:LEU:HD12	1.55	0.86
3:C:473:ASP:CB	14:T:26:PRO:HB3	2.05	0.86
13:O:145:LEU:CD2	13:O:175:PRO:HG2	2.06	0.86
2:b:5079:SER:HB3	2:b:5083:GLU:H	1.41	0.86
4:d:5186:GLN:HB2	20:d:5354:CLA:HBC1	1.58	0.86
16:v:5159:GLY:O	16:v:5161:VAL:N	2.08	0.86
17:X:26:UNK:NE2	17:X:26:UNK:CG	2.44	0.86
20:b:5518:CLA:HAB	4:d:5123:ILE:HG23	1.56	0.86
15:u:5072:TYR:HB3	15:u:5073:PRO:HD3	1.58	0.85
20:c:5493:CLA:HBD	20:c:5493:CLA:HBA1	1.57	0.85
3:c:5346:THR:O	13:o:5040:GLY:HA2	1.75	0.85
3:c:5473:ASP:CB	14:t:5026:PRO:HB3	2.05	0.85
2:b:5124:ARG:HG3	2:b:5124:ARG:HH11	1.41	0.85
10:K:45:PHE:O	10:K:46:ARG:OXT	1.95	0.85
2:B:124:ARG:HH11	2:B:124:ARG:HG3	1.42	0.85
13:o:5056:TYR:O	13:o:5161:SER:HA	1.77	0.84
16:V:38:LEU:HD13	16:V:45:ILE:HD11	1.57	0.84
2:b:5263:THR:HG22	2:b:5448:ARG:HH22	1.41	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ASN:ND2	1:A:79:THR:HG23	1.93	0.84
1:A:306:VAL:HG23	1:A:306:VAL:O	1.77	0.84
14:T:29:ILE:H	14:T:29:ILE:HD12	1.43	0.84
1:a:5279:PRO:HB2	21:a:5561:PHO:HBC1	1.57	0.84
20:b:5518:CLA:H42	4:d:5127:LEU:HD11	1.59	0.84
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.59	0.83
3:c:5116:VAL:HG11	24:c:5505:BCR:H323	1.59	0.83
13:o:5092:VAL:CG1	13:o:5093:PRO:HD2	2.08	0.83
2:B:79:SER:HB3	2:B:83:GLU:H	1.43	0.83
20:C:493:CLA:HBD	20:C:493:CLA:HBA1	1.59	0.83
2:B:368:VAL:HG11	2:B:381:ILE:HD12	1.60	0.83
18:Z:5:PHE:HA	18:Z:57:LEU:HD13	1.59	0.83
1:A:279:PRO:HB2	21:A:561:PHO:HBC1	1.58	0.83
7:H:38:PHE:HB2	24:H:107:BCR:H10C	1.61	0.83
3:C:209:ILE:HG23	24:C:506:BCR:H382	1.61	0.83
15:U:72:TYR:HB3	15:U:73:PRO:HD3	1.58	0.83
7:h:5038:PHE:HB2	24:h:5107:BCR:H10C	1.60	0.83
8:I:34:ARG:HE	8:I:34:ARG:N	1.76	0.83
3:c:5254:THR:HG22	3:c:5255:THR:H	1.44	0.83
17:x:5012:UNK:HG3	18:z:5017:PHE:HE1	1.44	0.83
20:B:518:CLA:H42	4:D:127:LEU:HD11	1.60	0.83
2:B:263:THR:HG22	2:B:448:ARG:HH22	1.44	0.83
1:a:5225:ARG:NH1	2:b:5483:ASP:HA	1.94	0.82
17:x:5026:UNK:NE2	17:x:5026:UNK:CG	2.46	0.82
13:O:92:VAL:HG13	13:O:93:PRO:HD2	1.60	0.82
1:a:5324:ALA:HB2	4:d:5329:MET:HE3	1.61	0.82
3:C:166:ILE:HG23	3:C:245:ILE:HG23	1.62	0.82
3:C:293:ASN:ND2	3:C:296:VAL:HG22	1.94	0.82
13:O:45:CYS:H	13:O:72:GLN:NE2	1.77	0.82
13:O:151:LEU:HD13	13:O:223:ILE:HD11	1.59	0.82
4:D:246:MET:HE2	4:D:264:LYS:HG3	1.61	0.82
4:d:5027:PHE:HD2	4:d:5028:VAL:HG23	1.44	0.81
14:t:5029:ILE:H	14:t:5029:ILE:HD12	1.45	0.81
1:A:258:LEU:HD12	4:D:128:ARG:HD3	1.62	0.81
2:B:220:ARG:HD3	2:B:221:PRO:HD2	1.62	0.81
3:C:406:SER:O	3:C:418:ASN:HB2	1.78	0.81
4:D:192:THR:HG23	20:D:354:CLA:HBC2	1.60	0.81
5:E:18:ARG:HG2	5:E:22:ILE:HD11	1.62	0.81
4:d:5161:PRO:HG2	4:d:5170:ALA:HB2	1.62	0.81
2:b:5263:THR:HG21	2:b:5448:ARG:NH1	1.95	0.81
5:e:5018:ARG:O	5:e:5022:ILE:HG13	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:5449:ARG:HH22	8:i:5027:ASP:HB3	1.46	0.81
16:v:5081:ARG:CZ	16:v:5157:GLY:HA3	2.11	0.81
3:c:5282:MET:HA	3:c:5285:ILE:HD12	1.61	0.81
10:k:5045:PHE:O	10:k:5046:ARG:OXT	1.99	0.81
16:v:5064:ALA:O	16:v:5068:VAL:HG13	1.79	0.81
6:f:5021:VAL:O	6:f:5025:THR:HG23	1.79	0.81
24:C:504:BCR:H353	24:X:130:BCR:H321	1.62	0.81
2:b:5068:ARG:NH2	20:b:5514:CLA:HED1	1.96	0.81
3:C:116:VAL:HG11	24:C:505:BCR:H323	1.62	0.80
3:c:5209:ILE:HG23	24:c:5506:BCR:H382	1.62	0.80
3:c:5405:ASN:HD22	30:c:5509:DGD:HD5	1.43	0.80
4:d:5266:TRP:HD1	28:d:5361:MGE:H3D	1.46	0.80
1:A:324:ALA:HB2	4:D:329:MET:HE3	1.61	0.80
6:F:21:VAL:O	6:F:25:THR:HG23	1.80	0.80
1:a:5258:LEU:HD12	4:d:5128:ARG:HD3	1.63	0.80
13:o:5098:THR:HG22	13:o:5099:ARG:N	1.95	0.80
3:C:464:GLU:HB2	3:C:467:LEU:HD12	1.61	0.80
4:D:351:ALA:O	4:D:352:LEU:OXT	1.99	0.80
15:u:5088:VAL:O	15:u:5091:VAL:HG23	1.81	0.80
13:O:73:PRO:HG3	13:O:102:THR:HB	1.63	0.80
3:c:5464:GLU:HB2	3:c:5467:LEU:HD12	1.61	0.80
1:A:201:GLY:HA3	1:A:286:THR:HG23	1.62	0.80
4:D:27:PHE:HD2	4:D:28:VAL:HG23	1.45	0.80
3:c:5342:MET:HE3	3:c:5352:GLY:HA2	1.63	0.80
15:u:5113:THR:CG2	15:u:5114:VAL:H	1.95	0.80
1:A:60:ILE:HG23	1:A:61:ASP:H	1.45	0.79
18:Z:49:ALA:O	18:Z:53:VAL:HG23	1.82	0.79
3:c:5406:SER:O	3:c:5418:ASN:HB2	1.82	0.79
13:o:5073:PRO:HG3	13:o:5102:THR:HB	1.64	0.79
1:A:41:LEU:O	1:A:45:THR:HG22	1.82	0.79
13:o:5045:CYS:H	13:o:5072:GLN:NE2	1.80	0.79
1:A:225:ARG:NH1	2:B:483:ASP:HA	1.96	0.79
3:c:5042:LEU:HD21	20:c:5501:CLA:H2A	1.63	0.79
4:D:161:PRO:HG2	4:D:170:ALA:HB2	1.63	0.79
1:a:5190:HIS:HA	1:a:5298:ASN:ND2	1.96	0.79
2:b:5220:ARG:HD3	2:b:5221:PRO:HD2	1.65	0.79
3:C:27:ASP:HB2	20:C:501:CLA:HED2	1.64	0.79
4:d:5246:MET:HE2	4:d:5264:LYS:HG3	1.63	0.79
13:O:56:TYR:O	13:O:161:SER:HA	1.82	0.79
4:d:5192:THR:HG23	20:d:5354:CLA:HBC2	1.65	0.79
3:C:365:TRP:HB3	3:C:391:ARG:HD3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:5201:GLY:HA3	1:a:5286:THR:HG23	1.64	0.78
1:a:5306:VAL:HG21	1:a:5316:THR:HG23	1.64	0.78
15:U:58:ASN:ND2	15:U:114:VAL:HG13	1.98	0.78
3:c:5166:ILE:HG23	3:c:5245:ILE:HG23	1.66	0.78
1:A:190:HIS:HA	1:A:298:ASN:ND2	1.98	0.78
1:a:5257:ARG:HH11	1:a:5257:ARG:HG3	1.47	0.78
3:c:5365:TRP:HB3	3:c:5391:ARG:HD3	1.66	0.78
13:O:98:THR:HG22	13:O:99:ARG:N	1.99	0.78
15:U:94:ILE:HB	15:U:97:LEU:HD11	1.66	0.78
3:C:42:LEU:HD21	20:C:501:CLA:H2A	1.66	0.78
2:b:5356:VAL:HG22	2:b:5370:LEU:HD21	1.64	0.78
13:o:5052:ALA:HB1	13:o:5230:VAL:H	1.47	0.78
3:C:405:ASN:HD22	30:C:509:DGD:HD5	1.48	0.78
3:C:346:THR:O	13:O:40:GLY:HA2	1.84	0.78
14:T:4:ILE:HG13	24:T:5104:BCR:H383	1.65	0.78
4:D:266:TRP:HD1	28:D:360:MGE:H3D	1.48	0.77
8:I:16:VAL:O	8:I:20:VAL:HG23	1.82	0.77
3:C:67:MET:HE1	20:C:494:CLA:ND	1.99	0.77
17:X:12:UNK:HG3	18:Z:17:PHE:HE1	1.49	0.77
5:E:18:ARG:O	5:E:22:ILE:HG13	1.85	0.77
3:C:39:ASN:HB2	20:C:498:CLA:HBA1	1.66	0.77
3:c:5293:ASN:ND2	3:c:5296:VAL:HG22	1.99	0.77
3:C:186:TYR:O	3:C:230:LEU:HD11	1.84	0.77
3:C:282:MET:HA	3:C:285:ILE:HD12	1.67	0.77
2:b:5027:THR:O	20:b:5515:CLA:HBC1	1.84	0.77
8:i:5016:VAL:O	8:i:5020:VAL:HG23	1.85	0.77
2:B:116:VAL:HG21	24:B:529:BCR:H271	1.67	0.77
1:a:5041:LEU:O	1:a:5045:THR:HG22	1.85	0.77
13:o:5178:ARG:HB2	13:o:5251:MET:HE3	1.65	0.77
13:O:155:THR:HG22	13:O:167:ASP:O	1.86	0.77
1:A:142:TRP:HZ2	3:C:447:ARG:HD2	1.50	0.76
1:a:5076:ASN:ND2	1:a:5079:THR:HG23	2.00	0.76
3:c:5188:THR:HG22	3:c:5364:PRO:HG2	1.67	0.76
15:U:88:VAL:O	15:U:91:VAL:HG23	1.85	0.76
2:b:5018:ARG:HD2	2:b:5115:TRP:CE3	2.20	0.76
4:d:5250:ASN:HD22	4:d:5262:SER:HB3	1.51	0.76
2:B:68:ARG:NH2	20:B:514:CLA:HED1	2.00	0.76
16:V:64:ALA:O	16:V:68:VAL:HG13	1.86	0.76
3:C:255:THR:HG23	3:C:256:PRO:HD2	1.68	0.76
1:A:257:ARG:HG3	1:A:257:ARG:HH11	1.51	0.76
21:A:562:PHO:HMC2	4:D:279:LEU:HD11	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:493:CLA:HMD2	20:C:493:CLA:H191	1.68	0.76
2:B:263:THR:HG21	2:B:448:ARG:NH1	1.99	0.76
15:U:113:THR:CG2	15:U:114:VAL:H	1.94	0.76
6:F:19:ARG:O	6:F:23:VAL:HG23	1.85	0.76
1:a:5022:THR:HG23	1:a:5136:ARG:HH11	1.49	0.76
1:a:5142:TRP:HZ2	3:c:5447:ARG:HD2	1.50	0.76
2:b:5263:THR:CG2	2:b:5448:ARG:HH12	1.97	0.76
2:B:18:ARG:HD2	2:B:115:TRP:CE3	2.21	0.75
13:o:5151:LEU:HD13	13:o:5223:ILE:HD11	1.69	0.75
3:C:342:MET:HE3	3:C:352:GLY:HA2	1.68	0.75
11:l:5014:ARG:HG2	12:m:5026:TYR:HE1	1.50	0.75
3:C:298:PRO:O	3:C:299:SER:HB3	1.85	0.75
21:a:5562:PHO:HBC1	4:d:5275:PRO:HB2	1.68	0.75
13:o:5178:ARG:HG3	13:o:5178:ARG:HH11	1.51	0.75
3:C:276:LEU:HD21	20:C:498:CLA:HBB1	1.69	0.75
1:a:5060:ILE:HG23	1:a:5061:ASP:N	2.01	0.75
4:d:5337:GLU:HG2	4:d:5339:PHE:CZ	2.21	0.75
4:D:266:TRP:CD1	28:D:360:MGE:H3D	2.22	0.75
6:F:34:LEU:HD22	9:J:24:ILE:HD13	1.69	0.75
8:i:5034:ARG:HE	8:i:5034:ARG:N	1.81	0.75
3:c:5027:ASP:HB2	20:c:5501:CLA:HED2	1.68	0.75
2:B:356:VAL:HG22	2:B:370:LEU:HD21	1.69	0.75
4:D:337:GLU:HG2	4:D:339:PHE:CZ	2.22	0.75
3:c:5067:MET:HE1	20:c:5494:CLA:ND	2.02	0.75
1:A:202:VAL:O	1:A:206:PHE:HB2	1.87	0.74
1:a:5272:HIS:CD2	4:d:5218:VAL:HG21	2.22	0.74
13:O:52:ALA:HB1	13:O:230:VAL:H	1.52	0.74
3:c:5103:GLY:HA3	3:c:5301:PHE:HE1	1.52	0.74
3:C:103:GLY:HA3	3:C:301:PHE:HE1	1.51	0.74
6:f:5019:ARG:O	6:f:5023:VAL:HG23	1.86	0.74
3:C:419:PHE:HA	30:C:508:DGD:HE5	1.70	0.74
3:c:5337:LEU:HD23	13:o:5131:PRO:HG3	1.69	0.74
13:o:5092:VAL:HG13	13:o:5093:PRO:HD2	1.67	0.74
20:A:558:CLA:HBB1	20:D:354:CLA:NB	2.02	0.74
3:C:204:LEU:O	3:C:205:ASP:HB3	1.85	0.74
2:b:5116:VAL:HG21	24:b:5529:BCR:H271	1.68	0.74
5:e:5027:ILE:HB	5:e:5028:PRO:HD3	1.70	0.74
4:d:5266:TRP:CD1	28:d:5361:MGE:H3D	2.22	0.74
3:C:241:GLY:C	3:C:243:ILE:H	1.96	0.74
3:c:5039:ASN:HB2	20:c:5498:CLA:HBA1	1.70	0.74
12:M:9:ILE:HD11	12:m:5009:ILE:HD11	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:5002:GLY:HA3	11:l:5011:GLU:OE1	1.88	0.73
1:A:334:ARG:NH2	13:O:185:PRO:HA	2.03	0.73
3:C:188:THR:HG22	3:C:364:PRO:HG2	1.69	0.73
7:H:11:LEU:C	7:H:13:PRO:HD2	2.14	0.73
13:O:178:ARG:HB2	13:O:251:MET:HE3	1.69	0.73
1:A:81:ALA:HB2	1:A:175:GLY:HA3	1.70	0.73
3:C:449:ARG:HH22	8:I:27:ASP:HB3	1.51	0.73
12:m:5025:LEU:O	12:m:5028:GLN:HG3	1.89	0.73
2:B:191:ASN:HD22	2:B:192:PRO:HD2	1.53	0.73
15:U:50:ALA:HB3	15:U:113:THR:HG21	1.70	0.73
1:A:309:ALA:HB3	16:V:28:GLU:HG3	1.68	0.73
2:b:5271:THR:CG2	2:b:5273:TYR:H	2.02	0.73
2:B:27:THR:O	20:B:515:CLA:HBC1	1.89	0.73
15:U:83:ALA:HB1	15:U:84:PRO:CD	2.19	0.72
13:O:144:LEU:H	13:O:144:LEU:HD23	1.54	0.72
20:a:5558:CLA:HBB1	20:d:5354:CLA:NB	2.03	0.72
2:B:306:PRO:HG2	2:B:309:LEU:HB2	1.71	0.72
4:D:330:ALA:HB3	4:D:331:PRO:HD3	1.71	0.72
21:A:562:PHO:HBC1	4:D:275:PRO:HB2	1.71	0.72
3:C:204:LEU:H	3:C:204:LEU:CD2	2.02	0.72
4:D:250:ASN:HD22	4:D:262:SER:HB3	1.53	0.72
5:E:17:VAL:O	5:E:21:VAL:HG23	1.89	0.72
15:u:5083:ALA:HB1	15:u:5084:PRO:CD	2.19	0.72
15:u:5094:ILE:HB	15:u:5097:LEU:HD11	1.71	0.72
3:C:62:PHE:HE2	10:K:29:PRO:HD3	1.54	0.72
3:c:5186:TYR:O	3:c:5230:LEU:HD11	1.89	0.72
15:u:5050:ALA:HB3	15:u:5113:THR:HG21	1.71	0.72
2:b:5191:ASN:HD22	2:b:5192:PRO:HD2	1.52	0.72
3:C:337:LEU:HD23	13:O:131:PRO:HG3	1.71	0.72
3:c:5298:PRO:O	3:c:5299:SER:HB3	1.90	0.72
3:C:464:GLU:CB	3:C:467:LEU:HD12	2.20	0.72
16:V:81:ARG:CZ	16:V:157:GLY:HA3	2.20	0.72
21:a:5562:PHO:HMC2	4:d:5279:LEU:HD11	1.70	0.72
24:c:5506:BCR:H332	8:i:5020:VAL:HG13	1.71	0.72
3:C:29:GLU:HB3	10:K:46:ARG:O	1.89	0.72
24:C:506:BCR:H332	8:I:20:VAL:HG13	1.71	0.72
3:c:5150:ASP:O	3:c:5153:ASP:HB3	1.90	0.72
20:c:5493:CLA:HMD2	20:c:5493:CLA:H191	1.72	0.72
5:e:5058:GLN:HE22	16:v:5028:GLU:HA	1.54	0.72
7:h:5011:LEU:C	7:h:5013:PRO:HD2	2.15	0.71
1:a:5224:ILE:HG22	2:b:5484:PRO:HG3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:5081:ALA:HB2	1:a:5175:GLY:HA3	1.72	0.71
3:C:293:ASN:ND2	3:C:296:VAL:H	1.87	0.71
3:C:334:PRO:HA	13:O:179:THR:HB	1.72	0.71
15:U:66:ILE:HG12	15:U:72:TYR:CG	2.25	0.71
2:B:271:THR:HG23	2:B:273:TYR:H	1.56	0.71
7:H:6:TRP:CE2	7:H:10:ILE:HD11	2.25	0.71
3:c:5453:ALA:HB1	8:i:5031:ASN:ND2	2.04	0.71
1:A:224:ILE:HG22	2:B:484:PRO:HG3	1.71	0.71
10:K:17:ILE:HD11	18:Z:6:GLN:HE21	1.56	0.71
2:B:471:ALA:HB2	4:D:130:PHE:CZ	2.26	0.71
1:A:260:PHE:CE1	1:A:263:ALA:HB2	2.25	0.71
3:C:293:ASN:HD22	3:C:296:VAL:HG22	1.55	0.71
2:b:5371:THR:HG22	2:b:5377:VAL:HA	1.73	0.71
1:a:5047:CYS:SG	1:a:5114:LEU:HD23	2.30	0.70
1:a:5202:VAL:O	1:a:5206:PHE:HB2	1.91	0.70
2:b:5471:ALA:HB2	4:d:5130:PHE:CZ	2.26	0.70
3:c:5466:VAL:CA	3:c:5469:MET:HE3	2.21	0.70
4:D:36:LEU:O	4:D:39:PRO:HD2	1.89	0.70
14:T:4:ILE:C	14:T:4:ILE:HD13	2.16	0.70
3:c:5363:GLY:O	3:c:5367:GLU:HG2	1.91	0.70
2:B:263:THR:CG2	2:B:448:ARG:HH12	2.02	0.70
3:C:56:HIS:C	3:C:58:GLY:H	1.99	0.70
3:C:466:VAL:CA	3:C:469:MET:HE3	2.21	0.70
1:a:5334:ARG:NH2	13:o:5185:PRO:HA	2.07	0.70
10:k:5017:ILE:CD1	18:z:5006:GLN:HE21	2.04	0.70
2:b:5306:PRO:HG2	2:b:5309:LEU:HB2	1.72	0.70
4:D:160:TYR:HB3	4:D:161:PRO:CD	2.19	0.70
4:D:267:LEU:HD23	4:D:267:LEU:C	2.17	0.70
1:A:306:VAL:HG21	1:A:316:THR:HG23	1.74	0.70
20:a:5558:CLA:H143	21:a:5561:PHO:H62	1.72	0.70
4:d:5036:LEU:O	4:d:5039:PRO:HD2	1.92	0.70
1:a:5072:LEU:CD2	14:t:5003:THR:HG21	2.21	0.70
15:u:5058:ASN:ND2	15:u:5114:VAL:HG13	2.07	0.70
16:v:5039:ASN:HD21	16:v:5041:GLU:HB2	1.55	0.70
1:A:272:HIS:CD2	4:D:218:VAL:HG21	2.26	0.70
7:h:5006:TRP:CE2	7:h:5010:ILE:HD11	2.26	0.70
10:k:5035:LEU:HD22	17:x:5017:UNK:CB	2.22	0.70
12:M:25:LEU:O	12:M:28:GLN:HG3	1.92	0.69
13:O:178:ARG:HH11	13:O:178:ARG:HG3	1.56	0.69
14:t:5004:ILE:HG13	24:t:104:BCR:H383	1.74	0.69
14:t:5004:ILE:C	14:t:5004:ILE:HD13	2.16	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:5253:GLY:O	1:a:5257:ARG:HD2	1.92	0.69
1:a:5260:PHE:CE1	1:a:5263:ALA:HB2	2.27	0.69
1:a:5306:VAL:HG23	1:a:5306:VAL:O	1.91	0.69
3:c:5255:THR:HG23	3:c:5256:PRO:HD2	1.74	0.69
2:B:124:ARG:HG3	2:B:124:ARG:NH1	2.07	0.69
21:A:562:PHO:H42	4:D:41:ALA:HB1	1.74	0.69
2:B:271:THR:CG2	2:B:273:TYR:H	2.04	0.69
2:B:371:THR:HG22	2:B:377:VAL:HA	1.73	0.69
1:a:5016:ARG:HD3	1:a:5017:PHE:N	2.07	0.69
4:d:5253:TRP:HA	4:d:5256:ILE:HG22	1.74	0.69
3:c:5293:ASN:ND2	3:c:5296:VAL:H	1.90	0.69
2:B:386:ALA:HB3	15:U:132:LEU:HD11	1.74	0.69
10:K:17:ILE:CD1	18:Z:6:GLN:HE21	2.05	0.69
1:a:5297:LEU:HD12	3:c:5428:THR:HG21	1.75	0.69
3:c:5334:PRO:HA	13:o:5179:THR:HB	1.74	0.69
18:Z:21:ILE:O	18:Z:25:VAL:HG23	1.91	0.69
13:o:5032:THR:H	13:o:5035:ASP:HB2	1.57	0.69
13:O:73:PRO:CG	13:O:102:THR:HB	2.22	0.69
2:b:5362:PHE:CE1	4:d:5184:PHE:HZ	2.10	0.69
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.75	0.69
3:C:453:ALA:HB1	8:I:31:ASN:ND2	2.08	0.69
20:C:495:CLA:HBD	20:C:495:CLA:HBA1	1.75	0.69
1:a:5309:ALA:HB3	16:v:5028:GLU:HG3	1.74	0.69
5:e:5015:THR:HG23	9:j:5008:ILE:O	1.93	0.69
1:A:305:SER:O	1:A:306:VAL:C	2.35	0.69
3:C:214:LEU:HD23	3:C:214:LEU:H	1.58	0.69
11:L:14:ARG:HG2	12:M:26:TYR:HE1	1.58	0.69
1:A:129:ARG:NH2	4:D:256:ILE:HA	2.08	0.68
18:Z:15:LEU:HD23	18:Z:50:LEU:HD12	1.75	0.68
2:b:5133:LEU:HA	7:h:5015:ASN:HD21	1.56	0.68
20:A:559:CLA:HED2	4:D:198:MET:SD	2.33	0.68
27:A:569:LMT:H92	2:b:5098:LEU:HD13	1.72	0.68
2:b:5356:VAL:HG22	2:b:5370:LEU:CD2	2.23	0.68
20:c:5501:CLA:H151	18:z:5020:VAL:HG13	1.76	0.68
2:B:126:PRO:HG3	7:H:12:ARG:NH2	2.09	0.68
3:C:84:GLN:HB2	3:C:86:LEU:HD22	1.75	0.68
1:A:22:THR:HG23	1:A:136:ARG:HH11	1.59	0.68
1:A:322:ASN:ND2	3:C:412:THR:HA	2.05	0.68
3:C:363:GLY:O	3:C:367:GLU:HG2	1.93	0.68
4:d:5267:LEU:HD23	4:d:5267:LEU:C	2.19	0.68
2:B:344:ALA:HB2	2:B:401:PHE:CE1	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:84:SER:HB2	5:E:68:ASP:HA	1.74	0.68
5:E:58:GLN:HE22	16:V:28:GLU:HA	1.58	0.68
1:a:5260:PHE:CZ	1:a:5263:ALA:HB2	2.29	0.68
21:a:5562:PHO:H42	4:d:5041:ALA:HB1	1.76	0.68
2:b:5353:GLU:HB3	2:b:5373:LYS:NZ	2.09	0.68
3:c:5204:LEU:O	3:c:5205:ASP:HB3	1.93	0.68
4:d:5089:LEU:HG	7:h:5050:ASN:OD1	1.93	0.68
2:B:362:PHE:CE1	4:D:184:PHE:HZ	2.11	0.68
24:C:505:BCR:H312	18:Z:55:GLY:HA2	1.75	0.68
4:D:36:LEU:C	4:D:39:PRO:HD2	2.19	0.68
3:c:5419:PHE:HA	30:c:5508:DGD:HE5	1.75	0.68
5:e:5060:GLN:HG3	5:e:5060:GLN:O	1.93	0.68
1:A:270:SER:HA	4:D:232:PHE:CE2	2.29	0.68
3:c:5248:GLY:O	3:c:5252:ILE:HG13	1.93	0.68
13:O:36:ILE:HG23	13:O:41:LEU:HB2	1.76	0.68
20:a:5559:CLA:HED2	4:d:5198:MET:SD	2.33	0.68
3:c:5029:GLU:HB3	10:k:5046:ARG:O	1.92	0.68
3:c:5090:PRO:O	3:c:5094:THR:HG23	1.94	0.68
12:M:9:ILE:HG13	12:m:5009:ILE:HG13	1.75	0.68
2:b:5231:MET:HG3	20:b:5520:CLA:HAC2	1.75	0.68
20:c:5495:CLA:HBD	20:c:5495:CLA:HBA1	1.76	0.68
4:d:5036:LEU:C	4:d:5039:PRO:HD2	2.18	0.68
15:u:5066:ILE:HG12	15:u:5072:TYR:CG	2.28	0.68
1:a:5049:VAL:O	1:a:5053:ILE:HG13	1.94	0.67
3:c:5293:ASN:HD22	3:c:5296:VAL:HG22	1.58	0.67
3:c:5464:GLU:CB	3:c:5467:LEU:HD12	2.23	0.67
5:e:5078:THR:O	5:e:5082:GLN:HG2	1.94	0.67
10:k:5017:ILE:HD11	18:z:5006:GLN:HE21	1.58	0.67
17:x:5051:UNK:O	17:x:5052:UNK:C	2.41	0.67
1:A:47:CYS:SG	1:A:114:LEU:HD23	2.34	0.67
5:E:4:THR:HG23	17:X:90:UNK:CD2	2.24	0.67
2:B:231:MET:HG3	20:B:520:CLA:HAC2	1.75	0.67
2:B:246:PHE:CD1	2:B:246:PHE:C	2.72	0.67
5:E:23:HIS:C	5:E:25:ILE:H	2.02	0.67
15:U:89:GLU:CD	15:U:89:GLU:H	2.02	0.67
1:A:72:LEU:CD2	14:T:3:THR:HG21	2.23	0.67
2:B:222:PRO:HG3	7:H:27:THR:H	1.60	0.67
3:C:124:VAL:HB	24:C:505:BCR:H362	1.77	0.67
1:a:5257:ARG:HH12	1:a:5261:GLN:CD	2.02	0.67
2:b:5246:PHE:C	2:b:5246:PHE:CD1	2.72	0.67
4:D:161:PRO:CG	4:D:170:ALA:HB2	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:261:PHE:O	4:D:262:SER:HB3	1.94	0.67
18:z:5021:ILE:O	18:z:5025:VAL:HG23	1.94	0.67
2:B:191:ASN:HD22	2:B:192:PRO:CD	2.07	0.67
4:D:89:LEU:HG	7:H:50:ASN:OD1	1.95	0.67
3:c:5062:PHE:HE2	10:k:5029:PRO:HD3	1.59	0.67
5:e:5010:PHE:HA	5:e:5013:ILE:HG22	1.77	0.67
13:o:5111:LEU:HD11	13:o:5119:LEU:HB3	1.77	0.67
13:O:234:THR:OG1	13:O:236:GLU:HG2	1.95	0.67
20:c:5495:CLA:CMD	20:c:5497:CLA:HAB	2.25	0.67
13:O:163:THR:H	13:O:166:THR:HG23	1.60	0.67
2:b:5126:PRO:HG3	7:h:5012:ARG:NH2	2.10	0.67
5:e:5017:VAL:O	5:e:5021:VAL:HG23	1.94	0.67
6:f:5034:LEU:HD22	9:j:5024:ILE:HD13	1.76	0.67
6:f:5037:ILE:HG22	9:j:5028:PHE:CE1	2.30	0.67
15:u:5089:GLU:H	15:u:5089:GLU:CD	2.03	0.67
16:v:5095:ILE:O	16:v:5099:VAL:HG23	1.95	0.67
1:A:297:LEU:HD12	3:C:428:THR:HG21	1.75	0.67
2:B:223:GLN:HA	7:H:21:VAL:HG21	1.75	0.67
3:C:150:ASP:O	3:C:153:ASP:HB3	1.96	0.67
5:E:40:THR:HG21	17:X:102:UNK:CB	2.25	0.67
17:X:54:UNK:HB1	17:X:57:UNK:CG2	2.25	0.67
1:a:5305:SER:O	1:a:5306:VAL:C	2.38	0.66
13:o:5036:ILE:HG23	13:o:5041:LEU:HB2	1.75	0.66
3:C:153:ASP:O	3:C:155:ASN:N	2.28	0.66
3:C:210:PHE:O	3:C:213:LEU:HB2	1.95	0.66
1:a:5188:ALA:HB2	1:a:5328:MET:HB2	1.77	0.66
2:b:5392:PHE:O	2:b:5393:GLU:HB2	1.96	0.66
2:b:5463:PHE:HZ	20:b:5518:CLA:HBB1	1.60	0.66
3:c:5449:ARG:NH2	8:i:5027:ASP:HB3	2.08	0.66
2:B:353:GLU:HB3	2:B:373:LYS:NZ	2.10	0.66
2:b:5271:THR:HG23	2:b:5273:TYR:H	1.59	0.66
1:A:60:ILE:HG23	1:A:61:ASP:N	2.09	0.66
10:K:35:LEU:HD22	17:X:17:UNK:CB	2.26	0.66
2:b:5018:ARG:HH11	2:b:5018:ARG:HG3	1.59	0.66
7:h:5012:ARG:N	7:h:5013:PRO:HD2	2.11	0.66
17:x:5054:UNK:HB1	17:x:5057:UNK:CG2	2.25	0.66
4:d:5062:GLY:H	4:d:5063:LEU:HD12	1.59	0.66
13:o:5144:LEU:HD23	13:o:5144:LEU:H	1.60	0.66
13:O:32:THR:H	13:O:35:ASP:HB2	1.61	0.66
1:a:5064:ARG:C	1:a:5066:PRO:HD3	2.20	0.66
3:c:5241:GLY:C	3:c:5243:ILE:H	2.04	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:5010:PHE:O	5:e:5013:ILE:HG22	1.95	0.66
3:C:159:THR:HG23	3:C:252:ILE:HG23	1.78	0.66
5:E:27:ILE:HB	5:E:28:PRO:HD3	1.78	0.66
10:k:5039:TRP:NE1	17:x:5031:UNK:HG3	2.08	0.66
13:o:5073:PRO:CG	13:o:5102:THR:HB	2.24	0.66
3:c:5370:ARG:HD3	13:o:5033:TYR:CD2	2.31	0.66
4:d:5084:SER:HB2	5:e:5068:ASP:HA	1.77	0.66
2:B:68:ARG:NH1	2:B:262:THR:HG23	2.11	0.66
20:B:515:CLA:H141	20:B:520:CLA:HMA1	1.77	0.66
3:c:5214:LEU:H	3:c:5214:LEU:HD23	1.61	0.66
1:a:5129:ARG:NH2	4:d:5256:ILE:HA	2.11	0.65
20:b:5515:CLA:H141	20:b:5520:CLA:HMA1	1.78	0.65
5:e:5022:ILE:HG23	17:x:5116:UNK:HA	1.78	0.65
6:f:5028:VAL:HB	6:f:5029:PRO:HD3	1.77	0.65
7:h:5029:PRO:O	7:h:5033:VAL:HG23	1.95	0.65
1:A:64:ARG:C	1:A:66:PRO:HD3	2.21	0.65
2:B:297:THR:CB	2:B:300:GLU:HG3	2.26	0.65
2:B:463:PHE:HZ	20:B:518:CLA:HBB1	1.61	0.65
5:E:10:PHE:O	5:E:13:ILE:HG22	1.95	0.65
13:O:77:LEU:HD12	13:O:77:LEU:N	2.10	0.65
24:X:130:BCR:HC8	24:X:130:BCR:H331	1.78	0.65
24:c:5505:BCR:H312	18:z:5055:GLY:HA2	1.76	0.65
10:K:23:ASP:OD2	17:X:6:UNK:NE2	2.34	0.65
3:c:5158:THR:HG22	3:c:5251:HIS:O	1.96	0.65
18:z:5015:LEU:HD23	18:z:5050:LEU:HD12	1.78	0.65
1:A:81:ALA:CB	1:A:175:GLY:HA3	2.25	0.65
2:B:356:VAL:HG22	2:B:370:LEU:CD2	2.25	0.65
5:E:22:ILE:HG23	17:X:116:UNK:HA	1.78	0.65
1:a:5094:TYR:OH	1:a:5104:GLU:HG2	1.97	0.65
1:a:5134:SER:HB2	1:a:5139:MET:HG3	1.79	0.65
3:c:5084:GLN:HB2	3:c:5086:LEU:HD22	1.77	0.65
16:v:5038:LEU:HD13	16:v:5045:ILE:CD1	2.24	0.65
2:b:5191:ASN:HD22	2:b:5192:PRO:CD	2.09	0.65
3:c:5035:TRP:NE1	3:c:5036:TRP:HD1	1.95	0.65
1:A:270:SER:HA	4:D:232:PHE:HE2	1.61	0.65
2:b:5124:ARG:HG3	2:b:5124:ARG:NH1	2.07	0.65
3:c:5056:HIS:C	3:c:5058:GLY:H	2.02	0.65
4:d:5068:LEU:HD13	6:f:5040:MET:HE2	1.79	0.65
10:K:28:ILE:O	10:K:31:LEU:HB2	1.97	0.65
1:a:5081:ALA:CB	1:a:5175:GLY:HA3	2.26	0.65
1:A:76:ASN:ND2	1:A:79:THR:H	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:GLY:HA3	2:B:266:GLU:OE1	1.96	0.65
17:X:51:UNK:O	17:X:52:UNK:C	2.44	0.65
3:c:5342:MET:HE3	3:c:5352:GLY:CA	2.27	0.65
3:c:5343:ARG:HB2	13:o:5101:THR:HG23	1.79	0.65
4:d:5229:ALA:O	4:d:5231:THR:HG23	1.97	0.65
16:v:5049:GLU:O	16:v:5053:LEU:HG	1.97	0.65
20:A:558:CLA:H143	21:A:561:PHO:H62	1.78	0.65
2:B:133:LEU:HA	7:H:15:ASN:HD21	1.62	0.65
1:a:5243:GLU:HA	4:d:5241:GLU:HA	1.79	0.65
3:c:5210:PHE:O	3:c:5213:LEU:HB2	1.97	0.65
5:e:5023:HIS:C	5:e:5025:ILE:H	2.05	0.65
1:A:94:TYR:OH	1:A:104:GLU:HG2	1.97	0.65
5:E:78:THR:O	5:E:82:GLN:HG2	1.97	0.65
2:b:5386:ALA:HB3	15:u:5132:LEU:HD11	1.77	0.65
24:x:5130:BCR:HC8	24:x:5130:BCR:H331	1.77	0.65
2:B:222:PRO:HG3	7:H:26:GLY:HA3	1.80	0.64
2:B:392:PHE:O	2:B:393:GLU:HB2	1.96	0.64
20:C:501:CLA:H151	18:Z:20:VAL:HG13	1.78	0.64
1:a:5257:ARG:HG3	1:a:5257:ARG:NH1	2.12	0.64
2:b:5010:THR:O	2:b:5013:ILE:HG13	1.97	0.64
2:b:5176:GLY:HA3	2:b:5266:GLU:OE1	1.96	0.64
3:c:5453:ALA:HA	8:i:5034:ARG:HA	1.80	0.64
16:v:5121:LEU:HD11	16:v:5138:LEU:HD11	1.79	0.64
1:A:260:PHE:CZ	1:A:263:ALA:HB2	2.33	0.64
4:D:253:TRP:HA	4:D:256:ILE:HG22	1.80	0.64
2:b:5223:GLN:HA	7:h:5021:VAL:HG21	1.78	0.64
4:d:5330:ALA:HB3	4:d:5331:PRO:HD3	1.80	0.64
3:C:265:ILE:HD13	20:C:495:CLA:HED1	1.78	0.64
16:v:5124:ALA:HB1	16:v:5131:ARG:HG3	1.79	0.64
3:C:449:ARG:NH2	8:I:27:ASP:HB3	2.12	0.64
2:b:5062:VAL:HG12	2:b:5066:MET:HE2	1.80	0.64
13:o:5077:LEU:N	13:o:5077:LEU:HD12	2.12	0.64
2:B:223:GLN:HE22	2:B:227:LYS:HD3	1.62	0.64
4:D:210:LEU:HD21	22:D:356:PQ9:H17	1.80	0.64
6:F:37:ILE:HG22	9:J:28:PHE:CE1	2.33	0.64
1:a:5315:ASN:O	4:d:5063:LEU:HB3	1.97	0.64
3:c:5204:LEU:H	3:c:5204:LEU:CD2	2.06	0.64
3:c:5265:ILE:HG22	3:c:5270:ALA:CB	2.28	0.64
20:C:495:CLA:CMD	20:C:497:CLA:HAB	2.27	0.64
16:V:119:PRO:HA	16:V:127:PHE:CD2	2.33	0.64
3:c:5107:ASP:OD1	3:c:5110:PRO:HD3	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:5279:LEU:HD22	20:d:5354:CLA:HBA2	1.80	0.64
10:k:5028:ILE:O	10:k:5031:LEU:HB2	1.97	0.64
13:o:5110:GLU:HG3	13:o:5110:GLU:O	1.97	0.64
16:v:5039:ASN:ND2	16:v:5041:GLU:HB2	2.12	0.64
2:B:223:GLN:HE22	2:B:227:LYS:CD	2.10	0.64
13:O:92:VAL:HG12	13:O:93:PRO:HD2	1.80	0.64
3:c:5276:LEU:HD21	20:c:5498:CLA:HBB1	1.79	0.64
1:A:134:SER:HB2	1:A:139:MET:HG3	1.79	0.63
1:A:187:GLN:HG3	1:A:325:ASN:OD1	1.98	0.63
16:V:95:ILE:O	16:V:99:VAL:HG23	1.97	0.63
3:c:5405:ASN:HD22	30:c:5509:DGD:C5D	2.11	0.63
5:e:5040:THR:HG21	17:x:5102:UNK:CB	2.28	0.63
3:C:34:ALA:HB2	4:D:230:SER:HB3	1.81	0.63
24:C:504:BCR:H343	24:C:504:BCR:H311	1.81	0.63
24:C:504:BCR:H391	10:K:36:ALA:HB2	1.79	0.63
7:H:12:ARG:N	7:H:13:PRO:HD2	2.13	0.63
13:O:184:ASP:HB2	13:O:185:PRO:HD2	1.80	0.63
3:c:5260:ALA:O	3:c:5264:PHE:HD2	1.81	0.63
4:d:5160:TYR:HB3	4:d:5161:PRO:CD	2.23	0.63
5:e:5014:ILE:CG2	9:j:5013:VAL:HG11	2.29	0.63
1:A:243:GLU:HA	4:D:241:GLU:HA	1.80	0.63
4:D:229:ALA:O	4:D:231:THR:HG23	1.97	0.63
16:V:49:GLU:O	16:V:53:LEU:HG	1.98	0.63
24:c:5504:BCR:H391	10:k:5036:ALA:HB2	1.79	0.63
4:d:5348:ARG:HH21	4:d:5352:LEU:C	2.06	0.63
7:h:5006:TRP:O	7:h:5010:ILE:HG13	1.97	0.63
7:h:5043:LEU:HD23	17:x:5060:UNK:CZ	2.29	0.63
1:a:5322:ASN:ND2	3:c:5412:THR:HA	2.06	0.63
20:c:5501:CLA:H171	18:z:5020:VAL:HA	1.81	0.63
18:z:5016:SER:O	18:z:5020:VAL:HG23	1.99	0.63
1:A:304:HIS:CD2	3:C:414:ILE:HD11	2.34	0.63
3:C:248:GLY:O	3:C:252:ILE:HG13	1.97	0.63
3:C:343:ARG:HB2	13:O:101:THR:HG23	1.80	0.63
2:b:5068:ARG:NH1	2:b:5262:THR:HG23	2.14	0.63
3:c:5223:TRP:CD2	3:c:5224:ILE:HG13	2.34	0.63
13:o:5168:PHE:N	13:o:5168:PHE:CD1	2.67	0.63
3:C:224:ILE:O	3:C:227:VAL:HG23	1.98	0.63
4:D:62:GLY:H	4:D:63:LEU:HD12	1.64	0.63
4:D:87:HIS:CD2	4:D:166:SER:HA	2.34	0.63
4:D:200:GLY:HA2	4:D:278:GLY:O	1.99	0.63
7:H:43:LEU:HD23	17:X:60:UNK:CZ	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:76:PHE:C	13:O:77:LEU:HD12	2.23	0.63
16:V:38:LEU:HD13	16:V:45:ILE:CD1	2.29	0.63
1:A:16:ARG:HD3	1:A:17:PHE:N	2.14	0.63
3:C:417:VAL:HG22	3:C:417:VAL:O	1.99	0.63
13:O:45:CYS:HB2	13:O:46:PRO:CD	2.27	0.63
15:U:82:ASN:HB2	15:U:85:TYR:OH	1.99	0.63
2:b:5055:MET:HE3	2:b:5080:ILE:HG12	1.81	0.63
3:c:5153:ASP:C	3:c:5155:ASN:H	2.06	0.63
29:c:5474:UNL:C15	22:d:5356:PQ9:H293	2.29	0.63
3:C:158:THR:HG22	3:C:251:HIS:O	1.99	0.63
7:H:6:TRP:O	7:H:10:ILE:HG13	1.99	0.63
13:o:5204:LYS:HB3	13:o:5206:GLU:HG2	1.81	0.63
12:M:28:GLN:OE1	12:m:5036:SER:OXT	2.16	0.62
13:o:5155:THR:HG22	13:o:5167:ASP:O	1.99	0.62
5:E:57:ALA:O	5:E:59:GLU:N	2.32	0.62
16:V:135:GLU:O	16:V:139:VAL:HG23	1.98	0.62
16:v:5031:PRO:HA	16:v:5034:LEU:HD12	1.79	0.62
9:J:15:THR:HG21	10:K:38:VAL:HG13	1.81	0.62
13:O:110:GLU:HG3	13:O:110:GLU:O	1.99	0.62
13:o:5076:PHE:C	13:o:5077:LEU:HD12	2.24	0.62
13:o:5145:LEU:O	13:o:5147:THR:HG22	1.98	0.62
2:B:55:MET:HE3	2:B:80:ILE:HG12	1.81	0.62
1:A:40:THR:HG21	1:A:121:LEU:HB3	1.81	0.62
2:b:5357:ARG:NH2	4:d:5337:GLU:HG3	2.14	0.62
5:E:60:GLN:C	5:E:62:SER:H	2.07	0.62
13:O:45:CYS:H	13:O:72:GLN:HE22	1.48	0.62
3:c:5400:PRO:C	3:c:5401:LEU:HD23	2.24	0.62
20:C:501:CLA:H171	18:Z:20:VAL:HA	1.79	0.62
3:c:5034:ALA:HB2	4:d:5230:SER:HB3	1.81	0.62
1:A:72:LEU:HD23	14:T:3:THR:HG21	1.82	0.62
2:B:2:GLY:HA3	11:L:11:GLU:OE1	2.00	0.62
4:D:103:ARG:NH1	5:E:77:GLU:HG3	2.15	0.62
13:O:183:LEU:HD22	13:O:187:GLY:O	1.99	0.62
16:v:5081:ARG:HH11	16:v:5081:ARG:HG3	1.64	0.62
3:c:5159:THR:HG23	3:c:5252:ILE:HG23	1.82	0.62
18:z:5005:PHE:CA	18:z:5057:LEU:HD13	2.28	0.62
3:C:55:ALA:HB1	24:C:504:BCR:H373	1.82	0.62
4:D:90:LEU:HD23	4:D:109:GLY:HA2	1.81	0.62
10:K:18:PHE:O	10:K:19:ASP:C	2.43	0.62
11:L:20:GLY:HA3	12:M:22:LEU:CD1	2.30	0.62
13:O:46:PRO:HB2	13:O:266:TYR:CG	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:c:5491:CLA:HMB2	24:c:5506:BCR:H403	1.82	0.62
13:o:5033:TYR:C	13:o:5035:ASP:H	2.08	0.62
1:A:253:GLY:O	1:A:257:ARG:HD2	2.00	0.61
2:B:357:ARG:NH2	4:D:337:GLU:HG3	2.14	0.61
17:X:28:UNK:CG2	18:Z:29:SER:HA	2.30	0.61
1:a:5025:ASP:HB3	4:d:5251:ARG:HH22	1.65	0.61
3:c:5230:LEU:O	3:c:5234:VAL:HG23	2.00	0.61
10:k:5023:ASP:OD2	17:x:5006:UNK:NE2	2.38	0.61
1:A:49:VAL:O	1:A:53:ILE:HG13	2.00	0.61
6:F:41:GLN:HE21	6:F:41:GLN:HA	1.64	0.61
1:a:5304:HIS:CD2	3:c:5414:ILE:HD11	2.36	0.61
13:o:5172:PHE:CE2	13:o:5223:ILE:HG12	2.35	0.61
13:o:5179:THR:CG2	13:o:5180:ALA:N	2.62	0.61
18:z:5015:LEU:O	18:z:5019:MET:HG2	2.00	0.61
2:B:329:PRO:CB	20:B:517:CLA:HED1	2.26	0.61
3:C:35:TRP:NE1	3:C:36:TRP:HD1	1.99	0.61
17:X:26:UNK:NE2	17:X:26:UNK:HG2	2.20	0.61
2:b:5263:THR:HG22	2:b:5448:ARG:NH2	2.12	0.61
2:b:5297:THR:CB	2:b:5300:GLU:HG3	2.29	0.61
13:o:5046:PRO:HB2	13:o:5266:TYR:CG	2.36	0.61
16:v:5135:GLU:O	16:v:5139:VAL:HG23	2.01	0.61
1:A:25:ASP:HB3	4:D:251:ARG:HH22	1.65	0.61
1:a:5187:GLN:HG3	1:a:5325:ASN:OD1	2.01	0.61
2:b:5031:ALA:HB3	2:b:5104:SER:HB3	1.80	0.61
2:b:5222:PRO:HG3	7:h:5027:THR:H	1.65	0.61
6:f:5031:ILE:HG13	32:f:5051:HEM:HMC2	1.81	0.61
11:l:5020:GLY:HA3	12:m:5022:LEU:CD1	2.30	0.61
6:F:41:GLN:HA	6:F:41:GLN:NE2	2.15	0.61
3:c:5103:GLY:HA3	3:c:5301:PHE:CE1	2.36	0.61
3:C:90:PRO:O	3:C:94:THR:HG23	2.01	0.61
6:F:31:ILE:HG13	32:F:51:HEM:HMC2	1.82	0.61
15:U:73:PRO:HB2	16:V:109:ASP:CG	2.26	0.61
16:V:39:ASN:HD21	16:V:41:GLU:HB2	1.64	0.61
20:c:5495:CLA:HMD2	20:c:5497:CLA:HAB	1.81	0.61
4:d:5100:ASP:OD1	4:d:5102:THR:HG22	2.01	0.61
13:o:5112:LYS:HE2	13:o:5114:ASN:HB3	1.82	0.61
1:A:142:TRP:CZ2	3:C:447:ARG:HD2	2.34	0.61
2:B:247:PHE:O	2:B:251:VAL:HG23	2.00	0.61
3:C:298:PRO:O	3:C:299:SER:CB	2.48	0.61
5:E:10:PHE:HA	5:E:13:ILE:HG22	1.83	0.61
7:H:21:VAL:HG22	7:H:22:ALA:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:36:SER:O	11:l:5010:VAL:HG23	2.00	0.61
15:U:73:PRO:HB2	16:V:109:ASP:OD2	2.01	0.61
1:a:5013:LEU:N	1:a:5013:LEU:HD23	2.15	0.61
3:c:5377:LEU:HB2	13:o:5106:GLN:HG2	1.83	0.61
10:k:5039:TRP:HE1	17:x:5031:UNK:CG	2.10	0.61
17:x:5028:UNK:CG2	18:z:5029:SER:HA	2.30	0.61
13:O:144:LEU:HD13	13:O:259:VAL:HG11	1.82	0.61
2:b:5134:ASP:H	7:h:5015:ASN:ND2	1.99	0.61
3:c:5428:THR:HG22	3:c:5429:SER:N	2.16	0.61
4:d:5090:LEU:HD23	4:d:5109:GLY:HA2	1.81	0.61
5:e:5004:THR:HG23	17:x:5090:UNK:CD2	2.30	0.61
15:u:5082:ASN:HB2	15:u:5085:TYR:OH	2.00	0.61
2:B:31:ALA:HB2	20:B:515:CLA:HBC3	1.83	0.61
5:E:14:ILE:CG2	9:J:13:VAL:HG11	2.31	0.61
6:F:28:VAL:HB	6:F:29:PRO:HD3	1.83	0.61
1:a:5222:SER:O	1:a:5246:TYR:HB2	2.00	0.61
3:c:5456:GLU:N	3:c:5456:GLU:OE1	2.33	0.61
4:d:5161:PRO:CG	4:d:5170:ALA:HB2	2.28	0.61
5:e:5076:VAL:O	5:e:5079:PHE:HB2	2.01	0.61
6:f:5041:GLN:HA	6:f:5041:GLN:HE21	1.66	0.61
10:k:5018:PHE:O	10:k:5019:ASP:C	2.44	0.61
15:u:5072:TYR:CB	15:u:5073:PRO:HD3	2.30	0.61
16:v:5104:ASN:HD21	16:v:5113:GLU:CD	2.09	0.61
2:B:185:TRP:HH2	2:B:203:ILE:HG21	1.66	0.61
3:C:342:MET:HE3	3:C:352:GLY:CA	2.31	0.61
29:C:474:UNL:C15	22:D:356:PQ9:H293	2.31	0.61
2:b:5223:GLN:HE22	2:b:5227:LYS:HD3	1.65	0.61
4:d:5337:GLU:HG2	4:d:5339:PHE:CE2	2.36	0.61
5:e:5058:GLN:NE2	16:v:5028:GLU:HA	2.16	0.61
5:e:5060:GLN:C	5:e:5062:SER:H	2.08	0.61
3:C:279:LEU:HA	3:C:282:MET:HE3	1.82	0.60
13:O:128:ASP:OD2	13:O:149:LYS:HG2	2.01	0.60
13:O:144:LEU:CD1	13:O:259:VAL:HG11	2.31	0.60
1:a:5040:THR:HG21	1:a:5121:LEU:HB3	1.82	0.60
4:d:5325:ILE:O	4:d:5329:MET:HB3	2.02	0.60
16:v:5119:PRO:HA	16:v:5127:PHE:CD2	2.36	0.60
1:A:257:ARG:HG3	1:A:257:ARG:NH1	2.16	0.60
2:B:271:THR:HG22	2:B:274:GLN:H	1.64	0.60
5:E:56:TYR:HB3	5:E:60:GLN:HG3	1.83	0.60
3:c:5279:LEU:HA	3:c:5282:MET:HE3	1.83	0.60
5:e:5036:LEU:HA	5:e:5039:SER:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:u:5066:ILE:HG22	15:u:5066:ILE:O	2.00	0.60
3:C:453:ALA:HA	8:I:34:ARG:HA	1.82	0.60
8:I:12:VAL:O	8:I:16:VAL:HG23	2.02	0.60
10:K:28:ILE:HB	10:K:29:PRO:HD3	1.83	0.60
15:U:66:ILE:O	15:U:66:ILE:HG22	2.01	0.60
3:c:5265:ILE:HD13	20:c:5495:CLA:HED1	1.83	0.60
20:C:491:CLA:HMB2	24:C:506:BCR:H403	1.82	0.60
5:E:36:LEU:HA	5:E:39:SER:HB3	1.82	0.60
2:b:5025:MET:HE3	24:b:5527:BCR:H23C	1.83	0.60
3:c:5223:TRP:CE3	3:c:5224:ILE:HG13	2.37	0.60
3:c:5298:PRO:O	3:c:5299:SER:CB	2.49	0.60
4:d:5120:PHE:HA	4:d:5123:ILE:HD12	1.84	0.60
9:j:5015:THR:HG21	10:k:5038:VAL:HG13	1.83	0.60
1:A:187:GLN:NE2	1:A:191:ASN:HA	2.16	0.60
2:B:137:LYS:O	2:B:141:ILE:HG13	2.02	0.60
2:B:263:THR:HG22	2:B:448:ARG:NH2	2.15	0.60
1:a:5076:ASN:C	1:a:5076:ASN:HD22	2.09	0.60
17:x:5007:UNK:O	17:x:5011:UNK:HG2	2.02	0.60
2:B:25:MET:HE3	24:B:527:BCR:H23C	1.82	0.60
2:B:223:GLN:HA	7:H:21:VAL:CG2	2.31	0.60
3:C:107:ASP:OD1	3:C:110:PRO:HD3	2.01	0.60
3:C:400:PRO:C	3:C:401:LEU:HD23	2.26	0.60
9:J:8:ILE:H	9:J:8:ILE:HD12	1.66	0.60
14:T:21:ILE:HD12	24:T:5104:BCR:H332	1.83	0.60
15:U:72:TYR:CB	15:U:73:PRO:HD3	2.30	0.60
3:c:5400:PRO:O	3:c:5401:LEU:HD23	2.01	0.60
3:c:5452:ALA:C	3:c:5454:GLY:N	2.55	0.60
18:z:5049:ALA:O	18:z:5053:VAL:HG23	2.01	0.60
7:H:49:TYR:CD2	30:H:208:DGD:HB22	2.37	0.60
2:b:5391:SER:OG	2:b:5394:GLN:HB2	2.01	0.60
4:d:5210:LEU:HD21	22:d:5356:PQ9:H17	1.84	0.60
15:u:5069:ARG:O	15:u:5070:GLY:C	2.45	0.60
1:A:315:ASN:O	4:D:63:LEU:HB3	2.02	0.60
2:B:10:THR:O	2:B:13:ILE:HG13	2.02	0.60
15:U:117:VAL:HG13	15:U:122:VAL:HG21	1.82	0.60
1:a:5306:VAL:O	1:a:5314:ILE:HB	2.01	0.60
4:d:5273:PHE:CZ	28:l:5210:MGE:H3B2	2.37	0.60
7:h:5062:TRP:CD1	30:h:5208:DGD:HE5	2.36	0.60
13:o:5092:VAL:HG12	13:o:5093:PRO:HD2	1.82	0.60
2:B:229:LEU:O	2:B:231:MET:N	2.35	0.60
4:D:176:ALA:C	4:D:178:ILE:H	2.10	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:5156:PHE:HB3	2:b:5162:PHE:HB3	1.82	0.60
3:c:5224:ILE:O	3:c:5227:VAL:HG23	2.02	0.60
17:x:5026:UNK:NE2	17:x:5026:UNK:HG2	2.22	0.60
3:c:5318:LEU:HD23	3:c:5318:LEU:C	2.27	0.60
2:B:229:LEU:O	2:B:230:ARG:C	2.44	0.59
2:B:233:ASN:HD22	2:B:233:ASN:C	2.10	0.59
3:C:230:LEU:O	3:C:234:VAL:HG23	2.01	0.59
4:D:49:LEU:O	4:D:53:THR:HG23	2.01	0.59
4:D:337:GLU:HG2	4:D:339:PHE:CE2	2.36	0.59
5:E:60:GLN:HG3	5:E:60:GLN:O	2.01	0.59
4:d:5060:THR:HG23	4:d:5061:HIS:N	2.17	0.59
1:A:306:VAL:O	1:A:314:ILE:HB	2.02	0.59
13:O:55:ALA:O	13:O:57:PRO:HD3	2.02	0.59
1:a:5060:ILE:CG2	1:a:5061:ASP:H	2.13	0.59
1:a:5270:SER:HA	4:d:5232:PHE:CE2	2.37	0.59
2:b:5223:GLN:HA	7:h:5021:VAL:CG2	2.32	0.59
4:d:5103:ARG:HD3	4:d:5106:GLN:OE1	2.01	0.59
3:C:153:ASP:C	3:C:155:ASN:H	2.08	0.59
3:C:428:THR:HG22	3:C:429:SER:N	2.17	0.59
3:C:458:GLY:HA2	4:D:222:LEU:O	2.02	0.59
9:J:15:THR:CG2	10:K:38:VAL:HG22	2.32	0.59
13:O:112:LYS:HE2	13:O:114:ASN:HB3	1.84	0.59
13:O:179:THR:CG2	13:O:180:ALA:N	2.65	0.59
16:V:159:GLY:O	16:V:160:LYS:C	2.45	0.59
1:a:5072:LEU:HD23	14:t:5003:THR:HG21	1.83	0.59
1:a:5142:TRP:CZ2	3:c:5447:ARG:HD2	2.35	0.59
2:b:5185:TRP:HH2	2:b:5203:ILE:HG21	1.67	0.59
13:o:5047:THR:HG22	13:o:5048:LEU:N	2.17	0.59
1:A:193:LEU:HD13	4:D:179:PHE:HB3	1.84	0.59
16:V:147:VAL:O	16:V:150:LYS:HB2	2.02	0.59
3:c:5362:ARG:HG3	3:c:5362:ARG:HH11	1.66	0.59
6:f:5041:GLN:HA	6:f:5041:GLN:NE2	2.17	0.59
4:D:60:THR:HG23	4:D:61:HIS:N	2.18	0.59
18:Z:14:ILE:O	18:Z:18:VAL:HG23	2.02	0.59
1:a:5072:LEU:HD21	14:t:5003:THR:HG21	1.84	0.59
13:o:5183:LEU:HD22	13:o:5187:GLY:O	2.01	0.59
1:A:326:LEU:CD2	3:C:412:THR:HB	2.33	0.59
18:Z:16:SER:O	18:Z:20:VAL:HG23	2.03	0.59
1:a:5326:LEU:CD2	3:c:5412:THR:HB	2.32	0.59
2:b:5031:ALA:HB2	20:b:5515:CLA:HBC3	1.84	0.59
2:b:5223:GLN:HE22	2:b:5227:LYS:CD	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:THR:C	2:B:12:LEU:H	2.10	0.59
7:H:62:TRP:CD1	30:H:208:DGD:HE5	2.37	0.59
4:d:5087:HIS:CD2	4:d:5166:SER:HA	2.37	0.59
16:v:5103:LYS:O	16:v:5122:ARG:HG3	2.03	0.59
18:z:5039:LEU:O	18:z:5042:LEU:HB3	2.02	0.59
2:B:4:PRO:HD2	2:B:7:ARG:HD2	1.84	0.59
1:a:5076:ASN:ND2	1:a:5079:THR:H	2.00	0.59
2:b:5471:ALA:O	2:b:5475:PHE:HB2	2.02	0.59
4:d:5039:PRO:O	4:d:5043:LEU:HB2	2.02	0.59
4:d:5261:PHE:O	4:d:5262:SER:HB3	2.02	0.59
2:B:384:ARG:NH1	15:U:132:LEU:HD22	2.18	0.59
7:H:29:PRO:O	7:H:33:VAL:HG23	2.02	0.59
13:O:230:VAL:HG12	13:O:231:ASP:N	2.17	0.59
2:b:5329:PRO:CB	20:b:5517:CLA:HED1	2.28	0.59
15:u:5117:VAL:HG13	15:u:5122:VAL:HG21	1.85	0.59
3:C:223:TRP:CD2	3:C:224:ILE:HG13	2.38	0.59
2:b:5233:ASN:C	2:b:5233:ASN:HD22	2.09	0.59
3:c:5315:MET:HE2	3:c:5319:ILE:HD11	1.83	0.59
13:o:5234:THR:OG1	13:o:5236:GLU:HG2	2.02	0.59
1:A:307:ILE:HD11	1:A:311:GLY:O	2.00	0.58
3:C:156:LYS:O	3:C:160:ILE:HG13	2.03	0.58
4:D:279:LEU:HD22	20:D:354:CLA:HBA2	1.85	0.58
2:b:5247:PHE:O	2:b:5251:VAL:HG23	2.03	0.58
5:e:5025:ILE:O	5:e:5029:ALA:HB2	2.03	0.58
14:t:5004:ILE:HD13	14:t:5004:ILE:O	2.03	0.58
2:B:156:PHE:HB3	2:B:162:PHE:HB3	1.84	0.58
4:D:39:PRO:O	4:D:43:LEU:HB2	2.03	0.58
10:K:45:PHE:O	10:K:46:ARG:C	2.46	0.58
13:O:204:LYS:HB3	13:O:206:GLU:HG2	1.85	0.58
2:b:5271:THR:HG22	2:b:5274:GLN:H	1.68	0.58
2:b:5344:ALA:HB2	2:b:5401:PHE:CE1	2.39	0.58
7:h:5021:VAL:HG22	7:h:5022:ALA:O	2.02	0.58
3:C:265:ILE:HG22	3:C:270:ALA:CB	2.33	0.58
3:C:315:MET:O	3:C:319:ILE:HG13	2.04	0.58
1:a:5062:GLY:HA3	3:c:5356:MET:SD	2.44	0.58
3:c:5055:ALA:HB1	24:c:5504:BCR:H373	1.83	0.58
4:d:5014:TRP:H	4:d:5014:TRP:CD1	2.21	0.58
5:e:5057:ALA:O	5:e:5059:GLU:N	2.36	0.58
1:A:131:TRP:CE3	1:A:132:GLU:N	2.72	0.58
2:B:98:LEU:HD13	27:a:5568:LMT:H92	1.85	0.58
3:C:456:GLU:N	3:C:456:GLU:OE1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:31:PRO:HA	16:V:34:LEU:HD12	1.85	0.58
3:c:5156:LYS:O	3:c:5160:ILE:HG13	2.04	0.58
16:v:5134:THR:HG23	16:v:5137:ASP:OD2	2.03	0.58
27:T:217:LMT:O3'	2:b:5043:ALA:HB1	2.04	0.58
1:a:5306:VAL:HG21	1:a:5316:THR:CG2	2.33	0.58
20:b:5513:CLA:H191	7:h:5039:LEU:HD13	1.85	0.58
4:d:5200:GLY:HA2	4:d:5278:GLY:O	2.04	0.58
4:d:5221:THR:HG22	4:d:5245:SER:H	1.68	0.58
8:i:5012:VAL:O	8:i:5016:VAL:HG23	2.03	0.58
15:u:5094:ILE:HG23	15:u:5095:PRO:HD2	1.85	0.58
18:Z:5:PHE:CA	18:Z:57:LEU:HD13	2.32	0.58
1:a:5330:VAL:HG12	4:d:5348:ARG:HA	1.84	0.58
3:c:5266:TRP:HB3	3:c:5271:TYR:OH	2.03	0.58
4:d:5049:LEU:O	4:d:5053:THR:HG23	2.04	0.58
13:o:5045:CYS:H	13:o:5072:GLN:HE22	1.49	0.58
13:o:5144:LEU:HD13	13:o:5259:VAL:HG11	1.86	0.58
13:o:5163:THR:H	13:o:5166:THR:HG23	1.68	0.58
15:u:5073:PRO:HB2	16:v:5109:ASP:CG	2.28	0.58
1:A:76:ASN:HD22	1:A:76:ASN:C	2.11	0.58
4:D:102:THR:O	4:D:105:CYS:HB2	2.04	0.58
2:b:5229:LEU:O	2:b:5230:ARG:C	2.47	0.58
3:c:5153:ASP:O	3:c:5155:ASN:N	2.34	0.58
24:c:5504:BCR:H311	24:c:5504:BCR:H343	1.85	0.58
15:u:5064:ALA:O	15:u:5067:GLN:HG2	2.04	0.58
4:D:120:PHE:HA	4:D:123:ILE:HD12	1.85	0.58
4:D:261:PHE:CE1	4:D:267:LEU:HA	2.39	0.58
17:X:7:UNK:O	17:X:11:UNK:HG2	2.04	0.58
2:b:5222:PRO:HG3	7:h:5026:GLY:HA3	1.84	0.58
3:c:5245:ILE:O	3:c:5249:ILE:HD13	2.04	0.58
9:j:5008:ILE:H	9:j:5008:ILE:HD12	1.68	0.58
17:x:5012:UNK:CG	18:z:5017:PHE:CE1	2.85	0.58
21:A:562:PHO:CMC	4:D:279:LEU:HD11	2.34	0.58
2:B:24:LEU:HD21	20:B:526:CLA:HAB	1.86	0.58
2:B:471:ALA:O	2:B:475:PHE:HB2	2.04	0.58
3:c:5188:THR:HG23	3:c:5300:GLU:OE2	2.04	0.58
2:B:31:ALA:HB3	2:B:104:SER:HB3	1.86	0.58
2:B:149:LEU:HG	20:B:513:CLA:CBC	2.28	0.58
3:C:318:LEU:HD23	3:C:318:LEU:C	2.28	0.58
20:C:495:CLA:HMD2	20:C:497:CLA:HAB	1.86	0.58
4:D:103:ARG:HD3	4:D:106:GLN:OE1	2.04	0.58
4:D:110:LEU:O	4:D:114:ILE:HG13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:151:LEU:CD1	13:O:223:ILE:HD11	2.34	0.58
13:O:152:VAL:O	13:O:152:VAL:HG13	2.04	0.58
13:o:5163:THR:HG23	13:o:5165:SER:H	1.68	0.58
16:v:5147:VAL:O	16:v:5150:LYS:HB2	2.04	0.58
1:A:62:GLY:HA3	3:C:356:MET:SD	2.44	0.57
3:C:193:GLY:O	3:C:194:GLY:C	2.47	0.57
3:C:452:ALA:C	3:C:454:GLY:N	2.56	0.57
13:O:65:ARG:HA	13:O:111:LEU:H	1.68	0.57
15:U:72:TYR:O	15:U:73:PRO:C	2.46	0.57
3:c:5124:VAL:HB	24:c:5505:BCR:H362	1.84	0.57
3:c:5332:GLN:HA	3:c:5338:GLY:HA2	1.85	0.57
16:v:5081:ARG:NE	16:v:5157:GLY:HA3	2.18	0.57
2:B:444:ARG:HG2	2:B:444:ARG:HH11	1.69	0.57
3:C:94:THR:HG22	3:C:298:PRO:HG2	1.86	0.57
3:C:241:GLY:O	3:C:243:ILE:N	2.38	0.57
1:a:5258:LEU:HD12	4:d:5128:ARG:CD	2.34	0.57
2:b:5133:LEU:HB3	2:b:5138:MET:HE1	1.87	0.57
4:d:5110:LEU:O	4:d:5114:ILE:HG13	2.03	0.57
10:k:5039:TRP:O	10:k:5043:VAL:HG23	2.04	0.57
1:A:217:SER:HA	4:D:272:LEU:HD12	1.86	0.57
4:D:343:GLU:HG2	16:V:161:VAL:HG11	1.86	0.57
6:F:34:LEU:HD22	9:J:24:ILE:CD1	2.32	0.57
13:O:142:ILE:HD12	13:O:142:ILE:N	2.19	0.57
1:a:5124:SER:O	1:a:5127:MET:HB3	2.04	0.57
2:b:5170:ASP:HB2	2:b:5171:PRO:CD	2.35	0.57
4:d:5176:ALA:C	4:d:5178:ILE:H	2.11	0.57
8:I:27:ASP:N	8:I:28:PRO:CD	2.67	0.57
9:J:14:ALA:HB1	24:X:130:BCR:H393	1.85	0.57
15:U:94:ILE:HG23	15:U:95:PRO:HD2	1.85	0.57
3:c:5280:SER:HB2	3:c:5437:PHE:HB3	1.86	0.57
13:o:5075:THR:HG22	13:o:5077:LEU:HD11	1.87	0.57
13:o:5101:THR:O	13:o:5101:THR:HG22	2.03	0.57
1:A:132:GLU:O	1:A:136:ARG:HG2	2.04	0.57
2:B:150:CYS:HA	20:B:513:CLA:HBC2	1.87	0.57
3:C:266:TRP:HB3	3:C:271:TYR:OH	2.04	0.57
18:Z:39:LEU:O	18:Z:42:LEU:HB3	2.05	0.57
2:b:5004:PRO:HD2	2:b:5007:ARG:HD2	1.86	0.57
2:b:5063:LEU:N	2:b:5064:PRO:HD2	2.19	0.57
2:b:5314:TYR:CE2	2:b:5316:GLY:HA3	2.39	0.57
2:B:191:ASN:ND2	7:H:60:VAL:HG12	2.20	0.57
3:C:44:ASN:O	3:C:45:LEU:HG	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:63:TRP:O	3:C:64:ALA:C	2.47	0.57
3:C:428:THR:CG2	30:C:508:DGD:HA91	2.35	0.57
4:D:239:GLN:O	4:D:240:ALA:HB3	2.05	0.57
4:D:273:PHE:CZ	28:L:210:MGE:H3B2	2.40	0.57
1:a:5036:ILE:O	1:a:5039:PRO:HD2	2.04	0.57
1:a:5330:VAL:CG1	4:d:5348:ARG:HA	2.34	0.57
3:c:5094:THR:HG22	3:c:5298:PRO:HG2	1.85	0.57
2:B:11:VAL:HG21	11:L:7:ARG:HD2	1.87	0.57
4:D:239:GLN:O	4:D:240:ALA:CB	2.53	0.57
5:E:15:THR:HG23	9:J:8:ILE:O	2.04	0.57
13:O:33:TYR:C	13:O:35:ASP:H	2.12	0.57
13:O:168:PHE:N	13:O:168:PHE:CD1	2.71	0.57
14:T:4:ILE:HD13	14:T:4:ILE:O	2.04	0.57
1:a:5054:ALA:O	1:a:5055:ALA:HB2	2.04	0.57
2:b:5011:VAL:HG21	11:l:5007:ARG:HD2	1.87	0.57
3:c:5027:ASP:O	10:k:5046:ARG:HD3	2.04	0.57
6:f:5040:MET:HA	6:f:5043:ILE:HG13	1.87	0.57
9:j:5014:ALA:HB1	24:x:5130:BCR:H393	1.86	0.57
13:o:5067:ALA:HB3	13:o:5268:SER:OG	2.05	0.57
18:z:5036:SER:CA	18:z:5039:LEU:HD12	2.32	0.57
4:D:14:TRP:HD1	4:D:15:PHE:N	2.03	0.57
4:D:348:ARG:HH21	4:D:352:LEU:C	2.12	0.57
13:O:172:PHE:CE2	13:O:223:ILE:HG12	2.39	0.57
1:a:5325:ASN:HA	1:a:5328:MET:HE3	1.87	0.57
1:a:5328:MET:HE1	4:d:5183:LEU:HD13	1.87	0.57
2:b:5010:THR:C	2:b:5012:LEU:H	2.13	0.57
3:c:5072:LEU:HD11	3:c:5108:THR:OG1	2.05	0.57
3:c:5281:MET:O	3:c:5285:ILE:HG13	2.04	0.57
4:d:5014:TRP:HD1	4:d:5015:PHE:N	2.03	0.57
4:d:5261:PHE:CE1	4:d:5267:LEU:HA	2.40	0.57
1:A:57:PRO:HG3	1:A:68:SER:HB3	1.86	0.57
1:A:222:SER:O	1:A:246:TYR:HB2	2.05	0.57
3:C:48:LYS:HE2	3:C:48:LYS:HA	1.87	0.57
6:F:40:MET:HA	6:F:43:ILE:HG13	1.84	0.57
9:J:15:THR:HG22	10:K:38:VAL:HG22	1.85	0.57
1:A:54:ALA:O	1:A:55:ALA:HB2	2.03	0.57
2:B:170:ASP:HB2	2:B:171:PRO:CD	2.35	0.57
4:D:348:ARG:NH2	4:D:352:LEU:OXT	2.37	0.57
5:E:58:GLN:NE2	16:V:28:GLU:HA	2.18	0.57
13:O:73:PRO:HG2	13:O:102:THR:OG1	2.05	0.57
1:a:5022:THR:HG23	1:a:5136:ARG:NH1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:GLU:C	3:C:31:SER:H	2.13	0.56
14:T:1:MET:C	14:T:4:ILE:HG22	2.30	0.56
2:b:5356:VAL:HA	2:b:5370:LEU:HD23	1.87	0.56
2:b:5368:VAL:HG11	2:b:5381:ILE:CD1	2.29	0.56
13:o:5145:LEU:HD23	13:o:5175:PRO:CG	2.31	0.56
2:B:138:MET:SD	20:B:525:CLA:HAC1	2.45	0.56
2:B:391:SER:OG	2:B:394:GLN:HB2	2.05	0.56
13:O:145:LEU:O	13:O:147:THR:HG22	2.05	0.56
3:c:5201:ASN:N	3:c:5202:PRO:HD3	2.19	0.56
4:d:5067:TYR:CD2	4:d:5076:VAL:HG11	2.40	0.56
13:o:5144:LEU:CD1	13:o:5259:VAL:HG11	2.35	0.56
1:A:201:GLY:HA3	1:A:286:THR:CG2	2.34	0.56
1:A:257:ARG:HH12	1:A:261:GLN:CD	2.13	0.56
2:B:262:THR:C	2:B:264:PRO:HD3	2.30	0.56
2:B:332:LYS:HB3	2:B:444:ARG:HE	1.70	0.56
3:C:315:MET:HE2	3:C:319:ILE:HD11	1.85	0.56
4:D:221:THR:HG22	4:D:245:SER:H	1.69	0.56
13:O:111:LEU:HD11	13:O:119:LEU:HB3	1.85	0.56
13:O:163:THR:H	13:O:166:THR:CG2	2.18	0.56
13:O:206:GLU:CD	13:O:206:GLU:H	2.13	0.56
2:b:5150:CYS:HA	20:b:5513:CLA:HBC2	1.86	0.56
2:b:5326:ARG:HB3	2:b:5444:ARG:HH11	1.70	0.56
3:c:5048:LYS:HA	3:c:5048:LYS:HE2	1.87	0.56
1:A:213:ALA:O	1:A:217:SER:HB2	2.06	0.56
2:B:62:VAL:HG12	2:B:66:MET:HE2	1.87	0.56
3:C:56:HIS:C	3:C:58:GLY:N	2.59	0.56
8:I:19:PHE:CE1	8:I:23:PHE:HE2	2.24	0.56
24:T:5104:BCR:H393	20:b:5517:CLA:HAC2	1.86	0.56
16:V:39:ASN:ND2	16:V:41:GLU:HB2	2.20	0.56
2:b:5138:MET:SD	20:b:5525:CLA:HAC1	2.45	0.56
4:d:5103:ARG:NH1	5:e:5077:GLU:HG3	2.21	0.56
4:d:5239:GLN:O	4:d:5240:ALA:HB3	2.05	0.56
17:x:5085:UNK:C	17:x:5086:UNK:OD1	2.54	0.56
3:C:27:ASP:O	10:K:46:ARG:HD3	2.06	0.56
3:C:72:LEU:HD11	3:C:108:THR:OG1	2.05	0.56
3:C:198:VAL:HG12	3:C:200:THR:HG23	1.87	0.56
3:c:5056:HIS:C	3:c:5058:GLY:N	2.63	0.56
6:f:5018:VAL:HG13	6:f:5019:ARG:N	2.21	0.56
4:D:14:TRP:CD1	4:D:14:TRP:H	2.21	0.56
3:c:5052:ALA:HB1	20:c:5499:CLA:HAB	1.88	0.56
4:d:5102:THR:O	4:d:5105:CYS:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:5239:GLN:O	4:d:5240:ALA:CB	2.53	0.56
13:o:5172:PHE:HE2	13:o:5223:ILE:HG12	1.70	0.56
13:o:5206:GLU:H	13:o:5206:GLU:CD	2.13	0.56
1:A:29:TYR:HD1	1:A:133:LEU:HB2	1.69	0.56
2:B:55:MET:HE3	2:B:80:ILE:CG1	2.36	0.56
2:B:366:PHE:CD1	2:B:367:PRO:HD2	2.41	0.56
3:C:315:MET:CE	3:C:319:ILE:HD11	2.35	0.56
8:I:11:VAL:O	8:I:15:PHE:HD1	1.89	0.56
15:U:77:LYS:O	15:U:81:LYS:HB2	2.06	0.56
16:V:81:ARG:HG3	16:V:81:ARG:HH11	1.71	0.56
1:a:5213:ALA:O	1:a:5217:SER:HB2	2.05	0.56
1:a:5217:SER:HA	4:d:5272:LEU:HD12	1.88	0.56
2:b:5414:PRO:HB2	2:b:5415:PRO:CD	2.32	0.56
3:c:5293:ASN:HD21	3:c:5296:VAL:H	1.54	0.56
15:u:5073:PRO:HB2	16:v:5109:ASP:OD2	2.05	0.56
2:B:353:GLU:HB3	2:B:373:LYS:HZ3	1.71	0.56
2:B:380:ASP:C	2:B:380:ASP:OD2	2.47	0.56
4:D:103:ARG:HH12	5:E:77:GLU:HG3	1.70	0.56
9:J:33:TYR:O	9:J:34:ALA:HB3	2.04	0.56
15:U:69:ARG:O	15:U:70:GLY:C	2.47	0.56
2:b:5031:ALA:O	2:b:5032:GLY:C	2.48	0.56
1:A:13:LEU:N	1:A:13:LEU:HD23	2.21	0.56
3:C:293:ASN:HD21	3:C:296:VAL:H	1.51	0.56
4:D:178:ILE:HG22	4:D:179:PHE:N	2.21	0.56
2:b:5024:LEU:HD13	2:b:5111:ALA:HA	1.88	0.56
3:c:5460:ASP:O	3:c:5461:ARG:C	2.49	0.56
20:c:5503:CLA:HMB3	24:c:5505:BCR:H402	1.88	0.56
1:A:221:SER:HA	4:D:139:ARG:HB2	1.86	0.56
2:B:63:LEU:N	2:B:64:PRO:HD2	2.21	0.56
2:B:467:ILE:HD13	4:D:126:MET:SD	2.46	0.56
1:a:5159:LEU:C	1:a:5162:PRO:HD2	2.31	0.56
2:b:5392:PHE:O	2:b:5393:GLU:CB	2.53	0.56
3:C:194:GLY:O	3:C:195:ASP:HB2	2.06	0.55
3:C:332:GLN:HA	3:C:338:GLY:HA2	1.88	0.55
16:V:107:THR:HG22	16:V:108:TYR:H	1.69	0.55
16:V:119:PRO:HG3	16:V:127:PHE:CD1	2.41	0.55
2:b:5018:ARG:HG3	2:b:5018:ARG:NH1	2.20	0.55
2:b:5231:MET:C	2:b:5233:ASN:H	2.15	0.55
3:c:5458:GLY:HA2	4:d:5222:LEU:O	2.06	0.55
4:d:5077:ALA:HB2	4:d:5174:GLY:HA3	1.87	0.55
10:k:5045:PHE:O	10:k:5046:ARG:C	2.48	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:5033:TYR:C	13:o:5035:ASP:N	2.64	0.55
13:o:5110:GLU:OE2	13:o:5112:LYS:HB2	2.06	0.55
13:o:5128:ASP:OD2	13:o:5149:LYS:HG2	2.06	0.55
2:B:31:ALA:O	2:B:32:GLY:C	2.49	0.55
3:C:260:ALA:O	3:C:264:PHE:HD2	1.89	0.55
3:C:348:GLU:OE2	13:O:37:VAL:HA	2.06	0.55
10:K:39:TRP:O	10:K:43:VAL:HG23	2.05	0.55
15:U:57:LEU:HD22	15:U:79:ILE:HG21	1.89	0.55
16:V:103:LYS:O	16:V:122:ARG:HG3	2.07	0.55
1:a:5131:TRP:CE3	1:a:5132:GLU:N	2.74	0.55
1:a:5238:LYS:O	1:a:5241:GLN:HB3	2.06	0.55
1:a:5270:SER:HA	4:d:5232:PHE:HE2	1.69	0.55
2:b:5137:LYS:O	2:b:5141:ILE:HG13	2.06	0.55
2:b:5366:PHE:CD1	2:b:5367:PRO:HD2	2.42	0.55
5:e:5056:TYR:HB3	5:e:5060:GLN:HG3	1.88	0.55
8:i:5034:ARG:O	8:i:5035:LYS:C	2.49	0.55
3:C:284:PHE:HB3	30:C:507:DGD:HA51	1.87	0.55
13:O:163:THR:HG23	13:O:165:SER:H	1.71	0.55
16:V:124:ALA:HB1	16:V:131:ARG:HG3	1.87	0.55
1:a:5136:ARG:HH22	8:i:5027:ASP:CG	2.15	0.55
2:b:5221:PRO:O	7:h:5021:VAL:HG23	2.06	0.55
2:b:5353:GLU:HB3	2:b:5373:LYS:HZ1	1.69	0.55
30:c:5509:DGD:HD2	9:j:5032:ALA:O	2.06	0.55
4:d:5223:PHE:CZ	4:d:5245:SER:HB3	2.41	0.55
11:l:5014:ARG:HG3	11:l:5014:ARG:NH1	2.21	0.55
13:o:5142:ILE:HD12	13:o:5142:ILE:N	2.21	0.55
1:A:38:ILE:O	1:A:42:LEU:HG	2.07	0.55
2:B:283:GLU:OE1	2:B:286:ARG:HD2	2.07	0.55
5:E:13:ILE:HD13	32:F:51:HEM:O1D	2.07	0.55
6:F:18:VAL:HG13	6:F:19:ARG:N	2.22	0.55
15:U:72:TYR:CB	15:U:73:PRO:CD	2.84	0.55
1:a:5029:TYR:HD1	1:a:5133:LEU:HB2	1.70	0.55
1:a:5244:GLU:HG3	1:a:5246:TYR:H	1.71	0.55
20:b:5525:CLA:H112	20:b:5525:CLA:H162	1.87	0.55
3:c:5418:ASN:HB3	30:c:5509:DGD:HE2	1.88	0.55
4:d:5251:ARG:HG3	4:d:5255:GLN:HE21	1.72	0.55
10:k:5028:ILE:HB	10:k:5029:PRO:HD3	1.89	0.55
1:A:224:ILE:CG2	2:B:484:PRO:HG3	2.35	0.55
1:A:258:LEU:HD12	4:D:128:ARG:CD	2.34	0.55
4:D:68:LEU:HD13	6:F:40:MET:HE2	1.87	0.55
3:c:5428:THR:CG2	30:c:5508:DGD:HA91	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:o:5184:ASP:HB2	13:o:5185:PRO:HD2	1.87	0.55
1:A:27:ARG:HG3	1:A:27:ARG:NH1	2.22	0.55
1:A:116:ILE:HG13	1:A:117:PHE:N	2.21	0.55
1:A:184:ILE:HD11	4:D:186:GLN:CD	2.32	0.55
1:a:5057:PRO:HG3	1:a:5068:SER:HB3	1.89	0.55
2:b:5024:LEU:HD21	20:b:5526:CLA:HAB	1.89	0.55
2:b:5380:ASP:C	2:b:5380:ASP:OD2	2.50	0.55
3:c:5084:GLN:HB2	3:c:5086:LEU:CD2	2.37	0.55
4:d:5180:ARG:C	4:d:5180:ARG:HD3	2.32	0.55
5:e:5028:PRO:O	5:e:5032:ILE:HG13	2.07	0.55
8:i:5024:LEU:C	8:i:5026:GLY:H	2.13	0.55
10:k:5026:PRO:O	10:k:5029:PRO:HD2	2.06	0.55
1:A:264:SER:OG	1:A:265:PHE:N	2.40	0.55
2:B:246:PHE:C	2:B:246:PHE:HD1	2.15	0.55
3:C:209:ILE:CG2	24:C:506:BCR:H382	2.35	0.55
15:U:99:GLU:HA	15:U:102:LYS:HE3	1.89	0.55
3:c:5048:LYS:HE2	3:c:5133:ALA:HA	1.89	0.55
8:i:5027:ASP:N	8:i:5028:PRO:CD	2.69	0.55
10:k:5015:TYR:C	10:k:5017:ILE:H	2.15	0.55
11:l:5002:GLU:HB3	11:l:5003:PRO:HD2	1.87	0.55
15:u:5050:ALA:HB1	15:u:5113:THR:HG21	1.87	0.55
16:v:5107:THR:HG22	16:v:5108:TYR:H	1.71	0.55
2:B:18:ARG:HH11	2:B:18:ARG:HG3	1.70	0.55
2:B:231:MET:C	2:B:233:ASN:H	2.15	0.55
2:B:233:ASN:C	2:B:233:ASN:ND2	2.64	0.55
20:B:513:CLA:H191	7:H:39:LEU:HD13	1.89	0.55
10:K:39:TRP:NE1	17:X:31:UNK:HG3	2.12	0.55
13:O:47:THR:HG22	13:O:48:LEU:N	2.22	0.55
18:Z:23:VAL:HB	18:Z:24:PRO:HD3	1.89	0.55
2:b:5467:ILE:HD13	4:d:5126:MET:SD	2.47	0.55
12:m:5033:GLN:C	12:m:5035:SER:H	2.15	0.55
13:o:5118:SER:HB3	13:o:5157:PRO:HA	1.89	0.55
2:B:68:ARG:HH11	2:B:262:THR:HG23	1.70	0.55
3:C:37:ALA:HA	20:C:498:CLA:O1A	2.06	0.55
13:O:145:LEU:HD23	13:O:175:PRO:CG	2.34	0.55
21:a:5562:PHO:CMC	4:d:5279:LEU:HD11	2.37	0.55
11:l:5014:ARG:HD3	12:m:5026:TYR:OH	2.07	0.55
3:C:416:SER:O	3:C:417:VAL:CG1	2.55	0.54
9:J:14:ALA:CB	24:X:130:BCR:H393	2.38	0.54
1:a:5224:ILE:CG2	2:b:5484:PRO:HG3	2.37	0.54
2:b:5165:GLY:HA3	2:b:5179:GLN:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:5262:THR:C	2:b:5264:PRO:HD3	2.31	0.54
2:b:5377:VAL:HG11	4:d:5342:PRO:HG2	1.90	0.54
2:b:5384:ARG:NH1	15:u:5132:LEU:HD22	2.22	0.54
24:b:5527:BCR:H322	28:b:5530:MGE:H2G	1.90	0.54
3:c:5158:THR:O	3:c:5251:HIS:HB3	2.07	0.54
4:d:5136:VAL:HG12	4:d:5136:VAL:O	2.07	0.54
13:o:5216:PHE:C	13:o:5216:PHE:CD2	2.84	0.54
1:A:244:GLU:HG3	1:A:246:TYR:H	1.71	0.54
20:B:517:CLA:HAC2	24:t:104:BCR:H393	1.87	0.54
4:D:346:LEU:O	4:D:348:ARG:HG3	2.07	0.54
13:O:75:THR:HG22	13:O:77:LEU:HD11	1.88	0.54
13:O:92:VAL:CG1	13:O:93:PRO:CD	2.82	0.54
13:O:216:PHE:C	13:O:216:PHE:CD2	2.85	0.54
1:a:5257:ARG:HH12	1:a:5261:GLN:NE2	2.05	0.54
2:b:5233:ASN:C	2:b:5233:ASN:ND2	2.64	0.54
4:d:5040:CYS:O	4:d:5041:ALA:C	2.50	0.54
10:k:5019:ASP:N	10:k:5020:PRO:HD2	2.22	0.54
18:z:5019:MET:SD	18:z:5043:GLY:HA3	2.47	0.54
24:B:527:BCR:H322	28:B:530:MGE:H2G	1.89	0.54
3:C:91:HIS:HB3	20:C:493:CLA:HBA2	1.88	0.54
30:C:509:DGD:HD2	9:J:32:ALA:O	2.06	0.54
10:K:43:VAL:HG12	10:K:46:ARG:HG3	1.90	0.54
2:b:5233:ASN:ND2	2:b:5235:GLU:H	2.04	0.54
5:e:5032:ILE:O	5:e:5036:LEU:HG	2.08	0.54
15:u:5072:TYR:O	15:u:5073:PRO:C	2.50	0.54
16:v:5128:PRO:O	16:v:5129:LYS:C	2.47	0.54
2:B:286:ARG:C	2:B:286:ARG:HD3	2.33	0.54
2:B:377:VAL:HG11	4:D:342:PRO:HG2	1.89	0.54
3:C:405:ASN:HD22	30:C:509:DGD:C5D	2.19	0.54
16:V:104:ASN:HD21	16:V:113:GLU:CD	2.14	0.54
1:a:5040:THR:HG22	1:a:5118:HIS:O	2.07	0.54
4:d:5054:PHE:HB3	5:e:5047:PHE:CD1	2.42	0.54
5:e:5069:ARG:O	5:e:5070:PHE:HB2	2.07	0.54
3:C:55:ALA:HB1	24:C:504:BCR:C37	2.37	0.54
4:D:325:ILE:O	4:D:329:MET:HB3	2.08	0.54
5:E:25:ILE:O	5:E:29:ALA:HB2	2.08	0.54
15:U:72:TYR:HB3	15:U:73:PRO:CD	2.35	0.54
8:i:5013:THR:O	8:i:5017:LEU:HG	2.08	0.54
9:j:5014:ALA:CB	24:x:5130:BCR:H393	2.37	0.54
15:u:5099:GLU:HA	15:u:5102:LYS:HE3	1.90	0.54
1:A:72:LEU:HD21	14:T:3:THR:HG21	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:221:PRO:O	7:H:21:VAL:HG23	2.08	0.54
3:C:52:ALA:HB1	20:C:499:CLA:HAB	1.89	0.54
3:C:75:PHE:CE2	3:C:77:PRO:HA	2.43	0.54
3:C:223:TRP:CE3	3:C:224:ILE:HG13	2.43	0.54
3:C:277:GLY:C	20:C:495:CLA:HBC2	2.33	0.54
3:C:418:ASN:HB3	30:C:509:DGD:HE2	1.89	0.54
4:D:160:TYR:CB	4:D:161:PRO:HD3	2.26	0.54
13:O:216:PHE:C	13:O:216:PHE:HD2	2.15	0.54
3:c:5198:VAL:HG12	3:c:5200:THR:HG23	1.89	0.54
11:l:5014:ARG:HG2	12:m:5026:TYR:CE1	2.37	0.54
13:o:5152:VAL:O	13:o:5152:VAL:HG13	2.07	0.54
16:v:5081:ARG:HG3	16:v:5081:ARG:NH1	2.23	0.54
1:A:149:ALA:HB3	1:A:150:PRO:CD	2.33	0.54
2:B:392:PHE:O	2:B:393:GLU:CB	2.54	0.54
15:U:57:LEU:HD22	15:U:79:ILE:CG2	2.37	0.54
1:a:5201:GLY:HA3	1:a:5286:THR:CG2	2.36	0.54
3:c:5033:PHE:CD1	4:d:5229:ALA:HB3	2.43	0.54
3:c:5034:ALA:HB2	4:d:5230:SER:CB	2.37	0.54
20:c:5493:CLA:HBA1	20:c:5493:CLA:CBD	2.35	0.54
13:o:5216:PHE:C	13:o:5216:PHE:HD2	2.15	0.54
1:A:174:LEU:HD22	21:A:561:PHO:H152	1.89	0.54
5:E:76:VAL:O	5:E:79:PHE:HB2	2.07	0.54
2:b:5191:ASN:ND2	7:h:5060:VAL:HG12	2.23	0.54
3:C:201:ASN:N	3:C:202:PRO:HD3	2.22	0.54
4:D:100:ASP:OD1	4:D:102:THR:HG22	2.07	0.54
1:a:5027:ARG:NH1	1:a:5027:ARG:O	2.40	0.54
2:b:5283:GLU:OE1	2:b:5286:ARG:HD2	2.08	0.54
20:b:5520:CLA:H151	20:b:5520:CLA:OBD	2.07	0.54
3:c:5405:ASN:ND2	30:c:5509:DGD:HD5	2.20	0.54
1:A:159:LEU:C	1:A:162:PRO:HD2	2.32	0.54
3:C:276:LEU:CD2	20:C:498:CLA:HBB1	2.37	0.54
4:D:67:TYR:CD2	4:D:76:VAL:HG11	2.43	0.54
4:D:251:ARG:HG3	4:D:255:GLN:HE21	1.73	0.54
8:I:24:LEU:C	8:I:26:GLY:H	2.16	0.54
12:M:26:TYR:O	12:M:29:THR:HB	2.08	0.54
1:a:5116:ILE:HG13	1:a:5117:PHE:N	2.22	0.54
1:a:5269:ARG:NH1	4:d:5234:ALA:HB3	2.23	0.54
2:b:5256:MET:O	2:b:5448:ARG:NH1	2.40	0.54
2:b:5332:LYS:HB3	2:b:5444:ARG:HE	1.72	0.54
3:c:5161:LEU:HG	3:c:5165:LEU:HD12	1.90	0.54
3:c:5348:GLU:OE2	13:o:5037:VAL:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:h:5049:TYR:CD2	30:h:5208:DGD:HB22	2.43	0.54
3:C:99:VAL:HG23	3:C:100:GLY:H	1.72	0.53
4:D:45:LEU:HD13	4:D:49:LEU:HD12	1.90	0.53
4:D:90:LEU:HD12	4:D:96:GLU:HG3	1.89	0.53
16:V:102:MET:HE1	16:V:142:ALA:HB2	1.90	0.53
1:a:5307:ILE:HD11	1:a:5311:GLY:O	2.08	0.53
2:b:5061:PHE:CZ	20:b:5517:CLA:HBB1	2.43	0.53
13:o:5065:ARG:HA	13:o:5111:LEU:H	1.72	0.53
1:A:159:LEU:O	1:A:163:ILE:HG13	2.08	0.53
2:B:256:MET:O	2:B:448:ARG:NH1	2.36	0.53
16:V:128:PRO:O	16:V:129:LYS:C	2.51	0.53
1:a:5184:ILE:HD11	4:d:5186:GLN:CD	2.34	0.53
2:b:5229:LEU:O	2:b:5231:MET:N	2.41	0.53
2:b:5311:PHE:HA	2:b:5430:PHE:CZ	2.44	0.53
2:b:5360:PRO:O	2:b:5362:PHE:N	2.42	0.53
3:c:5044:ASN:O	3:c:5045:LEU:HG	2.08	0.53
3:c:5046:SER:HA	3:c:5049:LEU:HB3	1.90	0.53
3:c:5417:VAL:O	3:c:5417:VAL:HG22	2.07	0.53
8:i:5019:PHE:CE1	8:i:5023:PHE:HE2	2.27	0.53
13:o:5055:ALA:O	13:o:5057:PRO:HD3	2.07	0.53
15:u:5057:LEU:HD22	15:u:5079:ILE:HG21	1.89	0.53
1:A:223:LEU:HD13	4:D:265:ARG:HD3	1.91	0.53
2:B:242:ILE:HG22	2:B:466:HIS:HB2	1.90	0.53
2:B:414:PRO:HB2	2:B:415:PRO:CD	2.32	0.53
3:C:241:GLY:C	3:C:243:ILE:N	2.64	0.53
4:D:54:PHE:HB3	5:E:47:PHE:CD1	2.44	0.53
17:X:72:UNK:O	17:X:73:UNK:C	2.57	0.53
4:d:5090:LEU:HD12	4:d:5096:GLU:HG3	1.90	0.53
4:d:5219:GLU:OE1	4:d:5219:GLU:HA	2.09	0.53
4:d:5313:THR:OG1	4:d:5315:TYR:HB3	2.09	0.53
16:v:5128:PRO:O	16:v:5130:MET:N	2.42	0.53
2:B:124:ARG:O	7:H:12:ARG:NH2	2.42	0.53
2:B:135:LEU:HA	2:B:138:MET:HE2	1.91	0.53
3:C:84:GLN:HB2	3:C:86:LEU:CD2	2.37	0.53
3:C:158:THR:O	3:C:251:HIS:HB3	2.07	0.53
3:C:367:GLU:HB2	3:C:368:PRO:HD3	1.90	0.53
11:L:11:GLU:HG2	11:L:12:LEU:N	2.24	0.53
11:L:14:ARG:NH1	11:L:14:ARG:HG3	2.22	0.53
12:M:33:GLN:C	12:M:35:SER:H	2.16	0.53
14:T:29:ILE:H	14:T:29:ILE:CD1	2.18	0.53
2:b:5086:ILE:C	2:b:5086:ILE:HD12	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:5263:THR:HG22	2:b:5263:THR:O	2.08	0.53
3:c:5284:PHE:HB3	30:c:5507:DGD:HA51	1.89	0.53
15:u:5057:LEU:HD22	15:u:5079:ILE:CG2	2.38	0.53
2:B:259:GLY:O	2:B:260:SER:CB	2.56	0.53
4:D:14:TRP:HD1	4:D:15:PHE:H	1.55	0.53
5:E:51:ARG:O	5:E:53:ASP:N	2.41	0.53
10:K:14:ALA:HB2	18:Z:61:VAL:HG11	1.90	0.53
12:M:36:SER:OXT	12:m:5028:GLN:OE1	2.26	0.53
13:O:92:VAL:HG12	13:O:93:PRO:CD	2.37	0.53
1:a:5072:LEU:HD22	27:t:5217:LMT:O3'	2.08	0.53
2:b:5214:LEU:O	2:b:5218:LEU:HG	2.08	0.53
3:c:5337:LEU:HD23	13:o:5131:PRO:CG	2.36	0.53
28:d:5359:MGE:O3D	9:j:5037:GLY:HA3	2.09	0.53
13:o:5047:THR:HG22	13:o:5048:LEU:H	1.72	0.53
1:A:286:THR:HB	20:A:558:CLA:O1D	2.09	0.53
2:B:18:ARG:HD2	2:B:115:TRP:CD2	2.44	0.53
3:C:48:LYS:HE2	3:C:133:ALA:HA	1.90	0.53
13:O:162:ILE:HA	13:O:166:THR:HG21	1.90	0.53
1:a:5176:ILE:HD13	20:a:5559:CLA:HED3	1.89	0.53
2:b:5031:ALA:HB2	20:b:5515:CLA:CBC	2.39	0.53
2:b:5220:ARG:HD2	7:h:5020:LYS:O	2.09	0.53
3:c:5029:GLU:HG3	3:c:5030:SER:N	2.23	0.53
3:c:5075:PHE:CE2	3:c:5077:PRO:HA	2.43	0.53
4:d:5027:PHE:CD2	4:d:5028:VAL:HG23	2.35	0.53
4:d:5351:ALA:O	4:d:5352:LEU:OXT	2.27	0.53
10:k:5043:VAL:HG12	10:k:5046:ARG:HG3	1.91	0.53
17:x:5086:UNK:OD1	17:x:5086:UNK:N	2.41	0.53
18:z:5014:ILE:O	18:z:5018:VAL:HG23	2.08	0.53
1:A:40:THR:HG22	1:A:118:HIS:O	2.09	0.53
1:A:314:ILE:O	1:A:314:ILE:CG2	2.55	0.53
4:D:172:SER:O	4:D:173:PHE:HB2	2.08	0.53
10:K:15:TYR:C	10:K:17:ILE:H	2.17	0.53
16:V:74:THR:O	16:V:75:ASN:HB2	2.07	0.53
3:c:5029:GLU:C	3:c:5031:SER:H	2.17	0.53
4:d:5176:ALA:C	4:d:5178:ILE:N	2.67	0.53
1:A:124:SER:O	1:A:127:MET:HB3	2.09	0.53
1:A:238:LYS:O	1:A:241:GLN:HB3	2.09	0.53
3:C:29:GLU:HG3	3:C:30:SER:N	2.22	0.53
4:D:180:ARG:C	4:D:180:ARG:HD3	2.33	0.53
4:D:221:THR:HG22	4:D:221:THR:O	2.08	0.53
3:c:5055:ALA:HB1	24:c:5504:BCR:C37	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:ILE:C	2:B:86:ILE:HD12	2.33	0.53
2:B:133:LEU:HB3	2:B:138:MET:HE1	1.89	0.53
3:C:370:ARG:HD3	13:O:33:TYR:CD2	2.44	0.53
3:C:377:LEU:HB2	13:O:106:GLN:HG2	1.91	0.53
2:b:5028:ALA:O	2:b:5104:SER:HB2	2.09	0.53
3:c:5438:LEU:HD11	20:c:5495:CLA:HBB1	1.91	0.53
4:d:5060:THR:HG23	4:d:5061:HIS:H	1.73	0.53
10:k:5014:ALA:HB1	18:z:5005:PHE:HE2	1.74	0.53
14:t:5001:MET:C	14:t:5004:ILE:HG22	2.33	0.53
15:u:5058:ASN:OD1	15:u:5084:PRO:HA	2.09	0.53
16:v:5125:ASP:HA	16:v:5131:ARG:HH21	1.74	0.53
1:A:141:PRO:O	1:A:143:ILE:N	2.38	0.53
1:A:176:ILE:HD13	20:A:559:CLA:HED3	1.91	0.53
21:A:561:PHO:NC	4:D:209:LEU:HD12	2.24	0.53
16:V:160:LYS:O	16:V:161:VAL:C	2.52	0.53
1:a:5264:SER:OG	1:a:5265:PHE:N	2.41	0.53
3:c:5091:HIS:HB3	20:c:5493:CLA:HBA2	1.91	0.53
4:d:5178:ILE:HG22	4:d:5179:PHE:N	2.23	0.53
4:d:5221:THR:HG22	4:d:5221:THR:O	2.08	0.53
13:o:5045:CYS:HB2	13:o:5046:PRO:CD	2.31	0.53
14:t:5029:ILE:HD12	14:t:5029:ILE:N	2.20	0.53
1:A:27:ARG:HG3	1:A:27:ARG:HH11	1.75	0.52
1:A:36:ILE:O	1:A:39:PRO:HD2	2.09	0.52
1:A:330:VAL:CG1	4:D:348:ARG:HA	2.38	0.52
2:B:102:VAL:HA	24:B:528:BCR:C40	2.39	0.52
2:B:476:ARG:HH11	2:B:476:ARG:HG3	1.74	0.52
3:C:362:ARG:HH11	3:C:362:ARG:HG3	1.71	0.52
28:D:360:MGE:H241	14:T:13:ILE:HG21	1.90	0.52
5:E:32:ILE:O	5:E:36:LEU:HG	2.10	0.52
9:J:19:MET:O	9:J:23:VAL:HG23	2.09	0.52
10:K:31:LEU:HB3	24:X:130:BCR:C15	2.39	0.52
1:a:5132:GLU:O	1:a:5136:ARG:HG2	2.08	0.52
2:b:5444:ARG:HH11	2:b:5444:ARG:HG2	1.72	0.52
2:b:5463:PHE:CZ	20:b:5518:CLA:HBB1	2.41	0.52
20:b:5519:CLA:HBA2	7:h:5031:MET:SD	2.49	0.52
3:c:5063:TRP:O	3:c:5064:ALA:C	2.51	0.52
4:d:5068:LEU:HD21	5:e:5044:TYR:CD1	2.44	0.52
28:d:5361:MGE:H241	14:t:5013:ILE:HG21	1.91	0.52
13:o:5225:LEU:HD12	13:o:5225:LEU:N	2.23	0.52
3:C:318:LEU:HD23	3:C:318:LEU:O	2.10	0.52
7:H:45:ILE:O	7:H:46:LEU:C	2.51	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:33:TYR:C	13:O:35:ASP:N	2.66	0.52
13:O:56:TYR:CD1	13:O:235:GLY:HA2	2.44	0.52
15:U:98:THR:C	15:U:100:ARG:H	2.16	0.52
2:b:5068:ARG:HH11	2:b:5262:THR:HG23	1.72	0.52
2:b:5246:PHE:C	2:b:5246:PHE:HD1	2.16	0.52
3:c:5095:LEU:HA	3:c:5185:LEU:HD22	1.90	0.52
20:c:5501:CLA:H42	10:k:5039:TRP:CD1	2.44	0.52
4:d:5343:GLU:HG2	16:v:5161:VAL:HG11	1.91	0.52
4:d:5346:LEU:O	4:d:5348:ARG:HG3	2.09	0.52
16:v:5119:PRO:HG3	16:v:5127:PHE:CD1	2.44	0.52
1:A:328:MET:HE1	4:D:183:LEU:HD13	1.91	0.52
2:B:124:ARG:HD3	2:B:130:GLU:C	2.33	0.52
2:B:134:ASP:H	7:H:15:ASN:ND2	2.07	0.52
2:B:263:THR:HG22	2:B:263:THR:O	2.08	0.52
2:B:357:ARG:HH22	4:D:337:GLU:HG3	1.74	0.52
2:B:391:SER:OG	2:B:394:GLN:NE2	2.43	0.52
3:C:103:GLY:HA3	3:C:301:PHE:CE1	2.37	0.52
2:b:5124:ARG:O	7:h:5012:ARG:NH2	2.42	0.52
2:b:5179:GLN:HA	2:b:5179:GLN:HE21	1.75	0.52
3:c:5277:GLY:C	20:c:5495:CLA:HBC2	2.34	0.52
6:f:5034:LEU:HD22	9:j:5024:ILE:CD1	2.38	0.52
9:j:5015:THR:HG22	10:k:5038:VAL:HG22	1.91	0.52
13:o:5052:ALA:HB1	13:o:5230:VAL:N	2.21	0.52
13:o:5145:LEU:CD2	13:o:5175:PRO:CG	2.85	0.52
13:o:5241:PHE:CD1	13:o:5241:PHE:C	2.87	0.52
13:o:5259:VAL:HG12	13:o:5260:LYS:N	2.25	0.52
1:A:103:ASP:OD1	1:A:103:ASP:N	2.40	0.52
3:C:56:HIS:O	3:C:58:GLY:N	2.42	0.52
4:D:93:TRP:HZ2	20:D:355:CLA:O1A	1.93	0.52
5:E:69:ARG:O	5:E:70:PHE:HB2	2.09	0.52
17:X:12:UNK:CG	18:Z:17:PHE:CE1	2.90	0.52
2:b:5124:ARG:HD3	2:b:5130:GLU:C	2.34	0.52
2:b:5413:ASP:OD1	2:b:5415:PRO:HD2	2.10	0.52
4:d:5272:LEU:HD23	4:d:5272:LEU:C	2.33	0.52
13:o:5073:PRO:HG2	13:o:5102:THR:OG1	2.10	0.52
13:o:5083:LYS:O	13:o:5084:ASN:CB	2.57	0.52
15:u:5072:TYR:CB	15:u:5073:PRO:CD	2.86	0.52
3:C:33:PHE:CD1	4:D:229:ALA:HB3	2.45	0.52
1:a:5076:ASN:HD22	1:a:5076:ASN:H	1.57	0.52
1:a:5299:GLY:O	3:c:5403:SER:HB2	2.08	0.52
20:a:5560:CLA:HAB	20:d:5354:CLA:H72	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:5102:VAL:HA	24:b:5528:BCR:C40	2.40	0.52
16:v:5039:ASN:OD1	16:v:5043:LYS:N	2.42	0.52
16:v:5063:CYS:O	16:v:5064:ALA:C	2.51	0.52
4:D:272:LEU:C	4:D:272:LEU:HD23	2.35	0.52
16:V:81:ARG:NE	16:V:157:GLY:HA3	2.24	0.52
2:b:5055:MET:HE3	2:b:5080:ILE:CG1	2.39	0.52
3:c:5075:PHE:HE2	3:c:5077:PRO:HA	1.75	0.52
4:d:5093:TRP:HZ2	20:d:5355:CLA:O1A	1.92	0.52
12:m:5031:SER:C	12:m:5033:GLN:H	2.16	0.52
2:B:220:ARG:HD2	7:H:20:LYS:O	2.10	0.52
3:C:197:ARG:NH2	3:C:231:GLU:OE2	2.35	0.52
4:D:136:VAL:O	4:D:136:VAL:HG12	2.09	0.52
1:a:5193:LEU:HD13	4:d:5179:PHE:HB3	1.92	0.52
2:b:5476:ARG:HH11	2:b:5476:ARG:HG3	1.74	0.52
3:c:5315:MET:CE	3:c:5319:ILE:HD11	2.40	0.52
4:d:5251:ARG:HE	4:d:5255:GLN:NE2	2.08	0.52
10:k:5014:ALA:HB2	18:z:5061:VAL:HG11	1.92	0.52
28:l:5210:MGE:H5A2	12:m:5022:LEU:HD21	1.92	0.52
16:v:5102:MET:HE1	16:v:5142:ALA:HB2	1.91	0.52
17:x:5072:UNK:O	17:x:5073:UNK:C	2.57	0.52
2:B:214:LEU:O	2:B:218:LEU:HG	2.09	0.52
2:B:311:PHE:HA	2:B:430:PHE:CZ	2.44	0.52
3:C:42:LEU:HD13	20:C:501:CLA:HMA2	1.92	0.52
8:I:13:THR:O	8:I:17:LEU:HG	2.09	0.52
16:V:134:THR:HG23	16:V:137:ASP:OD2	2.10	0.52
2:b:5271:THR:HB	2:b:5274:GLN:HG3	1.92	0.52
3:c:5281:MET:HG3	28:i:5201:MGE:H231	1.92	0.52
4:d:5067:TYR:CE2	4:d:5076:VAL:HG11	2.45	0.52
5:e:5051:ARG:O	5:e:5053:ASP:N	2.43	0.52
13:o:5109:GLY:HA3	13:o:5122:VAL:O	2.10	0.52
14:t:5004:ILE:HB	27:t:5217:LMT:O6'	2.09	0.52
18:z:5023:VAL:HB	18:z:5024:PRO:HD3	1.91	0.52
1:A:63:ILE:CG2	3:C:335:THR:HG21	2.40	0.52
1:A:93:PHE:CD1	1:A:95:PRO:HD3	2.45	0.52
1:A:129:ARG:C	1:A:131:TRP:H	2.17	0.52
2:B:362:PHE:HE2	4:D:164:GLN:NE2	2.08	0.52
16:V:121:LEU:HD11	16:V:138:LEU:HD11	1.91	0.52
16:V:125:ASP:HA	16:V:131:ARG:HH21	1.74	0.52
1:a:5286:THR:HB	20:a:5558:CLA:O1D	2.09	0.52
2:b:5357:ARG:HH22	4:d:5337:GLU:HG3	1.74	0.52
1:A:27:ARG:NH1	1:A:27:ARG:O	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:VAL:HG12	4:D:348:ARG:HA	1.91	0.52
2:B:137:LYS:HD2	7:H:14:LEU:O	2.10	0.52
2:B:314:TYR:CE2	2:B:316:GLY:HA3	2.45	0.52
3:C:116:VAL:HG21	24:C:505:BCR:C32	2.40	0.52
3:C:280:SER:HB2	3:C:437:PHE:HB3	1.92	0.52
11:L:2:GLU:HB3	11:L:3:PRO:HD2	1.92	0.52
13:O:118:SER:HB3	13:O:157:PRO:HA	1.90	0.52
16:V:33:VAL:O	16:V:33:VAL:HG12	2.10	0.52
1:a:5187:GLN:NE2	1:a:5191:ASN:HA	2.25	0.52
1:a:5314:ILE:O	1:a:5314:ILE:CG2	2.57	0.52
3:c:5099:VAL:HG23	3:c:5100:GLY:H	1.75	0.52
3:c:5267:SER:O	3:c:5271:TYR:CD2	2.63	0.52
13:o:5092:VAL:HG12	13:o:5093:PRO:CD	2.40	0.52
4:D:14:TRP:CD1	4:D:15:PHE:N	2.78	0.51
9:J:24:ILE:HG23	9:J:25:VAL:N	2.24	0.51
13:O:110:GLU:OE2	13:O:112:LYS:HB2	2.10	0.51
18:Z:57:LEU:O	18:Z:61:VAL:HG23	2.10	0.51
1:a:5095:PRO:HD2	1:a:5098:GLU:HG3	1.92	0.51
2:b:5263:THR:CG2	2:b:5448:ARG:NH1	2.63	0.51
2:B:413:ASP:OD1	2:B:415:PRO:HD2	2.09	0.51
4:D:40:CYS:O	4:D:41:ALA:C	2.53	0.51
4:D:223:PHE:CZ	4:D:245:SER:HB3	2.44	0.51
13:O:144:LEU:HD23	13:O:144:LEU:N	2.23	0.51
1:a:5129:ARG:HH21	4:d:5256:ILE:HG13	1.76	0.51
2:b:5135:LEU:HA	2:b:5138:MET:HE2	1.92	0.51
3:c:5459:ILE:HD12	4:d:5245:SER:OG	2.10	0.51
4:d:5103:ARG:HH12	5:e:5077:GLU:HG3	1.76	0.51
4:d:5126:MET:HA	4:d:5129:GLN:OE1	2.09	0.51
1:A:76:ASN:HD22	1:A:76:ASN:H	1.58	0.51
1:A:272:HIS:CG	4:D:218:VAL:HG11	2.45	0.51
2:B:463:PHE:CZ	20:B:518:CLA:HBB1	2.43	0.51
13:O:172:PHE:HE2	13:O:223:ILE:HG12	1.75	0.51
16:V:59:PHE:HA	16:V:63:CYS:SG	2.50	0.51
16:V:63:CYS:O	16:V:64:ALA:C	2.54	0.51
3:c:5229:ASN:HD22	3:c:5231:GLU:HG2	1.75	0.51
7:h:5044:ILE:O	7:h:5048:ILE:HG13	2.10	0.51
11:l:5014:ARG:HG3	11:l:5014:ARG:HH11	1.76	0.51
18:z:5001:MET:HE3	18:z:5060:PHE:CG	2.46	0.51
1:A:192:ILE:HG23	1:A:193:LEU:N	2.25	0.51
3:C:62:PHE:HE2	10:K:28:ILE:HB	1.75	0.51
20:C:493:CLA:HBA1	20:C:493:CLA:CBD	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:76:UNK:O	17:X:77:UNK:C	2.57	0.51
1:a:5221:SER:HA	4:d:5139:ARG:HB2	1.91	0.51
1:a:5304:HIS:CD2	1:a:5313:VAL:HG21	2.46	0.51
1:a:5340:PRO:HG3	15:u:5133:TYR:CG	2.45	0.51
6:f:5011:VAL:HG12	6:f:5012:SER:N	2.26	0.51
13:o:5184:ASP:OD2	13:o:5188:ARG:HB2	2.11	0.51
17:x:5027:UNK:O	17:x:5028:UNK:O	2.29	0.51
1:A:326:LEU:HD21	3:C:412:THR:HB	1.93	0.51
2:B:229:LEU:HD11	20:B:519:CLA:O1A	2.11	0.51
3:C:55:ALA:C	24:C:504:BCR:H373	2.35	0.51
3:C:95:LEU:HA	3:C:185:LEU:HD22	1.93	0.51
3:C:281:MET:O	3:C:285:ILE:HG13	2.10	0.51
3:C:460:ASP:O	3:C:461:ARG:C	2.52	0.51
14:T:4:ILE:HB	27:T:217:LMT:O6'	2.11	0.51
1:a:5143:ILE:HD11	4:d:5217:THR:HA	1.92	0.51
2:b:5188:ASP:C	2:b:5190:PHE:H	2.18	0.51
2:b:5403:GLY:O	2:b:5407:ASN:HB2	2.11	0.51
3:c:5367:GLU:HB2	3:c:5368:PRO:HD3	1.93	0.51
3:c:5438:LEU:CD2	30:c:5507:DGD:HAH2	2.41	0.51
5:e:5013:ILE:HD13	32:f:5051:HEM:O1D	2.10	0.51
16:v:5159:GLY:O	16:v:5160:LYS:C	2.52	0.51
1:A:254:TYR:CD2	4:D:132:ILE:HG22	2.45	0.51
2:B:24:LEU:HD13	2:B:111:ALA:HA	1.92	0.51
2:B:233:ASN:ND2	2:B:235:GLU:H	2.08	0.51
10:K:39:TRP:HE1	17:X:31:UNK:CG	2.14	0.51
14:T:29:ILE:HD12	14:T:29:ILE:N	2.18	0.51
1:a:5064:ARG:O	1:a:5066:PRO:HD3	2.10	0.51
1:a:5093:PHE:CD1	1:a:5095:PRO:HD3	2.46	0.51
1:a:5210:LEU:HD13	21:a:5562:PHO:ND	2.25	0.51
2:b:5018:ARG:HD2	2:b:5115:TRP:CD2	2.44	0.51
4:d:5176:ALA:HA	4:d:5179:PHE:CD2	2.46	0.51
7:h:5059:ASN:OD1	7:h:5059:ASN:O	2.28	0.51
1:A:129:ARG:HH21	4:D:256:ILE:HG13	1.75	0.51
3:C:34:ALA:HB2	4:D:230:SER:CB	2.41	0.51
3:C:438:LEU:HD11	20:C:495:CLA:HBB1	1.92	0.51
4:D:176:ALA:C	4:D:178:ILE:N	2.66	0.51
10:K:14:ALA:HB1	18:Z:5:PHE:HE2	1.76	0.51
13:O:80:GLU:O	13:O:81:GLU:C	2.53	0.51
13:O:109:GLY:HA3	13:O:122:VAL:O	2.11	0.51
1:a:5140:ARG:HH22	25:a:5567:LHG:P	2.34	0.51
3:c:5035:TRP:CG	3:c:5036:TRP:N	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:5037:ALA:HA	20:c:5498:CLA:O1A	2.11	0.51
3:c:5116:VAL:HG21	24:c:5505:BCR:C32	2.40	0.51
9:j:5038:SER:OG	9:j:5039:SER:N	2.43	0.51
13:o:5230:VAL:HG12	13:o:5231:ASP:N	2.25	0.51
17:x:5076:UNK:O	17:x:5077:UNK:C	2.57	0.51
18:z:5020:VAL:O	18:z:5024:PRO:HG2	2.10	0.51
2:B:190:PHE:HE2	7:H:41:PHE:HE1	1.59	0.51
13:O:178:ARG:HD2	13:O:182:PHE:CD1	2.45	0.51
14:T:4:ILE:HG23	14:T:5:THR:N	2.25	0.51
1:a:5062:GLY:O	1:a:5063:ILE:O	2.28	0.51
1:a:5141:PRO:O	1:a:5143:ILE:N	2.37	0.51
3:c:5140:LEU:HB2	3:c:5148:GLY:HA2	1.92	0.51
8:i:5027:ASP:O	8:i:5028:PRO:C	2.54	0.51
13:o:5075:THR:HG22	13:o:5077:LEU:CD1	2.41	0.51
15:u:5077:LYS:O	15:u:5081:LYS:HB2	2.11	0.51
1:A:95:PRO:HD2	1:A:98:GLU:HG3	1.93	0.51
3:C:226:SER:HA	30:C:507:DGD:HE62	1.93	0.51
3:C:358:PHE:C	3:C:360:ASP:H	2.18	0.51
3:C:438:LEU:CD2	30:C:507:DGD:HAH2	2.41	0.51
3:C:449:ARG:HG3	3:C:449:ARG:O	2.10	0.51
6:F:11:VAL:HG12	6:F:12:SER:N	2.26	0.51
1:a:5232:SER:OG	1:a:5235:TYR:CD1	2.64	0.51
3:c:5194:GLY:O	3:c:5195:ASP:HB2	2.11	0.51
13:o:5059:ASP:C	13:o:5061:SER:H	2.18	0.51
13:o:5081:GLU:O	13:o:5082:PRO:C	2.51	0.51
14:t:5004:ILE:HG23	14:t:5005:THR:N	2.25	0.51
1:A:143:ILE:HD11	4:D:217:THR:HA	1.93	0.51
2:B:175:THR:HG22	2:B:175:THR:O	2.11	0.51
2:B:326:ARG:HH21	4:D:297:ASP:CG	2.19	0.51
3:C:48:LYS:HE2	3:C:132:HIS:O	2.11	0.51
5:E:59:GLU:O	5:E:60:GLN:C	2.53	0.51
8:I:4:LEU:O	8:I:8:VAL:HG23	2.11	0.51
15:U:59:ASN:O	15:U:60:THR:C	2.54	0.51
1:a:5228:THR:OG1	1:a:5231:GLU:HG2	2.11	0.51
1:a:5326:LEU:HD23	3:c:5412:THR:HB	1.93	0.51
4:d:5274:VAL:HG13	22:d:5356:PQ9:H251	1.93	0.51
13:o:5065:ARG:HG2	13:o:5066:ILE:N	2.25	0.51
16:v:5109:ASP:CG	16:v:5111:GLU:HB2	2.36	0.51
1:A:64:ARG:O	1:A:66:PRO:HD3	2.10	0.50
2:B:326:ARG:HB3	2:B:444:ARG:HH11	1.75	0.50
20:B:517:CLA:H202	11:L:27:LEU:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:219:GLU:OE1	4:D:219:GLU:HA	2.09	0.50
17:X:85:UNK:C	17:X:86:UNK:OD1	2.59	0.50
1:a:5174:LEU:HD22	21:a:5561:PHO:H152	1.93	0.50
2:b:5012:LEU:HD12	20:b:5522:CLA:HBB1	1.93	0.50
3:c:5190:ALA:HB3	3:c:5193:GLY:C	2.36	0.50
13:o:5144:LEU:HD23	13:o:5144:LEU:N	2.25	0.50
20:B:525:CLA:H112	20:B:525:CLA:H162	1.93	0.50
3:C:140:LEU:HB2	3:C:148:GLY:HA2	1.93	0.50
3:C:146:PHE:HD2	3:C:147:PHE:CE1	2.29	0.50
3:C:372:PRO:O	13:O:36:ILE:HD12	2.11	0.50
4:D:63:LEU:HD12	4:D:63:LEU:N	2.26	0.50
6:F:45:ARG:OXT	6:F:45:ARG:HG2	2.11	0.50
21:a:5561:PHO:NC	4:d:5209:LEU:HD12	2.26	0.50
2:b:5474:LEU:HD11	20:b:5518:CLA:HAA1	1.93	0.50
3:c:5042:LEU:HD13	20:c:5501:CLA:HMA2	1.92	0.50
3:c:5078:GLU:HA	3:c:5078:GLU:OE2	2.11	0.50
3:c:5410:VAL:HG12	3:c:5412:THR:H	1.77	0.50
4:d:5126:MET:HE1	4:d:5147:SER:HA	1.94	0.50
4:d:5223:PHE:CE1	4:d:5245:SER:HB3	2.46	0.50
9:j:5019:MET:O	9:j:5023:VAL:HG23	2.11	0.50
16:v:5134:THR:N	16:v:5137:ASP:OD2	2.44	0.50
1:A:26:ASN:O	1:A:27:ARG:C	2.54	0.50
1:A:42:LEU:HA	1:A:45:THR:HG22	1.92	0.50
20:A:560:CLA:HAB	20:D:354:CLA:H72	1.93	0.50
3:C:150:ASP:HB3	3:C:153:ASP:CB	2.32	0.50
15:U:64:ALA:O	15:U:67:GLN:HG2	2.10	0.50
1:a:5159:LEU:O	1:a:5163:ILE:HG13	2.12	0.50
2:b:5228:ALA:O	2:b:5230:ARG:NH1	2.44	0.50
20:b:5513:CLA:H2	20:b:5515:CLA:H91	1.93	0.50
3:c:5449:ARG:HG3	3:c:5449:ARG:O	2.11	0.50
5:e:5059:GLU:O	5:e:5060:GLN:C	2.54	0.50
6:f:5011:VAL:HG12	6:f:5012:SER:H	1.76	0.50
15:u:5072:TYR:CG	15:u:5073:PRO:N	2.79	0.50
4:D:27:PHE:CD2	4:D:28:VAL:HG23	2.36	0.50
13:O:145:LEU:CD2	13:O:175:PRO:CG	2.86	0.50
14:T:15:ALA:HB2	24:T:5104:BCR:H14C	1.92	0.50
1:a:5254:TYR:CD2	4:d:5132:ILE:HG22	2.46	0.50
2:b:5137:LYS:HD2	7:h:5014:LEU:O	2.12	0.50
2:b:5271:THR:HG22	2:b:5273:TYR:H	1.75	0.50
4:d:5096:GLU:H	4:d:5096:GLU:CD	2.19	0.50
13:o:5074:THR:HB	13:o:5262:GLN:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:t:5004:ILE:HB	27:t:5217:LMT:C6'	2.42	0.50
1:A:22:THR:HG23	1:A:136:ARG:NH1	2.26	0.50
1:A:62:GLY:O	1:A:63:ILE:O	2.29	0.50
2:B:24:LEU:HB3	2:B:111:ALA:HB2	1.93	0.50
2:B:368:VAL:HG11	2:B:381:ILE:CD1	2.37	0.50
3:C:245:ILE:O	3:C:249:ILE:HD13	2.12	0.50
4:D:77:ALA:HB2	4:D:174:GLY:HA3	1.93	0.50
10:K:19:ASP:N	10:K:20:PRO:HD2	2.26	0.50
10:K:37:PHE:HB3	24:X:130:BCR:C40	2.42	0.50
3:c:5296:VAL:HG23	3:c:5297:TYR:CD2	2.47	0.50
5:e:5031:PHE:CE1	6:f:5035:GLY:HA2	2.47	0.50
1:A:136:ARG:HH22	8:I:27:ASP:CG	2.19	0.50
2:B:215:PHE:C	2:B:215:PHE:CD2	2.89	0.50
10:K:43:VAL:HG21	17:X:31:UNK:HG3	1.93	0.50
12:M:15:VAL:O	12:M:19:SER:HB2	2.12	0.50
18:Z:36:SER:CA	18:Z:39:LEU:HD12	2.35	0.50
25:a:5567:LHG:HC61	3:c:5443:TRP:HH2	1.76	0.50
2:b:5286:ARG:C	2:b:5286:ARG:HD3	2.36	0.50
3:c:5472:LEU:C	3:c:5473:ASP:CG	2.79	0.50
4:d:5014:TRP:HD1	4:d:5015:PHE:H	1.59	0.50
9:j:5015:THR:CG2	10:k:5038:VAL:HG22	2.41	0.50
1:A:72:LEU:HD22	27:T:217:LMT:O3'	2.12	0.50
2:B:15:ASP:O	2:B:17:GLY:N	2.45	0.50
2:B:297:THR:H	2:B:300:GLU:CD	2.20	0.50
2:B:315:ILE:HG22	2:B:426:PHE:HB3	1.94	0.50
2:B:341:LYS:O	2:B:406:LEU:HB2	2.11	0.50
3:C:178:LYS:HD2	3:C:182:PHE:O	2.11	0.50
4:D:60:THR:HG23	4:D:61:HIS:H	1.77	0.50
13:O:147:THR:HG21	13:O:175:PRO:HD2	1.93	0.50
13:O:265:PHE:CD1	13:O:265:PHE:C	2.90	0.50
1:a:5042:LEU:HA	1:a:5045:THR:HG22	1.93	0.50
3:c:5197:ARG:NH2	3:c:5231:GLU:OE2	2.39	0.50
13:o:5147:THR:HG21	13:o:5175:PRO:HD2	1.94	0.50
16:v:5059:PHE:CE1	16:v:5063:CYS:HB2	2.46	0.50
6:F:40:MET:C	6:F:42:PHE:H	2.20	0.50
3:c:5346:THR:HG21	13:o:5038:GLY:HA2	1.94	0.50
4:d:5126:MET:HE2	4:d:5146:PHE:HB3	1.93	0.50
13:o:5032:THR:N	13:o:5035:ASP:HB2	2.27	0.50
15:u:5072:TYR:HB3	15:u:5073:PRO:CD	2.36	0.50
15:u:5073:PRO:HB3	16:v:5107:THR:HG21	1.93	0.50
1:A:299:GLY:O	3:C:403:SER:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:463:PHE:CZ	2:B:467:ILE:HD12	2.46	0.50
16:V:128:PRO:O	16:V:130:MET:N	2.45	0.50
1:a:5078:ILE:O	1:a:5177:SER:HB2	2.12	0.50
1:a:5191:ASN:ND2	1:a:5194:MET:HB2	2.27	0.50
1:a:5196:PRO:HA	1:a:5199:GLN:OE1	2.12	0.50
1:a:5306:VAL:CG2	1:a:5316:THR:HG23	2.40	0.50
2:b:5175:THR:HG22	2:b:5175:THR:O	2.11	0.50
3:c:5358:PHE:C	3:c:5360:ASP:H	2.20	0.50
3:c:5391:ARG:HG3	3:c:5391:ARG:NH1	2.26	0.50
4:d:5014:TRP:CD1	4:d:5015:PHE:N	2.79	0.50
15:u:5098:THR:C	15:u:5100:ARG:H	2.18	0.50
2:B:31:ALA:HB2	20:B:515:CLA:CBC	2.42	0.49
4:D:35:ILE:HG22	4:D:35:ILE:O	2.12	0.49
4:D:96:GLU:CD	4:D:96:GLU:H	2.20	0.49
4:D:313:THR:OG1	4:D:315:TYR:HB3	2.11	0.49
5:E:6:GLY:C	5:E:7:GLU:HG2	2.36	0.49
7:H:59:ASN:O	7:H:59:ASN:OD1	2.29	0.49
15:U:73:PRO:HB3	16:V:107:THR:HG21	1.94	0.49
18:Z:2:THR:O	18:Z:3:ILE:C	2.55	0.49
1:a:5013:LEU:HD23	1:a:5013:LEU:H	1.76	0.49
1:a:5190:HIS:ND1	1:a:5298:ASN:ND2	2.60	0.49
3:c:5146:PHE:HD2	3:c:5147:PHE:CE1	2.30	0.49
3:c:5193:GLY:O	3:c:5194:GLY:C	2.55	0.49
4:d:5148:ALA:CB	4:d:5149:PRO:HD3	2.34	0.49
7:h:5005:THR:O	7:h:5008:GLY:N	2.45	0.49
10:k:5013:GLU:O	10:k:5016:ALA:HB3	2.11	0.49
13:o:5178:ARG:HD2	13:o:5182:PHE:CD1	2.46	0.49
15:u:5083:ALA:HB1	15:u:5084:PRO:HD2	1.94	0.49
2:B:98:LEU:O	2:B:99:ALA:C	2.55	0.49
3:C:180:MET:HE3	3:C:202:PRO:CD	2.42	0.49
3:C:416:SER:O	3:C:417:VAL:HG12	2.11	0.49
13:O:73:PRO:CG	13:O:102:THR:CB	2.90	0.49
15:U:55:ILE:HG21	15:U:65:PHE:CE2	2.46	0.49
16:V:144:HIS:CE1	16:V:148:GLU:OE2	2.65	0.49
1:a:5131:TRP:CZ2	20:c:5495:CLA:HAA1	2.48	0.49
2:b:5024:LEU:HB3	2:b:5111:ALA:HB2	1.93	0.49
20:b:5517:CLA:H202	11:l:5027:LEU:HD11	1.94	0.49
3:c:5453:ALA:CB	8:i:5031:ASN:ND2	2.73	0.49
13:o:5070:CYS:O	13:o:5265:PHE:HB2	2.12	0.49
18:z:5005:PHE:HE1	18:z:5054:VAL:HG13	1.77	0.49
2:B:7:ARG:O	2:B:8:VAL:C	2.55	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:171:PRO:HD3	7:H:65:LEU:C	2.37	0.49
2:B:474:LEU:HD11	20:B:518:CLA:HAA1	1.94	0.49
3:C:46:SER:HA	3:C:49:LEU:HB3	1.93	0.49
4:D:55:VAL:HG12	4:D:56:THR:N	2.26	0.49
4:D:240:ALA:HB1	4:D:241:GLU:OE1	2.12	0.49
5:E:47:PHE:O	5:E:49:THR:N	2.45	0.49
9:J:12:ILE:O	9:J:16:VAL:HG23	2.12	0.49
1:a:5129:ARG:C	1:a:5131:TRP:H	2.20	0.49
5:e:5051:ARG:O	5:e:5054:SER:N	2.44	0.49
10:k:5037:PHE:HB3	24:x:5130:BCR:C40	2.42	0.49
12:m:5009:ILE:HD12	12:m:5009:ILE:N	2.28	0.49
13:o:5178:ARG:HG3	13:o:5178:ARG:NH1	2.24	0.49
3:C:188:THR:HG23	3:C:300:GLU:OE2	2.13	0.49
3:C:452:ALA:C	3:C:454:GLY:H	2.21	0.49
4:D:102:THR:CG2	4:D:103:ARG:N	2.74	0.49
13:O:51:THR:O	13:O:52:ALA:O	2.30	0.49
1:a:5011:ALA:HB1	1:a:5015:GLU:OE2	2.12	0.49
1:a:5076:ASN:ND2	1:a:5076:ASN:C	2.71	0.49
1:a:5129:ARG:NH2	4:d:5256:ILE:HG13	2.26	0.49
1:a:5279:PRO:CG	4:d:5212:ALA:HB2	2.42	0.49
2:b:5242:ILE:HG22	2:b:5466:HIS:HB2	1.93	0.49
6:f:5045:ARG:HG2	6:f:5045:ARG:OXT	2.13	0.49
8:i:5011:VAL:O	8:i:5015:PHE:HD1	1.95	0.49
13:o:5151:LEU:HD12	13:o:5171:GLU:O	2.12	0.49
13:o:5231:ASP:O	13:o:5232:GLY:C	2.55	0.49
1:A:129:ARG:NH2	4:D:256:ILE:HG13	2.28	0.49
1:A:325:ASN:HA	1:A:328:MET:HE3	1.93	0.49
2:B:13:ILE:O	2:B:13:ILE:HG22	2.11	0.49
2:B:124:ARG:HD3	2:B:131:PRO:N	2.28	0.49
2:B:165:GLY:HA3	2:B:179:GLN:O	2.11	0.49
2:B:222:PRO:HG3	7:H:27:THR:N	2.26	0.49
3:C:199:ILE:N	3:C:199:ILE:HD12	2.27	0.49
3:C:318:LEU:HG	3:C:328:VAL:HG11	1.92	0.49
13:O:52:ALA:HB1	13:O:230:VAL:N	2.24	0.49
13:O:74:THR:HB	13:O:262:GLN:O	2.10	0.49
13:O:117:GLY:HA3	13:O:158:ASN:HA	1.95	0.49
2:b:5271:THR:HG22	2:b:5273:TYR:N	2.28	0.49
3:c:5362:ARG:HG3	3:c:5362:ARG:NH1	2.25	0.49
7:h:5054:ILE:HD12	7:h:5054:ILE:N	2.28	0.49
13:o:5049:ASP:O	13:o:5051:THR:N	2.45	0.49
13:o:5215:ARG:NH1	13:o:5252:GLY:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ILE:O	1:A:177:SER:HB2	2.12	0.49
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.95	0.49
2:B:271:THR:HB	2:B:274:GLN:HG3	1.95	0.49
3:C:78:GLU:HA	3:C:78:GLU:OE2	2.12	0.49
13:O:65:ARG:HG2	13:O:66:ILE:N	2.27	0.49
1:a:5078:ILE:HD13	11:l:5033:SER:CB	2.42	0.49
1:a:5326:LEU:HD21	3:c:5412:THR:HB	1.94	0.49
1:A:232:SER:OG	1:A:235:TYR:CD1	2.65	0.49
3:C:75:PHE:HE2	3:C:77:PRO:HA	1.78	0.49
3:C:459:ILE:HG21	3:C:464:GLU:HG2	1.94	0.49
4:D:100:ASP:OD1	4:D:100:ASP:C	2.55	0.49
6:F:41:GLN:NE2	6:F:41:GLN:CA	2.74	0.49
8:I:17:LEU:O	8:I:18:LEU:C	2.55	0.49
10:K:43:VAL:HG12	10:K:43:VAL:O	2.13	0.49
13:O:101:THR:O	13:O:101:THR:HG22	2.13	0.49
2:b:5149:LEU:HG	20:b:5513:CLA:CBC	2.30	0.49
2:b:5215:PHE:C	2:b:5215:PHE:CD2	2.91	0.49
3:c:5318:LEU:HG	3:c:5328:VAL:HG11	1.94	0.49
3:c:5465:PRO:O	3:c:5469:MET:HG3	2.12	0.49
9:j:5021:VAL:HA	9:j:5024:ILE:HG22	1.94	0.49
13:o:5036:ILE:O	13:o:5037:VAL:C	2.55	0.49
3:C:116:VAL:O	3:C:117:VAL:C	2.56	0.49
3:C:250:TRP:HE1	20:C:496:CLA:HED1	1.78	0.49
3:C:281:MET:HG3	28:I:201:MGE:H231	1.94	0.49
13:O:81:GLU:O	13:O:82:PRO:C	2.56	0.49
18:Z:28:ALA:O	18:Z:30:PRO:HD3	2.12	0.49
2:b:5230:ARG:NH1	2:b:5474:LEU:HD22	2.27	0.49
3:c:5150:ASP:HB3	3:c:5153:ASP:CB	2.31	0.49
13:o:5056:TYR:CD1	13:o:5235:GLY:HA2	2.48	0.49
13:o:5162:ILE:HA	13:o:5166:THR:HG21	1.94	0.49
13:o:5163:THR:H	13:o:5166:THR:CG2	2.26	0.49
6:F:40:MET:O	6:F:42:PHE:N	2.46	0.49
24:T:5104:BCR:H23C	24:T:5104:BCR:H403	1.95	0.49
15:U:73:PRO:HD2	16:V:109:ASP:HB3	1.94	0.49
1:a:5026:ASN:O	1:a:5027:ARG:C	2.54	0.49
2:b:5488:PRO:CB	17:x:5092:UNK:CB	2.91	0.49
20:b:5518:CLA:H51	20:b:5519:CLA:H101	1.95	0.49
3:c:5418:ASN:HB3	30:c:5509:DGD:C1E	2.43	0.49
13:o:5030:THR:HG22	13:o:5031:LEU:N	2.27	0.49
13:o:5032:THR:O	13:o:5036:ILE:HG13	2.12	0.49
16:v:5074:THR:O	16:v:5075:ASN:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:VAL:O	1:A:60:ILE:N	2.46	0.49
2:B:28:ALA:O	2:B:104:SER:HB2	2.13	0.49
3:C:162:GLY:O	3:C:166:ILE:HG13	2.12	0.49
3:C:269:GLU:CG	3:C:448:ALA:HB2	2.34	0.49
12:M:31:SER:C	12:M:33:GLN:H	2.21	0.49
1:a:5048:PHE:HA	1:a:5115:ILE:CD1	2.43	0.49
2:b:5326:ARG:HH21	4:d:5297:ASP:CG	2.20	0.49
20:b:5515:CLA:H141	20:b:5520:CLA:CMA	2.43	0.49
3:c:5062:PHE:HE2	10:k:5028:ILE:HB	1.77	0.49
15:u:5098:THR:C	15:u:5100:ARG:N	2.70	0.49
1:A:153:SER:CB	20:A:558:CLA:H43	2.43	0.48
2:B:206:GLY:O	2:B:210:ILE:HG13	2.13	0.48
2:B:488:PRO:CB	17:X:92:UNK:CB	2.90	0.48
3:C:369:LEU:HD21	3:C:384:ILE:HG12	1.95	0.48
4:D:57:SER:O	4:D:63:LEU:O	2.31	0.48
5:E:23:HIS:HA	5:E:26:THR:OG1	2.13	0.48
9:J:34:ALA:O	9:J:35:GLY:O	2.30	0.48
13:O:33:TYR:O	13:O:37:VAL:HG23	2.13	0.48
13:O:59:ASP:C	13:O:61:SER:H	2.21	0.48
13:O:75:THR:HG22	13:O:77:LEU:CD1	2.43	0.48
13:O:154:SER:O	13:O:168:PHE:HA	2.13	0.48
13:O:241:PHE:CD1	13:O:241:PHE:C	2.90	0.48
14:T:2:GLU:HB3	14:T:6:TYR:CE2	2.48	0.48
1:a:5038:ILE:O	1:a:5042:LEU:HG	2.13	0.48
3:c:5048:LYS:HE2	3:c:5132:HIS:O	2.13	0.48
3:c:5162:GLY:O	3:c:5166:ILE:HG13	2.13	0.48
13:o:5166:THR:O	13:o:5167:ASP:HB3	2.12	0.48
1:A:140:ARG:NH2	25:A:567:LHG:O5	2.46	0.48
1:A:279:PRO:CG	4:D:212:ALA:HB2	2.44	0.48
2:B:450:TRP:O	2:B:451:PHE:C	2.55	0.48
10:K:26:PRO:O	10:K:29:PRO:HD2	2.13	0.48
15:U:72:TYR:CG	15:U:73:PRO:N	2.79	0.48
3:c:5055:ALA:C	24:c:5504:BCR:H373	2.38	0.48
5:e:5023:HIS:C	5:e:5025:ILE:N	2.72	0.48
6:f:5040:MET:C	6:f:5042:PHE:H	2.21	0.48
13:o:5044:LYS:HA	13:o:5072:GLN:CD	2.38	0.48
11:L:14:ARG:HG2	12:M:26:TYR:CE1	2.44	0.48
1:a:5303:ASN:O	3:c:5415:ASN:OD1	2.31	0.48
3:c:5315:MET:O	3:c:5319:ILE:HG13	2.12	0.48
4:d:5191:TRP:HZ3	4:d:5194:ASN:ND2	2.11	0.48
15:u:5130:ASN:ND2	15:u:5132:LEU:HG	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:THR:OG1	1:A:231:GLU:HG2	2.13	0.48
2:B:18:ARG:HG3	2:B:18:ARG:NH1	2.28	0.48
20:B:520:CLA:OBD	20:B:520:CLA:H151	2.13	0.48
13:O:83:LYS:O	13:O:84:ASN:CB	2.60	0.48
13:O:264:VAL:HG12	13:O:265:PHE:N	2.29	0.48
1:a:5033:PHE:CE1	1:a:5128:GLY:HA3	2.49	0.48
3:c:5452:ALA:O	3:c:5453:ALA:C	2.56	0.48
5:e:5027:ILE:CB	5:e:5028:PRO:HD3	2.42	0.48
13:o:5098:THR:CG2	13:o:5099:ARG:H	2.01	0.48
15:u:5104:ILE:O	15:u:5107:GLU:N	2.46	0.48
20:B:513:CLA:H2	20:B:515:CLA:H91	1.95	0.48
4:D:312:GLU:HB2	13:O:185:PRO:HB3	1.96	0.48
16:V:39:ASN:OD1	16:V:43:LYS:N	2.46	0.48
18:Z:15:LEU:O	18:Z:19:MET:HG2	2.13	0.48
1:a:5025:ASP:HA	4:d:5251:ARG:NH2	2.29	0.48
2:b:5150:CYS:HB2	20:b:5513:CLA:CMC	2.43	0.48
2:b:5315:ILE:HG22	2:b:5426:PHE:HB3	1.96	0.48
2:b:5341:LYS:O	2:b:5406:LEU:HB2	2.14	0.48
3:c:5225:VAL:O	3:c:5225:VAL:HG12	2.13	0.48
3:c:5259:TRP:CD1	3:c:5259:TRP:H	2.32	0.48
3:c:5416:SER:O	3:c:5417:VAL:CG1	2.62	0.48
3:c:5449:ARG:HD3	20:c:5495:CLA:HED1	1.96	0.48
4:d:5103:ARG:HG3	5:e:5073:LYS:HE3	1.96	0.48
4:d:5240:ALA:HB1	4:d:5241:GLU:OE1	2.13	0.48
15:u:5082:ASN:O	15:u:5083:ALA:O	2.31	0.48
28:L:210:MGE:H5A2	12:M:22:LEU:HD21	1.94	0.48
13:O:231:ASP:O	13:O:232:GLY:C	2.56	0.48
1:a:5130:GLN:HA	4:d:5256:ILE:CD1	2.43	0.48
1:a:5292:THR:C	1:a:5294:ALA:H	2.21	0.48
2:b:5171:PRO:HD3	7:h:5065:LEU:C	2.38	0.48
3:c:5459:ILE:HG21	3:c:5464:GLU:HG2	1.96	0.48
10:k:5043:VAL:HG21	17:x:5031:UNK:HG3	1.96	0.48
2:B:188:ASP:C	2:B:190:PHE:H	2.22	0.48
2:B:353:GLU:HB3	2:B:373:LYS:HZ1	1.78	0.48
4:D:67:TYR:CE2	4:D:76:VAL:HG11	2.48	0.48
10:K:17:ILE:O	10:K:17:ILE:HG22	2.14	0.48
13:O:259:VAL:HG12	13:O:260:LYS:N	2.28	0.48
1:a:5212:CYS:CB	4:d:5211:CYS:HB2	2.34	0.48
1:a:5225:ARG:NH1	2:b:5484:PRO:HD3	2.29	0.48
1:a:5267:ASN:HB3	1:a:5270:SER:HB3	1.96	0.48
1:a:5329:GLU:O	1:a:5332:HIS:ND1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:5190:PHE:HE2	7:h:5041:PHE:HE1	1.62	0.48
2:b:5259:GLY:O	2:b:5260:SER:CB	2.61	0.48
2:b:5471:ALA:HB2	4:d:5130:PHE:HZ	1.77	0.48
3:c:5104:GLU:O	3:c:5105:VAL:C	2.57	0.48
3:c:5116:VAL:O	3:c:5117:VAL:C	2.57	0.48
3:c:5226:SER:HA	30:c:5507:DGD:HE62	1.94	0.48
8:i:5017:LEU:O	8:i:5018:LEU:C	2.57	0.48
13:o:5052:ALA:O	13:o:5053:ARG:CB	2.61	0.48
13:o:5070:CYS:SG	13:o:5071:LEU:N	2.87	0.48
3:C:116:VAL:HG13	3:C:117:VAL:N	2.29	0.48
28:D:358:MGE:O3D	9:J:37:GLY:HA3	2.14	0.48
7:H:41:PHE:CE1	7:H:45:ILE:HD11	2.49	0.48
17:X:86:UNK:OD1	17:X:86:UNK:N	2.45	0.48
1:a:5058:VAL:O	1:a:5060:ILE:N	2.47	0.48
1:a:5077:ILE:HD13	11:l:5029:LEU:HG	1.96	0.48
1:a:5272:HIS:CG	4:d:5218:VAL:HG11	2.48	0.48
2:b:5068:ARG:HH12	20:b:5514:CLA:CED	2.26	0.48
13:o:5154:SER:O	13:o:5168:PHE:HA	2.14	0.48
18:z:5057:LEU:O	18:z:5061:VAL:HG23	2.13	0.48
1:A:78:ILE:HD13	11:L:33:SER:CB	2.44	0.48
1:A:153:SER:HB3	20:A:558:CLA:H43	1.96	0.48
3:C:229:ASN:HD22	3:C:231:GLU:HG2	1.79	0.48
3:C:254:THR:HG22	3:C:255:THR:N	2.19	0.48
3:C:435:PHE:O	3:C:438:LEU:N	2.47	0.48
4:D:193:LEU:O	4:D:193:LEU:HG	2.13	0.48
1:a:5219:VAL:HG21	4:d:5268:HIS:CD2	2.49	0.48
2:b:5029:LEU:HD12	20:b:5524:CLA:HBB2	1.96	0.48
4:d:5049:LEU:HD13	24:d:5357:BCR:C15	2.44	0.48
20:d:5355:CLA:H3A	20:d:5355:CLA:HBA2	1.49	0.48
13:o:5032:THR:H	13:o:5035:ASP:CB	2.25	0.48
13:o:5153:ALA:HA	13:o:5169:LYS:O	2.14	0.48
1:A:77:ILE:HD13	11:L:29:LEU:HG	1.96	0.48
1:A:191:ASN:ND2	1:A:194:MET:HB2	2.28	0.48
2:B:61:PHE:CZ	20:B:517:CLA:HBB1	2.49	0.48
2:B:446:SER:HB2	2:B:447:PRO:CD	2.44	0.48
3:C:161:LEU:HG	3:C:165:LEU:HD12	1.95	0.48
3:C:205:ASP:OD2	3:C:205:ASP:C	2.57	0.48
3:C:206:PRO:O	3:C:207:ARG:C	2.57	0.48
3:C:346:THR:HG21	13:O:38:GLY:HA2	1.95	0.48
3:C:452:ALA:O	3:C:453:ALA:C	2.55	0.48
4:D:101:PHE:O	4:D:104:TRP:HB3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:302:GLU:OE1	13:O:186:LYS:HE2	2.13	0.48
7:H:5:THR:O	7:H:8:GLY:N	2.46	0.48
15:U:58:ASN:OD1	15:U:84:PRO:HA	2.14	0.48
15:U:73:PRO:HG2	16:V:109:ASP:N	2.29	0.48
18:Z:5:PHE:HE1	18:Z:54:VAL:HG13	1.79	0.48
18:Z:20:VAL:O	18:Z:24:PRO:HG2	2.14	0.48
1:a:5027:ARG:NH1	1:a:5027:ARG:HG3	2.27	0.48
2:b:5195:PRO:O	2:b:5198:VAL:N	2.47	0.48
3:c:5190:ALA:O	3:c:5193:GLY:N	2.46	0.48
4:d:5101:PHE:O	4:d:5104:TRP:HB3	2.14	0.48
6:f:5030:THR:HG22	6:f:5034:LEU:HD12	1.95	0.48
13:o:5114:ASN:O	13:o:5115:SER:O	2.32	0.48
14:t:5001:MET:HG2	14:t:5001:MET:O	2.14	0.48
15:u:5105:LEU:O	15:u:5109:LEU:HG	2.14	0.48
16:v:5064:ALA:O	16:v:5065:SER:C	2.57	0.48
3:C:337:LEU:HD23	13:O:131:PRO:CG	2.40	0.47
13:O:67:ALA:HB3	13:O:268:SER:OG	2.14	0.47
17:X:3:UNK:C	17:X:5:UNK:N	2.76	0.47
2:b:5350:GLU:CD	2:b:5350:GLU:N	2.71	0.47
2:b:5359:MET:HB2	2:b:5425:ILE:CG2	2.44	0.47
2:b:5391:SER:OG	2:b:5394:GLN:NE2	2.47	0.47
3:c:5276:LEU:CD2	20:c:5498:CLA:HBB1	2.44	0.47
4:d:5256:ILE:O	4:d:5256:ILE:HG12	2.14	0.47
11:l:5011:GLU:HG2	11:l:5012:LEU:N	2.29	0.47
13:o:5098:THR:CG2	13:o:5099:ARG:N	2.67	0.47
1:A:138:GLY:HA2	3:C:455:PHE:CZ	2.48	0.47
2:B:122:LEU:HD13	7:H:12:ARG:HA	1.96	0.47
2:B:191:ASN:HD22	2:B:191:ASN:C	2.20	0.47
4:D:126:MET:HE1	4:D:147:SER:HA	1.94	0.47
4:D:350:ASN:O	4:D:352:LEU:N	2.47	0.47
9:J:18:GLY:O	9:J:22:ILE:HG12	2.14	0.47
11:L:14:ARG:HG3	11:L:14:ARG:HH11	1.78	0.47
13:O:73:PRO:HG2	13:O:102:THR:CB	2.45	0.47
14:T:4:ILE:C	14:T:4:ILE:CD1	2.85	0.47
1:a:5140:ARG:NH2	25:a:5567:LHG:O5	2.47	0.47
1:a:5259:ILE:O	1:a:5260:PHE:HB3	2.13	0.47
2:b:5141:ILE:O	2:b:5144:PHE:HB3	2.14	0.47
2:b:5235:GLU:HG2	2:b:5235:GLU:O	2.14	0.47
20:b:5518:CLA:HMD1	20:b:5520:CLA:HAB	1.96	0.47
4:d:5103:ARG:O	4:d:5106:GLN:N	2.45	0.47
1:A:78:ILE:HD13	11:L:33:SER:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:TYR:HB3	1:A:162:PRO:HD3	1.96	0.47
1:A:303:ASN:O	3:C:415:ASN:OD1	2.32	0.47
25:A:567:LHG:HC61	3:C:443:TRP:HH2	1.77	0.47
2:B:12:LEU:HD12	20:B:522:CLA:HBB1	1.96	0.47
2:B:221:PRO:O	2:B:222:PRO:C	2.56	0.47
3:C:404:LEU:C	3:C:406:SER:H	2.23	0.47
5:E:23:HIS:C	5:E:25:ILE:N	2.69	0.47
2:b:5221:PRO:O	2:b:5222:PRO:C	2.57	0.47
2:b:5229:LEU:HD11	20:b:5519:CLA:O1A	2.14	0.47
3:c:5305:THR:HB	3:c:5308:GLU:HB2	1.95	0.47
3:c:5323:LYS:O	3:c:5324:LEU:HB2	2.14	0.47
4:d:5102:THR:CG2	4:d:5103:ARG:N	2.78	0.47
4:d:5120:PHE:CD1	4:d:5123:ILE:HD12	2.49	0.47
4:d:5171:PRO:HG3	4:d:5181:PHE:CE2	2.49	0.47
17:x:5004:UNK:O	17:x:5007:UNK:N	2.47	0.47
18:z:5002:THR:O	18:z:5003:ILE:C	2.58	0.47
2:B:191:ASN:HD22	2:B:192:PRO:N	2.12	0.47
2:B:262:THR:O	2:B:262:THR:CG2	2.61	0.47
3:C:62:PHE:CE2	10:K:28:ILE:HB	2.50	0.47
3:C:87:ILE:C	3:C:90:PRO:HD2	2.39	0.47
3:C:104:GLU:O	3:C:105:VAL:C	2.57	0.47
3:C:152:LYS:O	3:C:154:LYS:N	2.47	0.47
3:C:201:ASN:O	3:C:202:PRO:C	2.58	0.47
3:C:293:ASN:HD21	3:C:295:THR:HB	1.79	0.47
3:C:449:ARG:HD3	20:C:495:CLA:HED1	1.95	0.47
3:C:459:ILE:HD12	4:D:245:SER:OG	2.13	0.47
4:D:148:ALA:HB3	4:D:149:PRO:CD	2.36	0.47
4:D:213:ILE:HG23	4:D:214:HIS:N	2.28	0.47
6:F:11:VAL:HG12	6:F:12:SER:H	1.79	0.47
11:L:12:LEU:HD12	12:M:25:LEU:HD12	1.95	0.47
16:V:81:ARG:HG3	16:V:81:ARG:NH1	2.28	0.47
1:a:5192:ILE:HG23	1:a:5193:LEU:N	2.29	0.47
1:a:5234:ASN:ND2	4:d:5266:TRP:HB2	2.30	0.47
3:c:5229:ASN:HD22	3:c:5231:GLU:CG	2.27	0.47
15:u:5115:THR:HG22	15:u:5116:GLU:N	2.29	0.47
24:x:5130:BCR:HC31	18:z:5013:VAL:HG13	1.96	0.47
1:A:213:ALA:O	1:A:217:SER:CB	2.63	0.47
1:A:311:GLY:HA3	16:V:151:ILE:HG21	1.96	0.47
1:A:314:ILE:O	1:A:314:ILE:HG22	2.14	0.47
2:B:228:ALA:O	2:B:230:ARG:NH1	2.47	0.47
4:D:49:LEU:HD13	24:D:357:BCR:C15	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:88:SER:HB2	5:E:69:ARG:CZ	2.43	0.47
7:H:12:ARG:HG3	7:H:12:ARG:NH1	2.30	0.47
11:L:14:ARG:HD3	12:M:26:TYR:OH	2.15	0.47
13:O:147:THR:OG1	13:O:148:VAL:N	2.47	0.47
13:O:169:LYS:HG2	13:O:224:SER:HB2	1.96	0.47
14:T:4:ILE:HB	27:T:217:LMT:C6'	2.44	0.47
15:U:105:LEU:O	15:U:109:LEU:HG	2.15	0.47
16:V:134:THR:N	16:V:137:ASP:OD2	2.45	0.47
16:V:144:HIS:HE1	16:V:148:GLU:OE2	1.97	0.47
1:a:5213:ALA:O	1:a:5217:SER:CB	2.62	0.47
1:a:5225:ARG:HH12	2:b:5483:ASP:CA	2.16	0.47
20:a:5558:CLA:H201	28:d:5361:MGE:H232	1.95	0.47
5:e:5026:THR:O	5:e:5029:ALA:HB3	2.15	0.47
5:e:5060:GLN:C	5:e:5062:SER:N	2.72	0.47
6:f:5018:VAL:CG1	6:f:5019:ARG:N	2.77	0.47
13:o:5033:TYR:O	13:o:5037:VAL:HG23	2.14	0.47
2:B:179:GLN:HA	2:B:179:GLN:HE21	1.78	0.47
13:O:77:LEU:HB3	13:O:91:PHE:HB3	1.95	0.47
1:a:5149:ALA:HB3	1:a:5150:PRO:CD	2.37	0.47
1:a:5159:LEU:HD11	1:a:5163:ILE:HD11	1.96	0.47
1:a:5188:ALA:HB2	1:a:5328:MET:CB	2.43	0.47
1:a:5223:LEU:HD13	4:d:5265:ARG:HD3	1.96	0.47
1:a:5311:GLY:HA3	16:v:5151:ILE:HG21	1.97	0.47
2:b:5031:ALA:N	20:b:5515:CLA:HBC3	2.30	0.47
2:b:5217:ILE:HG22	2:b:5218:LEU:HD23	1.97	0.47
2:b:5235:GLU:OE1	2:b:5472:ARG:NH1	2.48	0.47
3:c:5042:LEU:HD11	20:c:5501:CLA:C1A	2.44	0.47
3:c:5180:MET:HE3	3:c:5202:PRO:CD	2.44	0.47
3:c:5334:PRO:O	13:o:5182:PHE:HB2	2.14	0.47
4:d:5035:ILE:O	4:d:5039:PRO:HG2	2.13	0.47
7:h:5041:PHE:CE1	7:h:5045:ILE:HD11	2.49	0.47
10:k:5017:ILE:O	10:k:5017:ILE:HG22	2.14	0.47
13:o:5264:VAL:HG12	13:o:5265:PHE:N	2.29	0.47
13:o:5265:PHE:CD1	13:o:5265:PHE:C	2.91	0.47
16:v:5133:LEU:HD23	16:v:5133:LEU:H	1.80	0.47
1:A:11:ALA:HB1	1:A:15:GLU:OE2	2.15	0.47
1:A:326:LEU:HD23	3:C:412:THR:HB	1.96	0.47
20:A:558:CLA:H201	28:D:360:MGE:H232	1.96	0.47
2:B:7:ARG:NH2	28:D:359:MGE:O3D	2.47	0.47
2:B:235:GLU:OE1	2:B:472:ARG:NH1	2.48	0.47
2:B:259:GLY:O	2:B:260:SER:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:259:TRP:H	3:C:259:TRP:CD1	2.30	0.47
20:C:501:CLA:H42	10:K:39:TRP:CD1	2.49	0.47
4:D:103:ARG:HG3	5:E:73:LYS:HE3	1.96	0.47
4:D:251:ARG:HE	4:D:255:GLN:NE2	2.12	0.47
7:H:12:ARG:HG3	7:H:12:ARG:HH11	1.80	0.47
7:H:54:ILE:HD12	7:H:54:ILE:N	2.30	0.47
9:J:33:TYR:CD2	9:J:33:TYR:N	2.83	0.47
13:O:79:LYS:HA	13:O:90:GLU:O	2.15	0.47
15:U:50:ALA:HB1	15:U:113:THR:HG21	1.91	0.47
15:U:98:THR:C	15:U:100:ARG:N	2.71	0.47
16:V:64:ALA:O	16:V:65:SER:C	2.57	0.47
17:X:75:UNK:O	17:X:79:UNK:HG2	2.15	0.47
18:Z:1:MET:HE3	18:Z:60:PHE:CG	2.50	0.47
2:b:5192:PRO:HG3	7:h:5049:TYR:CE1	2.49	0.47
2:b:5222:PRO:HG3	7:h:5027:THR:N	2.30	0.47
2:b:5353:GLU:HB3	2:b:5373:LYS:HZ3	1.78	0.47
2:b:5360:PRO:O	2:b:5361:ALA:C	2.58	0.47
3:c:5201:ASN:OD1	3:c:5201:ASN:O	2.33	0.47
3:c:5299:SER:OG	3:c:5304:PRO:HA	2.15	0.47
3:c:5372:PRO:O	13:o:5036:ILE:HD12	2.13	0.47
24:c:5505:BCR:C31	18:z:5055:GLY:HA2	2.44	0.47
4:d:5313:THR:C	4:d:5315:TYR:N	2.73	0.47
10:k:5015:TYR:O	10:k:5017:ILE:N	2.48	0.47
11:l:5020:GLY:HA3	12:m:5022:LEU:HD11	1.97	0.47
13:o:5073:PRO:CG	13:o:5102:THR:CB	2.92	0.47
1:A:29:TYR:CD1	1:A:133:LEU:HB2	2.49	0.47
1:A:196:PRO:HA	1:A:199:GLN:OE1	2.15	0.47
3:C:362:ARG:HG3	3:C:362:ARG:NH1	2.30	0.47
4:D:102:THR:HG23	4:D:103:ARG:N	2.29	0.47
6:F:41:GLN:HE21	6:F:41:GLN:CA	2.26	0.47
16:V:162:TYR:O	16:V:163:TYR:OXT	2.33	0.47
1:a:5140:ARG:HB2	4:d:5220:ASN:HA	1.97	0.47
1:a:5296:ASN:HB2	3:c:5400:PRO:O	2.15	0.47
3:c:5103:GLY:CA	3:c:5301:PHE:HE1	2.25	0.47
3:c:5292:PHE:HB3	30:c:5507:DGD:HD62	1.96	0.47
4:d:5029:PHE:CD2	4:d:5030:VAL:N	2.83	0.47
4:d:5057:SER:O	4:d:5063:LEU:O	2.32	0.47
4:d:5157:PHE:CE2	4:d:5171:PRO:HB2	2.50	0.47
4:d:5236:ASN:C	4:d:5238:THR:N	2.73	0.47
5:e:5047:PHE:O	5:e:5049:THR:N	2.48	0.47
16:v:5059:PHE:HA	16:v:5063:CYS:SG	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:v:5121:LEU:C	16:v:5123:SER:H	2.22	0.47
1:A:76:ASN:ND2	1:A:76:ASN:C	2.73	0.47
1:A:140:ARG:HH22	25:A:567:LHG:P	2.38	0.47
1:A:306:VAL:O	1:A:306:VAL:CG2	2.49	0.47
2:B:29:LEU:HD12	20:B:524:CLA:HBB2	1.95	0.47
3:C:296:VAL:HG23	3:C:297:TYR:CD2	2.50	0.47
4:D:68:LEU:HD21	5:E:44:TYR:CD1	2.50	0.47
4:D:199:MET:O	4:D:200:GLY:C	2.56	0.47
3:c:5334:PRO:HG2	4:d:5350:ASN:ND2	2.30	0.47
4:d:5093:TRP:CZ2	20:d:5355:CLA:O1A	2.68	0.47
4:d:5222:LEU:HA	4:d:5244:TYR:HA	1.97	0.47
8:i:5004:LEU:O	8:i:5008:VAL:HG23	2.15	0.47
9:j:5033:TYR:O	9:j:5034:ALA:HB3	2.14	0.47
13:o:5092:VAL:CG1	13:o:5093:PRO:CD	2.87	0.47
1:A:296:ASN:HB2	3:C:400:PRO:O	2.15	0.47
3:C:201:ASN:O	3:C:201:ASN:OD1	2.33	0.47
4:D:68:LEU:HB2	6:F:40:MET:HE2	1.96	0.47
4:D:214:HIS:HA	22:D:356:PQ9:O4	2.15	0.47
14:T:2:GLU:O	14:T:3:THR:C	2.57	0.47
15:U:73:PRO:HG2	16:V:109:ASP:H	1.80	0.47
16:V:133:LEU:HD23	16:V:133:LEU:H	1.80	0.47
17:X:58:UNK:O	17:X:62:UNK:HG2	2.15	0.47
1:a:5035:VAL:HG22	24:a:5566:BCR:HC42	1.96	0.47
2:b:5463:PHE:CZ	2:b:5467:ILE:HD12	2.50	0.47
3:c:5075:PHE:HZ	3:c:5105:VAL:HG21	1.79	0.47
3:c:5080:PRO:HG2	3:c:5083:GLU:OE2	2.15	0.47
6:f:5025:THR:O	6:f:5029:PRO:HG2	2.14	0.47
12:m:5015:VAL:O	12:m:5019:SER:HB2	2.13	0.47
2:B:169:SER:HA	2:B:176:GLY:HA2	1.97	0.46
3:C:255:THR:HG23	3:C:256:PRO:CD	2.41	0.46
8:I:6:ILE:O	8:I:10:ILE:HG12	2.15	0.46
13:O:225:LEU:N	13:O:225:LEU:HD12	2.29	0.46
1:a:5020:TRP:O	1:a:5021:VAL:C	2.58	0.46
1:a:5063:ILE:CG2	3:c:5335:THR:HG21	2.45	0.46
1:a:5078:ILE:HD13	11:l:5033:SER:HB2	1.97	0.46
1:a:5138:GLY:HA2	3:c:5455:PHE:CZ	2.50	0.46
2:b:5450:TRP:O	2:b:5451:PHE:C	2.58	0.46
3:c:5241:GLY:C	3:c:5243:ILE:N	2.73	0.46
3:c:5453:ALA:HB1	8:i:5031:ASN:HD22	1.76	0.46
11:l:5012:LEU:HD12	12:m:5025:LEU:HD12	1.97	0.46
13:o:5178:ARG:HH11	13:o:5178:ARG:CG	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:390:TYR:N	2:B:390:TYR:CD1	2.83	0.46
20:B:513:CLA:H162	7:H:38:PHE:HE2	1.80	0.46
3:C:180:MET:CE	3:C:202:PRO:HG2	2.45	0.46
3:C:415:ASN:O	3:C:416:SER:CB	2.64	0.46
3:C:453:ALA:CB	8:I:31:ASN:ND2	2.76	0.46
3:C:472:LEU:C	3:C:473:ASP:CG	2.83	0.46
13:O:45:CYS:N	13:O:72:GLN:NE2	2.56	0.46
13:O:215:ARG:NH1	13:O:252:GLY:O	2.48	0.46
15:U:104:ILE:O	15:U:107:GLU:N	2.49	0.46
1:a:5262:TYR:C	1:a:5264:SER:H	2.24	0.46
21:a:5561:PHO:HED2	4:d:5257:PHE:CE2	2.50	0.46
2:b:5446:SER:HB2	2:b:5447:PRO:CD	2.45	0.46
12:m:5026:TYR:O	12:m:5029:THR:HB	2.15	0.46
16:v:5147:VAL:O	16:v:5148:GLU:C	2.57	0.46
2:B:365:SER:HB2	13:O:198:ILE:HD11	1.97	0.46
3:C:89:ILE:N	3:C:90:PRO:CD	2.79	0.46
3:C:290:VAL:HG23	3:C:297:TYR:CE1	2.50	0.46
4:D:176:ALA:HA	4:D:179:PHE:CD2	2.50	0.46
4:D:222:LEU:HA	4:D:244:TYR:HA	1.97	0.46
8:I:32:PRO:O	8:I:33:LYS:HG3	2.14	0.46
9:J:21:VAL:HA	9:J:24:ILE:HG22	1.97	0.46
2:b:5098:LEU:O	2:b:5099:ALA:C	2.57	0.46
3:c:5265:ILE:HB	20:c:5495:CLA:HED3	1.98	0.46
4:d:5042:TYR:HE1	6:f:5026:LEU:HD23	1.80	0.46
4:d:5063:LEU:HD12	4:d:5063:LEU:N	2.30	0.46
13:o:5051:THR:O	13:o:5052:ALA:O	2.33	0.46
15:u:5073:PRO:HD2	16:v:5109:ASP:HB3	1.97	0.46
32:v:5552:HEM:HHA	32:v:5552:HEM:HAD2	1.56	0.46
1:A:38:ILE:HB	1:A:39:PRO:HD3	1.98	0.46
1:A:60:ILE:CG2	1:A:61:ASP:H	2.23	0.46
1:A:107:TYR:HD1	13:O:141:ARG:CZ	2.28	0.46
2:B:391:SER:C	2:B:392:PHE:O	2.56	0.46
3:C:61:VAL:O	3:C:62:PHE:C	2.57	0.46
4:D:223:PHE:CE1	4:D:245:SER:HB3	2.51	0.46
4:D:267:LEU:C	4:D:267:LEU:CD2	2.88	0.46
6:F:25:THR:O	6:F:29:PRO:HG2	2.15	0.46
13:O:44:LYS:HA	13:O:72:GLN:CD	2.40	0.46
13:O:47:THR:HG22	13:O:48:LEU:H	1.80	0.46
18:Z:19:MET:SD	18:Z:43:GLY:HA3	2.56	0.46
1:a:5013:LEU:H	1:a:5013:LEU:CD2	2.28	0.46
2:b:5007:ARG:O	2:b:5008:VAL:C	2.59	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:c:5113:VAL:O	3:c:5117:VAL:HG23	2.14	0.46
3:c:5209:ILE:CG2	24:c:5506:BCR:H382	2.39	0.46
3:c:5452:ALA:C	3:c:5454:GLY:H	2.21	0.46
4:d:5286:VAL:C	4:d:5288:GLY:N	2.71	0.46
13:o:5147:THR:OG1	13:o:5148:VAL:N	2.48	0.46
1:A:130:GLN:HA	4:D:256:ILE:CD1	2.46	0.46
1:A:183:MET:HB3	20:A:558:CLA:HBC2	1.98	0.46
1:A:234:ASN:ND2	4:D:266:TRP:HB2	2.31	0.46
1:A:303:ASN:O	1:A:304:HIS:HB2	2.15	0.46
3:C:76:ILE:HA	3:C:77:PRO:HD2	1.71	0.46
3:C:428:THR:CG2	3:C:429:SER:N	2.79	0.46
4:D:103:ARG:HH12	5:E:77:GLU:CG	2.29	0.46
15:U:113:THR:O	15:U:114:VAL:HG23	2.16	0.46
18:Z:5:PHE:HA	18:Z:57:LEU:CD1	2.40	0.46
1:a:5090:GLY:HA2	1:a:5167:SER:HB2	1.97	0.46
2:b:5318:ASN:ND2	2:b:5361:ALA:HB2	2.31	0.46
2:b:5418:LYS:O	2:b:5419:SER:C	2.59	0.46
3:c:5201:ASN:N	3:c:5202:PRO:CD	2.79	0.46
3:c:5318:LEU:HD23	3:c:5318:LEU:O	2.15	0.46
4:d:5172:SER:O	4:d:5173:PHE:HB2	2.16	0.46
7:h:5025:TRP:O	7:h:5026:GLY:C	2.57	0.46
13:o:5085:LYS:O	13:o:5087:GLN:N	2.49	0.46
15:u:5055:ILE:HG21	15:u:5065:PHE:CE2	2.50	0.46
1:A:96:ILE:HG12	1:A:105:TRP:CE2	2.51	0.46
2:B:263:THR:CG2	2:B:448:ARG:NH1	2.70	0.46
3:C:39:ASN:OD1	20:C:499:CLA:HBB2	2.16	0.46
3:C:120:ILE:C	3:C:122:SER:H	2.23	0.46
3:C:120:ILE:C	3:C:122:SER:N	2.73	0.46
3:C:418:ASN:HB3	30:C:509:DGD:C1E	2.45	0.46
3:C:419:PHE:CD1	3:C:419:PHE:C	2.93	0.46
4:D:126:MET:HE2	4:D:146:PHE:HB3	1.96	0.46
11:L:20:GLY:HA3	12:M:22:LEU:HD11	1.97	0.46
12:M:9:ILE:HD12	12:M:9:ILE:N	2.30	0.46
13:O:32:THR:O	13:O:36:ILE:HG13	2.14	0.46
13:O:223:ILE:CG2	13:O:243:SER:HB3	2.22	0.46
14:T:11:ALA:HB3	24:T:5104:BCR:H363	1.96	0.46
1:a:5321:ILE:HD11	4:d:5176:ALA:HB1	1.98	0.46
3:c:5152:LYS:O	3:c:5154:LYS:N	2.49	0.46
3:c:5153:ASP:C	3:c:5155:ASN:N	2.72	0.46
3:c:5293:ASN:HD21	3:c:5295:THR:HB	1.80	0.46
4:d:5292:ASN:OD1	4:d:5294:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j:5024:ILE:HG23	9:j:5025:VAL:N	2.29	0.46
9:j:5033:TYR:CD2	9:j:5033:TYR:N	2.84	0.46
13:o:5179:THR:HG22	13:o:5180:ALA:N	2.31	0.46
1:A:292:THR:C	1:A:294:ALA:H	2.23	0.46
20:B:518:CLA:HMD1	20:B:520:CLA:HAB	1.96	0.46
3:C:62:PHE:CE2	10:K:29:PRO:HD3	2.42	0.46
3:C:190:ALA:HB3	3:C:193:GLY:C	2.41	0.46
20:C:497:CLA:H142	24:C:506:BCR:H362	1.96	0.46
4:D:106:GLN:NE2	5:E:48:GLY:HA3	2.31	0.46
8:I:27:ASP:O	8:I:28:PRO:C	2.58	0.46
2:b:5007:ARG:NH2	28:d:5360:MGE:O3D	2.47	0.46
2:b:5362:PHE:HE2	4:d:5164:GLN:NE2	2.14	0.46
2:b:5433:ASP:OD1	2:b:5433:ASP:C	2.58	0.46
3:c:5062:PHE:CE2	10:k:5028:ILE:HB	2.51	0.46
3:c:5365:TRP:CZ3	3:c:5366:LEU:HD13	2.50	0.46
13:o:5079:LYS:HA	13:o:5090:GLU:O	2.16	0.46
1:A:57:PRO:HA	1:A:68:SER:HA	1.97	0.46
1:A:63:ILE:HG21	3:C:335:THR:HG21	1.97	0.46
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.96	0.46
1:A:210:LEU:HD12	1:A:210:LEU:O	2.16	0.46
2:B:10:THR:O	2:B:12:LEU:N	2.49	0.46
2:B:43:ALA:HB1	27:t:5217:LMT:O3'	2.16	0.46
2:B:359:MET:HB2	2:B:425:ILE:CG2	2.46	0.46
3:C:35:TRP:CG	3:C:36:TRP:N	2.84	0.46
13:O:56:TYR:C	13:O:161:SER:HA	2.41	0.46
14:T:1:MET:O	14:T:1:MET:HG2	2.14	0.46
2:b:5061:PHE:HZ	20:b:5517:CLA:HBB1	1.81	0.46
2:b:5262:THR:O	2:b:5262:THR:CG2	2.64	0.46
2:b:5278:SER:HB3	2:b:5281:GLN:HB3	1.98	0.46
2:b:5365:SER:HB2	13:o:5198:ILE:HD11	1.97	0.46
3:c:5416:SER:C	3:c:5417:VAL:HG12	2.41	0.46
4:d:5102:THR:HG23	4:d:5103:ARG:N	2.31	0.46
15:u:5113:THR:O	15:u:5114:VAL:HG23	2.16	0.46
16:v:5144:HIS:CE1	16:v:5148:GLU:OE2	2.69	0.46
2:B:149:LEU:HB2	20:B:514:CLA:H203	1.97	0.46
2:B:249:ALA:O	2:B:252:VAL:HG22	2.16	0.46
2:B:366:PHE:CG	2:B:367:PRO:HD2	2.51	0.46
15:U:83:ALA:HB1	15:U:84:PRO:HD2	1.97	0.46
2:b:5031:ALA:CA	20:b:5515:CLA:HBC3	2.46	0.46
3:c:5168:LEU:CD1	20:c:5497:CLA:H2	2.46	0.46
4:d:5087:HIS:C	4:d:5167:TRP:HE1	2.22	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:5134:ARG:NE	4:d:5134:ARG:HA	2.30	0.46
4:d:5191:TRP:O	4:d:5193:LEU:N	2.49	0.46
5:e:5006:GLY:O	5:e:5007:GLU:HG2	2.16	0.46
6:f:5040:MET:O	6:f:5042:PHE:N	2.49	0.46
15:u:5073:PRO:HG2	16:v:5109:ASP:N	2.30	0.46
15:u:5073:PRO:HG2	16:v:5109:ASP:H	1.80	0.46
1:A:60:ILE:CG2	1:A:61:ASP:N	2.79	0.46
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.96	0.46
20:B:518:CLA:H51	20:B:519:CLA:H101	1.97	0.46
4:D:159:ILE:O	4:D:160:TYR:C	2.58	0.46
4:D:229:ALA:O	4:D:231:THR:N	2.49	0.46
13:O:116:ASP:O	13:O:158:ASN:N	2.35	0.46
2:b:5087:ASP:CG	2:b:5087:ASP:O	2.59	0.46
20:b:5511:CLA:CAA	24:h:5107:BCR:H19C	2.46	0.46
4:d:5068:LEU:CD1	6:f:5040:MET:HE2	2.44	0.46
10:k:5046:ARG:HH22	17:x:5031:UNK:CG2	2.29	0.46
11:l:5014:ARG:HH11	11:l:5014:ARG:CG	2.29	0.46
14:t:5002:GLU:O	14:t:5003:THR:C	2.57	0.46
15:u:5056:ASP:HB3	15:u:5060:THR:H	1.80	0.46
16:v:5117:VAL:O	16:v:5117:VAL:HG12	2.15	0.46
1:A:126:TYR:O	1:A:130:GLN:HG3	2.16	0.45
1:A:163:ILE:HD13	30:C:507:DGD:HB22	1.97	0.45
1:A:190:HIS:ND1	1:A:298:ASN:ND2	2.64	0.45
1:A:340:PRO:HG3	15:U:133:TYR:CG	2.52	0.45
2:B:356:VAL:HA	2:B:370:LEU:HD23	1.96	0.45
3:C:410:VAL:HG12	3:C:412:THR:H	1.80	0.45
3:C:416:SER:C	3:C:417:VAL:HG12	2.41	0.45
4:D:78:VAL:HG11	4:D:114:ILE:HD12	1.98	0.45
4:D:236:ASN:C	4:D:238:THR:N	2.74	0.45
20:D:355:CLA:H3A	20:D:355:CLA:HBA2	1.53	0.45
5:E:60:GLN:C	5:E:62:SER:N	2.71	0.45
7:H:44:ILE:O	7:H:48:ILE:HG13	2.16	0.45
26:L:5213:SQD:H211	2:b:5029:LEU:HD23	1.97	0.45
13:O:114:ASN:O	13:O:115:SER:O	2.33	0.45
13:O:151:LEU:HD12	13:O:171:GLU:O	2.17	0.45
27:T:217:LMT:H3B	2:b:5044:THR:HG22	1.98	0.45
1:a:5082:VAL:HB	1:a:5174:LEU:HB2	1.98	0.45
2:b:5125:ASP:O	2:b:5128:THR:O	2.34	0.45
2:b:5172:TYR:O	2:b:5173:GLY:C	2.57	0.45
2:b:5220:ARG:HD2	7:h:5020:LYS:C	2.41	0.45
2:b:5390:TYR:N	2:b:5390:TYR:CD1	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:5413:ASP:O	2:b:5417:VAL:HG23	2.16	0.45
3:c:5473:ASP:O	14:t:5024:ARG:NE	2.44	0.45
4:d:5103:ARG:O	4:d:5104:TRP:C	2.59	0.45
24:t:104:BCR:H23C	24:t:104:BCR:H403	1.96	0.45
15:u:5059:ASN:O	15:u:5060:THR:C	2.60	0.45
16:v:5128:PRO:C	16:v:5130:MET:N	2.74	0.45
2:B:192:PRO:HG3	7:H:49:TYR:CE1	2.51	0.45
2:B:329:PRO:HD3	20:B:517:CLA:HED2	1.98	0.45
3:C:400:PRO:O	3:C:401:LEU:HD23	2.15	0.45
4:D:71:CYS:HB2	4:D:76:VAL:HG12	1.97	0.45
4:D:313:THR:C	4:D:315:TYR:N	2.72	0.45
4:D:323:GLU:HG2	13:O:194:TYR:OH	2.16	0.45
6:F:30:THR:HG22	6:F:34:LEU:HD12	1.98	0.45
13:O:70:CYS:SG	13:O:71:LEU:N	2.89	0.45
13:O:98:THR:CG2	13:O:99:ARG:H	2.04	0.45
1:a:5022:THR:O	1:a:5023:SER:C	2.60	0.45
3:c:5229:ASN:ND2	3:c:5232:ASP:OD1	2.42	0.45
5:e:5006:GLY:C	5:e:5007:GLU:HG2	2.41	0.45
9:j:5008:ILE:HD12	9:j:5008:ILE:N	2.30	0.45
13:o:5160:THR:O	13:o:5161:SER:O	2.33	0.45
1:A:306:VAL:HG21	1:A:316:THR:CG2	2.42	0.45
2:B:156:PHE:HB2	20:B:516:CLA:HAC1	1.99	0.45
2:B:413:ASP:O	2:B:417:VAL:HG23	2.16	0.45
20:B:511:CLA:CAA	24:H:107:BCR:H19C	2.47	0.45
3:C:331:ALA:O	3:C:338:GLY:HA2	2.17	0.45
3:C:453:ALA:HB1	8:I:31:ASN:HD22	1.81	0.45
11:L:14:ARG:HH11	11:L:14:ARG:CG	2.29	0.45
15:U:115:THR:HG22	15:U:116:GLU:N	2.32	0.45
2:b:5124:ARG:HA	2:b:5131:PRO:HA	1.98	0.45
2:b:5208:VAL:HG21	20:b:5512:CLA:HMC3	1.99	0.45
2:b:5314:TYR:CZ	2:b:5316:GLY:HA3	2.52	0.45
2:b:5364:GLU:HG3	4:d:5296:TYR:CE2	2.52	0.45
2:b:5383:PHE:O	13:o:5193:GLY:N	2.47	0.45
4:d:5218:VAL:HG12	4:d:5219:GLU:N	2.30	0.45
4:d:5286:VAL:O	4:d:5287:VAL:C	2.58	0.45
4:d:5312:GLU:HB2	13:o:5185:PRO:HB3	1.98	0.45
13:o:5117:GLY:HA3	13:o:5158:ASN:HA	1.98	0.45
13:o:5231:ASP:O	13:o:5231:ASP:OD1	2.33	0.45
1:A:22:THR:HG22	1:A:22:THR:O	2.16	0.45
1:A:214:MET:O	1:A:215:HIS:C	2.59	0.45
1:A:304:HIS:CD2	1:A:313:VAL:HG21	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:ASP:O	2:B:88:PRO:C	2.58	0.45
2:B:208:VAL:HG21	20:B:512:CLA:HMC3	1.98	0.45
2:B:235:GLU:HG2	2:B:235:GLU:O	2.16	0.45
3:C:75:PHE:HZ	3:C:105:VAL:HG21	1.81	0.45
3:C:334:PRO:HG2	4:D:350:ASN:ND2	2.32	0.45
18:Z:1:MET:HE3	18:Z:60:PHE:CD2	2.52	0.45
1:a:5029:TYR:OH	1:a:5132:GLU:OE2	2.31	0.45
1:a:5033:PHE:CD1	1:a:5128:GLY:HA3	2.51	0.45
3:c:5089:ILE:N	3:c:5090:PRO:CD	2.79	0.45
3:c:5135:ARG:CB	18:z:5027:TYR:CD1	3.00	0.45
3:c:5168:LEU:HD13	20:c:5497:CLA:H2	1.99	0.45
3:c:5269:GLU:CG	3:c:5448:ALA:HB2	2.34	0.45
3:c:5290:VAL:HG21	3:c:5426:LEU:HD13	1.98	0.45
4:d:5134:ARG:HA	4:d:5134:ARG:HE	1.82	0.45
15:u:5130:ASN:HD21	15:u:5132:LEU:HG	1.82	0.45
1:A:131:TRP:CZ2	20:C:495:CLA:HAA1	2.51	0.45
1:A:269:ARG:NH1	4:D:234:ALA:HB3	2.31	0.45
2:B:193:TYR:CE1	2:B:260:SER:N	2.84	0.45
3:C:139:THR:O	3:C:139:THR:HG23	2.16	0.45
3:C:299:SER:OG	3:C:304:PRO:HA	2.17	0.45
4:D:213:ILE:CG2	4:D:214:HIS:N	2.79	0.45
9:J:8:ILE:HD12	9:J:8:ILE:N	2.30	0.45
10:K:45:PHE:C	10:K:46:ARG:OXT	2.58	0.45
1:a:5029:TYR:CD1	1:a:5133:LEU:HB2	2.50	0.45
2:b:5476:ARG:HG3	2:b:5476:ARG:NH1	2.32	0.45
3:c:5120:ILE:C	3:c:5122:SER:N	2.75	0.45
3:c:5435:PHE:O	3:c:5438:LEU:N	2.48	0.45
20:c:5497:CLA:H142	24:c:5506:BCR:H362	1.98	0.45
4:d:5266:TRP:CZ3	4:d:5269:PHE:HD2	2.33	0.45
1:A:192:ILE:CG1	1:A:293:MET:HE1	2.40	0.45
1:A:210:LEU:HD13	21:A:562:PHO:ND	2.31	0.45
3:C:250:TRP:HE1	20:C:496:CLA:CED	2.30	0.45
4:D:60:THR:CG2	4:D:61:HIS:N	2.79	0.45
4:D:179:PHE:O	4:D:183:LEU:HG	2.17	0.45
4:D:191:TRP:HZ3	4:D:194:ASN:ND2	2.14	0.45
13:O:70:CYS:O	13:O:265:PHE:HB2	2.16	0.45
1:a:5303:ASN:O	1:a:5304:HIS:HB2	2.16	0.45
1:a:5323:ARG:HD2	1:a:5323:ARG:HA	1.68	0.45
3:c:5076:ILE:HA	3:c:5077:PRO:HD2	1.72	0.45
4:d:5024:ARG:O	4:d:5026:ARG:HG3	2.17	0.45
4:d:5092:LEU:HA	4:d:5104:TRP:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:5236:ASN:C	4:d:5238:THR:H	2.23	0.45
2:B:120:LEU:O	2:B:121:GLU:C	2.59	0.45
2:B:271:THR:HG22	2:B:274:GLN:N	2.31	0.45
10:K:46:ARG:HH22	17:X:31:UNK:CG2	2.30	0.45
15:U:50:ALA:O	15:U:53:GLU:HB2	2.17	0.45
15:U:92:LEU:HD11	15:U:109:LEU:HD11	1.98	0.45
1:a:5261:GLN:O	1:a:5264:SER:HB3	2.16	0.45
2:b:5385:ARG:O	2:b:5386:ALA:C	2.57	0.45
3:c:5147:PHE:N	3:c:5147:PHE:CD1	2.85	0.45
4:d:5059:TYR:HB3	5:e:5066:VAL:HG23	1.99	0.45
1:A:27:ARG:HA	1:A:27:ARG:HD2	1.78	0.45
1:A:259:ILE:O	1:A:260:PHE:HB3	2.17	0.45
2:B:124:ARG:NH1	2:B:124:ARG:CG	2.77	0.45
2:B:124:ARG:HE	2:B:131:PRO:HG3	1.82	0.45
3:C:79:LYS:O	3:C:80:PRO:C	2.60	0.45
3:C:264:PHE:CD2	3:C:264:PHE:N	2.85	0.45
3:C:349:ILE:HD13	13:O:127:ILE:CD1	2.47	0.45
7:H:55:LEU:HB2	7:H:58:VAL:HG21	1.98	0.45
13:O:32:THR:N	13:O:35:ASP:HB2	2.29	0.45
13:O:139:GLY:O	13:O:140:GLU:O	2.34	0.45
13:O:160:THR:O	13:O:161:SER:O	2.34	0.45
13:O:166:THR:O	13:O:167:ASP:HB3	2.16	0.45
1:a:5027:ARG:HG3	1:a:5027:ARG:HH11	1.81	0.45
2:b:5015:ASP:O	2:b:5017:GLY:N	2.50	0.45
3:c:5062:PHE:CE2	10:k:5029:PRO:HD3	2.47	0.45
4:d:5038:PHE:HZ	4:d:5128:ARG:NH2	2.15	0.45
4:d:5093:TRP:NE1	17:x:5063:UNK:CB	2.80	0.45
4:d:5140:PRO:C	4:d:5142:ASN:H	2.25	0.45
4:d:5246:MET:HE2	4:d:5264:LYS:CG	2.40	0.45
4:d:5335:PRO:HB2	5:e:5065:LEU:HD22	1.99	0.45
14:t:5029:ILE:H	14:t:5029:ILE:CD1	2.22	0.45
16:v:5059:PHE:CD2	16:v:5144:HIS:HD2	2.34	0.45
1:A:40:THR:CG2	1:A:118:HIS:O	2.65	0.45
1:A:159:LEU:HD11	1:A:163:ILE:HD11	1.99	0.45
2:B:175:THR:O	2:B:176:GLY:C	2.60	0.45
2:B:418:LYS:O	2:B:419:SER:C	2.59	0.45
20:B:514:CLA:O1A	20:B:515:CLA:HBA1	2.16	0.45
3:C:305:THR:CG2	3:C:307:PRO:HD2	2.31	0.45
4:D:266:TRP:CZ3	4:D:269:PHE:HD2	2.35	0.45
8:I:6:ILE:O	8:I:7:THR:C	2.60	0.45
15:U:56:ASP:HB3	15:U:60:THR:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:51:GLN:O	16:V:52:TYR:C	2.60	0.45
1:a:5077:ILE:HD11	14:t:5006:TYR:CD1	2.51	0.45
1:a:5191:ASN:HD21	1:a:5194:MET:HG3	1.82	0.45
1:a:5314:ILE:O	1:a:5314:ILE:HG22	2.16	0.45
2:b:5332:LYS:HG3	2:b:5444:ARG:HH21	1.81	0.45
3:c:5369:LEU:HD21	3:c:5384:ILE:HG12	1.98	0.45
4:d:5018:LEU:O	4:d:5019:ASP:C	2.60	0.45
4:d:5040:CYS:O	4:d:5043:LEU:N	2.50	0.45
1:A:22:THR:O	1:A:23:SER:C	2.60	0.45
2:B:10:THR:HG23	2:B:13:ILE:HD11	1.99	0.45
2:B:222:PRO:O	2:B:223:GLN:C	2.59	0.45
20:B:519:CLA:HBA2	7:H:31:MET:SD	2.57	0.45
4:D:130:PHE:HE2	4:D:140:PRO:HB2	1.81	0.45
4:D:244:TYR:OH	4:D:264:LYS:HD3	2.17	0.45
6:F:18:VAL:CG1	6:F:19:ARG:N	2.80	0.45
6:F:45:ARG:OXT	6:F:45:ARG:CG	2.64	0.45
13:O:184:ASP:OD2	13:O:188:ARG:HB2	2.17	0.45
1:a:5160:ILE:HD12	3:c:5431:PHE:CE1	2.52	0.45
20:b:5518:CLA:HBA1	20:b:5518:CLA:HBD	1.99	0.45
3:c:5059:LEU:HD11	24:c:5504:BCR:H372	1.98	0.45
4:d:5034:GLY:C	4:d:5036:LEU:H	2.25	0.45
4:d:5229:ALA:O	4:d:5231:THR:N	2.50	0.45
13:o:5120:THR:OG1	13:o:5154:SER:HB3	2.17	0.45
13:o:5250:ASP:O	13:o:5251:MET:C	2.60	0.45
16:v:5029:LEU:O	16:v:5029:LEU:HG	2.17	0.45
18:z:5001:MET:HE3	18:z:5060:PHE:CD2	2.51	0.45
2:B:364:GLU:HG3	4:D:296:TYR:CE2	2.52	0.44
20:B:517:CLA:H3A	20:B:517:CLA:HBA2	1.71	0.44
4:D:59:TYR:HB3	5:E:66:VAL:HG23	1.99	0.44
4:D:176:ALA:O	4:D:178:ILE:N	2.50	0.44
32:F:51:HEM:HHA	32:F:51:HEM:HAD2	1.67	0.44
13:O:190:LEU:HD13	13:O:214:LYS:O	2.16	0.44
20:a:5559:CLA:H41	4:d:5209:LEU:HD13	1.99	0.44
2:b:5010:THR:C	2:b:5012:LEU:N	2.75	0.44
2:b:5169:SER:HA	2:b:5176:GLY:HA2	1.99	0.44
3:c:5254:THR:HG22	3:c:5255:THR:N	2.23	0.44
3:c:5447:ARG:HG2	3:c:5447:ARG:HH11	1.82	0.44
28:d:5360:MGE:H3A2	28:l:5210:MGE:H3B1	2.00	0.44
9:j:5034:ALA:O	9:j:5035:GLY:O	2.34	0.44
17:x:5062:UNK:O	17:x:5066:UNK:N	2.50	0.44
2:B:462:PHE:HA	20:B:521:CLA:HMC2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:218:VAL:HG12	4:D:219:GLU:N	2.32	0.44
13:O:132:VAL:O	13:O:144:LEU:HD23	2.17	0.44
16:V:128:PRO:C	16:V:130:MET:N	2.75	0.44
1:a:5038:ILE:HB	1:a:5039:PRO:HD3	1.99	0.44
1:a:5207:GLY:O	1:a:5208:GLY:C	2.59	0.44
2:b:5451:PHE:C	2:b:5451:PHE:CD2	2.94	0.44
3:c:5029:GLU:C	3:c:5031:SER:N	2.75	0.44
4:d:5045:LEU:HD13	4:d:5049:LEU:HD12	1.99	0.44
4:d:5047:GLY:HA2	24:d:5357:BCR:H332	1.98	0.44
5:e:5083:LEU:HD12	5:e:5083:LEU:HA	1.85	0.44
13:o:5184:ASP:C	13:o:5184:ASP:OD1	2.60	0.44
16:v:5068:VAL:O	16:v:5071:ILE:HG12	2.18	0.44
17:x:5052:UNK:O	17:x:5054:UNK:N	2.50	0.44
1:A:160:ILE:HD12	3:C:431:PHE:CE1	2.51	0.44
1:A:324:ALA:CB	4:D:329:MET:HE3	2.41	0.44
4:D:302:GLU:OE1	13:O:186:LYS:CE	2.65	0.44
5:E:10:PHE:O	5:E:11:SER:C	2.59	0.44
12:M:33:GLN:O	12:M:35:SER:N	2.50	0.44
1:a:5096:ILE:HG12	1:a:5105:TRP:CE2	2.52	0.44
1:a:5183:MET:HB3	20:a:5558:CLA:HBC2	1.98	0.44
1:a:5278:TRP:HB3	1:a:5279:PRO:CD	2.46	0.44
2:b:5222:PRO:O	2:b:5223:GLN:C	2.61	0.44
3:c:5109:PHE:O	3:c:5110:PRO:C	2.60	0.44
4:d:5176:ALA:O	4:d:5178:ILE:N	2.49	0.44
5:e:5052:PRO:HB3	6:f:5045:ARG:O	2.18	0.44
10:k:5043:VAL:HG12	10:k:5043:VAL:O	2.18	0.44
13:o:5190:LEU:HD13	13:o:5214:LYS:O	2.17	0.44
17:x:5068:UNK:O	17:x:5072:UNK:N	2.50	0.44
1:A:90:GLY:HA2	1:A:167:SER:HB2	2.00	0.44
1:A:323:ARG:HA	1:A:323:ARG:HD2	1.64	0.44
2:B:74:SER:C	2:B:76:SER:N	2.74	0.44
2:B:124:ARG:HA	2:B:131:PRO:HA	1.99	0.44
3:C:265:ILE:HB	20:C:495:CLA:HED3	1.98	0.44
24:C:504:BCR:H11C	24:X:130:BCR:H322	1.99	0.44
4:D:34:GLY:C	4:D:36:LEU:H	2.25	0.44
4:D:92:LEU:HA	4:D:104:TRP:CD1	2.52	0.44
15:U:57:LEU:CD2	15:U:79:ILE:HG21	2.48	0.44
15:U:76:ALA:O	15:U:80:VAL:HG23	2.18	0.44
2:b:5012:LEU:CD1	20:b:5522:CLA:HBB1	2.47	0.44
2:b:5124:ARG:HD3	2:b:5131:PRO:N	2.33	0.44
2:b:5458:PHE:HB3	20:b:5514:CLA:HBC2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:5464:PHE:HD2	20:b:5521:CLA:HAC2	1.83	0.44
3:c:5391:ARG:HG3	3:c:5391:ARG:HH11	1.83	0.44
4:d:5060:THR:CG2	4:d:5061:HIS:N	2.80	0.44
5:e:5023:HIS:HA	5:e:5026:THR:OG1	2.17	0.44
13:o:5077:LEU:HB3	13:o:5091:PHE:HB3	1.99	0.44
16:v:5126:ILE:C	16:v:5128:PRO:HD3	2.43	0.44
18:z:5005:PHE:HA	18:z:5057:LEU:CD1	2.36	0.44
2:B:170:ASP:HB2	2:B:171:PRO:HD2	2.00	0.44
2:B:172:TYR:O	2:B:173:GLY:C	2.60	0.44
2:B:446:SER:HB2	2:B:447:PRO:HD2	1.97	0.44
3:C:109:PHE:O	3:C:110:PRO:C	2.59	0.44
3:C:257:PHE:N	3:C:257:PHE:CD1	2.85	0.44
4:D:24:ARG:O	4:D:26:ARG:HG3	2.17	0.44
5:E:28:PRO:O	5:E:32:ILE:HG13	2.18	0.44
5:E:49:THR:HA	5:E:50:PRO:HD3	1.82	0.44
10:K:15:TYR:O	10:K:17:ILE:N	2.50	0.44
16:V:63:CYS:SG	32:V:552:HEM:HAB	2.57	0.44
16:V:64:ALA:O	16:V:66:CYS:N	2.51	0.44
1:a:5130:GLN:HG2	4:d:5256:ILE:CD1	2.47	0.44
11:l:5002:GLU:HB3	11:l:5003:PRO:CD	2.47	0.44
13:o:5132:VAL:O	13:o:5144:LEU:HD23	2.17	0.44
14:t:5002:GLU:HB3	14:t:5006:TYR:CE2	2.52	0.44
20:A:558:CLA:HBD	20:A:559:CLA:HAC2	1.99	0.44
2:B:192:PRO:HD2	7:H:60:VAL:HG12	2.00	0.44
3:C:42:LEU:HD11	20:C:501:CLA:C1A	2.48	0.44
3:C:267:SER:O	3:C:271:TYR:CD2	2.70	0.44
3:C:292:PHE:HB3	30:C:507:DGD:HD62	1.99	0.44
4:D:60:THR:CG2	4:D:61:HIS:H	2.31	0.44
10:K:17:ILE:CD1	18:Z:6:GLN:NE2	2.78	0.44
10:K:21:LEU:HD11	24:X:130:BCR:HC42	1.99	0.44
1:a:5040:THR:CG2	1:a:5118:HIS:O	2.64	0.44
1:a:5126:TYR:O	1:a:5130:GLN:HG3	2.18	0.44
2:b:5156:PHE:HB2	20:b:5516:CLA:HAC1	1.99	0.44
3:c:5033:PHE:CE1	4:d:5229:ALA:CB	3.01	0.44
3:c:5404:LEU:HD23	3:c:5404:LEU:HA	1.81	0.44
3:c:5415:ASN:O	3:c:5416:SER:CB	2.65	0.44
4:d:5348:ARG:NH2	4:d:5352:LEU:OXT	2.49	0.44
8:i:5006:ILE:O	8:i:5010:ILE:HG12	2.17	0.44
16:v:5033:VAL:O	16:v:5033:VAL:HG12	2.17	0.44
1:A:13:LEU:HD23	1:A:13:LEU:H	1.83	0.44
21:A:561:PHO:HED2	4:D:257:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:385:ARG:O	2:B:386:ALA:C	2.60	0.44
3:C:269:GLU:O	3:C:272:LEU:HB3	2.18	0.44
3:C:420:VAL:HB	3:C:425:TRP:NE1	2.33	0.44
4:D:283:ALA:O	4:D:284:ILE:C	2.61	0.44
5:E:17:VAL:HA	9:J:8:ILE:HD11	2.00	0.44
5:E:26:THR:O	5:E:29:ALA:HB3	2.18	0.44
10:K:13:GLU:O	10:K:16:ALA:HB3	2.18	0.44
2:b:5010:THR:HG23	2:b:5013:ILE:HD11	1.99	0.44
2:b:5191:ASN:HD22	2:b:5191:ASN:C	2.24	0.44
2:b:5379:ALA:HA	2:b:5390:TYR:HB3	2.00	0.44
3:c:5033:PHE:HE1	4:d:5229:ALA:HB2	1.83	0.44
3:c:5171:GLY:O	3:c:5174:LEU:HB2	2.17	0.44
3:c:5201:ASN:O	3:c:5202:PRO:C	2.60	0.44
3:c:5374:GLY:O	3:c:5375:LEU:C	2.61	0.44
3:c:5420:VAL:HB	3:c:5425:TRP:NE1	2.33	0.44
4:d:5035:ILE:O	4:d:5035:ILE:HG22	2.18	0.44
4:d:5038:PHE:N	4:d:5039:PRO:CD	2.80	0.44
4:d:5055:VAL:HG12	4:d:5056:THR:N	2.33	0.44
4:d:5267:LEU:C	4:d:5267:LEU:CD2	2.89	0.44
4:d:5323:GLU:HG2	13:o:5194:TYR:OH	2.17	0.44
7:h:5012:ARG:N	7:h:5013:PRO:CD	2.80	0.44
10:k:5035:LEU:HD13	17:x:5017:UNK:CB	2.48	0.44
1:A:85:SER:HA	1:A:109:GLY:HA3	1.98	0.44
1:A:262:TYR:C	1:A:264:SER:H	2.26	0.44
2:B:476:ARG:HG3	2:B:476:ARG:NH1	2.33	0.44
3:C:135:ARG:O	3:C:136:GLY:O	2.35	0.44
4:D:329:MET:O	4:D:330:ALA:C	2.61	0.44
5:E:51:ARG:O	5:E:54:SER:N	2.48	0.44
1:a:5161:TYR:HB3	1:a:5162:PRO:HD3	1.99	0.44
25:a:5567:LHG:O1	3:c:5447:ARG:NE	2.50	0.44
2:b:5188:ASP:C	2:b:5190:PHE:N	2.74	0.44
2:b:5297:THR:H	2:b:5300:GLU:CD	2.26	0.44
20:b:5513:CLA:H162	7:h:5038:PHE:HE2	1.82	0.44
3:c:5033:PHE:HE1	4:d:5229:ALA:CB	2.31	0.44
3:c:5079:LYS:HB3	3:c:5084:GLN:NE2	2.33	0.44
4:d:5125:PHE:CD1	4:d:5125:PHE:C	2.96	0.44
5:e:5017:VAL:HA	9:j:5008:ILE:HD11	1.99	0.44
13:o:5250:ASP:C	13:o:5252:GLY:N	2.74	0.44
1:A:188:ALA:HB2	1:A:328:MET:CB	2.44	0.44
2:B:16:PRO:HG2	2:B:133:LEU:HD13	1.99	0.44
2:B:150:CYS:HB2	20:B:513:CLA:CMC	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:405:ASN:HB2	30:C:509:DGD:HG32	2.00	0.44
4:D:68:LEU:CD1	6:F:40:MET:HE2	2.48	0.44
4:D:126:MET:HA	4:D:129:GLN:OE1	2.17	0.44
4:D:289:LEU:CD2	4:D:294:ARG:HB3	2.48	0.44
13:O:52:ALA:HA	13:O:230:VAL:O	2.18	0.44
1:a:5163:ILE:HD13	30:c:5507:DGD:HB22	2.00	0.44
1:a:5184:ILE:HA	20:a:5558:CLA:HBC1	1.99	0.44
2:b:5226:TYR:HA	2:b:5231:MET:SD	2.57	0.44
3:c:5199:ILE:N	3:c:5199:ILE:HD12	2.33	0.44
3:c:5257:PHE:N	3:c:5257:PHE:CD1	2.86	0.44
4:d:5160:TYR:CB	4:d:5161:PRO:HD3	2.29	0.44
10:k:5021:LEU:HD11	24:x:5130:BCR:HC42	2.00	0.44
10:k:5031:LEU:HB3	24:x:5130:BCR:C15	2.47	0.44
16:v:5134:THR:O	16:v:5137:ASP:N	2.51	0.44
2:B:10:THR:C	2:B:12:LEU:N	2.73	0.43
2:B:341:LYS:HB3	2:B:406:LEU:HD12	2.00	0.43
2:B:450:TRP:O	2:B:453:PHE:N	2.51	0.43
3:C:225:VAL:O	3:C:225:VAL:HG12	2.18	0.43
3:C:321:ASP:OD2	15:U:129:ASN:HB2	2.18	0.43
4:D:21:TRP:CE2	4:D:26:ARG:NH2	2.78	0.43
10:K:15:TYR:OH	18:Z:58:ASN:HB2	2.17	0.43
11:L:7:ARG:HD2	11:L:7:ARG:HA	1.69	0.43
13:O:223:ILE:HG23	13:O:243:SER:CB	2.23	0.43
16:V:121:LEU:C	16:V:123:SER:H	2.24	0.43
1:a:5107:TYR:HD1	13:o:5141:ARG:CZ	2.31	0.43
2:b:5159:THR:HA	2:b:5181:VAL:O	2.18	0.43
3:c:5056:HIS:O	3:c:5058:GLY:N	2.51	0.43
8:i:5024:LEU:O	8:i:5026:GLY:N	2.46	0.43
28:l:5210:MGE:H102	12:m:5018:PRO:HB3	1.99	0.43
1:A:48:PHE:HA	1:A:115:ILE:CD1	2.48	0.43
1:A:60:ILE:C	1:A:61:ASP:O	2.58	0.43
1:A:83:VAL:HA	1:A:84:PRO:HD3	1.91	0.43
2:B:36:SER:OG	24:B:528:BCR:H362	2.18	0.43
2:B:193:TYR:HE1	2:B:260:SER:N	2.17	0.43
2:B:217:ILE:HG22	2:B:218:LEU:HD23	1.99	0.43
3:C:134:ILE:HD11	20:C:501:CLA:H92	2.00	0.43
20:C:498:CLA:H122	20:C:500:CLA:HED1	2.00	0.43
4:D:93:TRP:CZ2	20:D:355:CLA:O1A	2.71	0.43
4:D:256:ILE:O	4:D:256:ILE:HG12	2.19	0.43
4:D:263:ASN:HB3	28:D:360:MGE:O3D	2.19	0.43
7:H:19:GLY:O	7:H:21:VAL:HG12	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:117:VAL:O	16:V:117:VAL:HG12	2.17	0.43
1:a:5133:LEU:HD23	4:d:5252:PHE:CD2	2.53	0.43
3:c:5404:LEU:C	3:c:5406:SER:H	2.25	0.43
6:f:5040:MET:C	6:f:5042:PHE:N	2.76	0.43
10:k:5015:TYR:C	10:k:5017:ILE:N	2.76	0.43
18:z:5001:MET:O	18:z:5004:LEU:HB3	2.18	0.43
2:B:31:ALA:N	20:B:515:CLA:HBC3	2.33	0.43
2:B:90:PHE:HZ	2:B:98:LEU:HD23	1.83	0.43
20:B:524:CLA:HAA2	11:L:7:ARG:HH22	1.84	0.43
3:C:305:THR:HB	3:C:308:GLU:HB2	1.99	0.43
24:D:357:BCR:H383	28:D:358:MGE:H6B1	2.00	0.43
7:H:41:PHE:CZ	7:H:45:ILE:HD11	2.54	0.43
13:O:36:ILE:O	13:O:37:VAL:C	2.61	0.43
15:U:78:LEU:HD13	15:U:97:LEU:HD21	2.01	0.43
18:Z:12:LEU:HA	18:Z:50:LEU:HD13	1.99	0.43
1:a:5085:SER:HA	1:a:5109:GLY:HA3	1.99	0.43
2:b:5170:ASP:HB2	2:b:5171:PRO:HD2	2.00	0.43
2:b:5175:THR:O	2:b:5176:GLY:C	2.59	0.43
4:d:5199:MET:O	4:d:5200:GLY:C	2.61	0.43
13:o:5114:ASN:C	13:o:5114:ASN:HD22	2.26	0.43
14:t:5021:ILE:HD12	24:t:104:BCR:H332	2.00	0.43
1:A:76:ASN:HD21	1:A:79:THR:H	1.66	0.43
1:A:84:PRO:HA	1:A:112:TYR:CG	2.53	0.43
1:A:278:TRP:HB3	1:A:279:PRO:CD	2.48	0.43
2:B:318:ASN:ND2	2:B:361:ALA:HB2	2.34	0.43
2:B:332:LYS:HG3	2:B:444:ARG:HH21	1.84	0.43
20:B:520:CLA:H122	20:B:522:CLA:H43	2.00	0.43
4:D:120:PHE:CD1	4:D:123:ILE:HD12	2.53	0.43
4:D:157:PHE:CE2	4:D:171:PRO:HB2	2.53	0.43
13:O:184:ASP:C	13:O:184:ASP:OD1	2.60	0.43
17:X:4:UNK:O	17:X:7:UNK:N	2.51	0.43
2:b:5413:ASP:O	2:b:5414:PRO:C	2.59	0.43
3:c:5048:LYS:NZ	3:c:5133:ALA:C	2.76	0.43
3:c:5085:GLY:N	30:c:5508:DGD:HE4	2.33	0.43
3:c:5188:THR:HG23	3:c:5300:GLU:CD	2.42	0.43
20:c:5494:CLA:CHA	20:c:5494:CLA:HBA1	2.48	0.43
24:c:5506:BCR:C33	8:i:5020:VAL:HG13	2.45	0.43
4:d:5071:CYS:HB2	4:d:5076:VAL:HG12	2.01	0.43
4:d:5263:ASN:HB3	28:d:5361:MGE:O3D	2.18	0.43
12:m:5017:VAL:HG12	12:m:5018:PRO:N	2.33	0.43
12:m:5033:GLN:O	12:m:5035:SER:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:u:5089:GLU:CD	15:u:5089:GLU:N	2.75	0.43
1:A:32:TRP:CE2	8:I:22:GLY:HA3	2.53	0.43
3:C:33:PHE:HE1	4:D:229:ALA:HB2	1.82	0.43
5:E:6:GLY:O	5:E:7:GLU:HG2	2.18	0.43
13:O:153:ALA:HB1	13:O:168:PHE:HB3	2.00	0.43
24:X:130:BCR:HC31	18:Z:13:VAL:HG13	2.00	0.43
4:d:5130:PHE:HE2	4:d:5140:PRO:HB2	1.84	0.43
4:d:5214:HIS:HA	22:d:5356:PQ9:O4	2.18	0.43
5:e:5034:GLY:HA2	6:f:5032:PHE:CE1	2.53	0.43
13:o:5052:ALA:HA	13:o:5230:VAL:O	2.19	0.43
16:v:5064:ALA:HB1	16:v:5068:VAL:HG12	2.01	0.43
16:v:5144:HIS:HE1	16:v:5148:GLU:OE2	2.01	0.43
1:A:25:ASP:HA	4:D:251:ARG:NH2	2.32	0.43
1:A:219:VAL:HG21	4:D:268:HIS:CD2	2.54	0.43
1:A:225:ARG:NH1	2:B:484:PRO:HD3	2.34	0.43
1:A:284:TRP:O	1:A:287:ALA:HB3	2.18	0.43
2:B:271:THR:HG22	2:B:273:TYR:N	2.34	0.43
3:C:250:TRP:CD1	3:C:250:TRP:C	2.97	0.43
20:C:498:CLA:H191	30:C:509:DGD:HA91	2.00	0.43
4:D:148:ALA:CB	4:D:149:PRO:HD3	2.35	0.43
6:F:22:ALA:O	6:F:24:HIS:N	2.52	0.43
6:F:40:MET:C	6:F:42:PHE:N	2.74	0.43
13:O:168:PHE:O	13:O:224:SER:HA	2.19	0.43
1:a:5127:MET:HE3	20:c:5495:CLA:HMB2	2.00	0.43
2:b:5016:PRO:HG2	2:b:5133:LEU:HD13	2.00	0.43
2:b:5122:LEU:HD13	7:h:5012:ARG:HA	2.00	0.43
2:b:5362:PHE:CE1	4:d:5184:PHE:CZ	3.00	0.43
20:b:5513:CLA:H3A	20:b:5513:CLA:CGA	2.48	0.43
3:c:5056:HIS:O	3:c:5059:LEU:N	2.50	0.43
3:c:5120:ILE:C	3:c:5122:SER:H	2.26	0.43
3:c:5241:GLY:O	3:c:5243:ILE:N	2.51	0.43
4:d:5128:ARG:O	4:d:5129:GLN:C	2.61	0.43
4:d:5222:LEU:HD23	4:d:5244:TYR:HB3	2.01	0.43
18:z:5015:LEU:O	18:z:5015:LEU:HD12	2.18	0.43
1:A:35:VAL:HG22	24:A:566:BCR:HC42	2.00	0.43
2:B:208:VAL:HG21	20:B:512:CLA:CMC	2.48	0.43
2:B:230:ARG:C	2:B:231:MET:O	2.61	0.43
2:B:403:GLY:O	2:B:407:ASN:HB2	2.18	0.43
4:D:53:THR:HG22	4:D:67:TYR:CE1	2.53	0.43
4:D:263:ASN:O	4:D:264:LYS:C	2.61	0.43
5:E:19:TYR:C	5:E:19:TYR:CD1	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:114:ASN:C	13:O:114:ASN:HD22	2.25	0.43
2:b:5153:PHE:CZ	2:b:5158:LEU:HD21	2.53	0.43
20:c:5493:CLA:H191	20:c:5493:CLA:CMD	2.46	0.43
24:c:5504:BCR:H11C	24:x:5130:BCR:H322	2.00	0.43
4:d:5060:THR:CG2	4:d:5061:HIS:H	2.31	0.43
5:e:5019:TYR:CD1	5:e:5019:TYR:C	2.96	0.43
14:t:5004:ILE:C	14:t:5004:ILE:CD1	2.85	0.43
2:B:360:PRO:O	2:B:362:PHE:N	2.51	0.43
2:B:368:VAL:O	2:B:368:VAL:HG13	2.19	0.43
2:B:451:PHE:C	2:B:451:PHE:CD2	2.96	0.43
3:C:214:LEU:HD23	3:C:214:LEU:N	2.31	0.43
20:C:491:CLA:CAD	20:C:493:CLA:H12	2.49	0.43
4:D:178:ILE:CG2	4:D:179:PHE:N	2.81	0.43
13:O:231:ASP:O	13:O:231:ASP:OD1	2.37	0.43
2:b:5391:SER:C	2:b:5392:PHE:O	2.57	0.43
3:c:5134:ILE:HD11	20:c:5501:CLA:H92	2.01	0.43
3:c:5176:VAL:HG11	3:c:5238:ILE:HG12	2.01	0.43
3:c:5206:PRO:O	3:c:5207:ARG:C	2.62	0.43
16:v:5090:PRO:HD2	16:v:5092:ARG:NH2	2.34	0.43
18:z:5012:LEU:HA	18:z:5050:LEU:HD13	2.00	0.43
20:B:515:CLA:H141	20:B:520:CLA:CMA	2.45	0.43
3:C:33:PHE:CE1	4:D:229:ALA:CB	3.02	0.43
3:C:168:LEU:HD13	20:C:497:CLA:H2	2.01	0.43
3:C:180:MET:SD	3:C:202:PRO:HG2	2.57	0.43
3:C:385:GLN:HB2	3:C:387:TRP:CD1	2.54	0.43
24:C:505:BCR:C31	18:Z:55:GLY:HA2	2.46	0.43
4:D:85:MET:HE3	4:D:107:LEU:HB3	2.01	0.43
4:D:87:HIS:C	4:D:167:TRP:HE1	2.27	0.43
4:D:134:ARG:NE	4:D:134:ARG:HA	2.34	0.43
4:D:171:PRO:HG3	4:D:181:PHE:CE2	2.54	0.43
1:a:5063:ILE:HG21	3:c:5335:THR:HG21	2.01	0.43
3:c:5061:VAL:O	3:c:5062:PHE:C	2.62	0.43
4:d:5091:LEU:O	4:d:5094:GLY:N	2.37	0.43
4:d:5100:ASP:OD1	4:d:5100:ASP:C	2.60	0.43
7:h:5019:GLY:O	7:h:5021:VAL:HG12	2.19	0.43
16:v:5124:ALA:HB1	16:v:5131:ARG:CG	2.47	0.43
2:B:464:PHE:HD2	20:B:521:CLA:HAC2	1.83	0.43
20:B:515:CLA:HBA1	20:B:515:CLA:CHA	2.48	0.43
3:C:48:LYS:NZ	3:C:133:ALA:C	2.77	0.43
3:C:323:LYS:O	3:C:324:LEU:HB2	2.19	0.43
3:C:394:GLU:O	3:C:398:HIS:HD2	2.02	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:35:ILE:O	4:D:39:PRO:HG2	2.18	0.43
13:O:32:THR:H	13:O:35:ASP:CB	2.28	0.43
14:T:22:PHE:O	14:T:23:PHE:CD2	2.71	0.43
15:U:66:ILE:HD11	15:U:72:TYR:CZ	2.54	0.43
18:Z:22:GLY:O	18:Z:23:VAL:C	2.62	0.43
1:a:5121:LEU:HD12	1:a:5121:LEU:HA	1.89	0.43
1:a:5310:LYS:HB2	16:v:5028:GLU:CB	2.34	0.43
3:c:5135:ARG:O	3:c:5136:GLY:O	2.37	0.43
3:c:5166:ILE:HG13	3:c:5248:GLY:HA3	2.01	0.43
3:c:5204:LEU:O	3:c:5205:ASP:CB	2.64	0.43
10:k:5017:ILE:CD1	18:z:5006:GLN:NE2	2.78	0.43
13:o:5080:GLU:O	13:o:5081:GLU:C	2.62	0.43
16:v:5085:LEU:HD22	16:v:5092:ARG:HB2	2.00	0.43
3:C:417:VAL:O	3:C:417:VAL:HG13	2.18	0.42
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.01	0.42
4:D:205:LEU:HD12	4:D:205:LEU:HA	1.79	0.42
5:E:31:PHE:CE1	6:F:35:GLY:HA2	2.54	0.42
10:K:13:GLU:O	10:K:14:ALA:C	2.61	0.42
1:a:5141:PRO:HG2	1:a:5142:TRP:CD1	2.54	0.42
1:a:5192:ILE:C	1:a:5194:MET:N	2.74	0.42
1:a:5193:LEU:HD11	20:a:5558:CLA:HMC2	2.01	0.42
1:a:5293:MET:HG2	1:a:5298:ASN:HA	2.01	0.42
3:c:5033:PHE:HD1	4:d:5229:ALA:HB3	1.80	0.42
3:c:5055:ALA:HB2	3:c:5129:GLY:HA3	2.01	0.42
3:c:5305:THR:CG2	3:c:5307:PRO:HD2	2.30	0.42
4:d:5043:LEU:HD11	20:d:5355:CLA:HBC3	1.99	0.42
4:d:5085:MET:HE3	4:d:5107:LEU:HB3	2.00	0.42
4:d:5191:TRP:CE3	4:d:5289:LEU:HD11	2.53	0.42
4:d:5329:MET:O	4:d:5330:ALA:C	2.62	0.42
7:h:5045:ILE:O	7:h:5046:LEU:C	2.61	0.42
13:o:5106:GLN:N	13:o:5106:GLN:HE21	2.16	0.42
13:o:5168:PHE:O	13:o:5224:SER:HA	2.19	0.42
13:o:5169:LYS:HG2	13:o:5224:SER:HB2	2.00	0.42
15:u:5069:ARG:HG3	15:u:5070:GLY:N	2.34	0.42
16:v:5051:GLN:O	16:v:5052:TYR:C	2.60	0.42
17:x:5003:UNK:C	17:x:5005:UNK:N	2.78	0.42
1:A:206:PHE:CD1	21:A:562:PHO:HBB2	2.54	0.42
2:B:31:ALA:CA	20:B:515:CLA:HBC3	2.49	0.42
2:B:271:THR:CG2	2:B:273:TYR:N	2.79	0.42
2:B:271:THR:HG22	2:B:273:TYR:H	1.82	0.42
2:B:379:ALA:HA	2:B:390:TYR:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:GLU:O	3:C:31:SER:N	2.52	0.42
3:C:353:GLY:C	3:C:355:THR:N	2.77	0.42
3:C:452:ALA:O	3:C:454:GLY:N	2.52	0.42
4:D:103:ARG:O	4:D:104:TRP:C	2.63	0.42
4:D:249:ALA:O	4:D:250:ASN:C	2.61	0.42
8:I:7:THR:O	8:I:11:VAL:HG23	2.19	0.42
13:O:120:THR:OG1	13:O:154:SER:HB3	2.19	0.42
1:a:5016:ARG:HD3	1:a:5016:ARG:C	2.44	0.42
1:a:5153:SER:CB	20:a:5558:CLA:H43	2.49	0.42
1:a:5321:ILE:HG22	1:a:5322:ASN:N	2.32	0.42
2:b:5450:TRP:NE1	20:b:5517:CLA:HBA1	2.34	0.42
3:c:5075:PHE:CE2	3:c:5105:VAL:HG11	2.55	0.42
3:c:5205:ASP:HA	3:c:5206:PRO:HD2	1.88	0.42
30:c:5509:DGD:HG31	9:j:5033:TYR:CZ	2.53	0.42
4:d:5082:ALA:O	4:d:5085:MET:HB2	2.18	0.42
13:o:5073:PRO:HG2	13:o:5102:THR:CB	2.48	0.42
15:u:5057:LEU:CD2	15:u:5079:ILE:HG21	2.49	0.42
1:A:217:SER:OG	4:D:141:TYR:O	2.31	0.42
2:B:90:PHE:CZ	2:B:98:LEU:HD23	2.55	0.42
2:B:314:TYR:CZ	2:B:316:GLY:HA3	2.55	0.42
2:B:350:GLU:CD	2:B:350:GLU:N	2.76	0.42
20:B:518:CLA:HBD	20:B:518:CLA:HBA1	2.00	0.42
3:C:201:ASN:N	3:C:202:PRO:CD	2.82	0.42
4:D:40:CYS:O	4:D:43:LEU:N	2.52	0.42
4:D:42:TYR:HE1	6:F:26:LEU:HD23	1.85	0.42
11:L:12:LEU:CD1	12:M:25:LEU:HD12	2.49	0.42
13:O:30:THR:HG22	13:O:31:LEU:N	2.33	0.42
16:V:147:VAL:O	16:V:148:GLU:C	2.62	0.42
1:a:5320:ILE:HG21	4:d:5333:ASP:OD2	2.19	0.42
24:a:5566:BCR:H312	8:i:5015:PHE:CE2	2.54	0.42
2:b:5008:VAL:HG12	11:l:5010:VAL:HG13	2.01	0.42
3:c:5353:GLY:O	3:c:5356:MET:HG2	2.18	0.42
3:c:5385:GLN:HB2	3:c:5387:TRP:CD1	2.54	0.42
3:c:5472:LEU:H	3:c:5472:LEU:HD12	1.85	0.42
4:d:5126:MET:HE3	4:d:5146:PHE:HD2	1.84	0.42
4:d:5179:PHE:O	4:d:5183:LEU:HG	2.19	0.42
7:h:5012:ARG:NH1	7:h:5012:ARG:HG3	2.34	0.42
7:h:5059:ASN:OD1	7:h:5059:ASN:C	2.62	0.42
13:o:5259:VAL:CG1	13:o:5260:LYS:N	2.82	0.42
13:o:5261:ILE:HD12	13:o:5261:ILE:N	2.33	0.42
1:A:69:GLY:O	1:A:80:GLY:HA2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ARG:HH12	2:B:483:ASP:CA	2.19	0.42
1:A:261:GLN:O	1:A:264:SER:HB3	2.19	0.42
2:B:90:PHE:CD1	2:B:90:PHE:C	2.98	0.42
20:B:524:CLA:H102	24:B:527:BCR:H362	2.02	0.42
3:C:147:PHE:CD1	3:C:147:PHE:N	2.85	0.42
4:D:38:PHE:N	4:D:39:PRO:CD	2.83	0.42
4:D:103:ARG:HD3	4:D:103:ARG:HA	1.81	0.42
7:H:19:GLY:O	7:H:20:LYS:C	2.62	0.42
7:H:25:TRP:O	7:H:26:GLY:C	2.62	0.42
13:O:155:THR:HG22	13:O:167:ASP:C	2.42	0.42
16:V:107:THR:HG22	16:V:108:TYR:N	2.34	0.42
1:a:5206:PHE:CD1	21:a:5562:PHO:HBB2	2.54	0.42
1:a:5284:TRP:O	1:a:5287:ALA:HB3	2.18	0.42
2:b:5061:PHE:CZ	20:b:5514:CLA:HMA1	2.54	0.42
2:b:5087:ASP:O	2:b:5088:PRO:C	2.60	0.42
2:b:5230:ARG:C	2:b:5231:MET:O	2.62	0.42
2:b:5249:ALA:O	2:b:5252:VAL:HG22	2.19	0.42
2:b:5259:GLY:O	2:b:5260:SER:HB2	2.20	0.42
3:c:5264:PHE:CD2	3:c:5264:PHE:N	2.86	0.42
4:d:5088:SER:HB2	5:e:5069:ARG:CZ	2.50	0.42
1:A:20:TRP:O	1:A:21:VAL:C	2.62	0.42
2:B:8:VAL:HG12	11:L:10:VAL:HG13	2.02	0.42
2:B:125:ASP:O	2:B:128:THR:O	2.38	0.42
2:B:214:LEU:O	2:B:217:ILE:HB	2.18	0.42
2:B:271:THR:HG22	2:B:274:GLN:HG3	2.02	0.42
2:B:302:TRP:C	2:B:304:ALA:N	2.77	0.42
4:D:47:GLY:HA2	24:D:357:BCR:H332	2.01	0.42
13:O:115:SER:O	13:O:116:ASP:CG	2.63	0.42
27:T:217:LMT:H5'	2:b:5040:TYR:HD1	1.83	0.42
1:a:5071:LEU:C	1:a:5073:TYR:H	2.27	0.42
2:b:5074:SER:C	2:b:5076:SER:N	2.74	0.42
2:b:5359:MET:HB2	2:b:5425:ILE:HG23	2.00	0.42
20:b:5515:CLA:CHA	20:b:5515:CLA:HBA1	2.49	0.42
3:c:5079:LYS:O	3:c:5080:PRO:C	2.61	0.42
20:c:5491:CLA:CAD	20:c:5493:CLA:H12	2.49	0.42
6:f:5041:GLN:NE2	6:f:5041:GLN:CA	2.74	0.42
15:u:5104:ILE:O	15:u:5105:LEU:C	2.61	0.42
16:v:5121:LEU:C	16:v:5123:SER:N	2.77	0.42
2:B:7:ARG:O	2:B:10:THR:OG1	2.25	0.42
2:B:29:LEU:HD23	26:t:213:SQD:H211	2.00	0.42
2:B:159:THR:HA	2:B:181:VAL:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:516:CLA:H72	24:B:529:BCR:H311	2.02	0.42
3:C:37:ALA:O	3:C:38:GLY:C	2.63	0.42
3:C:113:VAL:O	3:C:117:VAL:HG23	2.20	0.42
3:C:171:GLY:HA3	20:C:502:CLA:H41	2.01	0.42
3:C:472:LEU:H	3:C:472:LEU:HD12	1.84	0.42
7:H:17:GLU:O	7:H:18:TYR:C	2.62	0.42
11:L:16:SER:O	11:L:17:LEU:C	2.60	0.42
15:U:58:ASN:HD21	15:U:114:VAL:HG13	1.79	0.42
16:V:134:THR:O	16:V:137:ASP:N	2.52	0.42
17:X:23:UNK:CG2	18:Z:25:VAL:HG11	2.50	0.42
17:X:54:UNK:O	17:X:55:UNK:C	2.66	0.42
1:a:5135:TYR:CE1	3:c:5449:ARG:O	2.72	0.42
2:b:5033:TRP:HA	2:b:5036:SER:HB2	2.01	0.42
2:b:5193:TYR:CE1	2:b:5260:SER:N	2.88	0.42
2:b:5446:SER:HB2	2:b:5447:PRO:HD2	2.01	0.42
3:c:5095:LEU:O	3:c:5185:LEU:HD23	2.19	0.42
3:c:5209:ILE:HG22	3:c:5210:PHE:N	2.35	0.42
3:c:5290:VAL:HG23	3:c:5297:TYR:CE1	2.55	0.42
4:d:5122:LEU:HB3	4:d:5150:ILE:CD1	2.50	0.42
4:d:5263:ASN:O	4:d:5266:TRP:N	2.50	0.42
13:o:5168:PHE:N	13:o:5168:PHE:HD1	2.15	0.42
13:o:5178:ARG:NH1	13:o:5178:ARG:CG	2.82	0.42
1:A:33:PHE:CE1	1:A:128:GLY:HA3	2.55	0.42
1:A:334:ARG:NH1	13:O:183:LEU:O	2.53	0.42
3:C:180:MET:HE3	3:C:202:PRO:CG	2.50	0.42
6:F:13:TYR:HA	6:F:14:PRO:HD3	1.88	0.42
16:V:124:ALA:HB1	16:V:131:ARG:CG	2.49	0.42
16:V:126:ILE:C	16:V:128:PRO:HD3	2.45	0.42
1:a:5025:ASP:CB	4:d:5251:ARG:HH22	2.32	0.42
1:a:5210:LEU:HD12	1:a:5210:LEU:O	2.19	0.42
1:a:5326:LEU:HD23	3:c:5412:THR:CB	2.49	0.42
2:b:5160:GLY:HA3	2:b:5180:PRO:HB3	2.02	0.42
2:b:5208:VAL:HG21	20:b:5512:CLA:CMC	2.49	0.42
2:b:5341:LYS:HB3	2:b:5406:LEU:HD12	2.01	0.42
3:c:5416:SER:O	3:c:5417:VAL:HG12	2.20	0.42
5:e:5035:TRP:CD1	5:e:5035:TRP:C	2.97	0.42
16:v:5064:ALA:C	16:v:5066:CYS:N	2.77	0.42
1:A:184:ILE:HA	20:A:558:CLA:HBC1	2.02	0.42
27:A:569:LMT:H111	2:b:5098:LEU:HD22	2.02	0.42
2:B:226:TYR:HA	2:B:231:MET:SD	2.60	0.42
2:B:326:ARG:NH2	4:D:297:ASP:OD1	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:PHE:HE1	4:D:229:ALA:CB	2.33	0.42
3:C:55:ALA:HB2	3:C:129:GLY:HA3	2.00	0.42
3:C:80:PRO:HG2	3:C:83:GLU:OE2	2.20	0.42
3:C:168:LEU:CD1	20:C:497:CLA:H2	2.49	0.42
3:C:190:ALA:O	3:C:193:GLY:N	2.52	0.42
20:C:503:CLA:HMB2	24:C:505:BCR:H402	2.02	0.42
4:D:222:LEU:HD23	4:D:244:TYR:HB3	2.02	0.42
4:D:286:VAL:C	4:D:288:GLY:N	2.75	0.42
7:H:54:ILE:O	7:H:55:LEU:HD23	2.20	0.42
12:M:15:VAL:O	12:M:19:SER:CB	2.68	0.42
32:V:552:HEM:HHA	32:V:552:HEM:HAD2	1.56	0.42
1:a:5029:TYR:CD2	1:a:5029:TYR:C	2.97	0.42
1:a:5077:ILE:H	1:a:5077:ILE:HG13	1.58	0.42
1:a:5292:THR:C	1:a:5294:ALA:N	2.78	0.42
1:a:5314:ILE:O	1:a:5315:ASN:O	2.38	0.42
2:b:5134:ASP:H	7:h:5015:ASN:HD22	1.67	0.42
4:d:5103:ARG:HG3	5:e:5073:LYS:HG3	2.01	0.42
4:d:5235:PHE:CE1	4:d:5237:PRO:HA	2.54	0.42
7:h:5028:THR:HB	7:h:5029:PRO:HD3	2.01	0.42
9:j:5018:GLY:O	9:j:5022:ILE:HG12	2.19	0.42
13:o:5141:ARG:C	13:o:5142:ILE:HD12	2.44	0.42
17:x:5090:UNK:CD1	17:x:5091:UNK:H	2.33	0.42
18:z:5028:ALA:O	18:z:5030:PRO:HD3	2.19	0.42
1:A:257:ARG:HH12	1:A:261:GLN:NE2	2.18	0.42
2:B:30:VAL:O	2:B:30:VAL:HG12	2.19	0.42
2:B:112:CYS:O	2:B:113:TRP:C	2.62	0.42
20:B:515:CLA:H152	20:B:520:CLA:HED1	2.02	0.42
3:C:33:PHE:HD1	4:D:229:ALA:HB3	1.82	0.42
7:H:9:ASP:C	7:H:11:LEU:N	2.78	0.42
7:H:12:ARG:N	7:H:13:PRO:CD	2.82	0.42
11:L:12:LEU:HD13	12:M:25:LEU:HB2	2.02	0.42
13:O:230:VAL:CG1	13:O:231:ASP:N	2.83	0.42
16:V:29:LEU:HG	16:V:29:LEU:O	2.18	0.42
17:X:15:UNK:O	17:X:19:UNK:N	2.52	0.42
2:b:5326:ARG:NH2	4:d:5297:ASP:OD1	2.48	0.42
4:d:5289:LEU:CD2	4:d:5294:ARG:HB3	2.50	0.42
24:d:5357:BCR:H16C	6:f:5033:PHE:CD2	2.55	0.42
24:d:5357:BCR:H383	28:d:5359:MGE:H6B1	2.01	0.42
7:h:5041:PHE:HB2	24:h:5107:BCR:C16	2.49	0.42
13:o:5218:LEU:HD22	15:u:5119:THR:HG21	2.01	0.42
2:B:45:PHE:HE2	2:B:47:PRO:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:GLU:OE2	2:B:188:ASP:HB3	2.19	0.42
3:C:138:GLU:O	3:C:139:THR:HB	2.20	0.42
3:C:405:ASN:ND2	30:C:509:DGD:HD5	2.26	0.42
4:D:90:LEU:CD1	4:D:96:GLU:HG3	2.50	0.42
4:D:93:TRP:NE1	17:X:63:UNK:CB	2.83	0.42
4:D:131:GLU:O	4:D:135:LEU:HG	2.20	0.42
4:D:274:VAL:HG13	22:D:356:PQ9:H251	2.02	0.42
5:E:37:PHE:CD1	5:E:42:LEU:HD23	2.55	0.42
13:O:98:THR:CG2	13:O:99:ARG:N	2.70	0.42
13:O:176:SER:O	13:O:177:TYR:C	2.61	0.42
1:a:5055:ALA:HA	1:a:5056:PRO:HD3	1.81	0.42
1:a:5057:PRO:HA	1:a:5068:SER:HA	2.01	0.42
2:b:5010:THR:O	2:b:5012:LEU:N	2.53	0.42
2:b:5410:THR:HG22	2:b:5411:PHE:N	2.35	0.42
4:d:5134:ARG:HE	4:d:5134:ARG:CA	2.33	0.42
11:l:5007:ARG:HD2	11:l:5007:ARG:HA	1.68	0.42
16:v:5152:LEU:HB3	16:v:5155:LYS:HB2	2.02	0.42
1:A:314:ILE:O	1:A:315:ASN:O	2.38	0.41
20:A:559:CLA:H41	4:D:209:LEU:HD13	2.01	0.41
20:C:493:CLA:H171	20:C:500:CLA:HBB2	2.01	0.41
4:D:270:PHE:HZ	22:D:356:PQ9:H243	1.85	0.41
13:O:45:CYS:CB	13:O:46:PRO:HD2	2.31	0.41
1:a:5206:PHE:HD2	1:a:5206:PHE:HA	1.71	0.41
20:a:5559:CLA:H161	28:d:5361:MGE:H252	2.02	0.41
9:j:5012:ILE:O	9:j:5016:VAL:HG23	2.19	0.41
1:A:54:ALA:HB2	1:A:72:LEU:HD12	2.03	0.41
25:A:567:LHG:O1	3:C:447:ARG:NE	2.53	0.41
2:B:314:TYR:OH	2:B:334:ASP:OD1	2.30	0.41
3:C:153:ASP:C	3:C:155:ASN:N	2.72	0.41
3:C:322:GLN:O	3:C:324:LEU:N	2.49	0.41
3:C:465:PRO:O	3:C:469:MET:HG3	2.20	0.41
3:C:466:VAL:HG21	4:D:248:THR:HG23	2.02	0.41
30:C:509:DGD:HE3	9:J:39:SER:OG	2.21	0.41
4:D:91:LEU:O	4:D:94:GLY:N	2.38	0.41
7:H:28:THR:HB	7:H:29:PRO:HD3	2.02	0.41
10:K:20:PRO:O	17:X:6:UNK:HG3	2.20	0.41
13:O:52:ALA:O	13:O:53:ARG:CB	2.68	0.41
13:O:66:ILE:HD12	13:O:121:PHE:CD1	2.55	0.41
14:T:8:PHE:O	14:T:9:ILE:C	2.62	0.41
1:a:5033:PHE:CD1	1:a:5128:GLY:C	2.98	0.41
1:a:5060:ILE:C	1:a:5061:ASP:O	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:5145:LEU:O	2:b:5146:ALA:C	2.63	0.41
2:b:5231:MET:C	2:b:5233:ASN:N	2.78	0.41
2:b:5377:VAL:HG11	4:d:5342:PRO:CG	2.50	0.41
20:b:5520:CLA:H122	20:b:5522:CLA:H43	2.01	0.41
3:c:5035:TRP:CD2	3:c:5036:TRP:N	2.88	0.41
3:c:5250:TRP:HE1	20:c:5496:CLA:HED1	1.85	0.41
4:d:5047:GLY:HA2	24:d:5357:BCR:C33	2.50	0.41
8:i:5006:ILE:O	8:i:5007:THR:C	2.63	0.41
13:o:5077:LEU:N	13:o:5077:LEU:CD1	2.82	0.41
15:u:5081:LYS:HG3	15:u:5081:LYS:O	2.19	0.41
16:v:5160:LYS:HA	16:v:5163:TYR:CD2	2.55	0.41
27:A:569:LMT:O1'	2:b:5043:ALA:HA	2.20	0.41
3:C:29:GLU:C	3:C:31:SER:N	2.72	0.41
20:C:493:CLA:H191	20:C:493:CLA:CMD	2.45	0.41
4:D:140:PRO:C	4:D:142:ASN:H	2.28	0.41
4:D:236:ASN:C	4:D:238:THR:H	2.27	0.41
8:I:33:LYS:HA	8:I:34:ARG:NH2	2.16	0.41
13:O:106:GLN:HE21	13:O:106:GLN:N	2.18	0.41
13:O:250:ASP:O	13:O:251:MET:C	2.61	0.41
15:U:69:ARG:HG3	15:U:70:GLY:N	2.33	0.41
16:V:75:ASN:N	16:V:76:PRO:HD3	2.35	0.41
20:a:5558:CLA:HBD	20:a:5559:CLA:HAC2	2.01	0.41
9:j:5018:GLY:HA3	24:x:5130:BCR:H371	2.03	0.41
14:t:5018:PHE:HB2	24:t:104:BCR:C8	2.50	0.41
2:B:27:THR:O	2:B:28:ALA:C	2.62	0.41
2:B:185:TRP:CD1	2:B:185:TRP:H	2.38	0.41
3:C:334:PRO:O	13:O:182:PHE:HB2	2.19	0.41
3:C:365:TRP:CZ3	3:C:366:LEU:HD13	2.55	0.41
4:D:263:ASN:O	4:D:266:TRP:N	2.52	0.41
5:E:53:ASP:OD2	5:E:53:ASP:C	2.63	0.41
7:H:9:ASP:C	7:H:11:LEU:H	2.28	0.41
17:X:52:UNK:O	17:X:54:UNK:N	2.54	0.41
1:a:5027:ARG:HA	1:a:5027:ARG:HD2	1.78	0.41
1:a:5285:PHE:O	1:a:5286:THR:C	2.59	0.41
3:c:5095:LEU:HA	3:c:5185:LEU:CD2	2.50	0.41
3:c:5205:ASP:OD2	3:c:5205:ASP:C	2.63	0.41
3:c:5321:ASP:OD2	15:u:5129:ASN:HB2	2.20	0.41
3:c:5342:MET:SD	3:c:5356:MET:HE2	2.59	0.41
3:c:5418:ASN:HB3	30:c:5509:DGD:C2E	2.50	0.41
3:c:5418:ASN:ND2	30:c:5508:DGD:HE1	2.34	0.41
4:d:5103:ARG:HH12	5:e:5077:GLU:CG	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:5041:GLN:NE2	9:j:5031:GLY:HA3	2.35	0.41
7:h:5012:ARG:HG3	7:h:5012:ARG:HH11	1.85	0.41
8:i:5031:ASN:HB2	8:i:5032:PRO:HD2	2.01	0.41
12:m:5030:GLU:O	12:m:5035:SER:HB3	2.21	0.41
14:t:5015:ALA:HB2	24:t:104:BCR:H14C	2.02	0.41
15:u:5039:LEU:HD23	15:u:5039:LEU:HA	1.85	0.41
17:x:5015:UNK:O	17:x:5019:UNK:N	2.53	0.41
17:x:5054:UNK:O	17:x:5055:UNK:C	2.67	0.41
1:A:267:ASN:HB3	1:A:270:SER:HB3	2.02	0.41
2:B:121:GLU:C	2:B:123:PHE:H	2.27	0.41
2:B:141:ILE:O	2:B:144:PHE:HB3	2.20	0.41
2:B:208:VAL:O	2:B:208:VAL:HG12	2.20	0.41
20:B:513:CLA:H3A	20:B:513:CLA:CGA	2.50	0.41
3:C:166:ILE:HG23	3:C:245:ILE:CG2	2.42	0.41
4:D:178:ILE:O	4:D:181:PHE:N	2.54	0.41
4:D:246:MET:HE2	4:D:264:LYS:CG	2.42	0.41
4:D:259:ILE:HG22	4:D:260:ALA:N	2.34	0.41
10:K:15:TYR:C	10:K:17:ILE:N	2.79	0.41
1:a:5017:PHE:CE1	1:a:5021:VAL:CG2	3.03	0.41
1:a:5054:ALA:O	1:a:5055:ALA:CB	2.68	0.41
1:a:5214:MET:O	1:a:5217:SER:HB3	2.20	0.41
2:b:5033:TRP:CE3	2:b:5034:ALA:HA	2.55	0.41
2:b:5185:TRP:HH2	2:b:5203:ILE:CG2	2.32	0.41
3:c:5089:ILE:HB	3:c:5090:PRO:HD3	2.03	0.41
3:c:5250:TRP:HE1	20:c:5496:CLA:CED	2.33	0.41
3:c:5370:ARG:HD3	13:o:5033:TYR:CE2	2.55	0.41
3:c:5418:ASN:HB3	30:c:5509:DGD:O6E	2.20	0.41
5:e:5035:TRP:O	5:e:5039:SER:HB2	2.20	0.41
13:o:5142:ILE:N	13:o:5142:ILE:CD1	2.82	0.41
13:o:5179:THR:HG23	13:o:5180:ALA:N	2.35	0.41
1:A:54:ALA:O	1:A:55:ALA:CB	2.69	0.41
2:B:302:TRP:C	2:B:304:ALA:H	2.28	0.41
2:B:359:MET:HB2	2:B:425:ILE:HG23	2.02	0.41
20:B:521:CLA:C4	20:B:524:CLA:HBC3	2.50	0.41
3:C:75:PHE:CE2	3:C:105:VAL:HG11	2.56	0.41
3:C:95:LEU:O	3:C:185:LEU:HD23	2.21	0.41
24:C:506:BCR:C33	8:I:20:VAL:HG13	2.46	0.41
6:F:17:THR:OG1	6:F:18:VAL:N	2.53	0.41
13:O:77:LEU:N	13:O:77:LEU:CD1	2.81	0.41
13:O:208:LEU:O	13:O:209:ALA:C	2.63	0.41
15:U:46:LYS:C	15:U:48:GLY:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:152:LEU:HB3	16:V:155:LYS:HB2	2.01	0.41
2:b:5052:LEU:HA	2:b:5052:LEU:HD23	1.84	0.41
2:b:5206:GLY:O	2:b:5210:ILE:HG13	2.20	0.41
15:u:5050:ALA:O	15:u:5053:GLU:HB2	2.21	0.41
16:v:5064:ALA:O	16:v:5066:CYS:N	2.53	0.41
18:z:5005:PHE:CE1	18:z:5054:VAL:HG13	2.54	0.41
2:B:231:MET:C	2:B:233:ASN:N	2.78	0.41
2:B:338:GLN:HB2	2:B:431:GLU:O	2.20	0.41
3:C:210:PHE:O	3:C:211:GLY:C	2.62	0.41
5:E:35:TRP:CD1	5:E:35:TRP:C	2.98	0.41
7:H:46:LEU:HD11	30:H:208:DGD:HA22	2.02	0.41
9:J:10:LEU:C	9:J:12:ILE:H	2.27	0.41
10:K:11:LEU:O	10:K:12:PRO:C	2.62	0.41
13:O:141:ARG:C	13:O:142:ILE:HD12	2.46	0.41
16:V:59:PHE:CD1	16:V:63:CYS:HB2	2.56	0.41
16:V:64:ALA:HB1	16:V:68:VAL:HG12	2.03	0.41
16:V:68:VAL:O	16:V:71:ILE:HG12	2.21	0.41
1:a:5153:SER:HB3	20:a:5558:CLA:HED1	2.03	0.41
1:a:5156:ALA:HA	1:a:5160:ILE:HB	2.03	0.41
2:b:5046:ASP:C	2:b:5046:ASP:OD1	2.63	0.41
3:c:5033:PHE:CD2	3:c:5040:ALA:HB3	2.56	0.41
4:d:5350:ASN:O	4:d:5351:ALA:HB3	2.20	0.41
5:e:5050:PRO:HB3	5:e:5054:SER:O	2.21	0.41
8:i:5030:ARG:H	8:i:5030:ARG:HG2	1.55	0.41
15:u:5041:ASN:OD1	15:u:5041:ASN:C	2.63	0.41
16:v:5079:ASP:OD1	16:v:5079:ASP:C	2.63	0.41
2:B:61:PHE:HZ	20:B:517:CLA:HBB1	1.85	0.41
2:B:191:ASN:ND2	2:B:191:ASN:C	2.79	0.41
3:C:163:PHE:CE1	3:C:252:ILE:HD13	2.56	0.41
3:C:174:LEU:O	3:C:177:ALA:HB3	2.21	0.41
3:C:418:ASN:HB3	30:C:509:DGD:C2E	2.51	0.41
15:U:98:THR:OG1	15:U:101:GLN:HG3	2.20	0.41
17:X:4:UNK:O	17:X:5:UNK:C	2.69	0.41
1:a:5340:PRO:HD3	15:u:5133:TYR:CZ	2.56	0.41
2:b:5390:TYR:O	2:b:5391:SER:C	2.63	0.41
20:b:5512:CLA:H201	4:d:5159:ILE:HG12	2.03	0.41
20:b:5517:CLA:HBA2	20:b:5517:CLA:H3A	1.68	0.41
3:c:5171:GLY:HA3	20:c:5502:CLA:H41	2.03	0.41
3:c:5182:PHE:CD2	3:c:5182:PHE:N	2.88	0.41
3:c:5216:SER:O	3:c:5221:GLU:O	2.39	0.41
4:d:5078:VAL:HG11	4:d:5114:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:e:5014:ILE:HG21	9:j:5013:VAL:HG11	2.00	0.41
14:t:5007:VAL:HG11	27:t:5217:LMT:H42	2.03	0.41
16:v:5107:THR:HG22	16:v:5108:TYR:N	2.35	0.41
1:A:130:GLN:HG2	4:D:256:ILE:CD1	2.51	0.41
1:A:321:ILE:HG22	1:A:322:ASN:N	2.35	0.41
2:B:188:ASP:C	2:B:190:PHE:N	2.77	0.41
2:B:272:ARG:HH12	4:D:164:GLN:HG3	1.86	0.41
2:B:413:ASP:O	2:B:414:PRO:C	2.64	0.41
3:C:42:LEU:HG	20:C:501:CLA:O1D	2.20	0.41
3:C:56:HIS:O	3:C:59:LEU:N	2.53	0.41
3:C:229:ASN:HD22	3:C:231:GLU:CG	2.34	0.41
20:C:502:CLA:HBA2	20:C:502:CLA:O2D	2.20	0.41
4:D:130:PHE:CE2	4:D:140:PRO:HB2	2.56	0.41
4:D:178:ILE:C	4:D:180:ARG:N	2.77	0.41
9:J:24:ILE:CG2	9:J:25:VAL:N	2.83	0.41
10:K:17:ILE:HD11	18:Z:6:GLN:NE2	2.31	0.41
10:K:43:VAL:HG21	17:X:31:UNK:CG	2.51	0.41
17:X:51:UNK:O	17:X:53:UNK:N	2.54	0.41
1:a:5022:THR:O	1:a:5022:THR:HG22	2.21	0.41
1:a:5054:ALA:HB2	1:a:5072:LEU:HD12	2.03	0.41
1:a:5065:GLU:OE1	1:a:5334:ARG:NH2	2.54	0.41
1:a:5324:ALA:CB	4:d:5329:MET:HE3	2.42	0.41
2:b:5011:VAL:O	2:b:5011:VAL:HG22	2.20	0.41
2:b:5036:SER:OG	24:b:5528:BCR:H362	2.21	0.41
2:b:5045:PHE:CE2	2:b:5047:PRO:HB3	2.56	0.41
2:b:5191:ASN:HD22	2:b:5192:PRO:N	2.19	0.41
2:b:5272:ARG:HH12	4:d:5164:GLN:HG3	1.86	0.41
2:b:5372:ASP:OD2	2:b:5372:ASP:C	2.62	0.41
3:c:5087:ILE:C	3:c:5090:PRO:HD2	2.46	0.41
3:c:5099:VAL:HG23	3:c:5196:VAL:CG2	2.51	0.41
3:c:5155:ASN:C	3:c:5157:MET:N	2.78	0.41
3:c:5163:PHE:CE1	3:c:5252:ILE:HD13	2.56	0.41
3:c:5218:PHE:CE2	28:i:5201:MGE:H3A2	2.55	0.41
3:c:5260:ALA:O	3:c:5264:PHE:CD2	2.68	0.41
3:c:5387:TRP:O	3:c:5391:ARG:HB2	2.21	0.41
24:c:5504:BCR:H20C	24:c:5504:BCR:H361	1.94	0.41
4:d:5090:LEU:CD1	4:d:5096:GLU:HG3	2.51	0.41
4:d:5249:ALA:O	4:d:5250:ASN:C	2.64	0.41
4:d:5302:GLU:OE1	4:d:5302:GLU:HA	2.19	0.41
4:d:5350:ASN:O	4:d:5352:LEU:N	2.54	0.41
5:e:5010:PHE:CA	5:e:5013:ILE:HG22	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:f:5051:HEM:HAD2	32:f:5051:HEM:HHA	1.62	0.41
10:k:5020:PRO:HA	17:x:5006:UNK:HG3	2.03	0.41
13:o:5096:LEU:HD21	13:o:5099:ARG:O	2.20	0.41
17:x:5051:UNK:O	17:x:5053:UNK:N	2.54	0.41
17:x:5058:UNK:O	17:x:5062:UNK:HG2	2.21	0.41
1:A:13:LEU:H	1:A:13:LEU:CD2	2.33	0.41
1:A:78:ILE:HD12	1:A:78:ILE:N	2.36	0.41
2:B:410:THR:HG22	2:B:411:PHE:N	2.36	0.41
3:C:146:PHE:CD2	3:C:147:PHE:CE1	3.09	0.41
3:C:438:LEU:HD21	30:C:507:DGD:HAH2	2.02	0.41
4:D:125:PHE:CD1	4:D:125:PHE:C	2.99	0.41
5:E:16:SER:OG	5:E:19:TYR:HB2	2.21	0.41
8:I:34:ARG:O	8:I:35:LYS:C	2.64	0.41
10:K:18:PHE:CD1	10:K:18:PHE:N	2.89	0.41
13:O:178:ARG:HG3	13:O:178:ARG:NH1	2.28	0.41
13:O:266:TYR:CG	13:O:267:ALA:N	2.88	0.41
16:V:58:LEU:HD13	16:V:137:ASP:HB3	2.02	0.41
1:a:5248:ILE:H	1:a:5248:ILE:HG13	1.60	0.41
1:a:5296:ASN:OD1	3:c:5401:LEU:CD2	2.69	0.41
21:a:5562:PHO:H93	4:d:5118:GLY:HA3	2.03	0.41
2:b:5025:MET:HE1	2:b:5108:PHE:CE1	2.56	0.41
2:b:5233:ASN:HD22	2:b:5234:ILE:N	2.19	0.41
20:b:5518:CLA:HBA1	20:b:5518:CLA:CHA	2.50	0.41
3:c:5116:VAL:HG13	3:c:5117:VAL:N	2.36	0.41
3:c:5269:GLU:OE2	20:c:5498:CLA:HED1	2.21	0.41
5:e:5016:SER:OG	5:e:5019:TYR:HB2	2.21	0.41
7:h:5014:LEU:HD23	7:h:5014:LEU:HA	1.86	0.41
10:k:5011:LEU:O	10:k:5012:PRO:C	2.63	0.41
13:o:5056:TYR:C	13:o:5161:SER:HA	2.42	0.41
15:u:5075:LEU:O	15:u:5078:LEU:HB2	2.21	0.41
18:z:5004:LEU:CD2	18:z:5057:LEU:HD21	2.50	0.41
18:z:5036:SER:HA	18:z:5039:LEU:CD1	2.36	0.41
1:A:23:SER:HB3	1:A:26:ASN:ND2	2.36	0.40
1:A:293:MET:HG2	1:A:298:ASN:HA	2.03	0.40
2:B:68:ARG:HH12	20:B:514:CLA:CED	2.33	0.40
2:B:220:ARG:HD2	7:H:20:LYS:C	2.44	0.40
20:B:518:CLA:HBA1	20:B:518:CLA:CHA	2.51	0.40
3:C:173:LEU:HD23	3:C:173:LEU:HA	1.86	0.40
20:C:494:CLA:CHA	20:C:494:CLA:HBA1	2.52	0.40
4:D:38:PHE:HZ	4:D:128:ARG:NH2	2.18	0.40
12:M:17:VAL:HG12	12:M:18:PRO:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:64:ALA:C	16:V:66:CYS:N	2.77	0.40
1:a:5023:SER:HB3	1:a:5026:ASN:ND2	2.36	0.40
1:a:5069:GLY:O	1:a:5080:GLY:HA2	2.20	0.40
1:a:5142:TRP:CD1	1:a:5142:TRP:H	2.39	0.40
2:b:5008:VAL:HG23	2:b:5009:HIS:N	2.35	0.40
2:b:5030:VAL:HG11	20:b:5522:CLA:H112	2.02	0.40
3:c:5165:LEU:HD13	3:c:5251:HIS:HD2	1.86	0.40
4:d:5122:LEU:HB3	4:d:5150:ILE:HD13	2.04	0.40
7:h:5041:PHE:CD1	7:h:5041:PHE:C	2.99	0.40
7:h:5046:LEU:HD11	30:h:5208:DGD:HA22	2.02	0.40
8:i:5032:PRO:O	8:i:5033:LYS:HG3	2.21	0.40
18:z:5047:TRP:O	18:z:5050:LEU:HB2	2.20	0.40
1:A:318:ALA:O	1:A:321:ILE:HB	2.21	0.40
21:A:561:PHO:HND	4:D:209:LEU:HD12	1.87	0.40
2:B:12:LEU:CD1	20:B:522:CLA:HBB1	2.51	0.40
2:B:121:GLU:C	2:B:123:PHE:N	2.78	0.40
3:C:40:ALA:C	3:C:42:LEU:H	2.29	0.40
3:C:40:ALA:C	3:C:42:LEU:N	2.77	0.40
3:C:205:ASP:HA	3:C:206:PRO:HD2	1.89	0.40
4:D:201:VAL:HG13	20:D:354:CLA:HMB1	2.03	0.40
7:H:59:ASN:OD1	7:H:59:ASN:C	2.64	0.40
8:I:31:ASN:HB2	8:I:32:PRO:HD2	2.03	0.40
13:O:142:ILE:N	13:O:142:ILE:CD1	2.84	0.40
1:a:5206:PHE:CE2	20:d:5354:CLA:HAA1	2.56	0.40
2:b:5031:ALA:CB	20:b:5515:CLA:HBC3	2.49	0.40
3:c:5033:PHE:CE2	3:c:5040:ALA:HB1	2.57	0.40
3:c:5433:LEU:HD13	20:c:5492:CLA:CHC	2.51	0.40
4:d:5053:THR:HG22	4:d:5067:TYR:CE1	2.56	0.40
4:d:5263:ASN:O	4:d:5264:LYS:C	2.64	0.40
10:k:5013:GLU:O	10:k:5014:ALA:C	2.65	0.40
11:l:5016:SER:O	11:l:5017:LEU:C	2.60	0.40
14:t:5002:GLU:O	14:t:5005:THR:N	2.54	0.40
16:v:5081:ARG:HG2	16:v:5157:GLY:HA2	2.03	0.40
18:z:5058:ASN:OD1	18:z:5058:ASN:C	2.64	0.40
1:A:191:ASN:HD21	1:A:194:MET:HG3	1.86	0.40
1:A:212:CYS:CB	4:D:211:CYS:HB2	2.31	0.40
2:B:223:GLN:NE2	2:B:227:LYS:HG3	2.36	0.40
8:I:30:ARG:H	8:I:30:ARG:HG2	1.60	0.40
10:K:27:VAL:O	10:K:28:ILE:C	2.65	0.40
13:O:184:ASP:O	13:O:186:LYS:N	2.55	0.40
15:U:69:ARG:HE	15:U:69:ARG:HB2	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:5025:MET:HE3	24:b:5527:BCR:C23	2.50	0.40
2:b:5027:THR:HG22	2:b:5107:LEU:HD13	2.04	0.40
4:d:5193:LEU:O	4:d:5193:LEU:HG	2.21	0.40
4:d:5251:ARG:O	4:d:5252:PHE:C	2.65	0.40
4:d:5270:PHE:HZ	22:d:5356:PQ9:H243	1.86	0.40
5:e:5072:ALA:O	5:e:5075:GLN:HB3	2.21	0.40
13:o:5179:THR:HG23	13:o:5180:ALA:H	1.85	0.40
1:A:33:PHE:CD1	1:A:128:GLY:HA3	2.56	0.40
1:A:206:PHE:HD2	1:A:206:PHE:HA	1.75	0.40
2:B:164:PRO:HD3	20:B:516:CLA:O1D	2.22	0.40
2:B:230:ARG:NH1	2:B:474:LEU:HD22	2.36	0.40
2:B:390:TYR:O	2:B:391:SER:C	2.61	0.40
2:B:471:ALA:HB2	4:D:130:PHE:HZ	1.79	0.40
3:C:374:GLY:O	3:C:375:LEU:C	2.64	0.40
4:D:103:ARG:O	4:D:106:GLN:N	2.55	0.40
28:D:360:MGE:H3G1	11:L:15:THR:CG2	2.52	0.40
5:E:10:PHE:HA	5:E:13:ILE:CG2	2.51	0.40
7:H:5:THR:O	7:H:6:TRP:C	2.65	0.40
13:O:204:LYS:HA	13:O:204:LYS:HD3	1.93	0.40
14:T:22:PHE:O	14:T:23:PHE:CG	2.75	0.40
16:V:132:ASN:O	16:V:133:LEU:C	2.64	0.40
17:X:62:UNK:O	17:X:66:UNK:N	2.55	0.40
17:X:85:UNK:OD1	17:X:85:UNK:N	2.54	0.40
1:a:5228:THR:HG23	1:a:5231:GLU:OE1	2.22	0.40
2:b:5030:VAL:HG13	20:b:5523:CLA:HMC2	2.03	0.40
2:b:5122:LEU:HD22	7:h:5011:LEU:HB2	2.03	0.40
2:b:5193:TYR:O	2:b:5195:PRO:HD3	2.22	0.40
2:b:5271:THR:CB	2:b:5274:GLN:HG3	2.52	0.40
2:b:5424:ALA:O	2:b:5425:ILE:C	2.64	0.40
20:b:5524:CLA:HAA2	11:l:5007:ARG:HH22	1.87	0.40
3:c:5042:LEU:HG	20:c:5501:CLA:O1D	2.21	0.40
3:c:5187:ASP:O	3:c:5190:ALA:HB2	2.21	0.40
3:c:5428:THR:CG2	3:c:5429:SER:N	2.79	0.40
4:d:5106:GLN:NE2	5:e:5048:GLY:HA3	2.36	0.40
6:f:5040:MET:HA	6:f:5043:ILE:CD1	2.51	0.40
10:k:5043:VAL:HG21	17:x:5031:UNK:CG	2.52	0.40
13:o:5176:SER:O	13:o:5177:TYR:C	2.64	0.40
17:x:5061:UNK:O	17:x:5062:UNK:C	2.67	0.40
1:A:27:ARG:HH11	1:A:27:ARG:C	2.29	0.40
1:A:131:TRP:CD2	1:A:132:GLU:N	2.89	0.40
1:A:255:PHE:CE2	22:A:564:PQ9:H151	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:PHE:CD1	1:A:260:PHE:C	2.99	0.40
1:A:272:HIS:CB	4:D:218:VAL:HG11	2.52	0.40
2:B:46:ASP:OD1	2:B:46:ASP:C	2.65	0.40
2:B:87:ASP:C	2:B:88:PRO:O	2.62	0.40
2:B:222:PRO:HG3	7:H:26:GLY:CA	2.50	0.40
3:C:188:THR:HG23	3:C:300:GLU:CD	2.46	0.40
3:C:252:ILE:O	3:C:252:ILE:HG22	2.21	0.40
8:I:24:LEU:O	8:I:26:GLY:N	2.48	0.40
15:U:54:LYS:HB3	15:U:111:HIS:O	2.21	0.40
1:a:5043:ALA:HA	24:a:5566:BCR:C16	2.51	0.40
2:b:5060:MET:HA	2:b:5060:MET:HE2	2.04	0.40
2:b:5068:ARG:CZ	20:b:5514:CLA:HED1	2.51	0.40
2:b:5143:LEU:O	2:b:5143:LEU:HD12	2.22	0.40
2:b:5433:ASP:OD2	2:b:5436:THR:OG1	2.33	0.40
3:c:5394:GLU:O	3:c:5398:HIS:HD2	2.04	0.40
4:d:5251:ARG:HE	4:d:5255:GLN:HE22	1.69	0.40
5:e:5049:THR:HA	5:e:5050:PRO:HD3	1.82	0.40
11:l:5014:ARG:NH1	11:l:5014:ARG:CG	2.85	0.40
14:t:5011:ALA:HB3	24:t:104:BCR:H363	2.02	0.40
15:u:5078:LEU:HD13	15:u:5097:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	333/344 (97%)	279 (84%)	39 (12%)	15 (4%)	2	12
1	a	333/344 (97%)	278 (84%)	38 (11%)	17 (5%)	1	10
2	B	486/510 (95%)	407 (84%)	60 (12%)	19 (4%)	2	14
2	b	486/510 (95%)	413 (85%)	56 (12%)	17 (4%)	3	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	445/473 (94%)	340 (76%)	80 (18%)	25 (6%)	1	8
3	c	445/473 (94%)	342 (77%)	77 (17%)	26 (6%)	1	8
4	D	338/352 (96%)	272 (80%)	50 (15%)	16 (5%)	2	11
4	d	338/352 (96%)	272 (80%)	52 (15%)	14 (4%)	2	13
5	E	80/84 (95%)	60 (75%)	14 (18%)	6 (8%)	1	4
5	e	80/84 (95%)	59 (74%)	15 (19%)	6 (8%)	1	4
6	F	33/45 (73%)	28 (85%)	3 (9%)	2 (6%)	1	7
6	f	33/45 (73%)	28 (85%)	3 (9%)	2 (6%)	1	7
7	H	62/66 (94%)	45 (73%)	11 (18%)	6 (10%)	0	2
7	h	62/66 (94%)	44 (71%)	12 (19%)	6 (10%)	0	2
8	I	33/38 (87%)	22 (67%)	10 (30%)	1 (3%)	3	19
8	i	33/38 (87%)	22 (67%)	10 (30%)	1 (3%)	3	19
9	J	32/40 (80%)	27 (84%)	2 (6%)	3 (9%)	0	2
9	j	32/40 (80%)	25 (78%)	4 (12%)	3 (9%)	0	2
10	K	35/37 (95%)	28 (80%)	5 (14%)	2 (6%)	1	8
10	k	35/37 (95%)	28 (80%)	4 (11%)	3 (9%)	0	3
11	L	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	1	8
11	l	35/37 (95%)	28 (80%)	4 (11%)	3 (9%)	0	3
12	M	34/36 (94%)	26 (76%)	6 (18%)	2 (6%)	1	7
12	m	34/36 (94%)	28 (82%)	4 (12%)	2 (6%)	1	7
13	O	240/247 (97%)	185 (77%)	38 (16%)	17 (7%)	1	4
13	o	240/247 (97%)	184 (77%)	39 (16%)	17 (7%)	1	4
14	T	28/32 (88%)	24 (86%)	4 (14%)	0	100	100
14	t	28/32 (88%)	26 (93%)	2 (7%)	0	100	100
15	U	96/104 (92%)	71 (74%)	18 (19%)	7 (7%)	1	4
15	u	96/104 (92%)	68 (71%)	21 (22%)	7 (7%)	1	4
16	V	135/137 (98%)	110 (82%)	18 (13%)	7 (5%)	1	9
16	v	135/137 (98%)	110 (82%)	18 (13%)	7 (5%)	1	9
18	Z	60/62 (97%)	47 (78%)	9 (15%)	4 (7%)	1	5
18	z	60/62 (97%)	46 (77%)	10 (17%)	4 (7%)	1	5
All	All	5010/5288 (95%)	4001 (80%)	740 (15%)	269 (5%)	1	9

All (269) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	11	ALA
1	A	63	ILE
1	A	141	PRO
1	A	142	TRP
1	A	315	ASN
2	B	230	ARG
2	B	260	SER
2	B	362	PHE
2	B	488	PRO
3	C	154	LYS
3	C	324	LEU
3	C	416	SER
4	D	239	GLN
4	D	240	ALA
4	D	257	PHE
4	D	262	SER
5	E	7	GLU
5	E	58	GLN
5	E	60	GLN
7	H	18	TYR
7	H	64	ALA
13	O	46	PRO
13	O	52	ALA
13	O	86	ARG
13	O	115	SER
13	O	140	GLU
13	O	175	PRO
15	U	72	TYR
15	U	73	PRO
15	U	83	ALA
16	V	133	LEU
16	V	160	LYS
1	a	5011	ALA
1	a	5012	ASN
1	a	5063	ILE
1	a	5141	PRO
1	a	5142	TRP
1	a	5315	ASN
2	b	5230	ARG
2	b	5260	SER
2	b	5362	PHE
2	b	5488	PRO

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Mol	Chain	Res	Type
3	c	5154	LYS
3	c	5226	SER
3	c	5324	LEU
3	c	5416	SER
4	d	5239	GLN
4	d	5240	ALA
4	d	5262	SER
5	e	5007	GLU
5	e	5058	GLN
5	e	5060	GLN
7	h	5018	TYR
7	h	5064	ALA
13	o	5046	PRO
13	o	5052	ALA
13	o	5086	ARG
13	o	5115	SER
13	o	5140	GLU
13	o	5175	PRO
15	u	5072	TYR
15	u	5073	PRO
15	u	5083	ALA
16	v	5133	LEU
16	v	5160	LYS
1	A	12	ASN
1	A	130	GLN
1	A	261	GLN
1	A	266	ASN
2	B	11	VAL
2	B	85	GLY
2	B	176	GLY
2	B	231	MET
3	C	57	ALA
3	C	136	GLY
3	C	139	THR
3	C	141	GLU
3	C	144	SER
3	C	207	ARG
3	C	209	ILE
3	C	226	SER
3	C	242	LEU
4	D	92	LEU
4	D	263	ASN

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Mol	Chain	Res	Type
5	E	48	GLY
7	H	26	GLY
8	I	25	SER
9	J	35	GLY
10	K	13	GLU
10	K	16	ALA
12	M	34	LYS
13	O	50	ASP
13	O	84	ASN
13	O	88	GLU
13	O	138	GLY
13	O	161	SER
15	U	70	GLY
18	Z	31	GLN
18	Z	32	ASP
1	a	5055	ALA
1	a	5130	GLN
1	a	5242	GLU
1	a	5266	ASN
2	b	5011	VAL
2	b	5085	GLY
3	c	5136	GLY
3	c	5141	GLU
3	c	5144	SER
3	c	5207	ARG
3	c	5209	ILE
4	d	5092	LEU
4	d	5192	THR
4	d	5252	PHE
4	d	5257	PHE
4	d	5263	ASN
5	e	5048	GLY
6	f	5041	GLN
7	h	5026	GLY
8	i	5025	SER
9	j	5035	GLY
10	k	5013	GLU
10	k	5016	ALA
12	m	5034	LYS
13	o	5050	ASP
13	o	5084	ASN
13	o	5088	GLU

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Mol	Chain	Res	Type
13	o	5138	GLY
13	o	5161	SER
13	o	5233	ARG
15	u	5070	GLY
18	z	5031	GLN
18	z	5032	ASP
1	A	55	ALA
1	A	59	ASP
1	A	242	GLU
1	A	306	VAL
2	B	228	ALA
3	C	39	ASN
3	C	194	GLY
3	C	221	GLU
4	D	25	ASP
4	D	192	THR
4	D	252	PHE
4	D	351	ALA
5	E	52	PRO
6	F	41	GLN
7	H	3	ARG
7	H	59	ASN
9	J	14	ALA
11	L	5	PRO
11	L	7	ARG
13	O	233	ARG
15	U	88	VAL
16	V	75	ASN
1	a	5059	ASP
1	a	5261	GLN
1	a	5306	VAL
2	b	5176	GLY
2	b	5228	ALA
3	c	5039	ASN
3	c	5057	ALA
3	c	5139	THR
3	c	5221	GLU
3	c	5242	LEU
4	d	5025	ASP
4	d	5041	ALA
4	d	5351	ALA
5	e	5052	PRO

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Mol	Chain	Res	Type
7	h	5059	ASN
9	j	5011	TRP
11	l	5005	PRO
11	l	5007	ARG
13	o	5167	ASP
13	o	5232	GLY
15	u	5088	VAL
16	v	5064	ALA
1	A	232	SER
1	A	260	PHE
2	B	91	TRP
2	B	485	GLU
3	C	30	SER
3	C	38	GLY
3	C	77	PRO
3	C	205	ASP
3	C	298	PRO
4	D	41	ALA
4	D	177	ALA
4	D	261	PHE
9	J	11	TRP
13	O	167	ASP
13	O	232	GLY
15	U	60	THR
16	V	65	SER
1	a	5260	PHE
2	b	5231	MET
2	b	5485	GLU
3	c	5194	GLY
3	c	5205	ASP
4	d	5062	GLY
7	h	5003	ARG
9	j	5014	ALA
16	v	5129	LYS
2	B	16	PRO
2	B	89	GLY
2	B	386	ALA
3	C	227	VAL
3	C	382	ASN
4	D	29	PHE
4	D	62	GLY
12	M	17	VAL

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Mol	Chain	Res	Type
13	O	139	GLY
16	V	129	LYS
1	a	5172	MET
1	a	5217	SER
2	b	5089	GLY
2	b	5122	LEU
2	b	5361	ALA
3	c	5030	SER
3	c	5077	PRO
3	c	5153	ASP
3	c	5227	VAL
3	c	5298	PRO
3	c	5382	ASN
4	d	5177	ALA
16	v	5075	ASN
2	B	361	ALA
3	C	243	ILE
13	O	185	PRO
3	c	5038	GLY
3	c	5134	ILE
4	d	5264	LYS
12	m	5017	VAL
13	o	5139	GLY
16	v	5065	SER
2	B	8	VAL
6	F	23	VAL
18	Z	24	PRO
2	b	5016	PRO
3	c	5243	ILE
13	o	5185	PRO
15	u	5066	ILE
2	B	414	PRO
3	C	105	VAL
3	C	134	ILE
13	O	117	GLY
2	b	5008	VAL
2	b	5414	PRO
18	z	5003	ILE
4	D	80	THR
18	Z	3	ILE
1	a	5060	ILE
3	c	5105	VAL

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Mol	Chain	Res	Type
6	f	5023	VAL
7	h	5058	VAL
18	z	5024	PRO
2	B	86	ILE
2	B	232	GLY
7	H	58	VAL
15	U	66	ILE
16	V	71	ILE
16	V	161	VAL
2	b	5086	ILE
10	k	5012	PRO
13	o	5117	GLY
5	E	25	ILE
5	e	5025	ILE
11	l	5003	PRO
15	u	5062	ILE
16	v	5071	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	269/280 (96%)	252 (94%)	17 (6%)	16	48
1	a	269/280 (96%)	253 (94%)	16 (6%)	18	50
2	B	378/407 (93%)	356 (94%)	22 (6%)	18	51
2	b	378/407 (93%)	353 (93%)	25 (7%)	15	46
3	C	341/374 (91%)	322 (94%)	19 (6%)	19	52
3	c	341/374 (91%)	320 (94%)	21 (6%)	16	49
4	D	273/283 (96%)	258 (94%)	15 (6%)	19	53
4	d	273/283 (96%)	255 (93%)	18 (7%)	15	46
5	E	68/73 (93%)	65 (96%)	3 (4%)	25	60
5	e	68/73 (93%)	65 (96%)	3 (4%)	25	60
6	F	27/39 (69%)	26 (96%)	1 (4%)	30	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	f	27/39 (69%)	26 (96%)	1 (4%)	30	64
7	H	50/55 (91%)	44 (88%)	6 (12%)	5	22
7	h	50/55 (91%)	44 (88%)	6 (12%)	5	22
8	I	32/35 (91%)	27 (84%)	5 (16%)	2	13
8	i	32/35 (91%)	27 (84%)	5 (16%)	2	13
9	J	22/28 (79%)	22 (100%)	0	100	100
9	j	22/28 (79%)	22 (100%)	0	100	100
10	K	29/30 (97%)	27 (93%)	2 (7%)	14	45
10	k	29/30 (97%)	27 (93%)	2 (7%)	14	45
11	L	34/35 (97%)	30 (88%)	4 (12%)	5	22
11	l	34/35 (97%)	30 (88%)	4 (12%)	5	22
12	M	32/33 (97%)	31 (97%)	1 (3%)	35	68
12	m	32/33 (97%)	31 (97%)	1 (3%)	35	68
13	O	181/208 (87%)	169 (93%)	12 (7%)	15	46
13	o	181/208 (87%)	170 (94%)	11 (6%)	17	49
14	T	26/29 (90%)	24 (92%)	2 (8%)	12	40
14	t	26/29 (90%)	24 (92%)	2 (8%)	12	40
15	U	83/89 (93%)	81 (98%)	2 (2%)	43	73
15	u	83/89 (93%)	81 (98%)	2 (2%)	43	73
16	V	117/117 (100%)	110 (94%)	7 (6%)	17	50
16	v	117/117 (100%)	109 (93%)	8 (7%)	14	45
18	Z	43/52 (83%)	42 (98%)	1 (2%)	44	74
18	z	43/52 (83%)	42 (98%)	1 (2%)	44	74
All	All	4010/4334 (92%)	3765 (94%)	245 (6%)	17	49

All (245) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	24	THR
1	A	30	VAL
1	A	35	VAL
1	A	76	ASN
1	A	143	ILE

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Mol	Chain	Res	Type
1	A	157	VAL
1	A	177	SER
1	A	206	PHE
1	A	210	LEU
1	A	232	SER
1	A	241	GLN
1	A	271	LEU
1	A	286	THR
1	A	292	THR
1	A	297	LEU
1	A	308	ASP
2	B	36	SER
2	B	81	THR
2	B	121	GLU
2	B	124	ARG
2	B	133	LEU
2	B	222	PRO
2	B	231	MET
2	B	233	ASN
2	B	245	VAL
2	B	246	PHE
2	B	262	THR
2	B	271	THR
2	B	309	LEU
2	B	350	GLU
2	B	354	LEU
2	B	362	PHE
2	B	390	TYR
2	B	399	VAL
2	B	414	PRO
2	B	425	ILE
2	B	467	ILE
2	B	478	VAL
3	C	27	ASP
3	C	29	GLU
3	C	86	LEU
3	C	165	LEU
3	C	191	PRO
3	C	204	LEU
3	C	214	LEU
3	C	240	ILE
3	C	244	CYS

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Mol	Chain	Res	Type
3	C	254	THR
3	C	265	ILE
3	C	289	PHE
3	C	298	PRO
3	C	355	THR
3	C	377	LEU
3	C	419	PHE
3	C	428	THR
3	C	472	LEU
3	C	473	ASP
4	D	14	TRP
4	D	63	LEU
4	D	90	LEU
4	D	96	GLU
4	D	98	GLN
4	D	130	PHE
4	D	164	GLN
4	D	178	ILE
4	D	191	TRP
4	D	218	VAL
4	D	241	GLU
4	D	250	ASN
4	D	294	ARG
4	D	323	GLU
4	D	346	LEU
5	E	4	THR
5	E	17	VAL
5	E	52	PRO
6	F	17	THR
7	H	7	LEU
7	H	21	VAL
7	H	27	THR
7	H	41	PHE
7	H	53	LEU
7	H	59	ASN
8	I	2	GLU
8	I	27	ASP
8	I	30	ARG
8	I	32	PRO
8	I	34	ARG
10	K	11	LEU
10	K	12	PRO

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Mol	Chain	Res	Type
11	L	3	PRO
11	L	10	VAL
11	L	14	ARG
11	L	16	SER
12	M	33	GLN
13	O	46	PRO
13	O	50	ASP
13	O	97	VAL
13	O	106	GLN
13	O	114	ASN
13	O	120	THR
13	O	160	THR
13	O	168	PHE
13	O	179	THR
13	O	206	GLU
13	O	216	PHE
13	O	223	ILE
14	T	4	ILE
14	T	29	ILE
15	U	61	ASN
15	U	119	THR
16	V	35	THR
16	V	37	PRO
16	V	47	LEU
16	V	81	ARG
16	V	107	THR
16	V	111	GLU
16	V	128	PRO
18	Z	58	ASN
1	a	5013	LEU
1	a	5030	VAL
1	a	5035	VAL
1	a	5076	ASN
1	a	5143	ILE
1	a	5157	VAL
1	a	5177	SER
1	a	5206	PHE
1	a	5210	LEU
1	a	5232	SER
1	a	5241	GLN
1	a	5271	LEU
1	a	5286	THR

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Mol	Chain	Res	Type
1	a	5292	THR
1	a	5297	LEU
1	a	5308	ASP
2	b	5013	ILE
2	b	5016	PRO
2	b	5036	SER
2	b	5081	THR
2	b	5121	GLU
2	b	5124	ARG
2	b	5130	GLU
2	b	5133	LEU
2	b	5222	PRO
2	b	5231	MET
2	b	5233	ASN
2	b	5245	VAL
2	b	5246	PHE
2	b	5262	THR
2	b	5271	THR
2	b	5309	LEU
2	b	5350	GLU
2	b	5354	LEU
2	b	5362	PHE
2	b	5390	TYR
2	b	5399	VAL
2	b	5425	ILE
2	b	5433	ASP
2	b	5467	ILE
2	b	5478	VAL
3	c	5027	ASP
3	c	5029	GLU
3	c	5086	LEU
3	c	5097	TRP
3	c	5165	LEU
3	c	5191	PRO
3	c	5204	LEU
3	c	5214	LEU
3	c	5240	ILE
3	c	5244	CYS
3	c	5254	THR
3	c	5262	ARG
3	c	5265	ILE
3	c	5289	PHE

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Mol	Chain	Res	Type
3	c	5298	PRO
3	c	5355	THR
3	c	5377	LEU
3	c	5419	PHE
3	c	5428	THR
3	c	5472	LEU
3	c	5473	ASP
4	d	5014	TRP
4	d	5037	LEU
4	d	5053	THR
4	d	5063	LEU
4	d	5090	LEU
4	d	5096	GLU
4	d	5098	GLN
4	d	5130	PHE
4	d	5164	GLN
4	d	5178	ILE
4	d	5191	TRP
4	d	5218	VAL
4	d	5219	GLU
4	d	5241	GLU
4	d	5250	ASN
4	d	5294	ARG
4	d	5323	GLU
4	d	5346	LEU
5	e	5004	THR
5	e	5017	VAL
5	e	5052	PRO
6	f	5017	THR
7	h	5007	LEU
7	h	5021	VAL
7	h	5027	THR
7	h	5041	PHE
7	h	5053	LEU
7	h	5059	ASN
8	i	5002	GLU
8	i	5027	ASP
8	i	5030	ARG
8	i	5032	PRO
8	i	5034	ARG
10	k	5011	LEU
10	k	5012	PRO

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Mol	Chain	Res	Type
11	l	5003	PRO
11	l	5010	VAL
11	l	5014	ARG
11	l	5016	SER
12	m	5033	GLN
13	o	5046	PRO
13	o	5050	ASP
13	o	5097	VAL
13	o	5106	GLN
13	o	5114	ASN
13	o	5120	THR
13	o	5168	PHE
13	o	5179	THR
13	o	5206	GLU
13	o	5216	PHE
13	o	5223	ILE
14	t	5004	ILE
14	t	5029	ILE
15	u	5061	ASN
15	u	5117	VAL
16	v	5035	THR
16	v	5037	PRO
16	v	5047	LEU
16	v	5063	CYS
16	v	5081	ARG
16	v	5107	THR
16	v	5111	GLU
16	v	5128	PRO
18	z	5058	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (117) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	19	ASN
1	A	75	ASN
1	A	76	ASN
1	A	118	HIS
1	A	165	GLN
1	A	181	ASN
1	A	187	GLN
1	A	191	ASN

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Mol	Chain	Res	Type
1	A	234	ASN
1	A	241	GLN
1	A	272	HIS
1	A	296	ASN
1	A	298	ASN
1	A	304	HIS
1	A	322	ASN
1	A	337	HIS
1	A	338	ASN
2	B	26	HIS
2	B	53	ASN
2	B	157	HIS
2	B	179	GLN
2	B	191	ASN
2	B	223	GLN
2	B	233	ASN
2	B	274	GLN
2	B	331	ASN
2	B	394	GLN
3	C	155	ASN
3	C	201	ASN
3	C	229	ASN
3	C	293	ASN
3	C	322	GLN
3	C	332	GLN
3	C	388	GLN
3	C	398	HIS
3	C	415	ASN
4	D	61	HIS
4	D	98	GLN
4	D	186	GLN
4	D	224	GLN
4	D	255	GLN
4	D	301	GLN
4	D	350	ASN
5	E	58	GLN
6	F	41	GLN
7	H	15	ASN
7	H	50	ASN
7	H	59	ASN
12	M	5	GLN
12	M	32	GLN

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Mol	Chain	Res	Type
13	O	72	GLN
13	O	106	GLN
13	O	108	GLN
13	O	114	ASN
13	O	130	GLN
13	O	262	GLN
15	U	108	ASN
16	V	104	ASN
16	V	144	HIS
18	Z	6	GLN
1	a	5012	ASN
1	a	5019	ASN
1	a	5075	ASN
1	a	5076	ASN
1	a	5118	HIS
1	a	5165	GLN
1	a	5181	ASN
1	a	5187	GLN
1	a	5191	ASN
1	a	5241	GLN
1	a	5272	HIS
1	a	5296	ASN
1	a	5298	ASN
1	a	5304	HIS
1	a	5322	ASN
1	a	5337	HIS
2	b	5026	HIS
2	b	5053	ASN
2	b	5157	HIS
2	b	5179	GLN
2	b	5191	ASN
2	b	5223	GLN
2	b	5233	ASN
2	b	5274	GLN
2	b	5331	ASN
2	b	5394	GLN
3	c	5155	ASN
3	c	5201	ASN
3	c	5229	ASN
3	c	5293	ASN
3	c	5332	GLN
3	c	5382	ASN

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Mol	Chain	Res	Type
3	c	5388	GLN
3	c	5398	HIS
4	d	5061	HIS
4	d	5098	GLN
4	d	5186	GLN
4	d	5224	GLN
4	d	5250	ASN
4	d	5255	GLN
4	d	5301	GLN
4	d	5350	ASN
5	e	5058	GLN
6	f	5041	GLN
7	h	5015	ASN
12	m	5005	GLN
13	o	5072	GLN
13	o	5106	GLN
13	o	5108	GLN
13	o	5114	ASN
13	o	5130	GLN
13	o	5262	GLN
15	u	5108	ASN
16	v	5104	ASN
16	v	5144	HIS
18	z	5006	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 180 ligands modelled in this entry, 4 are monoatomic and 34 are unknown - leaving 142 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	a	5563	1	59,63,73	1.48	9 (15%)	70,101,113	1.69	10 (14%)
20	CLA	B	524	2	60,64,73	1.50	7 (11%)	71,102,113	1.93	9 (12%)
28	MGE	D	358	-	47,47,48	1.22	5 (10%)	55,55,56	0.96	3 (5%)
27	LMT	T	217	-	36,36,36	1.40	5 (13%)	47,47,47	1.03	4 (8%)
30	DGD	C	507	-	54,54,67	1.35	8 (14%)	68,68,81	1.47	7 (10%)
20	CLA	C	497	-	69,73,73	1.31	10 (14%)	82,113,113	1.87	11 (13%)
20	CLA	B	521	2	69,73,73	1.31	9 (13%)	82,113,113	1.81	11 (13%)
24	BCR	H	107	-	41,41,41	2.11	6 (14%)	56,56,56	2.29	24 (42%)
20	CLA	b	5522	2	69,73,73	1.40	10 (14%)	82,113,113	1.68	7 (8%)
20	CLA	C	491	3	69,73,73	1.24	5 (7%)	82,113,113	1.62	9 (10%)
20	CLA	b	5511	-	45,49,73	1.66	10 (22%)	54,84,113	2.02	8 (14%)
20	CLA	d	5354	4	69,73,73	1.26	11 (15%)	82,113,113	1.68	11 (13%)
30	DGD	h	5208	-	55,55,67	1.39	9 (16%)	69,69,81	1.56	9 (13%)
20	CLA	C	503	3	54,58,73	1.72	8 (14%)	64,95,113	1.95	9 (14%)
20	CLA	c	5500	3	69,73,73	1.24	6 (8%)	82,113,113	1.70	12 (14%)
30	DGD	C	508	-	48,48,67	1.43	9 (18%)	62,62,81	1.67	11 (17%)
21	PHO	A	561	-	58,69,69	1.61	9 (15%)	55,99,99	2.06	16 (29%)
26	SQD	d	5358	-	52,54,54	2.58	29 (55%)	62,65,65	2.53	18 (29%)
27	LMT	t	5217	-	36,36,36	1.45	5 (13%)	47,47,47	1.00	3 (6%)
20	CLA	c	5493	3	69,73,73	1.35	7 (10%)	82,113,113	1.81	13 (15%)
28	MGE	I	201	-	48,48,48	1.10	5 (10%)	56,56,56	1.07	4 (7%)
26	SQD	t	213	-	45,47,54	2.81	23 (51%)	55,58,65	2.49	14 (25%)
28	MGE	D	359	-	41,41,48	1.25	5 (12%)	49,49,56	1.02	4 (8%)
20	CLA	B	526	2	69,73,73	1.49	12 (17%)	82,113,113	1.76	10 (12%)
20	CLA	b	5519	2	69,73,73	1.37	7 (10%)	82,113,113	1.73	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	a	5560	-	69,73,73	1.37	8 (11%)	82,113,113	1.75	10 (12%)
24	BCR	b	5528	-	41,41,41	1.74	6 (14%)	56,56,56	2.06	17 (30%)
24	BCR	c	5506	-	41,41,41	1.95	7 (17%)	56,56,56	2.16	20 (35%)
31	BCT	D	353	19	3,3,3	2.28	1 (33%)	2,3,3	0.32	0
30	DGD	H	208	-	55,55,67	1.48	10 (18%)	69,69,81	1.55	8 (11%)
20	CLA	B	517	-	69,73,73	1.53	7 (10%)	82,113,113	1.87	12 (14%)
20	CLA	c	5491	3	69,73,73	1.42	6 (8%)	82,113,113	1.84	11 (13%)
20	CLA	B	519	2	69,73,73	1.46	6 (8%)	82,113,113	1.73	11 (13%)
20	CLA	B	512	2	69,73,73	1.31	8 (11%)	82,113,113	1.63	11 (13%)
28	MGE	b	5530	-	48,48,48	1.19	8 (16%)	56,56,56	1.11	6 (10%)
32	HEM	v	5552	16	50,50,50	2.09	22 (44%)	67,82,82	1.98	14 (20%)
20	CLA	b	5512	2	69,73,73	1.23	6 (8%)	82,113,113	1.60	9 (10%)
20	CLA	b	5516	2	69,73,73	1.49	5 (7%)	82,113,113	1.85	8 (9%)
20	CLA	b	5518	2	69,73,73	1.41	6 (8%)	82,113,113	1.79	11 (13%)
28	MGE	B	530	-	48,48,48	1.21	6 (12%)	56,56,56	1.16	6 (10%)
20	CLA	C	500	3	69,73,73	1.29	8 (11%)	82,113,113	1.70	12 (14%)
20	CLA	b	5517	-	69,73,73	1.44	8 (11%)	82,113,113	1.77	9 (10%)
20	CLA	A	558	1	69,73,73	1.29	8 (11%)	82,113,113	1.64	10 (12%)
28	MGE	D	360	-	48,48,48	0.93	4 (8%)	56,56,56	1.12	4 (7%)
20	CLA	B	520	-	69,73,73	1.25	8 (11%)	82,113,113	1.66	11 (13%)
20	CLA	b	5520	-	69,73,73	1.25	9 (13%)	82,113,113	1.66	10 (12%)
21	PHO	A	562	-	58,69,69	1.73	8 (13%)	55,99,99	2.11	12 (21%)
20	CLA	C	501	3	69,73,73	1.47	9 (13%)	82,113,113	1.86	11 (13%)
20	CLA	B	522	2	69,73,73	1.29	10 (14%)	82,113,113	1.67	9 (10%)
20	CLA	c	5503	3	54,58,73	1.73	9 (16%)	64,95,113	1.96	6 (9%)
20	CLA	c	5495	3	69,73,73	1.59	8 (11%)	82,113,113	1.85	12 (14%)
20	CLA	B	513	2	69,73,73	1.44	11 (15%)	82,113,113	1.69	11 (13%)
26	SQD	A	5212	-	24,26,54	2.85	13 (54%)	34,37,65	2.65	11 (32%)
31	BCT	d	5353	19	3,3,3	2.70	1 (33%)	2,3,3	0.35	0
20	CLA	b	5514	2	69,73,73	1.45	10 (14%)	82,113,113	1.84	10 (12%)
27	LMT	M	5216	-	36,36,36	1.45	8 (22%)	47,47,47	0.92	2 (4%)
27	LMT	a	5568	-	36,36,36	1.46	6 (16%)	47,47,47	1.09	1 (2%)
27	LMT	m	216	-	36,36,36	1.45	7 (19%)	47,47,47	0.98	3 (6%)
30	DGD	c	5508	-	48,48,67	1.48	8 (16%)	62,62,81	1.71	10 (16%)
20	CLA	B	518	2	69,73,73	1.41	6 (8%)	82,113,113	1.82	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	C	506	-	41,41,41	1.74	8 (19%)	56,56,56	2.23	21 (37%)
20	CLA	D	354	4	69,73,73	1.24	7 (10%)	82,113,113	1.61	10 (12%)
24	BCR	C	504	-	41,41,41	1.87	6 (14%)	56,56,56	2.21	22 (39%)
22	PQ9	A	564	-	30,30,45	0.85	0	38,39,57	1.50	8 (21%)
24	BCR	A	566	-	41,41,41	1.63	8 (19%)	56,56,56	2.14	22 (39%)
20	CLA	c	5498	3	69,73,73	1.50	9 (13%)	82,113,113	1.80	12 (14%)
22	PQ9	D	356	-	30,30,45	0.91	1 (3%)	38,39,57	1.68	9 (23%)
20	CLA	b	5525	-	69,73,73	1.22	7 (10%)	82,113,113	1.78	9 (10%)
24	BCR	d	5357	-	41,41,41	2.02	8 (19%)	56,56,56	2.33	21 (37%)
24	BCR	x	5130	-	41,41,41	1.95	9 (21%)	56,56,56	2.52	24 (42%)
20	CLA	B	511	-	45,49,73	1.61	10 (22%)	54,84,113	1.94	8 (14%)
20	CLA	C	499	3	51,55,73	1.53	8 (15%)	60,91,113	1.95	8 (13%)
20	CLA	b	5513	2	69,73,73	1.30	8 (11%)	82,113,113	1.64	13 (15%)
20	CLA	c	5501	3	69,73,73	1.45	9 (13%)	82,113,113	1.84	9 (10%)
20	CLA	B	516	2	69,73,73	1.39	4 (5%)	82,113,113	1.81	7 (8%)
20	CLA	b	5515	2	69,73,73	1.28	10 (14%)	82,113,113	1.74	15 (18%)
20	CLA	b	5526	2	69,73,73	1.49	11 (15%)	82,113,113	1.77	11 (13%)
20	CLA	C	493	3	69,73,73	1.30	7 (10%)	82,113,113	1.82	13 (15%)
21	PHO	a	5561	-	58,69,69	1.60	11 (18%)	55,99,99	1.98	15 (27%)
20	CLA	A	563	1	59,63,73	1.46	10 (16%)	70,101,113	1.75	11 (15%)
20	CLA	C	498	3	69,73,73	1.31	7 (10%)	82,113,113	1.76	10 (12%)
26	SQD	a	212	-	24,26,54	3.09	13 (54%)	34,37,65	2.73	13 (38%)
27	LMT	A	569	-	36,36,36	1.54	6 (16%)	47,47,47	1.07	1 (2%)
24	BCR	h	5107	-	41,41,41	2.04	7 (17%)	56,56,56	2.30	25 (44%)
24	BCR	t	104	-	41,41,41	1.67	10 (24%)	56,56,56	2.28	23 (41%)
20	CLA	C	496	3	69,73,73	1.43	10 (14%)	82,113,113	1.78	13 (15%)
24	BCR	c	5504	-	41,41,41	2.18	5 (12%)	56,56,56	2.18	23 (41%)
24	BCR	b	5529	-	41,41,41	1.66	6 (14%)	56,56,56	2.15	21 (37%)
20	CLA	b	5523	2	69,73,73	1.29	9 (13%)	82,113,113	1.78	9 (10%)
20	CLA	a	5559	-	69,73,73	1.13	4 (5%)	82,113,113	1.66	9 (10%)
26	SQD	L	5213	-	45,47,54	2.81	24 (53%)	55,58,65	2.42	12 (21%)
20	CLA	b	5524	2	60,64,73	1.43	7 (11%)	71,102,113	1.82	8 (11%)
20	CLA	A	560	-	69,73,73	1.34	9 (13%)	82,113,113	1.72	10 (12%)
28	MGE	d	5361	-	48,48,48	1.04	4 (8%)	56,56,56	1.06	2 (3%)
20	CLA	B	523	2	69,73,73	1.36	8 (11%)	82,113,113	1.76	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	MGE	d	5359	-	47,47,48	1.14	5 (10%)	55,55,56	0.97	3 (5%)
24	BCR	a	5566	-	41,41,41	1.68	7 (17%)	56,56,56	2.14	23 (41%)
20	CLA	B	515	2	69,73,73	1.29	9 (13%)	82,113,113	1.77	14 (17%)
20	CLA	C	494	-	50,54,73	1.45	7 (14%)	59,90,113	2.05	7 (11%)
24	BCR	b	5527	-	41,41,41	1.57	8 (19%)	56,56,56	1.99	15 (26%)
26	SQD	A	568	-	52,54,54	2.59	31 (59%)	62,65,65	2.55	18 (29%)
20	CLA	C	502	3	55,59,73	1.66	13 (23%)	64,96,113	2.00	11 (17%)
24	BCR	D	357	-	41,41,41	1.96	8 (19%)	56,56,56	2.27	20 (35%)
28	MGE	i	5201	-	48,48,48	1.24	7 (14%)	56,56,56	1.08	4 (7%)
20	CLA	C	492	3	64,68,73	1.29	7 (10%)	76,107,113	1.82	11 (14%)
24	BCR	B	528	-	41,41,41	1.93	6 (14%)	56,56,56	2.02	17 (30%)
20	CLA	D	355	4	54,58,73	1.65	11 (20%)	64,95,113	1.94	11 (17%)
22	PQ9	a	5564	-	30,30,45	0.86	1 (3%)	38,39,57	1.46	6 (15%)
25	LHG	A	567	-	38,38,48	1.98	5 (13%)	41,44,54	1.51	4 (9%)
30	DGD	c	5507	-	54,54,67	1.47	9 (16%)	68,68,81	1.46	6 (8%)
21	PHO	a	5562	-	58,69,69	1.75	7 (12%)	55,99,99	2.06	13 (23%)
20	CLA	b	5521	2	69,73,73	1.17	5 (7%)	82,113,113	1.76	12 (14%)
20	CLA	C	495	3	69,73,73	1.50	11 (15%)	82,113,113	1.82	11 (13%)
32	HEM	F	51	6,5	50,50,50	2.08	16 (32%)	67,82,82	1.98	16 (23%)
32	HEM	f	5051	6,5	50,50,50	2.16	17 (34%)	67,82,82	2.05	13 (19%)
20	CLA	c	5502	-	55,59,73	1.71	12 (21%)	64,96,113	2.03	11 (17%)
24	BCR	X	130	-	41,41,41	1.93	8 (19%)	56,56,56	2.54	23 (41%)
24	BCR	T	5104	-	41,41,41	1.55	9 (21%)	56,56,56	2.31	25 (44%)
24	BCR	B	529	-	41,41,41	1.79	6 (14%)	56,56,56	2.22	21 (37%)
28	MGE	d	5360	-	41,41,48	1.19	6 (14%)	49,49,56	1.05	4 (8%)
20	CLA	B	514	2	69,73,73	1.43	8 (11%)	82,113,113	1.81	10 (12%)
20	CLA	c	5492	3	64,68,73	1.29	8 (12%)	76,107,113	1.84	9 (11%)
25	LHG	a	5567	-	38,38,48	2.02	5 (13%)	41,44,54	1.46	4 (9%)
32	HEM	V	552	16	50,50,50	1.97	17 (34%)	67,82,82	1.98	13 (19%)
20	CLA	c	5496	3	69,73,73	1.36	8 (11%)	82,113,113	1.73	11 (13%)
20	CLA	c	5499	3	51,55,73	1.45	7 (13%)	60,91,113	1.90	7 (11%)
22	PQ9	d	5356	-	30,30,45	0.82	0	38,39,57	1.66	6 (15%)
28	MGE	l	5210	-	48,48,48	0.90	4 (8%)	56,56,56	1.12	5 (8%)
28	MGE	L	210	-	48,48,48	0.99	3 (6%)	56,56,56	1.15	5 (8%)
24	BCR	C	505	-	41,41,41	1.98	9 (21%)	56,56,56	2.13	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	B	525	-	69,73,73	1.25	9 (13%)	82,113,113	1.75	9 (10%)
20	CLA	c	5497	-	69,73,73	1.31	10 (14%)	82,113,113	1.76	11 (13%)
20	CLA	a	5558	1	69,73,73	1.31	11 (15%)	82,113,113	1.58	11 (13%)
20	CLA	c	5494	-	50,54,73	1.39	6 (12%)	59,90,113	1.89	8 (13%)
30	DGD	c	5509	-	58,58,67	1.35	7 (12%)	72,72,81	1.39	6 (8%)
30	DGD	C	509	-	58,58,67	1.12	7 (12%)	72,72,81	1.40	5 (6%)
24	BCR	B	527	-	41,41,41	1.74	8 (19%)	56,56,56	2.08	16 (28%)
20	CLA	d	5355	4	54,58,73	1.65	11 (20%)	64,95,113	1.93	9 (14%)
24	BCR	c	5505	-	41,41,41	2.01	8 (19%)	56,56,56	2.14	19 (33%)
20	CLA	A	559	-	69,73,73	1.14	5 (7%)	82,113,113	1.63	8 (9%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	a	5563	1	-	7/27/103/115	-
20	CLA	B	524	2	-	9/29/105/115	-
28	MGE	D	358	-	-	14/42/62/63	0/1/1/1
27	LMT	T	217	-	-	1/21/61/61	0/2/2/2
30	DGD	C	507	-	3/3/13/13	20/42/82/95	0/2/2/2
20	CLA	C	497	-	-	9/39/115/115	-
20	CLA	B	521	2	-	9/39/115/115	-
24	BCR	H	107	-	-	4/29/63/63	0/2/2/2
20	CLA	b	5522	2	-	12/39/115/115	-
20	CLA	C	491	3	-	9/39/115/115	-
20	CLA	b	5511	-	-	4/10/86/115	-
30	DGD	h	5208	-	3/3/13/13	23/43/83/95	0/2/2/2
20	CLA	d	5354	4	-	8/39/115/115	-
20	CLA	C	503	3	-	7/21/97/115	-
20	CLA	c	5500	3	-	13/39/115/115	-
30	DGD	C	508	-	3/3/13/13	14/36/76/95	0/2/2/2
21	PHO	A	561	-	-	13/37/103/103	0/5/6/6
26	SQD	d	5358	-	-	23/49/69/69	0/1/1/1
27	LMT	t	5217	-	-	0/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	c	5493	3	-	12/39/115/115	-
28	MGE	I	201	-	-	24/43/63/63	0/1/1/1
26	SQD	t	213	-	-	20/42/62/69	0/1/1/1
28	MGE	D	359	-	-	18/36/56/63	0/1/1/1
20	CLA	B	526	2	-	12/39/115/115	-
20	CLA	b	5519	2	-	13/39/115/115	-
20	CLA	a	5560	-	-	9/39/115/115	-
24	BCR	b	5528	-	-	1/29/63/63	0/2/2/2
24	BCR	c	5506	-	-	4/29/63/63	0/2/2/2
30	DGD	H	208	-	3/3/13/13	23/43/83/95	0/2/2/2
20	CLA	B	517	-	-	14/39/115/115	-
20	CLA	c	5491	3	-	11/39/115/115	-
20	CLA	B	519	2	-	13/39/115/115	-
20	CLA	B	512	2	-	12/39/115/115	-
28	MGE	b	5530	-	-	21/43/63/63	0/1/1/1
32	HEM	v	5552	16	-	6/14/54/54	-
20	CLA	b	5512	2	-	12/39/115/115	-
20	CLA	b	5516	2	-	15/39/115/115	-
20	CLA	b	5518	2	-	16/39/115/115	-
28	MGE	B	530	-	-	21/43/63/63	0/1/1/1
20	CLA	C	500	3	-	13/39/115/115	-
20	CLA	b	5517	-	-	14/39/115/115	-
20	CLA	A	558	1	-	10/39/115/115	-
28	MGE	D	360	-	-	23/43/63/63	0/1/1/1
20	CLA	B	520	-	-	15/39/115/115	-
20	CLA	b	5520	-	-	13/39/115/115	-
21	PHO	A	562	-	-	9/37/103/103	0/5/6/6
20	CLA	C	501	3	-	15/39/115/115	-
20	CLA	B	522	2	-	12/39/115/115	-
20	CLA	c	5503	3	-	7/21/97/115	-
20	CLA	c	5495	3	-	18/39/115/115	-
20	CLA	B	513	2	-	14/39/115/115	-
26	SQD	A	5212	-	-	5/19/39/69	0/1/1/1
20	CLA	b	5514	2	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMT	M	5216	-	-	2/21/61/61	0/2/2/2
27	LMT	a	5568	-	-	3/21/61/61	0/2/2/2
30	DGD	c	5508	-	3/3/13/13	16/36/76/95	0/2/2/2
27	LMT	m	216	-	-	2/21/61/61	0/2/2/2
20	CLA	B	518	2	-	16/39/115/115	-
24	BCR	C	506	-	-	4/29/63/63	0/2/2/2
20	CLA	D	354	4	-	10/39/115/115	-
24	BCR	C	504	-	-	5/29/63/63	0/2/2/2
22	PQ9	A	564	-	-	8/23/43/61	0/1/1/1
24	BCR	A	566	-	-	4/29/63/63	0/2/2/2
20	CLA	c	5498	3	-	18/39/115/115	-
22	PQ9	D	356	-	-	11/23/43/61	0/1/1/1
20	CLA	b	5525	-	-	14/39/115/115	-
24	BCR	d	5357	-	-	3/29/63/63	0/2/2/2
24	BCR	x	5130	-	-	4/29/63/63	0/2/2/2
20	CLA	B	511	-	-	4/10/86/115	-
20	CLA	C	499	3	-	8/18/94/115	-
20	CLA	b	5513	2	-	12/39/115/115	-
20	CLA	c	5501	3	-	13/39/115/115	-
20	CLA	B	516	2	-	15/39/115/115	-
20	CLA	b	5515	2	-	19/39/115/115	-
20	CLA	b	5526	2	-	12/39/115/115	-
20	CLA	C	493	3	-	12/39/115/115	-
21	PHO	a	5561	-	-	13/37/103/103	0/5/6/6
20	CLA	A	563	1	-	7/27/103/115	-
20	CLA	C	498	3	-	18/39/115/115	-
26	SQD	a	212	-	-	6/19/39/69	0/1/1/1
27	LMT	A	569	-	-	1/21/61/61	0/2/2/2
24	BCR	h	5107	-	-	4/29/63/63	0/2/2/2
24	BCR	t	104	-	-	4/29/63/63	0/2/2/2
20	CLA	C	496	3	-	13/39/115/115	-
24	BCR	c	5504	-	-	5/29/63/63	0/2/2/2
24	BCR	b	5529	-	-	3/29/63/63	0/2/2/2
20	CLA	b	5523	2	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	a	5559	-	-	14/39/115/115	-
26	SQD	L	5213	-	-	21/42/62/69	0/1/1/1
20	CLA	b	5524	2	-	9/29/105/115	-
20	CLA	A	560	-	-	9/39/115/115	-
28	MGE	d	5361	-	-	23/43/63/63	0/1/1/1
20	CLA	B	523	2	-	15/39/115/115	-
28	MGE	d	5359	-	-	13/42/62/63	0/1/1/1
24	BCR	a	5566	-	-	4/29/63/63	0/2/2/2
20	CLA	B	515	2	-	19/39/115/115	-
20	CLA	C	494	-	-	9/17/93/115	-
24	BCR	b	5527	-	-	1/29/63/63	0/2/2/2
26	SQD	A	568	-	-	23/49/69/69	0/1/1/1
20	CLA	C	502	3	-	9/23/99/115	-
24	BCR	D	357	-	-	3/29/63/63	0/2/2/2
28	MGE	i	5201	-	-	22/43/63/63	0/1/1/1
20	CLA	C	492	3	-	11/33/109/115	-
24	BCR	B	528	-	-	1/29/63/63	0/2/2/2
20	CLA	D	355	4	-	11/21/97/115	-
22	PQ9	a	5564	-	-	8/23/43/61	0/1/1/1
25	LHG	A	567	-	-	16/43/43/53	-
30	DGD	c	5507	-	3/3/13/13	20/42/82/95	0/2/2/2
20	CLA	b	5521	2	-	9/39/115/115	-
21	PHO	a	5562	-	-	9/37/103/103	0/5/6/6
20	CLA	C	495	3	-	18/39/115/115	-
32	HEM	F	51	6,5	-	2/14/54/54	-
32	HEM	f	5051	6,5	-	2/14/54/54	-
20	CLA	c	5502	-	-	8/23/99/115	-
24	BCR	X	130	-	-	5/29/63/63	0/2/2/2
24	BCR	T	5104	-	-	4/29/63/63	0/2/2/2
24	BCR	B	529	-	-	3/29/63/63	0/2/2/2
28	MGE	d	5360	-	-	18/36/56/63	0/1/1/1
20	CLA	B	514	2	-	13/39/115/115	-
20	CLA	c	5492	3	-	11/33/109/115	-
25	LHG	a	5567	-	-	14/43/43/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	HEM	V	552	16	-	6/14/54/54	-
20	CLA	c	5496	3	-	13/39/115/115	-
20	CLA	c	5499	3	-	8/18/94/115	-
22	PQ9	d	5356	-	-	11/23/43/61	0/1/1/1
28	MGE	l	5210	-	-	23/43/63/63	0/1/1/1
28	MGE	L	210	-	-	23/43/63/63	0/1/1/1
24	BCR	C	505	-	-	3/29/63/63	0/2/2/2
20	CLA	B	525	-	-	14/39/115/115	-
20	CLA	c	5497	-	-	10/39/115/115	-
20	CLA	a	5558	1	-	11/39/115/115	-
20	CLA	c	5494	-	-	9/17/93/115	-
30	DGD	c	5509	-	3/3/13/13	19/46/86/95	0/2/2/2
30	DGD	C	509	-	3/3/13/13	20/46/86/95	0/2/2/2
24	BCR	B	527	-	-	1/29/63/63	0/2/2/2
20	CLA	d	5355	4	-	11/21/97/115	-
24	BCR	c	5505	-	-	3/29/63/63	0/2/2/2
20	CLA	A	559	-	-	14/39/115/115	-

All (1162) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	5495	CLA	MG-NA	8.38	2.26	2.06
25	A	567	LHG	P-O5	8.23	1.79	1.50
24	c	5504	BCR	C1-C6	8.20	1.64	1.53
20	B	517	CLA	MG-NA	8.14	2.25	2.06
25	a	5567	LHG	P-O5	8.13	1.79	1.50
26	A	568	SQD	C4-C3	8.02	1.73	1.52
26	t	213	SQD	C4-C3	7.98	1.73	1.52
26	a	212	SQD	C4-C3	7.96	1.73	1.52
20	c	5503	CLA	MG-NA	7.88	2.25	2.06
20	C	503	CLA	MG-NA	7.88	2.25	2.06
26	d	5358	SQD	C4-C3	7.69	1.72	1.52
26	L	5213	SQD	C4-C3	7.63	1.72	1.52
21	a	5562	PHO	C3B-C4B	7.57	1.49	1.41
20	b	5516	CLA	MG-NA	7.52	2.24	2.06
20	C	495	CLA	MG-NA	7.46	2.24	2.06
21	A	562	PHO	C3B-C4B	7.44	1.49	1.41
20	C	501	CLA	MG-NA	7.40	2.23	2.06
20	c	5498	CLA	MG-NA	7.30	2.23	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	D	355	CLA	MG-NA	7.17	2.23	2.06
20	B	516	CLA	MG-NA	7.16	2.23	2.06
24	c	5504	BCR	C30-C25	7.16	1.62	1.53
24	h	5107	BCR	C30-C25	7.14	1.62	1.53
20	c	5491	CLA	MG-NA	7.12	2.23	2.06
26	A	5212	SQD	C4-C3	7.11	1.70	1.52
24	H	107	BCR	C30-C25	7.07	1.62	1.53
20	B	524	CLA	MG-NA	7.02	2.23	2.06
20	b	5514	CLA	MG-NA	6.92	2.22	2.06
20	b	5518	CLA	MG-NA	6.73	2.22	2.06
24	B	528	BCR	C30-C25	6.71	1.62	1.53
20	c	5501	CLA	MG-NA	6.65	2.22	2.06
20	B	519	CLA	MG-NA	6.65	2.22	2.06
20	B	518	CLA	MG-NA	6.64	2.22	2.06
24	d	5357	BCR	C1-C6	6.61	1.62	1.53
20	c	5502	CLA	MG-NA	6.54	2.21	2.06
20	B	514	CLA	MG-NA	6.50	2.21	2.06
20	C	499	CLA	MG-NA	6.47	2.21	2.06
26	L	5213	SQD	O7-S	6.45	1.63	1.45
20	b	5517	CLA	MG-NA	6.44	2.21	2.06
24	C	505	BCR	C30-C25	6.43	1.62	1.53
24	c	5505	BCR	C30-C25	6.37	1.61	1.53
24	C	504	BCR	C1-C6	6.29	1.61	1.53
20	d	5355	CLA	MG-NA	6.29	2.21	2.06
20	C	502	CLA	MG-NA	6.14	2.20	2.06
26	t	213	SQD	O7-S	6.11	1.62	1.45
24	b	5528	BCR	C30-C25	6.06	1.61	1.53
26	d	5358	SQD	O7-S	6.03	1.62	1.45
24	B	528	BCR	C1-C6	5.99	1.61	1.53
21	a	5561	PHO	C1B-C2B	5.96	1.46	1.39
24	A	566	BCR	C1-C6	5.94	1.61	1.53
21	a	5562	PHO	C1B-C2B	5.89	1.46	1.39
21	A	561	PHO	C1B-C2B	5.85	1.46	1.39
24	H	107	BCR	C1-C6	5.80	1.61	1.53
20	C	496	CLA	MG-NA	5.79	2.20	2.06
30	H	208	DGD	O3G-C1D	5.76	1.49	1.40
21	A	562	PHO	C1B-C2B	5.73	1.45	1.39
26	a	212	SQD	O47-C7	5.72	1.47	1.35
24	B	527	BCR	C30-C25	5.70	1.61	1.53
20	C	498	CLA	MG-NA	5.59	2.19	2.06
24	D	357	BCR	C30-C25	5.57	1.60	1.53
20	b	5519	CLA	MG-NA	5.54	2.19	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	h	5107	BCR	C1-C6	5.52	1.60	1.53
26	A	5212	SQD	O7-S	5.51	1.60	1.45
20	b	5522	CLA	MG-NA	5.44	2.19	2.06
20	b	5524	CLA	MG-NA	5.43	2.19	2.06
20	b	5511	CLA	MG-NA	5.41	2.19	2.06
20	a	5560	CLA	MG-NA	5.36	2.19	2.06
24	c	5506	BCR	C30-C25	5.36	1.60	1.53
24	a	5566	BCR	C1-C6	5.36	1.60	1.53
24	C	504	BCR	C30-C25	5.33	1.60	1.53
24	B	529	BCR	C30-C25	5.28	1.60	1.53
20	c	5499	CLA	MG-NA	5.26	2.18	2.06
32	v	5552	HEM	CBC-CAC	5.24	1.55	1.30
24	x	5130	BCR	C1-C6	5.24	1.60	1.53
24	x	5130	BCR	C30-C25	5.24	1.60	1.53
24	X	130	BCR	C1-C6	5.23	1.60	1.53
21	A	561	PHO	C3B-C4B	5.22	1.46	1.41
20	B	526	CLA	MG-NA	5.15	2.18	2.06
20	C	493	CLA	MG-NA	5.15	2.18	2.06
24	b	5527	BCR	C30-C25	5.15	1.60	1.53
32	V	552	HEM	CBC-CAC	5.13	1.55	1.30
24	c	5505	BCR	C1-C6	5.10	1.60	1.53
24	X	130	BCR	C30-C25	5.10	1.60	1.53
24	H	107	BCR	C29-C30	5.09	1.65	1.54
24	b	5529	BCR	C30-C25	5.09	1.60	1.53
30	h	5208	DGD	O3G-C1D	5.08	1.48	1.40
26	a	212	SQD	O7-S	5.07	1.59	1.45
32	f	5051	HEM	CBC-CAC	5.05	1.54	1.30
32	F	51	HEM	FE-NB	5.00	2.10	1.94
32	F	51	HEM	CBC-CAC	4.99	1.54	1.30
20	B	523	CLA	MG-NA	4.94	2.18	2.06
26	t	213	SQD	C1-C2	4.94	1.67	1.52
20	c	5493	CLA	MG-NA	4.94	2.18	2.06
24	X	130	BCR	C5-C6	4.94	1.42	1.34
24	c	5506	BCR	C1-C6	4.92	1.60	1.53
32	f	5051	HEM	FE-NB	4.89	2.10	1.94
26	A	5212	SQD	O47-C7	4.82	1.45	1.35
24	x	5130	BCR	C5-C6	4.80	1.42	1.34
26	A	568	SQD	O7-S	4.79	1.58	1.45
25	a	5567	LHG	P-O3	4.79	1.78	1.59
20	a	5563	CLA	MG-NA	4.77	2.17	2.06
27	A	569	LMT	O1'-C1'	4.71	1.48	1.40
20	c	5492	CLA	MG-NA	4.68	2.17	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	D	357	BCR	C26-C25	4.68	1.42	1.34
31	d	5353	BCT	O1-C	4.65	1.41	1.25
24	a	5566	BCR	C30-C25	4.64	1.59	1.53
24	B	527	BCR	C26-C25	4.61	1.42	1.34
20	C	492	CLA	MG-NA	4.59	2.17	2.06
32	v	5552	HEM	FE-NC	4.58	2.10	1.95
20	A	560	CLA	MG-NA	4.57	2.17	2.06
24	C	506	BCR	C30-C25	4.55	1.59	1.53
26	L	5213	SQD	O48-C23	4.52	1.46	1.33
24	c	5505	BCR	C26-C25	4.50	1.42	1.34
24	B	529	BCR	C1-C6	4.49	1.59	1.53
21	a	5561	PHO	C3B-C4B	4.49	1.46	1.41
24	C	505	BCR	C26-C25	4.46	1.42	1.34
26	t	213	SQD	O5-C5	4.45	1.55	1.44
20	c	5497	CLA	MG-NC	4.43	2.16	2.06
24	B	529	BCR	C26-C25	4.42	1.41	1.34
30	c	5509	DGD	O3G-C1D	4.41	1.47	1.40
20	C	497	CLA	MG-NA	4.40	2.16	2.06
32	V	552	HEM	FE-NC	4.39	2.09	1.95
24	d	5357	BCR	C5-C6	4.39	1.41	1.34
24	b	5528	BCR	C1-C6	4.38	1.59	1.53
20	B	515	CLA	MG-NA	4.33	2.16	2.06
24	H	107	BCR	C26-C25	4.33	1.41	1.34
24	h	5107	BCR	C26-C25	4.32	1.41	1.34
32	f	5051	HEM	C4D-ND	-4.31	1.32	1.40
24	C	505	BCR	C1-C6	4.30	1.59	1.53
20	B	513	CLA	MG-NA	4.29	2.16	2.06
24	c	5506	BCR	C5-C6	4.28	1.41	1.34
24	t	104	BCR	C30-C25	4.27	1.59	1.53
28	B	530	MGE	O3G-C1D	4.26	1.47	1.40
21	a	5562	PHO	C3A-C2A	-4.25	1.51	1.54
24	C	506	BCR	C2-C1	4.25	1.63	1.54
20	b	5526	CLA	MG-NA	4.24	2.16	2.06
27	a	5568	LMT	O1'-C1'	4.24	1.47	1.40
26	a	212	SQD	C1-C2	4.24	1.64	1.52
21	A	562	PHO	C3A-C2A	-4.23	1.51	1.54
27	M	5216	LMT	O1'-C1'	4.23	1.47	1.40
24	D	357	BCR	C5-C6	4.23	1.41	1.34
30	c	5508	DGD	O6D-C1D	4.21	1.52	1.41
24	d	5357	BCR	C26-C25	4.20	1.41	1.34
20	B	521	CLA	MG-NA	4.20	2.16	2.06
20	A	563	CLA	MG-NA	4.20	2.16	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	c	5506	BCR	C26-C25	4.19	1.41	1.34
20	B	522	CLA	MG-NA	4.17	2.16	2.06
32	V	552	HEM	FE-NB	4.15	2.07	1.94
20	A	558	CLA	MG-NA	4.13	2.16	2.06
24	c	5504	BCR	C29-C30	4.13	1.63	1.54
32	f	5051	HEM	FE-NA	4.12	2.08	1.95
20	B	525	CLA	MG-NA	4.11	2.16	2.06
20	C	500	CLA	MG-NA	4.11	2.16	2.06
20	A	560	CLA	CAA-C2A	4.10	1.61	1.54
30	c	5507	DGD	O5D-C1E	4.09	1.47	1.40
24	h	5107	BCR	C29-C30	4.07	1.63	1.54
20	B	511	CLA	MG-NA	4.07	2.15	2.06
24	x	5130	BCR	C29-C30	4.06	1.63	1.54
32	F	51	HEM	FE-NA	4.06	2.08	1.95
24	h	5107	BCR	C2-C1	4.04	1.63	1.54
28	D	359	MGE	O3G-C1D	4.03	1.46	1.40
20	c	5494	CLA	CAA-C2A	4.02	1.61	1.54
24	c	5506	BCR	C2-C1	4.02	1.63	1.54
26	L	5213	SQD	O5-C5	4.02	1.54	1.44
24	C	505	BCR	C2-C1	4.01	1.63	1.54
26	A	568	SQD	O48-C23	4.01	1.45	1.33
26	d	5358	SQD	O47-C7	4.01	1.45	1.34
26	d	5358	SQD	O48-C23	4.00	1.45	1.33
26	d	5358	SQD	C1-C2	4.00	1.64	1.52
20	B	511	CLA	MG-NC	3.99	2.15	2.06
24	t	104	BCR	C1-C6	3.99	1.58	1.53
32	f	5051	HEM	CHB-C1B	-3.99	1.30	1.38
20	b	5513	CLA	MG-NA	3.97	2.15	2.06
24	D	357	BCR	C29-C30	3.96	1.63	1.54
24	d	5357	BCR	C30-C25	3.96	1.58	1.53
21	A	561	PHO	C3A-C2A	-3.96	1.51	1.54
30	c	5508	DGD	O3G-C1D	3.95	1.46	1.40
26	A	568	SQD	C1-C2	3.94	1.64	1.52
24	T	5104	BCR	C2-C1	3.94	1.63	1.54
31	D	353	BCT	O1-C	3.93	1.39	1.25
26	t	213	SQD	O48-C23	3.92	1.44	1.33
26	L	5213	SQD	C1-C2	3.91	1.64	1.52
20	C	497	CLA	MG-NC	3.91	2.15	2.06
25	A	567	LHG	P-O3	3.91	1.74	1.59
26	A	568	SQD	O47-C7	3.91	1.45	1.34
20	D	355	CLA	CAA-C2A	3.90	1.61	1.54
20	B	512	CLA	MG-NA	3.88	2.15	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	T	217	LMT	O1'-C1'	3.88	1.46	1.40
30	c	5507	DGD	C4D-C3D	3.88	1.62	1.52
32	v	5552	HEM	FE-NB	3.88	2.06	1.94
20	C	494	CLA	MG-NA	3.85	2.15	2.06
20	C	494	CLA	CAA-C2A	3.85	1.61	1.54
21	a	5561	PHO	C3A-C2A	-3.84	1.51	1.54
24	D	357	BCR	C1-C6	3.84	1.58	1.53
24	T	5104	BCR	C5-C6	3.83	1.40	1.34
20	C	491	CLA	MG-NA	3.82	2.15	2.06
24	d	5357	BCR	C29-C30	3.81	1.62	1.54
24	X	130	BCR	C29-C30	3.81	1.62	1.54
20	B	519	CLA	CAA-C2A	3.79	1.61	1.54
20	c	5501	CLA	CAA-C2A	3.78	1.61	1.54
24	B	528	BCR	C29-C30	3.78	1.62	1.54
25	a	5567	LHG	P-O6	3.78	1.74	1.59
20	c	5496	CLA	MG-NA	3.77	2.15	2.06
32	F	51	HEM	CMA-C3A	3.77	1.58	1.50
20	A	563	CLA	CHB-C1B	-3.76	1.31	1.39
32	F	51	HEM	FE-NC	3.76	2.07	1.95
26	a	212	SQD	O5-C5	3.75	1.53	1.44
24	C	506	BCR	C1-C6	3.75	1.58	1.53
24	H	107	BCR	C2-C1	3.75	1.62	1.54
25	A	567	LHG	O8-C23	3.75	1.44	1.33
24	c	5504	BCR	C2-C1	3.75	1.62	1.54
24	C	504	BCR	C29-C30	3.72	1.62	1.54
20	D	354	CLA	CHB-C1B	-3.72	1.31	1.39
32	f	5051	HEM	CBD-CAD	3.71	1.64	1.51
20	C	503	CLA	CAA-C2A	3.70	1.60	1.54
30	C	507	DGD	O5D-C1E	3.69	1.46	1.40
28	d	5361	MGE	O6D-C1D	3.66	1.51	1.41
32	F	51	HEM	C4D-ND	-3.66	1.33	1.40
20	B	516	CLA	CAA-C2A	3.66	1.60	1.54
25	A	567	LHG	P-O6	3.66	1.73	1.59
30	C	507	DGD	C4D-C3D	3.65	1.61	1.52
30	C	509	DGD	O3G-C1D	3.65	1.46	1.40
28	L	210	MGE	O6D-C1D	3.65	1.51	1.41
24	T	5104	BCR	C1-C6	3.64	1.58	1.53
24	C	506	BCR	C5-C6	3.64	1.40	1.34
28	D	358	MGE	O3G-C1D	3.63	1.46	1.40
28	L	210	MGE	O3G-C1D	3.63	1.46	1.40
20	B	513	CLA	CAA-C2A	3.62	1.60	1.54
20	b	5512	CLA	MG-NA	3.61	2.14	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	566	BCR	C5-C6	3.61	1.40	1.34
20	b	5518	CLA	C1D-ND	-3.61	1.33	1.37
24	D	357	BCR	C2-C1	3.61	1.62	1.54
26	t	213	SQD	O47-C7	3.61	1.44	1.34
20	B	518	CLA	CAA-C2A	3.60	1.60	1.54
20	c	5503	CLA	CAA-C2A	3.60	1.60	1.54
24	C	504	BCR	C26-C25	3.59	1.40	1.34
20	c	5500	CLA	MG-NA	3.59	2.14	2.06
20	b	5526	CLA	C4-C3	3.58	1.59	1.50
20	b	5525	CLA	MG-NA	3.58	2.14	2.06
20	B	523	CLA	C1D-ND	-3.57	1.33	1.37
25	a	5567	LHG	O8-C23	3.57	1.43	1.33
24	b	5529	BCR	C29-C30	3.57	1.62	1.54
24	b	5528	BCR	C29-C30	3.57	1.62	1.54
30	c	5509	DGD	O6D-C1D	3.56	1.51	1.41
20	b	5520	CLA	MG-NC	3.56	2.14	2.06
24	C	505	BCR	C29-C30	3.56	1.62	1.54
24	x	5130	BCR	C2-C1	3.56	1.62	1.54
32	f	5051	HEM	FE-NC	3.56	2.06	1.95
24	t	104	BCR	C5-C6	3.55	1.40	1.34
26	t	213	SQD	C20-C19	-3.55	1.34	1.51
20	b	5526	CLA	CAA-C2A	3.54	1.60	1.54
24	b	5529	BCR	C1-C6	3.54	1.58	1.53
20	B	522	CLA	CAA-C2A	3.53	1.60	1.54
32	v	5552	HEM	C4D-ND	-3.53	1.34	1.40
28	D	358	MGE	O6D-C1D	3.52	1.50	1.41
20	b	5519	CLA	MG-NC	3.52	2.14	2.06
24	C	506	BCR	C26-C25	3.51	1.40	1.34
30	c	5509	DGD	O5D-C1E	3.51	1.46	1.40
26	t	213	SQD	O8-S	3.51	1.60	1.47
26	A	568	SQD	O3-C3	3.51	1.51	1.43
26	L	5213	SQD	O8-S	3.50	1.60	1.47
20	a	5563	CLA	CHB-C1B	-3.50	1.31	1.39
20	b	5522	CLA	CAA-C2A	3.50	1.60	1.54
26	a	212	SQD	O8-S	3.50	1.60	1.47
24	A	566	BCR	C2-C1	3.50	1.62	1.54
20	c	5493	CLA	MG-NC	3.49	2.14	2.06
26	A	5212	SQD	O5-C5	3.49	1.52	1.44
26	d	5358	SQD	O5-C5	3.49	1.52	1.44
24	B	528	BCR	C26-C25	3.49	1.40	1.34
24	c	5505	BCR	C2-C1	3.49	1.62	1.54
24	B	527	BCR	C29-C30	3.48	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	L	5213	SQD	C12-C11	-3.47	1.34	1.51
20	c	5496	CLA	CAA-C2A	3.47	1.60	1.54
24	b	5529	BCR	C2-C1	3.46	1.62	1.54
20	c	5499	CLA	CAA-C2A	3.46	1.60	1.54
20	d	5354	CLA	CHB-C1B	-3.46	1.31	1.39
27	t	5217	LMT	O1'-C1'	3.46	1.46	1.40
25	A	567	LHG	O7-C7	3.46	1.44	1.34
24	b	5527	BCR	C29-C30	3.46	1.62	1.54
30	H	208	DGD	C4E-C5E	3.46	1.60	1.53
25	a	5567	LHG	O7-C7	3.46	1.44	1.34
26	L	5213	SQD	C17-C16	-3.44	1.34	1.51
26	L	5213	SQD	C11-C10	-3.44	1.34	1.51
20	b	5517	CLA	CAA-C2A	3.43	1.60	1.54
24	B	529	BCR	C2-C1	3.43	1.61	1.54
26	A	5212	SQD	O8-S	3.43	1.60	1.47
24	c	5505	BCR	C5-C6	3.42	1.40	1.34
24	d	5357	BCR	C2-C1	3.41	1.61	1.54
20	b	5526	CLA	C5-C3	3.41	1.58	1.51
26	L	5213	SQD	C20-C19	-3.40	1.34	1.51
20	B	513	CLA	C1D-ND	-3.40	1.33	1.37
32	F	51	HEM	CHB-C1B	-3.40	1.31	1.38
28	b	5530	MGE	O6D-C1D	3.39	1.50	1.41
20	a	5559	CLA	MG-NA	3.38	2.14	2.06
26	A	5212	SQD	C1-C2	3.37	1.62	1.52
24	c	5505	BCR	C29-C30	3.37	1.61	1.54
20	b	5520	CLA	MG-NA	3.36	2.14	2.06
24	B	527	BCR	C5-C6	3.36	1.40	1.34
21	a	5562	PHO	C4D-CHA	3.36	1.44	1.39
20	b	5523	CLA	C1D-ND	-3.35	1.33	1.37
26	t	213	SQD	C19-C18	-3.35	1.35	1.51
20	B	512	CLA	CHB-C1B	-3.35	1.31	1.39
28	B	530	MGE	O6D-C1D	3.34	1.50	1.41
26	a	212	SQD	O6-C1	3.32	1.45	1.40
26	A	568	SQD	O6-C44	-3.32	1.38	1.43
20	a	5558	CLA	CHB-C1B	-3.32	1.32	1.39
26	t	213	SQD	C14-C13	-3.31	1.35	1.51
20	a	5558	CLA	MG-NA	3.31	2.14	2.06
20	C	491	CLA	CAA-C2A	3.30	1.60	1.54
26	L	5213	SQD	C19-C18	-3.30	1.35	1.51
26	L	5213	SQD	O47-C7	3.30	1.43	1.34
30	C	508	DGD	O5D-C1E	3.29	1.45	1.40
20	B	526	CLA	C5-C3	3.29	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	D	360	MGE	O3G-C1D	3.29	1.45	1.40
26	A	5212	SQD	O3-C3	3.28	1.51	1.43
20	c	5495	CLA	CAA-C2A	3.28	1.60	1.54
20	c	5502	CLA	MG-NC	3.27	2.14	2.06
24	X	130	BCR	C2-C1	3.26	1.61	1.54
28	b	5530	MGE	O3G-C1D	3.26	1.45	1.40
24	c	5506	BCR	C29-C30	3.26	1.61	1.54
24	t	104	BCR	C2-C1	3.26	1.61	1.54
20	B	519	CLA	MG-NC	3.26	2.14	2.06
26	L	5213	SQD	O3-C3	3.26	1.51	1.43
20	b	5515	CLA	MG-NA	3.26	2.14	2.06
20	b	5516	CLA	CAA-C2A	3.25	1.60	1.54
28	d	5359	MGE	O3G-C1D	3.25	1.45	1.40
24	A	566	BCR	C30-C25	3.25	1.57	1.53
28	i	5201	MGE	O6D-C5D	3.25	1.52	1.44
26	A	568	SQD	C17-C16	-3.24	1.35	1.51
20	A	560	CLA	CHB-C1B	-3.24	1.32	1.39
26	t	213	SQD	C15-C14	-3.24	1.35	1.51
26	L	5213	SQD	C18-C17	-3.24	1.35	1.51
20	b	5515	CLA	CAA-C2A	3.23	1.60	1.54
20	b	5514	CLA	CAA-C2A	3.22	1.60	1.54
26	a	212	SQD	O3-C3	3.22	1.50	1.43
30	c	5507	DGD	O6D-C1D	3.21	1.50	1.41
24	d	5357	BCR	C38-C26	3.21	1.56	1.50
28	d	5361	MGE	O3G-C1D	3.21	1.45	1.40
26	L	5213	SQD	C13-C12	-3.21	1.35	1.51
20	b	5523	CLA	MG-NA	3.21	2.13	2.06
30	C	508	DGD	O6D-C1D	3.20	1.50	1.41
20	b	5512	CLA	MG-NC	3.20	2.13	2.06
20	B	520	CLA	MG-NA	3.20	2.13	2.06
26	t	213	SQD	O3-C3	3.20	1.50	1.43
20	B	512	CLA	MG-NC	3.20	2.13	2.06
20	b	5522	CLA	C1D-ND	-3.19	1.33	1.37
20	d	5354	CLA	CAA-CBA	-3.19	1.43	1.52
20	C	500	CLA	CAA-C2A	3.18	1.59	1.54
26	t	213	SQD	C12-C11	-3.17	1.36	1.51
20	C	498	CLA	CHB-C1B	-3.17	1.32	1.39
26	t	213	SQD	C11-C10	-3.17	1.36	1.51
24	B	528	BCR	C2-C1	3.17	1.61	1.54
20	b	5511	CLA	MG-NC	3.17	2.13	2.06
24	c	5505	BCR	C38-C26	3.17	1.56	1.50
24	B	529	BCR	C29-C30	3.17	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	558	CLA	CHB-C1B	-3.17	1.32	1.39
20	b	5521	CLA	CHB-C1B	-3.17	1.32	1.39
20	D	354	CLA	CAA-CBA	-3.17	1.43	1.52
20	C	496	CLA	MG-NB	3.16	2.12	2.05
20	a	5563	CLA	CAA-C2A	3.16	1.59	1.54
24	a	5566	BCR	C5-C6	3.16	1.39	1.34
20	c	5501	CLA	MG-NC	3.15	2.13	2.06
20	c	5494	CLA	MG-NC	3.15	2.13	2.06
20	B	511	CLA	C4B-NB	3.15	1.42	1.37
26	A	568	SQD	C12-C11	-3.15	1.36	1.51
26	t	213	SQD	C17-C16	-3.14	1.36	1.51
20	B	517	CLA	CAA-C2A	3.13	1.59	1.54
28	D	359	MGE	O6D-C1D	3.13	1.49	1.41
21	a	5561	PHO	C4-C3	3.13	1.58	1.50
20	B	513	CLA	CHB-C1B	-3.12	1.32	1.39
20	B	520	CLA	CAA-C2A	3.12	1.59	1.54
24	a	5566	BCR	C2-C1	3.11	1.61	1.54
20	b	5513	CLA	CAA-C2A	3.11	1.59	1.54
26	A	568	SQD	O5-C5	3.10	1.52	1.44
20	C	502	CLA	MG-NC	3.10	2.13	2.06
24	C	504	BCR	C2-C1	3.10	1.61	1.54
26	L	5213	SQD	C15-C14	-3.10	1.36	1.51
24	b	5527	BCR	C2-C1	3.09	1.61	1.54
20	b	5515	CLA	CHB-C1B	-3.09	1.32	1.39
28	l	5210	MGE	O6D-C1D	3.09	1.49	1.41
24	c	5504	BCR	C26-C25	3.09	1.39	1.34
20	a	5560	CLA	CAA-C2A	3.08	1.59	1.54
20	b	5512	CLA	CHB-C1B	-3.08	1.32	1.39
20	b	5519	CLA	CAA-C2A	3.08	1.59	1.54
20	C	499	CLA	C1D-ND	-3.08	1.33	1.37
20	B	513	CLA	C1D-C2D	-3.08	1.39	1.45
20	B	526	CLA	C4-C3	3.08	1.58	1.50
20	B	526	CLA	CAA-C2A	3.08	1.59	1.54
26	t	213	SQD	C13-C12	-3.08	1.36	1.51
20	C	502	CLA	CAA-C2A	3.07	1.59	1.54
27	m	216	LMT	C3B-C2B	3.07	1.60	1.52
26	L	5213	SQD	C16-C15	-3.07	1.36	1.51
26	A	568	SQD	C16-C15	-3.07	1.36	1.51
20	B	521	CLA	CAA-C2A	3.06	1.59	1.54
20	B	520	CLA	CHB-C1B	-3.06	1.32	1.39
20	c	5496	CLA	MG-NC	3.05	2.13	2.06
20	b	5523	CLA	CAA-C2A	3.05	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	5358	SQD	C17-C16	-3.05	1.36	1.51
20	b	5525	CLA	MG-NC	3.05	2.13	2.06
26	d	5358	SQD	O6-C44	-3.04	1.38	1.43
26	L	5213	SQD	C14-C13	-3.04	1.36	1.51
20	b	5514	CLA	C1D-C2D	-3.04	1.39	1.45
20	b	5511	CLA	C4C-C3C	3.04	1.50	1.45
26	A	568	SQD	C15-C14	-3.04	1.36	1.51
30	C	507	DGD	O6D-C1D	3.03	1.49	1.41
28	d	5359	MGE	O6D-C1D	3.02	1.49	1.41
24	b	5528	BCR	C2-C1	3.02	1.61	1.54
32	f	5051	HEM	CMA-C3A	3.01	1.56	1.50
26	A	568	SQD	C11-C10	-3.01	1.36	1.51
20	B	526	CLA	CHB-C1B	-3.00	1.32	1.39
20	a	5559	CLA	C1D-ND	-3.00	1.33	1.37
24	X	130	BCR	C26-C25	3.00	1.39	1.34
30	C	508	DGD	O1G-C1A	3.00	1.42	1.33
20	c	5496	CLA	CHB-C1B	-3.00	1.32	1.39
26	t	213	SQD	C16-C15	-2.99	1.36	1.51
24	C	505	BCR	C5-C6	2.99	1.39	1.34
26	A	5212	SQD	O6-C1	2.99	1.45	1.40
20	c	5491	CLA	CAA-C2A	2.99	1.59	1.54
24	t	104	BCR	C29-C30	2.99	1.60	1.54
26	L	5213	SQD	O5-C1	2.99	1.49	1.41
20	a	5558	CLA	MG-NC	2.99	2.13	2.06
20	c	5496	CLA	C4C-C3C	2.98	1.50	1.45
20	B	515	CLA	CHB-C1B	-2.98	1.32	1.39
24	C	506	BCR	C29-C30	2.98	1.60	1.54
20	b	5524	CLA	MG-NB	2.98	2.11	2.05
20	c	5500	CLA	CAA-C2A	2.98	1.59	1.54
26	L	5213	SQD	O6-C1	2.97	1.45	1.40
26	t	213	SQD	C18-C17	-2.97	1.37	1.51
20	c	5500	CLA	MG-NC	2.97	2.13	2.06
20	b	5526	CLA	C1-C2	2.96	1.57	1.49
20	c	5493	CLA	CAA-C2A	2.96	1.59	1.54
26	d	5358	SQD	O3-C3	2.95	1.50	1.43
21	A	561	PHO	CAA-CBA	-2.95	1.44	1.52
20	b	5521	CLA	CAA-C2A	2.95	1.59	1.54
32	V	552	HEM	CHB-C1B	-2.95	1.32	1.38
21	a	5561	PHO	C1D-C2D	2.94	1.42	1.39
27	a	5568	LMT	O5'-C1'	2.94	1.49	1.41
20	b	5518	CLA	CAA-C2A	2.94	1.59	1.54
20	B	511	CLA	CMD-C2D	2.94	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	H	208	DGD	O5D-C1E	2.94	1.45	1.40
20	B	518	CLA	C1D-ND	-2.94	1.34	1.37
20	c	5494	CLA	CHB-C1B	-2.93	1.32	1.39
30	C	508	DGD	O3G-C1D	2.93	1.45	1.40
20	a	5558	CLA	CHC-C1C	2.92	1.44	1.38
20	C	494	CLA	CHB-C1B	-2.92	1.32	1.39
32	V	552	HEM	C4D-ND	-2.91	1.35	1.40
20	C	503	CLA	MG-NC	2.91	2.13	2.06
20	D	354	CLA	MG-NC	2.91	2.13	2.06
28	d	5360	MGE	O6D-C1D	2.91	1.49	1.41
24	x	5130	BCR	C26-C25	2.91	1.39	1.34
20	C	500	CLA	CHB-C1B	-2.89	1.32	1.39
28	D	358	MGE	O6D-C5D	2.89	1.51	1.44
27	A	569	LMT	O5'-C1'	2.89	1.49	1.41
20	a	5559	CLA	CHB-C1B	-2.89	1.32	1.39
28	D	358	MGE	C4D-C3D	2.88	1.59	1.52
20	a	5560	CLA	CHB-C1B	-2.88	1.33	1.39
20	B	525	CLA	CHB-C1B	-2.88	1.33	1.39
20	d	5355	CLA	CAA-C2A	2.88	1.59	1.54
28	d	5360	MGE	C4D-C3D	2.88	1.59	1.52
28	i	5201	MGE	C4D-C5D	2.87	1.59	1.53
26	d	5358	SQD	C32-C31	-2.87	1.37	1.51
20	a	5560	CLA	MG-NC	2.87	2.13	2.06
24	t	104	BCR	C26-C25	2.87	1.39	1.34
20	b	5524	CLA	MG-NC	2.87	2.13	2.06
20	b	5511	CLA	C1C-C2C	2.87	1.50	1.44
26	A	568	SQD	C13-C12	-2.86	1.37	1.51
24	b	5527	BCR	C5-C6	2.86	1.39	1.34
30	c	5507	DGD	O3G-C1D	2.86	1.45	1.40
27	A	569	LMT	C1'-C2'	2.86	1.60	1.52
20	b	5521	CLA	MG-NC	2.85	2.13	2.06
26	d	5358	SQD	C20-C19	-2.85	1.37	1.51
26	A	568	SQD	C14-C13	-2.85	1.37	1.51
20	c	5497	CLA	CHB-C1B	-2.85	1.33	1.39
24	H	107	BCR	C5-C6	2.85	1.39	1.34
20	C	495	CLA	C1C-C2C	2.85	1.50	1.44
30	C	507	DGD	O3G-C1D	2.85	1.44	1.40
20	B	522	CLA	CHC-C1C	2.85	1.44	1.38
20	c	5497	CLA	CAA-C2A	2.84	1.59	1.54
24	D	357	BCR	C19-C18	-2.84	1.39	1.46
32	f	5051	HEM	CAA-C2A	2.83	1.58	1.51
30	c	5507	DGD	C3E-C2E	2.83	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	5521	CLA	MG-NA	2.83	2.13	2.06
27	t	5217	LMT	O1B-C1B	2.83	1.49	1.41
20	B	517	CLA	CHB-C1B	-2.82	1.33	1.39
20	b	5511	CLA	CMD-C2D	2.82	1.56	1.50
20	b	5516	CLA	CHB-C1B	-2.82	1.33	1.39
30	C	508	DGD	C4E-C3E	2.82	1.59	1.52
30	h	5208	DGD	O6D-C5D	2.81	1.51	1.44
20	B	514	CLA	CAA-C2A	2.81	1.59	1.54
30	c	5508	DGD	C4D-C3D	2.81	1.59	1.52
20	A	558	CLA	CAA-CBA	-2.80	1.44	1.52
28	i	5201	MGE	O2G-C1B	2.80	1.42	1.34
20	b	5525	CLA	CAA-C2A	2.80	1.59	1.54
20	b	5522	CLA	CHB-C1B	-2.80	1.33	1.39
24	B	527	BCR	C2-C1	2.80	1.60	1.54
20	b	5526	CLA	CHB-C1B	-2.80	1.33	1.39
20	C	495	CLA	CAA-C2A	2.79	1.59	1.54
26	d	5358	SQD	C11-C10	-2.79	1.37	1.51
24	b	5527	BCR	C26-C25	2.79	1.39	1.34
30	C	509	DGD	O6D-C1D	2.78	1.49	1.41
20	A	563	CLA	MG-NC	2.78	2.12	2.06
32	F	51	HEM	CAA-C2A	2.78	1.58	1.51
26	d	5358	SQD	C12-C11	-2.78	1.38	1.51
26	d	5358	SQD	C33-C32	-2.78	1.38	1.51
32	v	5552	HEM	CHB-C1B	-2.78	1.32	1.38
28	b	5530	MGE	O6D-C5D	2.77	1.51	1.44
20	B	521	CLA	CHB-C1B	-2.77	1.33	1.39
21	A	562	PHO	C3D-CAD	-2.77	1.42	1.47
20	A	560	CLA	MG-NC	2.77	2.12	2.06
20	B	513	CLA	C5-C3	2.77	1.57	1.51
20	B	511	CLA	C4C-C3C	2.77	1.49	1.45
20	b	5514	CLA	C1D-ND	-2.77	1.34	1.37
24	C	505	BCR	C38-C26	2.77	1.55	1.50
20	A	559	CLA	MG-NA	2.77	2.12	2.06
32	V	552	HEM	CMA-C3A	2.77	1.56	1.50
20	C	493	CLA	CAA-C2A	2.77	1.59	1.54
27	m	216	LMT	O1'-C1'	2.77	1.44	1.40
20	A	558	CLA	MG-NC	2.77	2.12	2.06
26	d	5358	SQD	C15-C14	-2.76	1.38	1.51
28	d	5360	MGE	O1G-C1A	2.76	1.41	1.33
20	a	5558	CLA	CAA-CBA	-2.76	1.44	1.52
32	v	5552	HEM	FE-ND	2.76	2.03	1.94
20	c	5492	CLA	C4-C3	2.76	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	566	BCR	C29-C30	2.75	1.60	1.54
20	C	496	CLA	MG-NC	2.75	2.12	2.06
26	d	5358	SQD	C19-C18	-2.74	1.38	1.51
20	B	521	CLA	MG-NC	2.74	2.12	2.06
30	h	5208	DGD	O6E-C1E	2.74	1.48	1.41
20	c	5498	CLA	C3B-C4B	2.74	1.50	1.42
20	B	525	CLA	MG-NC	2.74	2.12	2.06
24	b	5529	BCR	C26-C25	2.74	1.39	1.34
20	c	5502	CLA	CAA-C2A	2.74	1.59	1.54
20	C	496	CLA	C4C-C3C	2.74	1.49	1.45
20	B	522	CLA	MG-NC	2.74	2.12	2.06
20	c	5493	CLA	CHB-C1B	-2.74	1.33	1.39
20	C	492	CLA	CHB-C1B	-2.74	1.33	1.39
20	d	5355	CLA	MG-NC	2.73	2.12	2.06
20	c	5502	CLA	C3B-C4B	2.73	1.50	1.42
20	C	494	CLA	MG-NB	2.73	2.11	2.05
26	A	568	SQD	C33-C32	-2.73	1.38	1.51
20	B	513	CLA	MG-NC	2.73	2.12	2.06
26	t	213	SQD	C21-C20	-2.73	1.34	1.51
24	C	504	BCR	C5-C6	2.72	1.39	1.34
24	b	5528	BCR	C5-C6	2.72	1.39	1.34
28	d	5359	MGE	C4D-C3D	2.72	1.59	1.52
30	h	5208	DGD	O5D-C1E	2.72	1.44	1.40
24	t	104	BCR	C23-C22	-2.72	1.40	1.46
26	d	5358	SQD	C16-C15	-2.72	1.38	1.51
20	a	5558	CLA	CAA-C2A	2.72	1.59	1.54
20	C	496	CLA	CAA-C2A	2.72	1.59	1.54
30	c	5508	DGD	O1G-C1A	2.71	1.41	1.33
20	a	5560	CLA	CHD-C1D	2.71	1.43	1.38
20	b	5517	CLA	CHB-C1B	-2.71	1.33	1.39
26	A	568	SQD	O8-S	2.71	1.57	1.47
28	I	201	MGE	O2G-C1B	2.70	1.41	1.34
24	b	5529	BCR	C5-C6	2.70	1.39	1.34
27	t	5217	LMT	O5B-C1B	2.70	1.48	1.41
21	A	562	PHO	C4-C3	2.70	1.57	1.50
20	C	501	CLA	CAA-C2A	2.69	1.59	1.54
20	b	5525	CLA	CHB-C1B	-2.69	1.33	1.39
32	V	552	HEM	FE-NA	2.68	2.04	1.95
20	d	5354	CLA	MG-NA	2.68	2.12	2.06
30	C	508	DGD	C1E-C2E	2.68	1.60	1.52
32	v	5552	HEM	CMA-C3A	2.68	1.56	1.50
26	A	568	SQD	C32-C31	-2.68	1.38	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	5358	SQD	O8-S	2.68	1.57	1.47
32	v	5552	HEM	CAA-C2A	2.67	1.58	1.51
20	d	5355	CLA	CHB-C1B	-2.67	1.33	1.39
30	H	208	DGD	O6D-C1D	2.67	1.48	1.41
20	C	500	CLA	MG-NC	2.67	2.12	2.06
20	B	525	CLA	CAA-C2A	2.67	1.58	1.54
20	b	5513	CLA	CHB-C1B	-2.67	1.33	1.39
24	B	529	BCR	C5-C6	2.66	1.39	1.34
26	a	212	SQD	C8-C7	2.66	1.58	1.49
20	C	501	CLA	MG-NC	2.66	2.12	2.06
20	c	5502	CLA	CMD-C2D	2.66	1.56	1.50
24	T	5104	BCR	C29-C30	2.66	1.60	1.54
21	A	561	PHO	C3D-CAD	-2.65	1.42	1.47
20	B	519	CLA	CMD-C2D	2.65	1.56	1.50
20	c	5503	CLA	C1C-C2C	2.65	1.49	1.44
32	v	5552	HEM	C1C-C2C	2.65	1.50	1.45
21	a	5561	PHO	C3D-CAD	-2.65	1.42	1.47
20	b	5524	CLA	CHB-C1B	-2.65	1.33	1.39
20	a	5563	CLA	C5-C3	2.65	1.56	1.51
30	C	507	DGD	C3E-C2E	2.65	1.59	1.52
26	A	5212	SQD	O5-C1	2.65	1.48	1.41
20	C	491	CLA	CHB-C1B	-2.65	1.33	1.39
28	d	5360	MGE	O6D-C5D	2.65	1.50	1.44
20	c	5500	CLA	C4-C3	2.64	1.57	1.50
20	B	520	CLA	C4C-C3C	2.64	1.49	1.45
24	T	5104	BCR	C29-C28	-2.64	1.46	1.52
21	A	561	PHO	C1D-C2D	2.64	1.42	1.39
20	A	559	CLA	CAA-C2A	2.64	1.58	1.54
20	B	522	CLA	C1D-ND	-2.64	1.34	1.37
30	C	508	DGD	C3D-C2D	2.64	1.59	1.52
26	d	5358	SQD	C14-C13	-2.64	1.38	1.51
20	b	5517	CLA	MG-NC	2.63	2.12	2.06
32	F	51	HEM	CBD-CAD	2.63	1.61	1.51
20	C	501	CLA	C1C-C2C	2.63	1.49	1.44
21	A	562	PHO	C4A-C3A	-2.63	1.46	1.51
26	A	568	SQD	C19-C18	-2.62	1.38	1.51
26	d	5358	SQD	C36-C35	-2.62	1.38	1.51
20	B	514	CLA	MG-NC	2.62	2.12	2.06
20	D	354	CLA	MG-NB	2.62	2.11	2.05
20	C	498	CLA	CHC-C1C	2.62	1.43	1.38
30	C	509	DGD	O6D-C5D	2.62	1.50	1.44
28	D	359	MGE	C4D-C3D	2.62	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	H	208	DGD	O6D-C5D	2.62	1.50	1.44
26	a	212	SQD	O5-C1	2.61	1.48	1.41
20	B	524	CLA	CHB-C1B	-2.61	1.33	1.39
20	c	5494	CLA	MG-NA	2.61	2.12	2.06
27	T	217	LMT	O5B-C1B	2.60	1.48	1.41
26	A	568	SQD	C18-C17	-2.60	1.38	1.51
30	c	5509	DGD	O6D-C5D	2.60	1.50	1.44
20	B	517	CLA	C1D-ND	-2.60	1.34	1.37
20	b	5520	CLA	CAA-C2A	2.60	1.58	1.54
20	c	5498	CLA	CAA-C2A	2.60	1.58	1.54
24	t	104	BCR	C29-C28	-2.60	1.46	1.52
30	H	208	DGD	C1E-C2E	2.60	1.60	1.52
20	c	5493	CLA	CMB-C2B	2.60	1.56	1.50
28	I	201	MGE	O6D-C5D	2.60	1.50	1.44
21	a	5561	PHO	CAA-CBA	-2.59	1.45	1.52
30	C	508	DGD	C4D-C3D	2.59	1.59	1.52
20	c	5498	CLA	MG-NB	2.59	2.10	2.05
30	c	5507	DGD	C1E-C2E	2.59	1.60	1.52
20	B	516	CLA	MG-NC	2.59	2.12	2.06
20	A	559	CLA	CHB-C1B	-2.59	1.33	1.39
26	L	5213	SQD	O6-C44	-2.59	1.39	1.43
26	L	5213	SQD	C21-C20	-2.59	1.35	1.51
26	A	568	SQD	C35-C34	-2.58	1.38	1.51
28	i	5201	MGE	O6D-C1D	2.58	1.48	1.41
32	F	51	HEM	C3C-C4C	2.58	1.50	1.46
20	c	5498	CLA	CHC-C1C	2.58	1.43	1.38
26	t	213	SQD	O5-C1	2.58	1.48	1.41
20	b	5513	CLA	C4-C3	2.58	1.57	1.50
28	B	530	MGE	O2G-C1B	2.57	1.41	1.34
20	C	500	CLA	CMD-C2D	2.57	1.56	1.50
26	A	568	SQD	C34-C33	-2.57	1.39	1.51
32	v	5552	HEM	CAD-C3D	-2.57	1.44	1.51
24	c	5506	BCR	C19-C18	-2.57	1.40	1.46
28	d	5359	MGE	O6D-C5D	2.57	1.50	1.44
27	A	569	LMT	O5B-C5B	2.57	1.50	1.44
24	b	5527	BCR	C19-C18	-2.56	1.40	1.46
32	V	552	HEM	CHA-C4D	2.56	1.43	1.38
20	B	524	CLA	MG-NB	2.56	2.10	2.05
26	d	5358	SQD	C13-C12	-2.56	1.39	1.51
20	B	523	CLA	C1D-C2D	-2.56	1.40	1.45
30	c	5508	DGD	C1E-C2E	2.55	1.60	1.52
24	b	5527	BCR	C1-C6	2.55	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	502	CLA	CMB-C2B	2.55	1.56	1.50
32	f	5051	HEM	FE-ND	2.54	2.02	1.94
30	C	507	DGD	O6D-C5D	2.54	1.50	1.44
20	b	5520	CLA	CHB-C1B	-2.54	1.33	1.39
26	A	568	SQD	C20-C19	-2.54	1.39	1.51
26	d	5358	SQD	O5-C1	2.54	1.48	1.41
20	c	5496	CLA	C1C-C2C	2.53	1.49	1.44
26	d	5358	SQD	C35-C34	-2.53	1.39	1.51
21	a	5562	PHO	C3D-CAD	-2.53	1.42	1.47
20	c	5492	CLA	CHB-C1B	-2.53	1.33	1.39
20	D	354	CLA	C1D-C2D	-2.52	1.40	1.45
24	a	5566	BCR	C29-C30	2.52	1.59	1.54
20	c	5498	CLA	CHB-C1B	-2.52	1.33	1.39
20	A	563	CLA	C4-C3	2.52	1.56	1.50
27	T	217	LMT	O1B-C1B	2.52	1.48	1.41
20	B	526	CLA	MG-NC	2.52	2.12	2.06
20	B	520	CLA	C4-C3	2.51	1.56	1.50
20	B	516	CLA	CHB-C1B	-2.51	1.33	1.39
32	v	5552	HEM	CBA-CGA	-2.51	1.44	1.50
28	D	360	MGE	O6D-C1D	2.51	1.48	1.41
20	C	493	CLA	C1D-ND	-2.51	1.34	1.37
20	c	5494	CLA	MG-NB	2.51	2.10	2.05
28	B	530	MGE	C1D-C2D	2.51	1.59	1.52
26	A	568	SQD	C36-C35	-2.51	1.39	1.51
20	B	514	CLA	C1D-C2D	-2.51	1.40	1.45
20	C	497	CLA	C4-C3	2.51	1.56	1.50
26	a	212	SQD	O6-C44	-2.51	1.39	1.43
32	v	5552	HEM	FE-NA	2.51	2.03	1.95
20	C	495	CLA	C1D-C2D	-2.50	1.40	1.45
28	B	530	MGE	O6D-C5D	2.50	1.50	1.44
32	v	5552	HEM	C1A-NA	2.50	1.44	1.39
20	b	5513	CLA	MG-NC	2.50	2.12	2.06
20	d	5354	CLA	MG-NC	2.50	2.12	2.06
30	H	208	DGD	O6E-C1E	2.50	1.48	1.41
24	A	566	BCR	C26-C25	2.50	1.38	1.34
20	B	523	CLA	CHB-C1B	-2.50	1.33	1.39
20	b	5515	CLA	C4-C3	2.50	1.56	1.50
26	d	5358	SQD	C34-C33	-2.49	1.39	1.51
24	T	5104	BCR	C23-C22	-2.49	1.40	1.46
24	X	130	BCR	C33-C5	2.49	1.54	1.50
20	C	493	CLA	CHB-C1B	-2.49	1.33	1.39
20	b	5514	CLA	CHC-C1C	2.49	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	V	552	HEM	C1C-NC	-2.49	1.34	1.39
27	t	5217	LMT	O1B-C4'	2.49	1.50	1.43
20	A	563	CLA	C1D-ND	-2.49	1.34	1.37
20	d	5355	CLA	CMD-C2D	2.49	1.55	1.50
20	b	5522	CLA	CHC-C1C	2.48	1.43	1.38
20	c	5502	CLA	CHC-C1C	2.48	1.43	1.38
32	f	5051	HEM	CAC-C3C	2.48	1.54	1.47
20	C	492	CLA	C4-C3	2.48	1.56	1.50
28	I	201	MGE	O3G-C1D	2.48	1.44	1.40
20	C	500	CLA	C4C-C3C	2.48	1.49	1.45
20	c	5500	CLA	CMD-C2D	2.48	1.55	1.50
32	v	5552	HEM	CBD-CAD	2.47	1.60	1.51
20	b	5526	CLA	MG-NC	2.47	2.12	2.06
20	A	563	CLA	C5-C3	2.47	1.56	1.51
20	b	5523	CLA	MG-NC	2.47	2.12	2.06
24	T	5104	BCR	C30-C25	2.47	1.56	1.53
27	A	569	LMT	O5B-C1B	2.47	1.48	1.41
24	B	527	BCR	C1-C6	2.47	1.56	1.53
20	c	5502	CLA	C4-C3	2.46	1.56	1.50
26	d	5358	SQD	C18-C17	-2.46	1.39	1.51
20	C	491	CLA	C4-C3	2.46	1.56	1.50
20	B	513	CLA	C4-C3	2.46	1.56	1.50
27	T	217	LMT	O1B-C4'	2.46	1.50	1.43
20	c	5497	CLA	MG-NB	2.46	2.10	2.05
20	B	523	CLA	CHB-C4A	2.46	1.43	1.37
20	B	514	CLA	C4-C3	2.46	1.56	1.50
20	C	491	CLA	MG-NC	2.46	2.12	2.06
30	c	5508	DGD	O5D-C1E	2.45	1.44	1.40
27	t	5217	LMT	C1B-C2B	2.45	1.59	1.52
20	B	517	CLA	CMB-C2B	2.45	1.55	1.50
20	a	5563	CLA	MG-NB	2.45	2.10	2.05
20	C	494	CLA	MG-NC	2.45	2.12	2.06
20	c	5502	CLA	CMB-C2B	2.45	1.55	1.50
20	d	5355	CLA	CHC-C1C	2.45	1.43	1.38
20	c	5496	CLA	C4-C3	2.44	1.56	1.50
27	A	569	LMT	C1B-C2B	2.44	1.59	1.52
20	b	5515	CLA	MG-NC	2.44	2.12	2.06
26	A	5212	SQD	O6-C44	-2.44	1.39	1.43
20	C	502	CLA	MG-NB	2.44	2.10	2.05
27	a	5568	LMT	C1'-C2'	2.43	1.59	1.52
32	v	5552	HEM	C3B-C2B	2.43	1.42	1.37
20	B	511	CLA	C1C-C2C	2.43	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	b	5512	CLA	CAA-CBA	-2.43	1.45	1.52
28	I	201	MGE	O6D-C1D	2.42	1.48	1.41
20	A	559	CLA	C1D-ND	-2.42	1.34	1.37
20	c	5501	CLA	C1C-C2C	2.42	1.49	1.44
26	d	5358	SQD	C8-C7	2.41	1.57	1.50
20	d	5354	CLA	C1D-C2D	-2.41	1.40	1.45
20	B	511	CLA	C3C-C2C	2.41	1.42	1.36
26	A	568	SQD	O5-C1	2.41	1.48	1.41
20	c	5500	CLA	CHB-C1B	-2.40	1.34	1.39
20	C	495	CLA	CHC-C1C	2.40	1.43	1.38
32	f	5051	HEM	C1A-NA	2.40	1.44	1.39
20	A	558	CLA	CHC-C1C	2.40	1.43	1.38
20	B	521	CLA	MG-NB	2.40	2.10	2.05
32	v	5552	HEM	C1A-C2A	2.40	1.49	1.44
27	M	5216	LMT	O5'-C1'	2.40	1.48	1.41
20	c	5495	CLA	MG-NC	2.40	2.12	2.06
20	B	525	CLA	C3B-C4B	2.39	1.49	1.42
20	b	5511	CLA	C3C-C2C	2.39	1.41	1.36
20	B	522	CLA	CHB-C1B	-2.39	1.34	1.39
20	C	492	CLA	CAA-C2A	2.39	1.58	1.54
20	D	354	CLA	CHC-C1C	2.39	1.43	1.38
21	a	5562	PHO	C4A-C3A	-2.39	1.47	1.51
32	f	5051	HEM	C1A-C2A	2.39	1.49	1.44
20	b	5518	CLA	CHC-C1C	2.38	1.43	1.38
20	C	502	CLA	CHC-C1C	2.38	1.43	1.38
32	v	5552	HEM	CHA-C4D	2.38	1.43	1.38
30	c	5507	DGD	O6D-C5D	2.38	1.50	1.44
21	a	5562	PHO	C4-C3	2.38	1.56	1.50
27	m	216	LMT	O5'-C1'	2.38	1.48	1.41
20	B	512	CLA	CHD-C1D	2.38	1.43	1.38
20	B	526	CLA	CMB-C2B	2.38	1.55	1.50
20	c	5503	CLA	C1-C2	2.37	1.55	1.49
32	F	51	HEM	O2A-CGA	2.37	1.38	1.30
20	c	5502	CLA	C1B-C2B	2.37	1.48	1.43
26	a	212	SQD	O48-C23	2.37	1.44	1.33
32	v	5552	HEM	CBA-CAA	-2.37	1.43	1.51
20	c	5497	CLA	C4-C3	2.36	1.56	1.50
20	C	498	CLA	C3B-C4B	2.36	1.49	1.42
24	B	528	BCR	C5-C6	2.36	1.38	1.34
20	C	502	CLA	CHB-C1B	-2.36	1.34	1.39
20	c	5499	CLA	C4C-C3C	2.36	1.49	1.45
32	v	5552	HEM	C1C-NC	-2.36	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	a	5558	CLA	CMB-C2B	2.36	1.55	1.50
20	C	501	CLA	CHB-C4A	2.36	1.43	1.37
20	A	558	CLA	CMB-C2B	2.36	1.55	1.50
27	m	216	LMT	O5B-C1B	2.35	1.47	1.41
21	A	561	PHO	C4-C3	2.35	1.56	1.50
20	c	5503	CLA	CMD-C2D	2.35	1.55	1.50
30	c	5509	DGD	C4E-C5E	2.35	1.58	1.53
20	c	5499	CLA	CHB-C1B	-2.35	1.34	1.39
32	V	552	HEM	CBA-CAA	-2.35	1.43	1.51
20	b	5520	CLA	C4C-C3C	2.35	1.49	1.45
20	b	5513	CLA	C5-C3	2.35	1.56	1.51
28	d	5361	MGE	O6D-C5D	2.35	1.50	1.44
20	c	5491	CLA	C4-C3	2.34	1.56	1.50
30	C	507	DGD	C4D-C5D	2.34	1.58	1.53
20	B	515	CLA	CAA-C2A	2.34	1.58	1.54
28	I	201	MGE	C4D-C3D	2.34	1.58	1.52
20	c	5495	CLA	CHC-C1C	2.34	1.43	1.38
20	B	523	CLA	CAA-C2A	2.34	1.58	1.54
20	c	5495	CLA	C1C-C2C	2.34	1.49	1.44
20	b	5525	CLA	MG-NB	2.34	2.10	2.05
28	i	5201	MGE	C2A-C1A	2.34	1.57	1.50
20	B	514	CLA	CHB-C1B	-2.34	1.34	1.39
20	B	518	CLA	MG-NB	2.33	2.10	2.05
20	c	5494	CLA	CHC-C1C	2.33	1.43	1.38
20	D	355	CLA	MG-NC	2.33	2.11	2.06
30	C	509	DGD	O1G-C1A	2.33	1.40	1.33
26	A	568	SQD	C8-C7	2.33	1.57	1.50
20	A	563	CLA	CHC-C1C	2.33	1.43	1.38
20	D	355	CLA	CHD-C1D	2.33	1.42	1.38
20	c	5499	CLA	MG-NC	2.33	2.11	2.06
20	A	558	CLA	C1D-C2D	-2.33	1.40	1.45
20	B	515	CLA	MG-NB	2.33	2.10	2.05
20	c	5498	CLA	C4-C3	2.32	1.56	1.50
32	V	552	HEM	CAA-C2A	2.32	1.57	1.51
28	b	5530	MGE	C4D-C5D	2.32	1.58	1.53
20	c	5503	CLA	C4-C3	2.32	1.56	1.50
20	b	5525	CLA	CHC-C1C	2.32	1.43	1.38
20	c	5502	CLA	CHB-C1B	-2.32	1.34	1.39
26	d	5358	SQD	C24-C23	2.32	1.57	1.50
20	b	5511	CLA	C4B-NB	2.32	1.40	1.37
28	d	5360	MGE	O3G-C1D	2.32	1.44	1.40
20	B	526	CLA	C1-C2	2.31	1.55	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	V	552	HEM	CBD-CAD	2.31	1.60	1.51
20	b	5525	CLA	CHB-C4A	2.31	1.43	1.37
20	c	5501	CLA	CHC-C1C	2.31	1.43	1.38
20	B	518	CLA	CHC-C1C	2.31	1.43	1.38
20	c	5492	CLA	CAA-C2A	2.31	1.58	1.54
20	C	495	CLA	CHB-C4A	2.31	1.43	1.37
20	d	5355	CLA	MG-NB	2.31	2.10	2.05
24	B	527	BCR	C38-C26	2.31	1.54	1.50
28	i	5201	MGE	O3G-C1D	2.31	1.44	1.40
20	c	5493	CLA	CHC-C1C	2.30	1.43	1.38
20	B	514	CLA	C1D-ND	-2.30	1.34	1.37
20	C	500	CLA	C1D-ND	-2.30	1.34	1.37
20	d	5355	CLA	C3B-C4B	2.30	1.49	1.42
20	b	5517	CLA	CHC-C1C	2.30	1.43	1.38
20	d	5354	CLA	C3B-C4B	2.30	1.49	1.42
20	B	513	CLA	CMB-C2B	2.30	1.55	1.50
20	B	524	CLA	CAA-C2A	2.30	1.58	1.54
20	b	5523	CLA	C1D-C2D	-2.29	1.40	1.45
20	c	5497	CLA	C1D-C2D	-2.29	1.40	1.45
20	b	5515	CLA	C1D-ND	-2.29	1.34	1.37
30	c	5507	DGD	O6E-C5E	2.29	1.50	1.44
20	A	563	CLA	CAA-C2A	2.29	1.58	1.54
20	b	5523	CLA	C5-C3	2.29	1.56	1.51
30	c	5508	DGD	C4E-C3E	2.28	1.58	1.52
20	b	5524	CLA	C1D-ND	-2.28	1.34	1.37
20	C	493	CLA	CMB-C2B	2.28	1.55	1.50
28	D	360	MGE	O6D-C5D	2.28	1.50	1.44
24	B	527	BCR	C19-C18	-2.28	1.41	1.46
20	b	5522	CLA	MG-NB	2.28	2.10	2.05
20	b	5523	CLA	CHB-C1B	-2.28	1.34	1.39
24	C	506	BCR	C35-C13	2.27	1.55	1.50
20	b	5526	CLA	CAA-CBA	-2.27	1.46	1.52
20	c	5497	CLA	MG-NA	2.27	2.11	2.06
20	B	512	CLA	MG-NB	2.27	2.10	2.05
28	b	5530	MGE	O2G-C1B	2.27	1.40	1.34
26	t	213	SQD	O6-C1	2.27	1.44	1.40
24	t	104	BCR	C35-C13	2.27	1.55	1.50
24	D	357	BCR	C38-C26	2.27	1.54	1.50
28	b	5530	MGE	O1G-C1G	-2.27	1.40	1.45
20	b	5513	CLA	CMB-C2B	2.27	1.55	1.50
24	h	5107	BCR	C5-C6	2.26	1.38	1.34
20	C	494	CLA	CMB-C2B	2.26	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	492	CLA	C5-C3	2.26	1.56	1.51
20	A	560	CLA	CMB-C2B	2.26	1.55	1.50
20	c	5495	CLA	C4-C3	2.26	1.56	1.50
26	A	568	SQD	C37-C36	-2.26	1.37	1.51
20	B	520	CLA	MG-NC	2.25	2.11	2.06
20	d	5354	CLA	C1D-ND	-2.25	1.34	1.37
20	C	498	CLA	MG-NB	2.25	2.10	2.05
20	b	5519	CLA	C1C-C2C	2.25	1.49	1.44
20	c	5492	CLA	C1C-NC	-2.25	1.34	1.37
20	B	511	CLA	CMC-C2C	2.25	1.55	1.50
20	C	503	CLA	CMB-C2B	2.25	1.55	1.50
20	b	5515	CLA	C3A-C2A	-2.25	1.48	1.54
20	b	5524	CLA	CMB-C2B	2.25	1.55	1.50
20	b	5511	CLA	CHB-C4A	2.24	1.43	1.37
20	B	521	CLA	CHC-C1C	2.24	1.43	1.38
20	C	497	CLA	CHB-C1B	-2.24	1.34	1.39
28	l	5210	MGE	C4D-C3D	2.24	1.58	1.52
32	f	5051	HEM	CBD-CGD	2.24	1.55	1.50
20	a	5560	CLA	MG-NB	2.24	2.10	2.05
20	c	5491	CLA	CHB-C1B	-2.24	1.34	1.39
20	b	5515	CLA	CAA-CBA	-2.24	1.46	1.52
26	A	568	SQD	O6-C1	2.24	1.43	1.40
22	a	5564	PQ9	C11-C2	2.24	1.54	1.51
20	C	501	CLA	CHC-C1C	2.24	1.43	1.38
30	C	507	DGD	O6E-C5E	2.24	1.49	1.44
20	B	513	CLA	C3B-C4B	2.24	1.49	1.42
30	h	5208	DGD	C1D-C2D	2.24	1.59	1.52
20	a	5560	CLA	C4-C3	2.24	1.56	1.50
20	B	526	CLA	C2-C3	2.24	1.38	1.33
20	C	493	CLA	MG-NC	2.24	2.11	2.06
20	C	495	CLA	C4C-C3C	2.24	1.48	1.45
27	a	5568	LMT	O5B-C1B	2.24	1.47	1.41
30	C	509	DGD	O2G-C1B	2.24	1.40	1.34
24	a	5566	BCR	C26-C25	2.23	1.38	1.34
20	C	502	CLA	C4-C3	2.23	1.56	1.50
20	b	5517	CLA	C1-C2	2.23	1.55	1.49
20	b	5514	CLA	CHB-C1B	-2.23	1.34	1.39
20	b	5521	CLA	MG-NB	2.23	2.10	2.05
20	b	5524	CLA	CHC-C1C	2.23	1.42	1.38
27	M	5216	LMT	C1B-C2B	2.23	1.59	1.52
20	b	5519	CLA	CHB-C1B	-2.23	1.34	1.39
22	D	356	PQ9	C3-C4	2.22	1.50	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	5503	CLA	CMB-C2B	2.22	1.55	1.50
20	b	5520	CLA	C1D-C2D	-2.22	1.40	1.45
20	C	499	CLA	CHB-C4A	2.22	1.43	1.37
28	b	5530	MGE	C4D-C3D	2.22	1.58	1.52
20	d	5355	CLA	C1C-C2C	2.22	1.49	1.44
20	c	5503	CLA	MG-NC	2.22	2.11	2.06
20	B	522	CLA	C3B-C4B	2.22	1.49	1.42
20	B	518	CLA	C4-C3	2.22	1.56	1.50
20	c	5495	CLA	C1D-C2D	-2.22	1.40	1.45
20	C	502	CLA	C3B-C4B	2.22	1.49	1.42
20	C	499	CLA	C1D-C2D	-2.22	1.40	1.45
30	h	5208	DGD	C3E-C2E	2.22	1.58	1.52
20	B	515	CLA	MG-NC	2.22	2.11	2.06
20	B	524	CLA	CHC-C1C	2.22	1.42	1.38
20	A	558	CLA	CAA-C2A	2.21	1.58	1.54
20	B	526	CLA	CHD-C1D	2.21	1.42	1.38
27	M	5216	LMT	C3B-C2B	2.21	1.58	1.52
28	B	530	MGE	C4D-C5D	2.21	1.57	1.53
30	h	5208	DGD	O6D-C1D	2.21	1.47	1.41
20	B	526	CLA	CAA-CBA	-2.21	1.46	1.52
20	c	5501	CLA	C3B-C4B	2.21	1.49	1.42
20	c	5503	CLA	CHB-C4A	2.21	1.43	1.37
20	B	515	CLA	C1D-ND	-2.21	1.35	1.37
20	b	5513	CLA	C1D-ND	-2.21	1.35	1.37
20	B	512	CLA	CMB-C2B	2.21	1.55	1.50
32	F	51	HEM	CAC-C3C	2.21	1.53	1.47
20	d	5355	CLA	CHB-C4A	2.20	1.43	1.37
20	d	5354	CLA	C3A-C4A	-2.20	1.44	1.51
20	a	5559	CLA	CAA-C2A	2.20	1.58	1.54
20	B	515	CLA	C4-C3	2.20	1.56	1.50
28	D	359	MGE	O1G-C1A	2.20	1.39	1.33
27	M	5216	LMT	C1'-C2'	2.20	1.59	1.52
28	L	210	MGE	C4D-C3D	2.20	1.58	1.52
20	C	501	CLA	CMB-C2B	2.19	1.55	1.50
28	d	5361	MGE	O2G-C1B	2.19	1.40	1.34
32	V	552	HEM	FE-ND	2.19	2.01	1.94
20	b	5522	CLA	C3B-C4B	2.19	1.49	1.42
20	C	492	CLA	C1D-C2D	-2.19	1.41	1.45
20	C	499	CLA	MG-NC	2.19	2.11	2.06
32	V	552	HEM	CAD-C3D	-2.19	1.45	1.51
32	f	5051	HEM	C1C-NC	-2.19	1.35	1.39
20	C	497	CLA	CAA-C2A	2.19	1.58	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	499	CLA	CAA-C2A	2.19	1.58	1.54
20	B	525	CLA	CHB-C4A	2.19	1.43	1.37
32	F	51	HEM	CMD-C2D	2.19	1.55	1.50
20	b	5517	CLA	C1D-ND	-2.19	1.35	1.37
20	B	513	CLA	C3D-C4D	-2.18	1.39	1.44
32	V	552	HEM	C1A-NA	2.18	1.43	1.39
20	c	5502	CLA	CHB-C4A	2.18	1.43	1.37
20	b	5522	CLA	CMB-C2B	2.18	1.55	1.50
20	b	5514	CLA	MG-NC	2.18	2.11	2.06
24	T	5104	BCR	C37-C22	2.17	1.55	1.50
20	B	521	CLA	C4-C3	2.17	1.56	1.50
20	B	520	CLA	C1D-ND	-2.17	1.35	1.37
20	C	503	CLA	C4-C3	2.17	1.56	1.50
24	c	5505	BCR	C19-C18	-2.17	1.41	1.46
30	c	5508	DGD	O6D-C5D	2.17	1.49	1.44
20	D	355	CLA	CHC-C1C	2.17	1.42	1.38
26	t	213	SQD	C22-C21	-2.17	1.34	1.50
28	b	5530	MGE	C1D-C2D	2.17	1.58	1.52
20	b	5526	CLA	MG-NB	2.17	2.10	2.05
30	c	5507	DGD	C4D-C5D	2.17	1.57	1.53
20	a	5558	CLA	CBA-CGA	-2.17	1.44	1.50
26	A	5212	SQD	C8-C7	2.16	1.56	1.49
20	A	563	CLA	MG-NB	2.16	2.10	2.05
28	D	358	MGE	O2G-C1B	2.16	1.40	1.34
27	a	5568	LMT	C1B-C2B	2.16	1.58	1.52
21	a	5561	PHO	CMC-C2C	2.16	1.53	1.50
32	v	5552	HEM	CMB-C2B	2.16	1.55	1.50
20	D	355	CLA	C4-C3	2.16	1.56	1.50
20	c	5492	CLA	MG-NC	2.16	2.11	2.06
20	c	5501	CLA	CMB-C2B	2.16	1.55	1.50
20	c	5498	CLA	C1C-C2C	2.16	1.48	1.44
20	C	498	CLA	CAA-C2A	2.16	1.58	1.54
20	b	5518	CLA	CHB-C1B	-2.15	1.34	1.39
20	c	5491	CLA	MG-NC	2.15	2.11	2.06
20	c	5492	CLA	C1D-C2D	-2.15	1.41	1.45
20	D	355	CLA	C1C-C2C	2.15	1.48	1.44
27	m	216	LMT	O5'-C5'	2.15	1.49	1.44
28	d	5359	MGE	C4D-C5D	2.15	1.57	1.53
32	v	5552	HEM	C2A-C3A	2.15	1.44	1.38
20	b	5522	CLA	C4-C3	2.15	1.56	1.50
24	A	566	BCR	C29-C28	-2.15	1.47	1.52
30	h	5208	DGD	C4E-C3E	2.15	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	c	5493	CLA	C1B-C2B	2.15	1.48	1.43
20	C	494	CLA	CMD-C2D	2.15	1.55	1.50
20	B	521	CLA	CBA-CGA	-2.15	1.44	1.50
20	a	5560	CLA	C1D-ND	-2.15	1.35	1.37
20	B	519	CLA	CHB-C4A	2.14	1.43	1.37
20	D	355	CLA	CHB-C4A	2.14	1.43	1.37
30	H	208	DGD	C1D-C2D	2.14	1.58	1.52
26	t	213	SQD	O6-C44	-2.14	1.40	1.43
20	a	5563	CLA	C4-C3	2.14	1.55	1.50
28	D	359	MGE	O6D-C5D	2.14	1.49	1.44
20	C	496	CLA	C1C-C2C	2.14	1.48	1.44
26	L	5213	SQD	C8-C7	2.14	1.56	1.50
20	B	520	CLA	C1D-C2D	-2.14	1.41	1.45
20	b	5518	CLA	C3B-C4B	2.14	1.49	1.42
20	C	503	CLA	CHD-C1D	2.14	1.42	1.38
20	b	5523	CLA	CHB-C4A	2.13	1.43	1.37
21	A	562	PHO	C4D-CHA	2.13	1.42	1.39
20	B	515	CLA	C3A-C2A	-2.13	1.48	1.54
20	b	5523	CLA	CAA-CBA	-2.13	1.46	1.52
27	a	5568	LMT	O5B-C5B	2.13	1.49	1.44
20	d	5354	CLA	MG-NB	2.13	2.10	2.05
20	b	5520	CLA	C1C-C2C	2.13	1.48	1.44
20	A	559	CLA	MG-NC	2.12	2.11	2.06
24	a	5566	BCR	C29-C28	-2.12	1.47	1.52
24	A	566	BCR	C19-C18	-2.12	1.41	1.46
27	m	216	LMT	C4B-C3B	2.12	1.57	1.52
20	c	5496	CLA	MG-NB	2.12	2.10	2.05
21	a	5561	PHO	C1D-ND	-2.12	1.34	1.38
24	x	5130	BCR	C35-C13	2.12	1.55	1.50
20	B	514	CLA	CHB-C4A	2.12	1.43	1.37
20	B	524	CLA	CMB-C2B	2.12	1.55	1.50
20	C	495	CLA	C4-C3	2.12	1.55	1.50
20	d	5354	CLA	CHC-C1C	2.12	1.42	1.38
20	b	5512	CLA	C4C-C3C	2.12	1.48	1.45
24	d	5357	BCR	C19-C18	-2.12	1.41	1.46
20	C	502	CLA	C4C-C3C	2.11	1.48	1.45
32	V	552	HEM	C1D-C2D	-2.11	1.40	1.44
28	D	360	MGE	O2G-C1B	2.11	1.40	1.34
20	A	563	CLA	CHD-C1D	2.11	1.42	1.38
20	C	501	CLA	CMD-C2D	2.11	1.55	1.50
21	A	562	PHO	C4D-ND	-2.11	1.35	1.38
20	c	5499	CLA	C1C-C2C	2.11	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	a	5561	PHO	CBA-CGA	-2.11	1.44	1.50
20	B	517	CLA	CHC-C1C	2.11	1.42	1.38
24	C	505	BCR	C19-C18	-2.11	1.41	1.46
20	C	502	CLA	C4B-NB	2.11	1.40	1.37
20	C	497	CLA	C1D-C2D	-2.11	1.41	1.45
28	d	5360	MGE	O2G-C1B	2.11	1.40	1.34
27	M	5216	LMT	O5B-C1B	2.11	1.47	1.41
20	C	495	CLA	MG-NC	2.11	2.11	2.06
24	C	506	BCR	C19-C18	-2.11	1.41	1.46
20	d	5354	CLA	CBA-CGA	-2.10	1.44	1.50
27	M	5216	LMT	C4B-C5B	2.10	1.57	1.53
26	d	5358	SQD	C37-C36	-2.10	1.38	1.51
20	c	5492	CLA	CMB-C2B	2.10	1.55	1.50
20	b	5512	CLA	CMB-C2B	2.10	1.55	1.50
20	C	497	CLA	CHC-C1C	2.10	1.42	1.38
24	b	5527	BCR	C23-C22	-2.10	1.41	1.46
20	b	5517	CLA	CMB-C2B	2.10	1.55	1.50
20	B	522	CLA	MG-NB	2.10	2.10	2.05
32	f	5051	HEM	CHC-C1C	2.10	1.42	1.38
20	D	355	CLA	CMD-C2D	2.10	1.55	1.50
20	A	560	CLA	C4C-C3C	2.10	1.48	1.45
20	d	5355	CLA	C1-C2	2.10	1.55	1.49
24	b	5528	BCR	C26-C25	2.10	1.38	1.34
32	V	552	HEM	C3D-C2D	2.10	1.41	1.36
26	A	568	SQD	C21-C20	-2.09	1.38	1.51
20	C	500	CLA	C4-C3	2.09	1.55	1.50
24	x	5130	BCR	C33-C5	2.09	1.54	1.50
20	C	497	CLA	CMB-C2B	2.09	1.55	1.50
24	h	5107	BCR	C38-C26	2.09	1.54	1.50
30	H	208	DGD	O6E-C5E	2.09	1.49	1.44
20	C	496	CLA	CHD-C1D	2.09	1.42	1.38
20	D	354	CLA	C1C-C2C	2.09	1.48	1.44
30	C	509	DGD	C3D-C2D	2.09	1.57	1.52
20	c	5502	CLA	CHD-C1D	2.09	1.42	1.38
20	a	5563	CLA	C1D-ND	-2.09	1.35	1.37
20	A	560	CLA	MG-NB	2.09	2.09	2.05
20	C	499	CLA	CHB-C1B	-2.08	1.34	1.39
20	B	511	CLA	C1B-C2B	2.08	1.48	1.43
24	X	130	BCR	C24-C23	2.08	1.39	1.33
24	x	5130	BCR	C24-C23	2.08	1.39	1.33
28	i	5201	MGE	C3D-C2D	2.08	1.57	1.52
20	C	499	CLA	C4C-C3C	2.08	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	508	DGD	O6D-C5D	2.08	1.49	1.44
30	H	208	DGD	C4E-C3E	2.08	1.57	1.52
20	c	5501	CLA	MG-NB	2.07	2.09	2.05
20	b	5511	CLA	C3A-C2A	-2.07	1.52	1.54
20	A	560	CLA	C4-C3	2.07	1.55	1.50
28	l	5210	MGE	O6D-C5D	2.07	1.49	1.44
20	b	5514	CLA	MG-NB	2.07	2.09	2.05
20	C	498	CLA	C4-C3	2.07	1.55	1.50
20	B	512	CLA	CAA-CBA	-2.07	1.46	1.52
20	b	5520	CLA	C4-C3	2.07	1.55	1.50
20	B	519	CLA	C4-C3	2.07	1.55	1.50
20	c	5497	CLA	CHC-C1C	2.06	1.42	1.38
20	b	5515	CLA	MG-NB	2.06	2.09	2.05
20	c	5491	CLA	C1B-C2B	2.06	1.48	1.43
32	v	5552	HEM	C1D-C2D	-2.06	1.40	1.44
20	b	5516	CLA	C1D-ND	-2.06	1.35	1.37
26	A	568	SQD	C24-C23	2.06	1.56	1.50
20	b	5526	CLA	CHB-C4A	2.06	1.42	1.37
20	b	5519	CLA	C5-C3	2.06	1.55	1.51
20	c	5499	CLA	CMB-C2B	2.06	1.55	1.50
20	b	5519	CLA	CHB-C4A	2.06	1.42	1.37
20	C	502	CLA	C1B-C2B	2.06	1.48	1.43
27	m	216	LMT	C1'-C2'	2.06	1.58	1.52
20	C	496	CLA	C1-C2	2.05	1.55	1.49
30	h	5208	DGD	C4E-C5E	2.05	1.57	1.53
32	F	51	HEM	FE-ND	2.05	2.01	1.94
30	c	5509	DGD	O1G-C1A	2.05	1.39	1.33
20	B	525	CLA	CHC-C1C	2.05	1.42	1.38
20	c	5495	CLA	CHB-C1B	-2.05	1.34	1.39
20	a	5563	CLA	C3B-C4B	2.04	1.48	1.42
20	C	496	CLA	C2-C3	2.04	1.37	1.33
20	a	5558	CLA	C1D-ND	-2.04	1.35	1.37
20	B	525	CLA	C1B-C2B	2.04	1.47	1.43
20	C	496	CLA	CHB-C1B	-2.04	1.34	1.39
20	B	526	CLA	CMD-C2D	2.04	1.55	1.50
20	c	5497	CLA	C4C-C3C	2.04	1.48	1.45
20	b	5520	CLA	CMD-C2D	2.04	1.55	1.50
20	c	5497	CLA	C1-C2	2.04	1.55	1.49
21	a	5561	PHO	C1-C2	2.04	1.55	1.49
20	C	503	CLA	CHC-C1C	2.04	1.42	1.38
20	b	5514	CLA	C4-C3	2.04	1.55	1.50
27	M	5216	LMT	O5B-C5B	2.04	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	d	5358	SQD	C21-C20	-2.04	1.39	1.51
24	t	104	BCR	C19-C18	-2.04	1.41	1.46
20	C	497	CLA	CHD-C1D	2.03	1.42	1.38
26	A	568	SQD	C22-C21	-2.03	1.35	1.50
28	l	5210	MGE	O3G-C1D	2.03	1.43	1.40
20	b	5511	CLA	CMC-C2C	2.03	1.54	1.50
26	A	5212	SQD	C44-C45	2.03	1.57	1.50
20	B	523	CLA	MG-NB	2.03	2.09	2.05
32	F	51	HEM	C1C-C2C	2.03	1.49	1.45
26	a	212	SQD	C44-C45	2.03	1.57	1.50
26	A	5212	SQD	C24-C23	2.03	1.56	1.49
20	C	495	CLA	C1D-ND	-2.03	1.35	1.37
20	B	525	CLA	CMD-C2D	2.03	1.54	1.50
20	B	524	CLA	C1D-ND	-2.03	1.35	1.37
20	b	5515	CLA	C5-C3	2.03	1.55	1.51
20	D	355	CLA	CHB-C1B	-2.02	1.34	1.39
20	C	493	CLA	C4-C3	2.02	1.55	1.50
20	b	5526	CLA	C2-C3	2.02	1.37	1.33
20	C	503	CLA	C3B-C4B	2.02	1.48	1.42
20	C	492	CLA	MG-NC	2.02	2.11	2.06
20	B	523	CLA	C5-C3	2.02	1.55	1.51
26	L	5213	SQD	C22-C21	-2.02	1.35	1.50
20	b	5522	CLA	CMD-C2D	2.02	1.54	1.50
20	B	522	CLA	CHB-C4A	2.02	1.42	1.37
20	B	521	CLA	C1C-C2C	2.02	1.48	1.44
21	A	561	PHO	C1D-ND	-2.02	1.35	1.38
20	c	5498	CLA	C1D-ND	-2.02	1.35	1.37
20	a	5563	CLA	MG-NC	2.02	2.11	2.06
20	b	5514	CLA	CHB-C4A	2.02	1.42	1.37
20	B	512	CLA	C3B-C4B	2.01	1.48	1.42
20	C	495	CLA	C5-C3	2.01	1.55	1.51
20	D	355	CLA	C1-C2	2.01	1.54	1.49
24	C	505	BCR	C23-C22	-2.01	1.41	1.46
20	B	522	CLA	CMB-C2B	2.01	1.54	1.50
20	c	5501	CLA	C1B-C2B	2.01	1.47	1.43
21	A	561	PHO	CMC-C2C	2.01	1.53	1.50
30	C	509	DGD	O5D-C1E	2.01	1.43	1.40
20	B	511	CLA	CHB-C1B	-2.01	1.34	1.39
20	B	515	CLA	CAA-CBA	-2.01	1.46	1.52
20	b	5516	CLA	C1D-C2D	-2.01	1.41	1.45
20	a	5558	CLA	C1C-C2C	2.01	1.48	1.44
24	T	5104	BCR	C26-C25	2.01	1.37	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	C	502	CLA	C1C-C2C	2.01	1.48	1.44
20	A	560	CLA	CHD-C1D	2.01	1.42	1.38
20	B	517	CLA	CHB-C4A	2.01	1.42	1.37
20	C	497	CLA	MG-NB	2.01	2.09	2.05
27	T	217	LMT	C1B-C2B	2.01	1.58	1.52
20	a	5558	CLA	C1D-C2D	-2.00	1.41	1.45
32	f	5051	HEM	CAD-C3D	-2.00	1.46	1.51
30	c	5509	DGD	O6E-C5E	2.00	1.49	1.44
32	F	51	HEM	CAD-C3D	-2.00	1.46	1.51
20	C	501	CLA	C4-C3	2.00	1.55	1.50

All (1531) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	5501	CLA	C4A-NA-C1A	12.96	112.59	106.68
20	b	5514	CLA	C4A-NA-C1A	12.90	112.56	106.68
20	C	501	CLA	C4A-NA-C1A	12.84	112.54	106.68
20	B	514	CLA	C4A-NA-C1A	12.74	112.49	106.68
20	B	524	CLA	C4A-NA-C1A	12.52	112.39	106.68
20	c	5491	CLA	C4A-NA-C1A	12.43	112.35	106.68
20	c	5503	CLA	C4A-NA-C1A	12.34	112.31	106.68
20	C	497	CLA	C4A-NA-C1A	12.21	112.25	106.68
20	b	5516	CLA	C4A-NA-C1A	12.21	112.25	106.68
20	C	503	CLA	C4A-NA-C1A	12.17	112.23	106.68
20	B	518	CLA	C4A-NA-C1A	12.15	112.22	106.68
20	B	521	CLA	C4A-NA-C1A	12.13	112.21	106.68
20	b	5525	CLA	C4A-NA-C1A	12.10	112.20	106.68
20	c	5502	CLA	C4A-NA-C1A	12.09	112.20	106.68
20	B	517	CLA	C4A-NA-C1A	12.08	112.19	106.68
20	c	5492	CLA	C4A-NA-C1A	12.08	112.19	106.68
20	B	523	CLA	C4A-NA-C1A	12.04	112.17	106.68
20	c	5498	CLA	C4A-NA-C1A	12.00	112.15	106.68
20	b	5523	CLA	C4A-NA-C1A	11.99	112.15	106.68
20	c	5495	CLA	C4A-NA-C1A	11.97	112.14	106.68
20	B	516	CLA	C4A-NA-C1A	11.95	112.13	106.68
20	C	494	CLA	C4A-NA-C1A	11.90	112.11	106.68
20	d	5355	CLA	C4A-NA-C1A	11.88	112.10	106.68
20	b	5518	CLA	C4A-NA-C1A	11.81	112.07	106.68
20	D	355	CLA	C4A-NA-C1A	11.72	112.03	106.68
20	C	502	CLA	C4A-NA-C1A	11.70	112.02	106.68
20	C	493	CLA	C4A-NA-C1A	11.65	112.00	106.68
20	b	5511	CLA	C4A-NA-C1A	11.60	111.97	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	492	CLA	C4A-NA-C1A	11.58	111.96	106.68
20	C	498	CLA	C4A-NA-C1A	11.56	111.95	106.68
20	C	496	CLA	C4A-NA-C1A	11.54	111.94	106.68
20	b	5524	CLA	C4A-NA-C1A	11.53	111.94	106.68
20	B	525	CLA	C4A-NA-C1A	11.53	111.94	106.68
20	C	499	CLA	C4A-NA-C1A	11.49	111.92	106.68
20	b	5521	CLA	C4A-NA-C1A	11.43	111.89	106.68
20	b	5517	CLA	C4A-NA-C1A	11.41	111.89	106.68
20	c	5493	CLA	C4A-NA-C1A	11.38	111.87	106.68
20	C	495	CLA	C4A-NA-C1A	11.37	111.87	106.68
20	B	526	CLA	C4A-NA-C1A	11.27	111.82	106.68
20	c	5499	CLA	C4A-NA-C1A	11.20	111.79	106.68
20	c	5496	CLA	C4A-NA-C1A	11.16	111.77	106.68
20	B	519	CLA	C4A-NA-C1A	11.12	111.75	106.68
20	b	5522	CLA	C4A-NA-C1A	11.11	111.75	106.68
20	b	5519	CLA	C4A-NA-C1A	11.05	111.72	106.68
20	a	5560	CLA	C4A-NA-C1A	11.03	111.71	106.68
20	c	5497	CLA	C4A-NA-C1A	10.97	111.68	106.68
20	B	511	CLA	C4A-NA-C1A	10.92	111.66	106.68
20	C	500	CLA	C4A-NA-C1A	10.88	111.64	106.68
20	b	5526	CLA	C4A-NA-C1A	10.87	111.64	106.68
20	c	5500	CLA	C4A-NA-C1A	10.81	111.61	106.68
20	B	522	CLA	C4A-NA-C1A	10.73	111.57	106.68
20	A	560	CLA	C4A-NA-C1A	10.61	111.52	106.68
20	c	5494	CLA	C4A-NA-C1A	10.60	111.52	106.68
20	B	520	CLA	C4A-NA-C1A	10.57	111.50	106.68
20	a	5559	CLA	C4A-NA-C1A	10.46	111.45	106.68
20	C	491	CLA	C4A-NA-C1A	10.41	111.43	106.68
20	b	5520	CLA	C4A-NA-C1A	10.36	111.41	106.68
20	A	559	CLA	C4A-NA-C1A	10.35	111.40	106.68
20	A	563	CLA	C4A-NA-C1A	10.26	111.36	106.68
20	B	513	CLA	C4A-NA-C1A	10.21	111.34	106.68
20	B	515	CLA	C4A-NA-C1A	10.16	111.31	106.68
20	d	5354	CLA	C4A-NA-C1A	10.13	111.30	106.68
20	B	512	CLA	C4A-NA-C1A	9.91	111.20	106.68
21	A	562	PHO	C4D-CHA-CBD	-9.84	103.73	108.45
20	b	5515	CLA	C4A-NA-C1A	9.76	111.13	106.68
20	a	5563	CLA	C4A-NA-C1A	9.68	111.09	106.68
20	b	5513	CLA	C4A-NA-C1A	9.60	111.06	106.68
20	A	558	CLA	C4A-NA-C1A	9.53	111.03	106.68
21	a	5562	PHO	C4D-CHA-CBD	-9.50	103.90	108.45
20	b	5512	CLA	C4A-NA-C1A	9.42	110.98	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	D	354	CLA	C4A-NA-C1A	9.20	110.88	106.68
20	a	5558	CLA	C4A-NA-C1A	9.07	110.82	106.68
21	a	5561	PHO	C4D-CHA-CBD	-8.89	104.19	108.45
21	A	561	PHO	C4D-CHA-CBD	-8.78	104.25	108.45
26	A	5212	SQD	O5-C1-O6	8.77	130.76	110.04
26	a	212	SQD	O5-C1-O6	8.39	129.88	110.04
26	A	568	SQD	O5-C1-O6	8.36	129.81	110.04
26	d	5358	SQD	O5-C1-O6	8.09	129.16	110.04
26	L	5213	SQD	O5-C1-O6	8.06	129.09	110.04
32	f	5051	HEM	CAD-C3D-C2D	7.90	142.66	127.87
26	t	213	SQD	O6-C1-C2	7.87	120.22	108.27
26	t	213	SQD	O5-C1-O6	7.72	128.28	110.04
30	c	5507	DGD	O6E-C5E-C4E	7.71	123.60	109.70
32	F	51	HEM	CAD-C3D-C2D	7.68	142.26	127.87
32	V	552	HEM	CAD-C3D-C2D	7.61	142.12	127.87
30	H	208	DGD	O6E-C5E-C4E	7.54	123.29	109.70
26	L	5213	SQD	O6-C1-C2	7.49	119.65	108.27
32	v	5552	HEM	CAD-C3D-C2D	7.48	141.87	127.87
30	c	5508	DGD	O6E-C5E-C4E	7.47	123.17	109.70
26	d	5358	SQD	O6-C1-C2	7.41	119.53	108.27
32	f	5051	HEM	CAD-C3D-C4D	-7.40	111.81	124.70
30	C	507	DGD	O6E-C5E-C4E	7.31	122.88	109.70
30	C	508	DGD	O6E-C5E-C4E	7.31	122.87	109.70
26	A	568	SQD	O6-C1-C2	7.24	119.27	108.27
30	C	509	DGD	O6E-C5E-C4E	7.22	122.70	109.70
30	c	5509	DGD	O6E-C5E-C4E	7.19	122.66	109.70
30	h	5208	DGD	O6E-C5E-C4E	7.19	122.65	109.70
32	F	51	HEM	CAD-C3D-C4D	-7.11	112.31	124.70
32	V	552	HEM	CAD-C3D-C4D	-7.09	112.35	124.70
32	v	5552	HEM	CAD-C3D-C4D	-7.02	112.46	124.70
26	a	212	SQD	O6-C1-C2	6.87	118.71	108.27
24	D	357	BCR	C38-C26-C25	6.71	131.80	124.48
24	X	130	BCR	C33-C5-C6	6.70	131.79	124.48
24	T	5104	BCR	C38-C26-C25	6.67	131.77	124.48
26	A	5212	SQD	O6-C1-C2	6.64	118.36	108.27
24	d	5357	BCR	C33-C5-C6	6.51	131.58	124.48
24	c	5505	BCR	C38-C26-C25	6.48	131.55	124.48
24	d	5357	BCR	C38-C26-C25	6.46	131.54	124.48
24	B	529	BCR	C38-C26-C25	6.44	131.51	124.48
24	x	5130	BCR	C33-C5-C6	6.41	131.48	124.48
24	t	104	BCR	C38-C26-C25	6.33	131.39	124.48
24	D	357	BCR	C33-C5-C6	6.17	131.22	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	567	LHG	C25-C24-C23	6.12	136.10	113.69
26	d	5358	SQD	C25-C24-C23	6.11	136.09	113.69
24	B	527	BCR	C38-C26-C25	6.06	131.09	124.48
26	A	568	SQD	C10-C9-C8	6.02	135.25	113.13
25	a	5567	LHG	C25-C24-C23	6.02	135.74	113.69
24	B	528	BCR	C38-C26-C25	5.97	131.00	124.48
26	t	213	SQD	C10-C9-C8	5.97	135.07	113.13
24	C	505	BCR	C38-C26-C25	5.97	131.00	124.48
26	d	5358	SQD	C10-C9-C8	5.96	135.02	113.13
26	L	5213	SQD	C10-C9-C8	5.94	134.96	113.13
24	C	506	BCR	C38-C26-C25	5.88	130.90	124.48
24	h	5107	BCR	C38-C26-C25	5.85	130.87	124.48
26	t	213	SQD	C25-C24-C23	5.83	135.06	113.69
24	c	5506	BCR	C38-C26-C25	5.76	130.77	124.48
24	B	527	BCR	C33-C5-C6	5.76	130.77	124.48
26	L	5213	SQD	C25-C24-C23	5.75	134.76	113.69
26	A	568	SQD	C25-C24-C23	5.74	134.74	113.69
24	A	566	BCR	C33-C5-C6	5.73	130.73	124.48
24	C	504	BCR	C38-C26-C25	5.72	130.73	124.48
24	b	5527	BCR	C33-C5-C6	5.70	130.71	124.48
24	b	5528	BCR	C38-C26-C25	5.69	130.70	124.48
24	t	104	BCR	C33-C5-C6	5.69	130.70	124.48
24	T	5104	BCR	C33-C5-C6	5.69	130.69	124.48
24	X	130	BCR	C7-C8-C9	5.67	134.63	126.23
24	a	5566	BCR	C38-C26-C25	5.64	130.63	124.48
24	b	5529	BCR	C38-C26-C25	5.63	130.63	124.48
24	A	566	BCR	C38-C26-C25	5.63	130.62	124.48
24	B	529	BCR	C33-C5-C6	5.60	130.59	124.48
24	a	5566	BCR	C33-C5-C6	5.58	130.57	124.48
24	H	107	BCR	C38-C26-C25	5.57	130.56	124.48
24	x	5130	BCR	C7-C8-C9	5.52	134.40	126.23
24	c	5504	BCR	C38-C26-C25	5.52	130.51	124.48
24	b	5527	BCR	C38-C26-C25	5.50	130.49	124.48
24	C	506	BCR	C33-C5-C6	5.50	130.48	124.48
24	C	505	BCR	C33-C5-C6	5.43	130.41	124.48
24	X	130	BCR	C11-C10-C9	5.40	134.85	127.28
24	x	5130	BCR	C38-C26-C25	5.39	130.36	124.48
24	c	5506	BCR	C33-C5-C6	5.38	130.35	124.48
22	d	5356	PQ9	C11-C2-C1	5.35	121.32	116.91
20	B	515	CLA	CAA-C2A-C3A	-5.34	98.56	113.00
24	X	130	BCR	C38-C26-C25	5.32	130.29	124.48
32	f	5051	HEM	CHA-C4D-ND	5.30	130.92	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	H	107	BCR	C33-C5-C6	5.17	130.13	124.48
24	c	5505	BCR	C33-C5-C6	5.11	130.06	124.48
24	b	5529	BCR	C33-C5-C6	5.08	130.03	124.48
24	h	5107	BCR	C33-C5-C6	5.04	129.99	124.48
20	b	5515	CLA	CAA-C2A-C3A	-5.01	99.47	113.00
32	V	552	HEM	CHA-C4D-ND	4.98	130.53	124.37
24	C	504	BCR	C33-C5-C6	4.98	129.92	124.48
22	D	356	PQ9	C11-C2-C1	4.95	120.98	116.91
24	b	5528	BCR	C33-C5-C6	4.94	129.88	124.48
24	x	5130	BCR	C11-C10-C9	4.93	134.19	127.28
26	A	568	SQD	O7-S-C6	4.88	114.04	106.76
24	T	5104	BCR	C29-C30-C25	4.79	117.39	110.44
32	v	5552	HEM	CHA-C4D-ND	4.74	130.23	124.37
24	c	5504	BCR	C33-C5-C6	4.72	129.64	124.48
24	B	528	BCR	C33-C5-C6	4.69	129.60	124.48
26	a	212	SQD	O7-S-C6	4.63	113.66	106.76
20	C	494	CLA	CED-O2D-CGD	4.56	126.25	115.92
24	b	5529	BCR	C29-C30-C25	4.47	116.94	110.44
24	c	5505	BCR	C23-C24-C25	4.47	138.93	127.00
21	A	561	PHO	O2D-CGD-CBD	4.46	115.84	110.95
26	A	568	SQD	O8-S-C6	-4.40	97.49	105.97
24	C	505	BCR	C23-C24-C25	4.39	138.71	127.00
21	A	561	PHO	C1-C2-C3	4.37	133.36	126.20
24	t	104	BCR	C29-C30-C25	4.37	116.79	110.44
24	C	506	BCR	C8-C7-C6	4.34	138.60	127.00
26	a	212	SQD	C44-O6-C1	4.33	123.07	113.80
30	c	5508	DGD	C3G-O3G-C1D	-4.32	104.53	113.80
24	X	130	BCR	C8-C9-C10	-4.32	112.22	119.01
28	D	360	MGE	O6D-C5D-C6D	4.29	117.08	106.44
24	x	5130	BCR	C8-C9-C10	-4.26	112.31	119.01
21	A	562	PHO	O2D-CGD-CBD	4.23	115.60	110.95
24	d	5357	BCR	C29-C30-C25	4.21	116.56	110.44
24	x	5130	BCR	C29-C30-C25	4.18	116.50	110.44
24	x	5130	BCR	C23-C24-C25	4.17	138.13	127.00
32	F	51	HEM	CHA-C4D-ND	4.17	129.52	124.37
24	X	130	BCR	C23-C24-C25	4.16	138.10	127.00
20	c	5494	CLA	CED-O2D-CGD	4.15	125.33	115.92
32	F	51	HEM	CBD-CAD-C3D	-4.15	101.06	112.53
26	a	212	SQD	O8-S-C6	-4.14	97.98	105.97
20	b	5526	CLA	CED-O2D-CGD	4.12	125.26	115.92
30	h	5208	DGD	O3G-C1D-C2D	4.12	114.53	108.27
24	h	5107	BCR	C29-C30-C25	4.11	116.41	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	509	DGD	O6D-C5D-C6D	4.11	114.84	106.69
24	X	130	BCR	C2-C1-C6	4.10	116.40	110.44
24	c	5506	BCR	C8-C7-C6	4.10	137.95	127.00
26	d	5358	SQD	O8-S-C6	-4.09	98.07	105.97
20	c	5502	CLA	CAA-C2A-C3A	-4.09	101.96	113.00
24	t	104	BCR	C8-C7-C6	4.06	137.84	127.00
20	C	495	CLA	CAA-C2A-C3A	-4.06	102.03	113.00
21	a	5561	PHO	O2D-CGD-CBD	4.05	115.40	110.95
20	C	497	CLA	C7-C6-C5	-4.05	102.48	113.26
20	c	5495	CLA	CAA-C2A-C3A	-4.04	102.09	113.00
26	t	213	SQD	O7-S-C6	4.03	112.78	106.76
20	B	511	CLA	CAA-C2A-C3A	-4.03	107.00	116.23
20	b	5511	CLA	CAA-C2A-C3A	-4.02	107.01	116.23
28	L	210	MGE	C3G-O3G-C1D	-4.02	105.18	113.80
24	X	130	BCR	C29-C30-C25	4.01	116.27	110.44
28	D	360	MGE	O2G-C1B-C2B	4.01	120.16	111.48
28	l	5210	MGE	C3G-O3G-C1D	-4.01	105.20	113.80
24	C	505	BCR	C2-C1-C6	4.01	116.26	110.44
24	C	505	BCR	C29-C30-C25	4.00	116.25	110.44
30	c	5509	DGD	O6D-C5D-C6D	4.00	114.62	106.69
24	c	5505	BCR	C29-C30-C25	4.00	116.25	110.44
24	b	5528	BCR	C29-C30-C25	4.00	116.24	110.44
20	C	494	CLA	CAA-C2A-C3A	-3.99	102.21	113.00
24	a	5566	BCR	C29-C30-C25	3.98	116.22	110.44
24	x	5130	BCR	C2-C1-C6	3.97	116.21	110.44
20	D	354	CLA	C1-C2-C3	3.97	132.70	126.20
26	L	5213	SQD	O48-C23-C24	3.97	123.94	111.83
24	B	528	BCR	C30-C25-C26	-3.96	117.23	122.64
32	f	5051	HEM	CBD-CAD-C3D	-3.95	101.61	112.53
26	d	5358	SQD	O7-S-C6	3.95	112.66	106.76
26	A	5212	SQD	O7-S-C6	3.95	112.66	106.76
20	c	5493	CLA	CAA-C2A-C3A	-3.95	102.32	113.00
24	b	5529	BCR	C2-C1-C6	3.95	116.17	110.44
20	c	5494	CLA	CAA-C2A-C3A	-3.95	102.33	113.00
24	C	504	BCR	C24-C23-C22	3.95	132.07	126.23
20	C	493	CLA	CAA-C2A-C3A	-3.93	102.37	113.00
26	d	5358	SQD	C31-C30-C29	3.93	134.21	114.37
26	t	213	SQD	O48-C23-C24	3.92	123.78	111.83
24	b	5528	BCR	C2-C1-C6	3.91	116.12	110.44
30	H	208	DGD	O3G-C1D-C2D	3.91	114.21	108.27
26	A	5212	SQD	C44-O6-C1	3.91	122.17	113.80
30	C	508	DGD	C3G-O3G-C1D	-3.91	105.42	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	d	5361	MGE	O6D-C5D-C6D	3.90	116.12	106.44
24	T	5104	BCR	C8-C7-C6	3.90	137.42	127.00
24	A	566	BCR	C29-C30-C25	3.90	116.10	110.44
20	C	502	CLA	CAA-C2A-C3A	-3.90	102.47	113.00
28	d	5361	MGE	O2G-C1B-C2B	3.89	119.90	111.48
24	D	357	BCR	C2-C1-C6	3.85	116.04	110.44
24	H	107	BCR	C29-C30-C25	3.85	116.03	110.44
20	b	5519	CLA	CED-O2D-CGD	3.84	124.63	115.92
26	A	568	SQD	C31-C30-C29	3.84	133.77	114.37
24	B	529	BCR	C29-C30-C25	3.83	116.00	110.44
20	c	5497	CLA	C7-C6-C5	-3.82	103.09	113.26
24	B	529	BCR	C2-C1-C6	3.81	115.98	110.44
24	d	5357	BCR	C30-C25-C26	-3.81	117.42	122.64
24	T	5104	BCR	C30-C25-C26	-3.81	117.43	122.64
24	c	5506	BCR	C29-C30-C25	3.81	115.97	110.44
24	T	5104	BCR	C24-C23-C22	3.80	131.85	126.23
24	T	5104	BCR	C33-C5-C4	-3.79	105.51	113.60
32	v	5552	HEM	C2A-C1A-NA	-3.79	105.94	110.15
24	d	5357	BCR	C1-C6-C5	-3.79	117.46	122.64
27	a	5568	LMT	C1-O1'-C1'	-3.79	107.21	113.68
20	c	5491	CLA	CED-O2D-CGD	3.79	124.50	115.92
24	T	5104	BCR	C38-C26-C27	-3.78	105.53	113.60
24	c	5504	BCR	C24-C23-C22	3.78	131.83	126.23
25	A	567	LHG	O8-C23-C24	3.78	123.35	111.83
32	v	5552	HEM	CBD-CAD-C3D	-3.77	102.11	112.53
26	A	5212	SQD	C45-O47-C7	3.77	124.50	117.85
26	A	568	SQD	C11-C10-C9	3.76	133.38	114.37
24	x	5130	BCR	C33-C5-C4	-3.76	105.58	113.60
24	B	529	BCR	C38-C26-C27	-3.76	105.58	113.60
20	b	5520	CLA	C7-C6-C5	-3.76	103.25	113.26
27	A	569	LMT	C1-O1'-C1'	-3.75	107.27	113.68
20	C	496	CLA	CED-O2D-CGD	3.75	124.42	115.92
22	d	5356	PQ9	C11-C2-C3	-3.75	118.97	123.39
24	D	357	BCR	C38-C26-C27	-3.74	105.62	113.60
24	C	506	BCR	C23-C24-C25	3.74	136.99	127.00
24	d	5357	BCR	C38-C26-C27	-3.74	105.63	113.60
20	B	518	CLA	O2A-CGA-CBA	3.73	123.22	111.83
24	h	5107	BCR	C11-C10-C9	3.73	132.51	127.28
24	C	506	BCR	C2-C1-C6	3.73	115.86	110.44
20	c	5492	CLA	CED-O2D-CGD	3.73	124.37	115.92
24	d	5357	BCR	C2-C1-C6	3.73	115.85	110.44
24	H	107	BCR	C11-C10-C9	3.72	132.50	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	5504	BCR	C1-C6-C5	-3.72	117.55	122.64
30	C	508	DGD	O5D-C1E-C2E	3.72	113.92	108.27
24	D	357	BCR	C1-C6-C5	-3.72	117.56	122.64
20	c	5503	CLA	CED-O2D-CGD	3.71	124.34	115.92
22	A	564	PQ9	C11-C12-C13	-3.71	120.43	126.83
20	b	5518	CLA	O2A-CGA-CBA	3.71	123.15	111.83
21	a	5562	PHO	C7-C6-C5	-3.71	103.37	113.26
26	d	5358	SQD	O48-C23-C24	3.70	123.12	111.83
26	t	213	SQD	O8-S-C6	-3.70	98.83	105.97
24	H	107	BCR	C30-C25-C26	-3.70	117.58	122.64
24	C	504	BCR	C1-C6-C5	-3.70	117.59	122.64
24	D	357	BCR	C33-C5-C4	-3.69	105.72	113.60
24	c	5505	BCR	C2-C1-C6	3.69	115.80	110.44
24	X	130	BCR	C33-C5-C4	-3.69	105.73	113.60
26	t	213	SQD	C11-C10-C9	3.69	133.00	114.37
24	D	357	BCR	C30-C25-C26	-3.68	117.60	122.64
21	a	5562	PHO	O2D-CGD-CBD	3.68	114.99	110.95
26	d	5358	SQD	C11-C10-C9	3.68	132.98	114.37
24	h	5107	BCR	C23-C24-C25	3.68	136.82	127.00
20	B	513	CLA	CAA-C2A-C3A	-3.68	103.06	113.00
20	b	5516	CLA	O2A-CGA-CBA	3.67	123.03	111.83
24	C	506	BCR	C29-C30-C25	3.67	115.77	110.44
24	b	5528	BCR	C30-C25-C26	-3.67	117.63	122.64
24	b	5527	BCR	C2-C1-C6	3.66	115.76	110.44
24	t	104	BCR	C33-C5-C4	-3.65	105.81	113.60
20	C	497	CLA	C1-C2-C3	3.65	132.17	126.20
20	B	517	CLA	C1-C2-C3	3.64	132.16	126.20
24	c	5506	BCR	C30-C25-C26	-3.64	117.67	122.64
24	d	5357	BCR	C33-C5-C4	-3.63	105.85	113.60
30	h	5208	DGD	C1E-O6E-C5E	3.63	120.81	113.72
20	a	5560	CLA	CAA-C2A-C3A	-3.63	103.19	113.00
24	x	5130	BCR	C16-C17-C18	3.63	132.36	127.28
28	d	5360	MGE	O6D-C5D-C6D	3.63	115.42	106.44
26	a	212	SQD	C45-O47-C7	3.62	124.24	117.85
22	D	356	PQ9	C11-C2-C3	-3.62	119.12	123.39
24	C	504	BCR	C38-C26-C27	-3.60	105.91	113.60
20	A	560	CLA	CAA-C2A-C3A	-3.60	103.26	113.00
24	t	104	BCR	C30-C25-C26	-3.60	117.71	122.64
24	X	130	BCR	C30-C25-C26	-3.60	117.71	122.64
24	x	5130	BCR	C30-C25-C26	-3.60	117.72	122.64
20	B	517	CLA	O2A-CGA-CBA	3.60	122.80	111.83
20	C	492	CLA	CED-O2D-CGD	3.59	124.07	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	5521	CLA	C7-C6-C5	-3.59	103.69	113.26
24	c	5504	BCR	C2-C1-C6	3.59	115.65	110.44
24	C	505	BCR	C33-C5-C4	-3.59	105.95	113.60
24	D	357	BCR	C29-C30-C25	3.58	115.64	110.44
21	a	5561	PHO	C1-C2-C3	3.58	132.06	126.20
22	d	5356	PQ9	C24-C23-C25	3.57	121.42	115.23
24	C	506	BCR	C38-C26-C27	-3.57	105.99	113.60
24	H	107	BCR	C23-C24-C25	3.56	136.52	127.00
28	d	5359	MGE	O2G-C1B-C2B	3.56	119.19	111.48
24	D	357	BCR	C23-C24-C25	3.56	136.51	127.00
20	B	521	CLA	C7-C6-C5	-3.56	103.78	113.26
30	C	507	DGD	C1E-O6E-C5E	3.56	120.66	113.72
24	a	5566	BCR	C30-C25-C26	-3.55	117.78	122.64
24	H	107	BCR	C38-C26-C27	-3.55	106.03	113.60
24	B	528	BCR	C2-C1-C6	3.54	115.59	110.44
20	B	520	CLA	C7-C6-C5	-3.54	103.82	113.26
24	b	5527	BCR	C23-C24-C25	3.54	136.46	127.00
20	B	516	CLA	C1-C2-C3	3.54	131.99	126.20
24	h	5107	BCR	C30-C25-C26	-3.53	117.81	122.64
25	a	5567	LHG	O8-C23-C24	3.53	122.60	111.83
30	c	5508	DGD	O2G-C1B-C2B	3.53	119.11	111.48
20	A	558	CLA	C1-C2-C3	3.53	131.97	126.20
26	A	568	SQD	O48-C23-C24	3.52	122.58	111.83
24	B	528	BCR	C38-C26-C27	-3.52	106.08	113.60
26	L	5213	SQD	C11-C10-C9	3.52	132.18	114.37
20	c	5500	CLA	C7-C6-C5	-3.52	103.88	113.26
24	B	528	BCR	C29-C30-C25	3.52	115.55	110.44
24	h	5107	BCR	C8-C7-C6	3.51	136.37	127.00
20	c	5501	CLA	C7-C6-C5	-3.51	103.91	113.26
20	c	5496	CLA	CED-O2D-CGD	3.51	123.87	115.92
32	V	552	HEM	C2A-C1A-NA	-3.50	106.27	110.15
20	c	5493	CLA	CED-O2D-CGD	3.50	123.85	115.92
26	A	5212	SQD	O8-S-C6	-3.50	99.22	105.97
24	C	504	BCR	C2-C1-C6	3.49	115.51	110.44
20	b	5513	CLA	CAA-C2A-C3A	-3.49	103.57	113.00
24	C	504	BCR	C33-C5-C4	-3.49	106.16	113.60
20	B	516	CLA	O2A-CGA-CBA	3.48	122.46	111.83
24	A	566	BCR	C30-C25-C26	-3.48	117.88	122.64
32	V	552	HEM	CBD-CAD-C3D	-3.48	102.91	112.53
24	b	5528	BCR	C23-C24-C25	3.48	136.29	127.00
22	D	356	PQ9	C24-C23-C25	3.48	121.26	115.23
32	v	5552	HEM	CBC-CAC-C3C	-3.48	110.16	127.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	H	107	BCR	C2-C1-C6	3.47	115.48	110.44
24	B	528	BCR	C23-C24-C25	3.47	136.26	127.00
20	C	503	CLA	CED-O2D-CGD	3.46	123.78	115.92
30	c	5508	DGD	O5D-C1E-C2E	3.46	113.53	108.27
20	B	519	CLA	CED-O2D-CGD	3.46	123.77	115.92
24	B	529	BCR	C23-C24-C25	3.46	136.24	127.00
20	b	5512	CLA	CAA-C2A-C3A	-3.46	103.65	113.00
20	B	526	CLA	CED-O2D-CGD	3.46	123.76	115.92
20	b	5516	CLA	CED-O2D-CGD	3.45	123.75	115.92
20	a	5558	CLA	CED-O2D-CGD	3.45	123.74	115.92
24	b	5529	BCR	C30-C25-C26	-3.45	117.93	122.64
24	c	5506	BCR	C23-C24-C25	3.45	136.21	127.00
24	C	506	BCR	C33-C5-C4	-3.44	106.25	113.60
20	b	5511	CLA	CMA-C3A-C2A	-3.44	108.33	116.23
20	b	5517	CLA	O2A-CGA-CBA	3.44	122.33	111.83
24	B	529	BCR	C30-C25-C26	-3.44	117.94	122.64
24	c	5506	BCR	C38-C26-C27	-3.44	106.27	113.60
20	b	5526	CLA	CAA-C2A-C3A	-3.43	103.72	113.00
30	c	5509	DGD	C1E-O6E-C5E	3.43	120.42	113.72
20	d	5355	CLA	C1-C2-C3	3.43	132.32	126.76
30	C	507	DGD	O6D-C5D-C6D	3.43	113.50	106.69
30	c	5507	DGD	O6D-C5D-C6D	3.43	113.49	106.69
24	c	5504	BCR	C38-C26-C27	-3.42	106.30	113.60
24	c	5506	BCR	C2-C1-C6	3.42	115.41	110.44
20	C	502	CLA	O2A-CGA-CBA	3.41	122.24	111.83
20	d	5354	CLA	CAA-C2A-C3A	-3.41	103.78	113.00
24	A	566	BCR	C38-C26-C27	-3.40	106.34	113.60
24	b	5527	BCR	C38-C26-C27	-3.40	106.35	113.60
20	B	522	CLA	O2A-CGA-CBA	3.40	122.19	111.83
24	b	5529	BCR	C23-C24-C25	3.40	136.07	127.00
24	A	566	BCR	C33-C5-C4	-3.39	106.37	113.60
24	a	5566	BCR	C38-C26-C27	-3.39	106.37	113.60
24	h	5107	BCR	C38-C26-C27	-3.39	106.37	113.60
28	B	530	MGE	C3G-O3G-C1D	-3.39	106.53	113.80
20	a	5559	CLA	CED-O2D-CGD	3.38	123.59	115.92
30	C	508	DGD	O2G-C1B-C2B	3.38	118.80	111.48
20	B	512	CLA	CAA-C2A-C3A	-3.38	103.86	113.00
24	c	5505	BCR	C38-C26-C27	-3.38	106.39	113.60
24	c	5506	BCR	C33-C5-C4	-3.38	106.39	113.60
20	B	513	CLA	O2A-CGA-CBA	3.38	122.13	111.83
24	C	504	BCR	C29-C30-C25	3.37	115.34	110.44
24	h	5107	BCR	C2-C1-C6	3.37	115.34	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	a	5566	BCR	C24-C23-C22	3.37	131.22	126.23
21	A	562	PHO	C7-C6-C5	-3.37	104.28	113.26
24	C	504	BCR	C30-C25-C26	-3.36	118.04	122.64
20	B	511	CLA	CMA-C3A-C2A	-3.36	108.53	116.23
20	c	5502	CLA	O2A-CGA-CBA	3.36	122.07	111.83
20	d	5354	CLA	C1-C2-C3	3.35	131.69	126.20
30	C	509	DGD	C1E-O6E-C5E	3.35	120.27	113.72
20	c	5493	CLA	O2A-CGA-CBA	3.35	122.06	111.83
20	C	493	CLA	O2A-CGA-CBA	3.35	122.06	111.83
21	A	561	PHO	CED-O2D-CGD	3.35	123.51	115.92
30	h	5208	DGD	O6D-C5D-C6D	3.35	113.33	106.69
24	D	357	BCR	C8-C7-C6	3.34	135.93	127.00
20	b	5517	CLA	C1-C2-C3	3.34	131.67	126.20
30	H	208	DGD	O2G-C1B-C2B	3.34	118.71	111.48
24	B	527	BCR	C2-C1-C6	3.34	115.29	110.44
28	i	5201	MGE	O2G-C1B-C2B	3.34	118.70	111.48
28	I	201	MGE	O2G-C1B-C2B	3.34	118.70	111.48
20	b	5513	CLA	O2A-CGA-CBA	3.34	122.01	111.83
30	C	508	DGD	C3G-C2G-C1G	-3.34	104.00	111.78
24	c	5505	BCR	C33-C5-C4	-3.34	106.48	113.60
20	c	5497	CLA	O2A-CGA-CBA	3.34	122.00	111.83
24	B	527	BCR	C38-C26-C27	-3.33	106.49	113.60
24	C	506	BCR	C30-C25-C26	-3.33	118.08	122.64
24	d	5357	BCR	C24-C23-C22	3.33	131.16	126.23
24	X	130	BCR	C38-C26-C27	-3.33	106.49	113.60
24	t	104	BCR	C24-C23-C22	3.33	131.16	126.23
21	a	5562	PHO	O2A-CGA-CBA	3.33	121.98	111.83
24	b	5529	BCR	C38-C26-C27	-3.32	106.51	113.60
24	b	5527	BCR	C33-C5-C4	-3.32	106.52	113.60
20	A	559	CLA	CAA-C2A-C3A	-3.32	104.04	113.00
20	b	5522	CLA	C7-C6-C5	-3.32	104.42	113.26
24	H	107	BCR	C1-C6-C5	-3.31	118.11	122.64
20	b	5512	CLA	CED-O2D-CGD	3.31	123.43	115.92
24	H	107	BCR	C33-C5-C4	-3.31	106.53	113.60
24	t	104	BCR	C38-C26-C27	-3.31	106.54	113.60
24	x	5130	BCR	C12-C13-C14	-3.31	113.81	119.01
24	d	5357	BCR	C23-C24-C25	3.31	135.83	127.00
24	B	527	BCR	C33-C5-C4	-3.30	106.55	113.60
32	V	552	HEM	CBC-CAC-C3C	-3.30	111.03	127.53
20	D	354	CLA	CAA-C2A-C3A	-3.30	104.08	113.00
28	D	359	MGE	O6D-C5D-C6D	3.30	114.62	106.44
21	A	562	PHO	O2A-CGA-CBA	3.30	121.89	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	5528	BCR	C1-C6-C5	-3.30	118.13	122.64
24	h	5107	BCR	C1-C6-C5	-3.29	118.14	122.64
28	B	530	MGE	O2G-C1B-C2B	3.29	118.60	111.48
24	x	5130	BCR	C38-C26-C27	-3.29	106.58	113.60
20	a	5559	CLA	CAA-C2A-C3A	-3.29	104.11	113.00
24	A	566	BCR	C24-C23-C22	3.29	131.10	126.23
28	D	359	MGE	O2G-C1B-C2B	3.29	118.59	111.48
24	H	107	BCR	C8-C7-C6	3.28	135.76	127.00
28	D	358	MGE	O2G-C1B-C2B	3.28	118.58	111.48
30	c	5508	DGD	C3G-C2G-C1G	-3.28	104.14	111.78
24	B	527	BCR	C23-C24-C25	3.28	135.75	127.00
20	b	5515	CLA	O2A-CGA-CBA	3.27	121.81	111.83
20	A	563	CLA	C1-C2-C3	3.27	131.55	126.20
24	b	5529	BCR	C33-C5-C4	-3.27	106.63	113.60
24	b	5527	BCR	C29-C30-C25	3.27	115.18	110.44
20	C	501	CLA	C7-C6-C5	-3.26	104.56	113.26
28	l	5210	MGE	O6D-C5D-C6D	3.26	114.52	106.44
20	b	5522	CLA	O2A-CGA-CBA	3.26	121.77	111.83
24	B	527	BCR	C30-C25-C26	-3.25	118.19	122.64
26	d	5358	SQD	C45-O47-C7	3.25	125.58	117.80
20	C	496	CLA	C1-C2-C3	3.25	131.52	126.20
24	B	529	BCR	C33-C5-C4	-3.24	106.69	113.60
24	b	5529	BCR	C1-C6-C5	-3.24	118.21	122.64
24	b	5529	BCR	C8-C7-C6	3.24	135.65	127.00
24	A	566	BCR	C23-C24-C25	3.24	135.65	127.00
28	b	5530	MGE	O2G-C1B-C2B	3.24	118.48	111.48
30	C	507	DGD	O2G-C1B-C2B	3.24	118.48	111.48
20	c	5497	CLA	C1-C2-C3	3.23	131.49	126.20
20	B	526	CLA	CAA-C2A-C3A	-3.23	104.27	113.00
24	B	527	BCR	C29-C30-C25	3.23	115.13	110.44
24	a	5566	BCR	C33-C5-C4	-3.23	106.72	113.60
22	a	5564	PQ9	C11-C12-C13	-3.22	121.28	126.83
20	b	5516	CLA	C1-C2-C3	3.22	131.48	126.20
24	H	107	BCR	C15-C14-C13	3.22	131.80	127.28
24	x	5130	BCR	C1-C6-C5	-3.22	118.23	122.64
32	f	5051	HEM	CHA-C4D-C3D	-3.22	119.29	125.23
24	d	5357	BCR	C8-C7-C6	3.22	135.60	127.00
20	c	5502	CLA	CED-O2D-CGD	3.22	123.22	115.92
20	B	524	CLA	CED-O2D-CGD	3.21	123.20	115.92
24	C	505	BCR	C16-C17-C18	3.21	131.78	127.28
24	c	5504	BCR	C33-C5-C4	-3.21	106.76	113.60
20	b	5515	CLA	CED-O2D-CGD	3.20	123.18	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	506	BCR	C35-C13-C12	3.20	122.98	118.09
24	X	130	BCR	C1-C6-C5	-3.20	118.27	122.64
24	c	5504	BCR	C32-C1-C6	3.19	115.25	110.24
20	D	355	CLA	C1-C2-C3	3.19	131.93	126.76
24	c	5505	BCR	C35-C13-C12	3.19	122.96	118.09
32	f	5051	HEM	C2A-C1A-NA	-3.19	106.62	110.15
24	a	5566	BCR	C23-C24-C25	3.19	135.51	127.00
24	b	5527	BCR	C1-C6-C5	-3.18	118.28	122.64
20	C	491	CLA	CED-O2D-CGD	3.18	123.13	115.92
20	C	497	CLA	O2A-CGA-CBA	3.18	121.53	111.83
21	A	561	PHO	C4A-C3A-C2A	3.18	105.87	102.84
21	A	562	PHO	C4A-C3A-C2A	3.18	105.87	102.84
30	c	5507	DGD	O2G-C1B-C2B	3.18	118.35	111.48
24	H	107	BCR	C24-C23-C22	3.17	130.93	126.23
30	h	5208	DGD	O2G-C1B-C2B	3.17	118.34	111.48
24	t	104	BCR	C2-C1-C6	3.17	115.04	110.44
20	C	495	CLA	C7-C6-C5	-3.17	104.83	113.26
30	c	5508	DGD	C1E-O6E-C5E	3.16	119.90	113.72
24	h	5107	BCR	C33-C5-C4	-3.16	106.86	113.60
24	c	5504	BCR	C23-C24-C25	3.16	135.44	127.00
24	h	5107	BCR	C32-C1-C6	3.16	115.20	110.24
24	C	506	BCR	C16-C17-C18	3.16	131.71	127.28
24	x	5130	BCR	C34-C9-C8	3.16	122.91	118.09
20	B	518	CLA	CED-O2D-CGD	3.15	123.07	115.92
20	b	5520	CLA	O2A-CGA-CBA	3.15	121.45	111.83
20	d	5354	CLA	O2A-CGA-CBA	3.15	121.45	111.83
24	B	528	BCR	C8-C7-C6	3.15	135.42	127.00
20	a	5558	CLA	C7-C6-C5	-3.15	104.87	113.26
20	B	525	CLA	C7-C6-C5	-3.15	104.87	113.26
30	c	5507	DGD	C1E-O6E-C5E	3.15	119.87	113.72
24	C	504	BCR	C23-C24-C25	3.15	135.40	127.00
20	b	5514	CLA	O2A-CGA-CBA	3.14	121.42	111.83
24	b	5528	BCR	C38-C26-C27	-3.14	106.90	113.60
21	a	5561	PHO	C7-C6-C5	-3.14	104.89	113.26
24	B	529	BCR	C1-C6-C5	-3.14	118.34	122.64
20	c	5491	CLA	O2A-CGA-CBA	3.14	121.41	111.83
24	C	505	BCR	C38-C26-C27	-3.14	106.90	113.60
20	B	522	CLA	C7-C6-C5	-3.14	104.90	113.26
24	b	5528	BCR	C33-C5-C4	-3.14	106.91	113.60
26	L	5213	SQD	O8-S-C6	-3.13	99.93	105.97
28	I	201	MGE	O6D-C5D-C6D	3.13	114.19	106.44
20	a	5563	CLA	C1-C2-C3	3.13	131.32	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	L	210	MGE	O6D-C5D-C6D	3.13	114.19	106.44
20	B	522	CLA	CED-O2D-CGD	3.12	123.00	115.92
28	b	5530	MGE	C3G-O3G-C1D	-3.12	107.10	113.80
20	b	5522	CLA	CED-O2D-CGD	3.12	123.00	115.92
24	B	529	BCR	C24-C23-C22	3.12	130.85	126.23
20	B	516	CLA	CED-O2D-CGD	3.12	122.99	115.92
24	c	5504	BCR	C29-C30-C25	3.11	114.96	110.44
20	B	512	CLA	CED-O2D-CGD	3.11	122.97	115.92
30	C	507	DGD	O5D-C1E-C2E	3.11	112.99	108.27
20	c	5493	CLA	C7-C6-C5	-3.10	104.99	113.26
20	A	558	CLA	C7-C6-C5	-3.10	104.99	113.26
20	B	520	CLA	CED-O2D-CGD	3.10	122.95	115.92
24	c	5504	BCR	C30-C25-C26	-3.10	118.40	122.64
32	F	51	HEM	CAB-C3B-C2B	-3.10	118.36	128.43
30	c	5509	DGD	O2G-C1B-C2B	3.09	118.18	111.48
20	C	493	CLA	CED-O2D-CGD	3.09	122.94	115.92
20	c	5495	CLA	CBA-CAA-C2A	3.09	123.00	113.79
20	B	521	CLA	CED-O2D-CGD	3.09	122.93	115.92
24	X	130	BCR	C34-C9-C8	3.09	122.81	118.09
24	c	5505	BCR	C1-C6-C5	-3.09	118.41	122.64
28	d	5360	MGE	O2G-C1B-C2B	3.09	118.16	111.48
32	F	51	HEM	C2A-C1A-NA	-3.09	106.73	110.15
30	H	208	DGD	O6D-C5D-C6D	3.09	112.81	106.69
24	B	527	BCR	C35-C13-C12	3.09	122.80	118.09
26	A	568	SQD	C32-C31-C30	3.08	129.96	114.37
20	C	495	CLA	O2A-CGA-CBA	3.08	121.23	111.83
20	B	518	CLA	CAA-C2A-C3A	-3.08	104.67	113.00
24	b	5528	BCR	C8-C7-C6	3.08	135.22	127.00
24	h	5107	BCR	C24-C23-C22	3.08	130.79	126.23
24	H	107	BCR	C12-C13-C14	-3.08	114.17	119.01
20	b	5524	CLA	CED-O2D-CGD	3.08	122.90	115.92
24	t	104	BCR	C11-C10-C9	3.08	131.59	127.28
20	c	5493	CLA	C1-C2-C3	3.07	131.23	126.20
20	c	5500	CLA	C1-C2-C3	3.07	131.23	126.20
32	f	5051	HEM	CAB-C3B-C2B	-3.07	118.45	128.43
20	C	495	CLA	CBA-CAA-C2A	3.07	122.93	113.79
21	a	5561	PHO	CED-O2D-CGD	3.06	122.86	115.92
24	t	104	BCR	C35-C13-C12	3.06	122.77	118.09
20	c	5495	CLA	C7-C6-C5	-3.06	105.10	113.26
30	C	509	DGD	O2G-C1B-C2B	3.06	118.10	111.48
21	a	5562	PHO	C4A-C3A-C2A	3.06	105.75	102.84
21	a	5562	PHO	CED-O2D-CGD	3.06	122.85	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	502	CLA	CED-O2D-CGD	3.06	122.85	115.92
30	C	508	DGD	C1E-O6E-C5E	3.05	119.68	113.72
20	d	5355	CLA	CED-O2D-CGD	3.05	122.83	115.92
20	b	5512	CLA	O2A-CGA-CBA	3.05	121.13	111.83
20	c	5496	CLA	C1-C2-C3	3.05	131.19	126.20
24	C	506	BCR	C1-C6-C5	-3.03	118.49	122.64
20	c	5498	CLA	CAA-C2A-C3A	-3.03	104.80	113.00
30	c	5507	DGD	O5D-C1E-C2E	3.03	112.88	108.27
20	a	5563	CLA	CED-O2D-CGD	3.03	122.79	115.92
24	B	529	BCR	C8-C7-C6	3.03	135.09	127.00
20	C	500	CLA	C7-C6-C5	-3.03	105.19	113.26
24	c	5504	BCR	C1-C6-C7	3.03	123.86	115.65
20	C	493	CLA	C7-C6-C5	-3.03	105.20	113.26
25	A	567	LHG	O7-C7-C8	3.02	118.02	111.48
20	c	5496	CLA	CAA-C2A-C3A	-3.02	104.83	113.00
20	D	354	CLA	O2A-CGA-CBA	3.02	121.05	111.83
20	b	5525	CLA	O2A-CGA-CBA	3.02	121.04	111.83
20	b	5518	CLA	CAA-C2A-C3A	-3.02	104.85	113.00
20	C	496	CLA	O2A-CGA-CBA	3.01	121.03	111.83
30	H	208	DGD	C1E-O6E-C5E	3.01	119.60	113.72
24	B	528	BCR	C1-C6-C5	-3.00	118.53	122.64
20	b	5526	CLA	C1-O2A-CGA	3.00	123.92	116.65
20	B	520	CLA	O2A-CGA-CBA	3.00	120.98	111.83
20	C	495	CLA	C1-C2-C3	3.00	131.11	126.20
26	t	213	SQD	C44-O6-C1	3.00	120.23	113.80
26	A	5212	SQD	C3-C4-C5	-3.00	104.79	110.23
24	c	5504	BCR	C40-C30-C25	3.00	114.94	110.24
20	C	499	CLA	O2A-CGA-CBA	3.00	120.97	111.83
20	c	5499	CLA	O2A-CGA-CBA	2.99	120.97	111.83
20	C	498	CLA	O2D-CGD-CBD	2.99	116.47	111.23
24	b	5527	BCR	C30-C25-C26	-2.99	118.55	122.64
20	C	501	CLA	C1-C2-C3	2.99	131.10	126.20
20	A	563	CLA	CAA-C2A-C3A	-2.99	104.92	113.00
20	B	524	CLA	C7-C6-C5	-2.99	105.30	113.26
24	T	5104	BCR	C2-C1-C6	2.99	114.78	110.44
20	C	492	CLA	O2A-CGA-CBA	2.98	120.93	111.83
26	t	213	SQD	C31-C30-C29	2.98	133.50	113.36
20	c	5495	CLA	C1-C2-C3	2.98	131.08	126.20
20	c	5498	CLA	CED-O2D-CGD	2.98	122.68	115.92
20	B	515	CLA	O2A-CGA-CBA	2.98	120.92	111.83
20	B	515	CLA	C7-C6-C5	-2.98	105.32	113.26
24	B	528	BCR	C24-C23-C22	2.98	130.64	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	5495	CLA	O2A-CGA-CBA	2.98	120.91	111.83
20	c	5499	CLA	CED-O2D-CGD	2.97	122.66	115.92
26	a	212	SQD	C3-C4-C5	-2.97	104.84	110.23
32	F	51	HEM	O2A-CGA-CBA	2.97	123.38	114.00
28	i	5201	MGE	O6D-C5D-C6D	2.97	113.80	106.44
20	c	5491	CLA	C7-C6-C5	-2.97	105.36	113.26
20	B	514	CLA	O2A-CGA-CBA	2.96	120.87	111.83
24	T	5104	BCR	C35-C13-C12	2.96	122.61	118.09
26	L	5213	SQD	O7-S-C6	2.96	111.17	106.76
20	c	5498	CLA	C3B-C4B-NB	-2.96	107.89	110.53
20	a	5558	CLA	C1-C2-C3	2.96	131.04	126.20
20	a	5560	CLA	CAA-CBA-CGA	2.96	121.60	113.21
22	A	564	PQ9	C16-C17-C18	-2.96	120.86	127.62
26	A	5212	SQD	O47-C7-C8	2.96	116.36	111.09
20	b	5517	CLA	C7-C6-C5	-2.95	105.39	113.26
20	b	5523	CLA	C1-C2-C3	2.95	131.02	126.20
24	H	107	BCR	C32-C1-C6	2.94	114.86	110.24
24	C	504	BCR	C35-C13-C12	2.94	122.58	118.09
20	b	5518	CLA	CED-O2D-CGD	2.94	122.59	115.92
20	b	5524	CLA	C7-C6-C5	-2.94	105.43	113.26
20	B	512	CLA	O2A-CGA-CBA	2.93	120.77	111.83
24	B	529	BCR	C7-C8-C9	2.93	130.57	126.23
26	A	568	SQD	C45-O47-C7	2.93	124.81	117.80
24	C	504	BCR	C32-C1-C6	2.93	114.83	110.24
20	D	355	CLA	CED-O2D-CGD	2.93	122.55	115.92
21	A	561	PHO	OBD-CAD-CBD	-2.93	121.53	125.82
26	a	212	SQD	O47-C7-C8	2.92	116.30	111.09
24	a	5566	BCR	C8-C7-C6	2.92	134.81	127.00
20	a	5563	CLA	O2A-CGA-CBA	2.92	120.75	111.83
20	a	5559	CLA	O2A-CGA-CBA	2.92	120.74	111.83
22	a	5564	PQ9	C16-C17-C18	-2.92	120.94	127.62
20	C	503	CLA	O2A-CGA-CBA	2.92	120.74	111.83
20	C	493	CLA	C1-C2-C3	2.92	130.98	126.20
20	B	525	CLA	O2A-CGA-CBA	2.92	120.73	111.83
21	A	562	PHO	C2D-C1D-ND	2.92	111.54	109.43
25	a	5567	LHG	O7-C7-C8	2.92	117.79	111.48
24	d	5357	BCR	C37-C22-C23	2.91	122.54	118.09
24	c	5505	BCR	C30-C25-C26	-2.91	118.66	122.64
20	b	5525	CLA	CED-O2D-CGD	2.91	122.52	115.92
20	b	5523	CLA	O2A-CGA-CBA	2.91	120.71	111.83
20	A	563	CLA	O2A-CGA-CBA	2.91	120.71	111.83
20	C	496	CLA	C7-C6-C5	-2.91	105.51	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	525	CLA	CED-O2D-CGD	2.91	122.51	115.92
20	B	526	CLA	O2A-CGA-CBA	2.91	120.70	111.83
24	b	5529	BCR	C24-C23-C22	2.90	130.53	126.23
20	C	497	CLA	O2D-CGD-CBD	2.90	116.30	111.23
20	b	5525	CLA	C7-C6-C5	-2.90	105.53	113.26
20	C	500	CLA	C1-C2-C3	2.90	130.95	126.20
24	B	527	BCR	C8-C7-C6	2.90	134.74	127.00
26	d	5358	SQD	C32-C31-C30	2.90	129.01	114.37
20	d	5354	CLA	C3B-C4B-NB	-2.90	107.94	110.53
20	A	558	CLA	CED-O2D-CGD	2.89	122.48	115.92
24	h	5107	BCR	C12-C13-C14	-2.89	114.46	119.01
24	C	505	BCR	C1-C6-C5	-2.89	118.69	122.64
21	a	5562	PHO	C2D-C1D-ND	2.88	111.51	109.43
20	c	5499	CLA	O2D-CGD-CBD	2.88	116.27	111.23
32	V	552	HEM	C4A-NA-C1A	2.88	110.52	105.82
20	b	5513	CLA	CED-O2D-CGD	2.88	122.45	115.92
32	v	5552	HEM	C4A-NA-C1A	2.88	110.51	105.82
24	t	104	BCR	C1-C6-C5	-2.88	118.70	122.64
20	C	497	CLA	CED-O2D-CGD	2.88	122.44	115.92
20	A	558	CLA	O2A-CGA-CBA	2.88	120.61	111.83
20	A	559	CLA	CED-O2D-CGD	2.87	122.44	115.92
20	a	5560	CLA	C7-C6-C5	-2.87	105.60	113.26
20	A	558	CLA	C3B-C4B-NB	-2.87	107.97	110.53
21	A	562	PHO	CAA-C2A-C3A	-2.87	105.25	113.00
21	A	561	PHO	C3B-C4B-NB	2.87	109.33	107.46
24	X	130	BCR	C12-C13-C14	-2.87	114.50	119.01
20	c	5497	CLA	CED-O2D-CGD	2.87	122.42	115.92
20	B	512	CLA	C7-C6-C5	-2.87	105.62	113.26
24	D	357	BCR	C12-C13-C14	-2.87	114.50	119.01
24	B	527	BCR	C1-C6-C5	-2.86	118.72	122.64
20	c	5501	CLA	CED-O2D-CGD	2.86	122.41	115.92
24	T	5104	BCR	C1-C6-C5	-2.86	118.73	122.64
20	D	355	CLA	O2A-CGA-CBA	2.86	120.54	111.83
21	A	562	PHO	OBD-CAD-CBD	-2.85	121.64	125.82
21	a	5562	PHO	CAA-C2A-C3A	-2.85	105.30	113.00
20	a	5563	CLA	CAA-C2A-C3A	-2.85	105.30	113.00
24	B	528	BCR	C33-C5-C4	-2.85	107.52	113.60
20	c	5496	CLA	C7-C6-C5	-2.85	105.67	113.26
24	c	5505	BCR	C16-C17-C18	2.85	131.27	127.28
26	L	5213	SQD	C31-C30-C29	2.85	132.59	113.36
28	D	358	MGE	O6D-C5D-C6D	2.85	113.49	106.44
20	B	518	CLA	C7-C6-C5	-2.85	105.68	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	513	CLA	CED-O2D-CGD	2.85	122.37	115.92
20	b	5514	CLA	C1-C2-C3	2.84	130.86	126.20
20	C	499	CLA	O2D-CGD-CBD	2.84	116.20	111.23
24	C	505	BCR	C35-C13-C12	2.84	122.43	118.09
20	A	560	CLA	CED-O2D-CGD	2.84	122.36	115.92
20	b	5520	CLA	CED-O2D-CGD	2.84	122.35	115.92
20	B	516	CLA	C7-C6-C5	-2.84	105.70	113.26
20	a	5558	CLA	O2A-CGA-CBA	2.84	120.49	111.83
32	F	51	HEM	CHA-C4D-C3D	-2.84	120.00	125.23
20	b	5526	CLA	C1-C2-C3	2.84	130.84	126.20
20	b	5519	CLA	C7-C6-C5	-2.83	105.71	113.26
20	A	560	CLA	CAA-CBA-CGA	2.83	121.26	113.21
24	b	5527	BCR	C16-C17-C18	2.83	131.24	127.28
24	d	5357	BCR	C36-C18-C19	2.83	122.41	118.09
21	a	5561	PHO	OBD-CAD-CBD	-2.83	121.68	125.82
20	C	498	CLA	CAA-C2A-C3A	-2.82	105.37	113.00
20	C	491	CLA	O2A-CGA-CBA	2.82	120.44	111.83
24	h	5107	BCR	C15-C14-C13	2.82	131.23	127.28
24	T	5104	BCR	C11-C10-C9	2.81	131.22	127.28
20	C	496	CLA	CAA-C2A-C3A	-2.81	105.40	113.00
26	d	5358	SQD	C36-C35-C34	2.81	128.58	114.37
20	C	498	CLA	C3B-C4B-NB	-2.81	108.02	110.53
20	D	354	CLA	C3B-C4B-NB	-2.81	108.02	110.53
24	C	504	BCR	C1-C6-C7	2.81	123.26	115.65
22	a	5564	PQ9	C19-C18-C20	2.81	120.10	115.23
22	a	5564	PQ9	C24-C23-C25	2.81	120.10	115.23
20	B	514	CLA	C7-C6-C5	-2.81	105.79	113.26
20	B	519	CLA	C7-C6-C5	-2.80	105.79	113.26
24	c	5506	BCR	C35-C13-C12	2.80	122.36	118.09
20	C	498	CLA	C7-C6-C5	-2.80	105.80	113.26
26	L	5213	SQD	C44-O6-C1	2.80	119.80	113.80
20	B	517	CLA	C7-C6-C5	-2.80	105.81	113.26
20	B	515	CLA	C2A-C3A-C4A	2.80	106.39	101.87
20	C	501	CLA	CED-O2D-CGD	2.80	122.26	115.92
28	L	210	MGE	O2G-C1B-C2B	2.79	117.53	111.48
20	B	515	CLA	CED-O2D-CGD	2.79	122.25	115.92
32	V	552	HEM	CHA-C4D-C3D	-2.79	120.08	125.23
20	c	5501	CLA	C3B-C4B-NB	-2.79	108.04	110.53
20	d	5354	CLA	O2D-CGD-CBD	2.79	116.11	111.23
21	A	562	PHO	CED-O2D-CGD	2.79	122.25	115.92
26	A	568	SQD	C36-C35-C34	2.79	128.47	114.37
20	B	526	CLA	C1-C2-C3	2.78	130.76	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	499	CLA	C2A-C1A-CHA	2.78	128.70	123.87
20	b	5519	CLA	C3B-C4B-NB	-2.78	108.05	110.53
20	b	5526	CLA	O2A-CGA-CBA	2.78	120.31	111.83
24	c	5505	BCR	C8-C7-C6	2.78	134.42	127.00
30	c	5508	DGD	O5D-C6D-C5D	2.78	115.68	109.42
20	A	558	CLA	CAA-C2A-C3A	-2.77	105.51	113.00
24	c	5506	BCR	C30-C25-C24	2.77	123.17	115.65
24	D	357	BCR	C24-C23-C22	2.77	130.34	126.23
24	T	5104	BCR	C23-C22-C21	-2.77	114.65	119.01
20	c	5502	CLA	C1-C2-C3	2.77	130.74	126.20
24	b	5529	BCR	C35-C13-C12	2.77	122.32	118.09
24	B	527	BCR	C24-C23-C22	2.77	130.33	126.23
20	b	5512	CLA	C7-C6-C5	-2.77	105.89	113.26
24	X	130	BCR	C16-C17-C18	2.77	131.16	127.28
21	A	561	PHO	C7-C6-C5	-2.77	105.89	113.26
20	C	498	CLA	CED-O2D-CGD	2.76	122.19	115.92
20	B	516	CLA	CBA-CAA-C2A	2.76	122.02	113.79
24	b	5527	BCR	C8-C7-C6	2.76	134.38	127.00
20	B	517	CLA	CAA-C2A-C3A	-2.76	105.54	113.00
20	c	5502	CLA	C3B-C4B-NB	-2.76	108.07	110.53
20	a	5558	CLA	CAA-C2A-C3A	-2.76	105.55	113.00
20	B	522	CLA	C3B-C4B-NB	-2.75	108.08	110.53
24	C	505	BCR	C30-C25-C26	-2.75	118.88	122.64
27	m	216	LMT	C1-O1'-C1'	-2.75	108.99	113.68
24	D	357	BCR	C35-C13-C12	2.74	122.28	118.09
30	h	5208	DGD	O6D-C5D-C4D	2.74	114.64	109.70
28	l	5210	MGE	O2G-C1B-C2B	2.74	117.42	111.48
20	B	524	CLA	O2A-CGA-CBA	2.74	120.20	111.83
20	b	5521	CLA	C6-C5-C3	2.74	120.15	113.47
22	D	356	PQ9	C19-C18-C20	2.74	119.99	115.23
22	A	564	PQ9	C19-C18-C20	2.74	119.98	115.23
22	A	564	PQ9	C24-C23-C25	2.74	119.98	115.23
30	H	208	DGD	O6D-C5D-C4D	2.74	114.63	109.70
28	B	530	MGE	O3G-C1D-C2D	2.74	112.43	108.27
20	b	5523	CLA	C2A-C3A-C4A	2.74	106.29	101.87
32	v	5552	HEM	CHA-C4D-C3D	-2.74	120.18	125.23
24	b	5528	BCR	C24-C23-C22	2.73	130.28	126.23
20	C	502	CLA	C3B-C4B-NB	-2.73	108.09	110.53
24	c	5506	BCR	C40-C30-C29	-2.73	98.46	108.95
26	A	5212	SQD	O48-C23-C24	2.73	123.98	112.38
20	b	5518	CLA	C7-C6-C5	-2.73	105.98	113.26
32	F	51	HEM	C4A-NA-C1A	2.73	110.27	105.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	x	5130	BCR	C35-C13-C12	2.73	122.26	118.09
20	B	523	CLA	O2A-CGA-CBA	2.73	120.15	111.83
20	B	519	CLA	C1-C2-C3	2.73	130.67	126.20
32	V	552	HEM	O2A-CGA-CBA	2.72	122.61	114.00
20	b	5526	CLA	C7-C6-C5	-2.72	106.01	113.26
20	B	512	CLA	C1-C2-C3	2.72	130.66	126.20
20	c	5497	CLA	O2D-CGD-CBD	2.72	115.98	111.23
20	b	5515	CLA	C7-C6-C5	-2.71	106.03	113.26
20	A	559	CLA	O2A-CGA-CBA	2.71	120.11	111.83
20	b	5516	CLA	CBA-CAA-C2A	2.71	121.86	113.79
24	A	566	BCR	C36-C18-C19	2.71	122.23	118.09
24	c	5506	BCR	C37-C22-C23	2.71	122.22	118.09
20	C	502	CLA	C2A-C3A-C4A	2.70	106.24	101.87
20	b	5516	CLA	C7-C6-C5	-2.70	106.06	113.26
20	B	519	CLA	CAA-C2A-C3A	-2.70	105.70	113.00
24	A	566	BCR	C35-C13-C12	2.70	122.21	118.09
20	C	492	CLA	C6-C5-C3	2.70	120.04	113.47
30	c	5509	DGD	C3G-C2G-C1G	-2.70	105.49	111.78
24	c	5504	BCR	C35-C13-C12	2.70	122.21	118.09
24	C	505	BCR	C19-C18-C17	-2.70	114.77	119.01
20	C	495	CLA	C6-C5-C3	2.70	120.04	113.47
24	h	5107	BCR	C35-C13-C12	2.70	122.21	118.09
22	D	356	PQ9	C16-C17-C18	-2.69	121.46	127.62
24	A	566	BCR	C1-C6-C5	-2.69	118.96	122.64
24	A	566	BCR	C16-C17-C18	2.69	131.05	127.28
24	t	104	BCR	C7-C8-C9	2.69	130.21	126.23
24	a	5566	BCR	C37-C22-C23	2.69	122.19	118.09
20	B	523	CLA	C1-C2-C3	2.68	130.59	126.20
26	a	212	SQD	O48-C23-C24	2.68	123.76	112.38
20	C	500	CLA	O2A-CGA-CBA	2.68	120.01	111.83
21	a	5561	PHO	C3B-C4B-NB	2.68	109.21	107.46
21	a	5562	PHO	OBD-CAD-CBD	-2.68	121.89	125.82
24	c	5506	BCR	C1-C6-C5	-2.68	118.98	122.64
30	c	5508	DGD	O6D-C5D-C6D	2.68	112.00	106.69
20	b	5519	CLA	C1-O2A-CGA	2.68	123.13	116.65
20	b	5521	CLA	CED-O2D-CGD	2.68	121.99	115.92
20	B	525	CLA	O2D-CGD-CBD	2.68	115.91	111.23
20	A	560	CLA	C7-C6-C5	-2.68	106.13	113.26
24	C	506	BCR	C40-C30-C29	-2.67	98.68	108.95
30	C	508	DGD	O5D-C6D-C5D	2.67	115.45	109.42
20	C	500	CLA	C2A-C3A-C4A	2.67	106.19	101.87
20	b	5523	CLA	C7-C6-C5	-2.67	106.14	113.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	527	BCR	C16-C17-C18	2.67	131.03	127.28
20	C	501	CLA	O2A-CGA-CBA	2.67	119.98	111.83
20	b	5521	CLA	CAA-C2A-C3A	-2.67	105.78	113.00
24	B	529	BCR	C35-C13-C12	2.67	122.17	118.09
20	b	5517	CLA	CAA-C2A-C3A	-2.67	105.79	113.00
20	C	499	CLA	CED-O2D-CGD	2.67	121.97	115.92
20	c	5496	CLA	O2A-CGA-CBA	2.66	119.96	111.83
20	b	5521	CLA	C2A-C3A-C4A	2.66	106.17	101.87
20	c	5499	CLA	C2A-C3A-C4A	2.66	106.17	101.87
24	d	5357	BCR	C12-C13-C14	-2.66	114.82	119.01
24	c	5506	BCR	C16-C17-C18	2.66	131.01	127.28
28	b	5530	MGE	O6D-C5D-C6D	2.66	113.03	106.44
20	c	5493	CLA	CMD-C2D-C1D	2.66	129.41	124.73
24	C	504	BCR	C37-C22-C23	2.65	122.14	118.09
20	b	5519	CLA	C1-C2-C3	2.65	130.54	126.20
24	d	5357	BCR	C7-C8-C9	2.65	130.16	126.23
20	c	5498	CLA	O2A-CGA-CBA	2.65	119.92	111.83
20	b	5514	CLA	C2A-C3A-C4A	2.65	106.15	101.87
24	a	5566	BCR	C2-C1-C6	2.65	114.29	110.44
20	c	5498	CLA	O2D-CGD-CBD	2.65	115.86	111.23
24	C	506	BCR	C19-C18-C17	-2.65	114.85	119.01
21	A	561	PHO	O1D-CGD-CBD	-2.64	120.71	124.72
20	A	560	CLA	C2A-C3A-C4A	2.64	106.14	101.87
20	d	5355	CLA	O2A-CGA-CBA	2.64	119.89	111.83
24	c	5506	BCR	C24-C23-C22	2.64	130.14	126.23
20	B	513	CLA	C1-C2-C3	2.64	130.53	126.20
20	d	5355	CLA	C3B-C4B-NB	-2.64	108.17	110.53
20	C	491	CLA	C7-C6-C5	-2.64	106.23	113.26
24	a	5566	BCR	C1-C6-C5	-2.64	119.03	122.64
20	b	5513	CLA	O2D-CGD-CBD	2.64	115.84	111.23
24	t	104	BCR	C23-C22-C21	-2.64	114.86	119.01
26	d	5358	SQD	C15-C14-C13	2.64	127.69	114.37
24	c	5504	BCR	C37-C22-C23	2.63	122.11	118.09
30	H	208	DGD	O5D-C1E-C2E	2.63	112.27	108.27
24	C	506	BCR	C12-C13-C14	-2.63	114.86	119.01
25	A	567	LHG	P-O6-C4	-2.63	106.26	121.35
20	b	5520	CLA	C1-C2-C3	2.63	130.51	126.20
20	a	5559	CLA	CMD-C2D-C1D	2.63	129.36	124.73
32	v	5552	HEM	O2A-CGA-CBA	2.63	122.30	114.00
27	T	217	LMT	C1-O1'-C1'	-2.63	109.19	113.68
24	C	504	BCR	C23-C22-C21	-2.63	114.88	119.01
20	a	5560	CLA	CED-O2D-CGD	2.63	121.87	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	520	CLA	C1-C2-C3	2.63	130.50	126.20
24	h	5107	BCR	C1-C6-C7	2.62	122.77	115.65
24	C	505	BCR	C8-C7-C6	2.62	134.00	127.00
24	X	130	BCR	C24-C23-C22	2.62	130.11	126.23
24	b	5529	BCR	C32-C1-C6	2.62	114.35	110.24
20	B	523	CLA	C7-C6-C5	-2.62	106.28	113.26
20	B	523	CLA	C6-C5-C3	2.62	119.85	113.47
20	D	355	CLA	O2D-CGD-CBD	2.62	115.81	111.23
24	A	566	BCR	C8-C7-C6	2.62	133.99	127.00
20	c	5503	CLA	C3B-C4B-NB	-2.61	108.20	110.53
20	c	5502	CLA	C2A-C3A-C4A	2.61	106.09	101.87
20	B	513	CLA	C3B-C4B-NB	-2.61	108.20	110.53
32	f	5051	HEM	C4A-NA-C1A	2.61	110.08	105.82
20	b	5513	CLA	C1-C2-C3	2.61	130.47	126.20
27	t	5217	LMT	C1-O1'-C1'	-2.61	109.23	113.68
24	a	5566	BCR	C36-C18-C19	2.61	122.07	118.09
24	A	566	BCR	C2-C1-C6	2.60	114.22	110.44
24	T	5104	BCR	C40-C30-C29	-2.60	98.95	108.95
30	C	509	DGD	C3G-C2G-C1G	-2.60	105.72	111.78
24	A	566	BCR	C7-C8-C9	2.60	130.08	126.23
24	H	107	BCR	C16-C17-C18	2.60	130.92	127.28
20	B	518	CLA	C3B-C4B-NB	-2.59	108.22	110.53
20	b	5515	CLA	CMD-C2D-C1D	2.59	129.28	124.73
20	b	5524	CLA	CAA-C2A-C3A	-2.58	106.02	113.00
20	b	5521	CLA	C3B-C4B-NB	-2.58	108.23	110.53
20	c	5498	CLA	C7-C6-C5	-2.58	106.39	113.26
20	A	563	CLA	CED-O2D-CGD	2.58	121.77	115.92
20	C	494	CLA	CBA-CAA-C2A	2.58	121.47	113.79
20	b	5522	CLA	C3B-C4B-NB	-2.58	108.23	110.53
20	d	5354	CLA	CED-O2D-CGD	2.58	121.76	115.92
28	d	5359	MGE	O6D-C5D-C6D	2.58	112.83	106.44
20	b	5519	CLA	CAA-C2A-C3A	-2.58	106.04	113.00
24	D	357	BCR	C37-C22-C23	2.57	122.02	118.09
20	C	493	CLA	CMD-C2D-C1D	2.57	129.26	124.73
26	A	568	SQD	O8-S-O7	2.57	117.83	111.40
32	f	5051	HEM	O2A-CGA-CBA	2.57	122.12	114.00
24	b	5527	BCR	C35-C13-C12	2.57	122.01	118.09
20	b	5524	CLA	C3B-C4B-NB	-2.57	108.24	110.53
20	C	499	CLA	C2A-C3A-C4A	2.57	106.01	101.87
20	b	5524	CLA	O2A-CGA-CBA	2.57	119.66	111.83
24	X	130	BCR	C30-C25-C24	2.57	122.61	115.65
20	C	498	CLA	O2A-CGA-CBA	2.56	119.65	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	5515	CLA	C6-C5-C3	2.56	119.71	113.47
20	c	5500	CLA	O2A-CGA-CBA	2.56	119.63	111.83
24	b	5529	BCR	C7-C8-C9	2.56	130.01	126.23
21	a	5561	PHO	O1D-CGD-CBD	-2.55	120.85	124.72
24	C	506	BCR	C30-C25-C24	2.55	122.57	115.65
20	A	560	CLA	C1-C2-C3	2.55	130.37	126.20
24	B	528	BCR	C32-C1-C6	2.55	114.24	110.24
26	L	5213	SQD	C3-C4-C5	-2.55	105.62	110.23
20	b	5511	CLA	C2A-C3A-C4A	2.54	104.57	101.59
24	B	527	BCR	C36-C18-C19	2.54	121.97	118.09
20	c	5492	CLA	CAA-C2A-C3A	-2.53	106.15	113.00
20	a	5563	CLA	C3B-C4B-NB	-2.53	108.27	110.53
20	b	5525	CLA	O2D-CGD-CBD	2.53	115.66	111.23
24	h	5107	BCR	C16-C17-C18	2.53	130.83	127.28
20	b	5512	CLA	C1-C2-C3	2.53	130.34	126.20
20	C	494	CLA	C2A-C3A-C4A	2.53	105.95	101.87
20	C	500	CLA	C3B-C4B-NB	-2.53	108.28	110.53
20	B	521	CLA	O2D-CGD-CBD	2.53	115.64	111.23
20	B	521	CLA	CAA-C2A-C3A	-2.53	106.17	113.00
20	B	526	CLA	C1-O2A-CGA	2.53	122.76	116.65
20	B	526	CLA	C7-C6-C5	-2.52	106.53	113.26
24	X	130	BCR	C35-C13-C12	2.52	121.94	118.09
27	t	5217	LMT	C3'-C4'-C5'	-2.52	105.33	110.93
20	c	5494	CLA	O2A-CGA-CBA	2.52	121.67	112.14
20	C	503	CLA	CAA-C2A-C3A	-2.52	106.18	113.00
20	B	525	CLA	C3B-C4B-NB	-2.52	108.28	110.53
20	A	558	CLA	C2A-C3A-C4A	2.52	105.94	101.87
20	C	495	CLA	CED-O2D-CGD	2.52	121.63	115.92
20	a	5560	CLA	CMD-C2D-C1D	2.52	129.16	124.73
24	a	5566	BCR	C16-C17-C18	2.52	130.81	127.28
21	a	5561	PHO	C2D-C1D-ND	2.52	111.25	109.43
20	B	517	CLA	C2A-C1A-CHA	2.51	128.23	123.87
22	d	5356	PQ9	C14-C13-C15	2.51	119.59	115.23
20	d	5354	CLA	C7-C6-C5	-2.51	106.57	113.26
20	B	521	CLA	C6-C5-C3	2.51	119.58	113.47
32	f	5051	HEM	CMD-C2D-C1D	2.51	128.96	125.03
24	X	130	BCR	C37-C22-C23	2.51	121.92	118.09
24	A	566	BCR	C37-C22-C23	2.51	121.92	118.09
24	d	5357	BCR	C16-C17-C18	2.51	130.79	127.28
20	c	5492	CLA	O2A-CGA-CBA	2.51	119.48	111.83
20	b	5520	CLA	C3B-C4B-NB	-2.51	108.29	110.53
24	T	5104	BCR	C23-C24-C25	2.51	133.69	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	494	CLA	O2A-CGA-CBA	2.51	121.61	112.14
24	B	528	BCR	C1-C6-C7	2.51	122.45	115.65
24	D	357	BCR	C16-C17-C18	2.51	130.79	127.28
30	C	508	DGD	O6D-C5D-C6D	2.51	111.66	106.69
24	C	504	BCR	C32-C1-C2	-2.50	99.33	108.95
24	c	5504	BCR	C30-C25-C24	2.50	122.44	115.65
24	C	505	BCR	C36-C18-C19	2.50	121.91	118.09
24	C	504	BCR	C7-C8-C9	2.50	129.94	126.23
24	T	5104	BCR	C7-C8-C9	2.50	129.93	126.23
24	t	104	BCR	C23-C24-C25	2.50	133.67	127.00
20	b	5515	CLA	C12-C11-C10	-2.50	102.08	113.28
20	A	558	CLA	CBA-CAA-C2A	2.50	121.22	113.79
20	c	5493	CLA	C12-C11-C10	-2.50	102.09	113.28
20	C	497	CLA	C3B-C4B-NB	-2.50	108.30	110.53
20	B	514	CLA	C2A-C3A-C4A	2.50	105.90	101.87
32	F	51	HEM	CBC-CAC-C3C	-2.49	115.06	127.53
24	T	5104	BCR	C37-C22-C23	2.49	121.90	118.09
20	B	513	CLA	C7-C6-C5	-2.49	106.62	113.26
20	C	501	CLA	C3B-C4B-NB	-2.49	108.31	110.53
24	C	506	BCR	C36-C18-C19	2.49	121.89	118.09
20	c	5495	CLA	C2A-C1A-CHA	2.49	128.19	123.87
20	B	521	CLA	C2A-C3A-C4A	2.49	105.89	101.87
24	C	505	BCR	C12-C13-C14	-2.49	115.10	119.01
20	B	524	CLA	CAA-C2A-C3A	-2.49	106.28	113.00
20	C	502	CLA	C1-C2-C3	2.49	130.27	126.20
30	C	507	DGD	O5D-C6D-C5D	2.48	115.02	109.42
20	c	5492	CLA	C6-C5-C3	2.48	119.52	113.47
22	d	5356	PQ9	C16-C17-C18	-2.48	121.94	127.62
24	b	5528	BCR	C1-C6-C7	2.48	122.38	115.65
25	a	5567	LHG	P-O6-C4	-2.48	107.14	121.35
20	b	5518	CLA	C3B-C4B-NB	-2.48	108.32	110.53
24	X	130	BCR	C32-C1-C2	-2.48	99.44	108.95
20	c	5501	CLA	O2A-CGA-CBA	2.47	119.38	111.83
24	c	5506	BCR	C19-C18-C17	-2.47	115.12	119.01
24	t	104	BCR	C12-C13-C14	-2.47	115.12	119.01
20	D	354	CLA	C2A-C3A-C4A	2.47	105.86	101.87
24	C	506	BCR	C37-C22-C23	2.46	121.85	118.09
24	C	504	BCR	C40-C30-C25	2.46	114.10	110.24
20	c	5495	CLA	C6-C5-C3	2.46	119.46	113.47
28	d	5360	MGE	C3G-O3G-C1D	-2.46	108.52	113.80
20	C	494	CLA	C2A-C1A-CHA	2.46	128.13	123.87
20	C	502	CLA	C2A-C1A-CHA	2.46	128.13	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	559	CLA	C2A-C3A-C4A	2.46	105.83	101.87
20	c	5494	CLA	CBA-CAA-C2A	2.45	121.10	113.79
24	H	107	BCR	C1-C6-C7	2.45	122.31	115.65
24	x	5130	BCR	C30-C25-C24	2.45	122.30	115.65
24	d	5357	BCR	C35-C13-C12	2.45	121.83	118.09
20	B	511	CLA	C2A-C3A-C4A	2.45	104.47	101.59
28	I	201	MGE	O1G-C1G-C2G	-2.45	101.33	108.40
24	B	529	BCR	C40-C30-C25	2.45	114.09	110.24
26	A	568	SQD	C15-C14-C13	2.45	126.76	114.37
28	i	5201	MGE	O1G-C1G-C2G	-2.45	101.33	108.40
21	A	561	PHO	O2A-CGA-CBA	2.45	119.31	111.83
20	C	495	CLA	C3B-C4B-NB	-2.45	108.34	110.53
20	a	5558	CLA	C2A-C3A-C4A	2.45	105.83	101.87
24	a	5566	BCR	C32-C1-C6	2.45	114.08	110.24
24	a	5566	BCR	C30-C25-C24	2.45	122.29	115.65
22	D	356	PQ9	C21-C22-C23	-2.45	122.03	127.62
20	C	496	CLA	C3B-C4B-NB	-2.44	108.35	110.53
20	c	5502	CLA	C2A-C1A-CHA	2.44	128.11	123.87
20	a	5558	CLA	CBA-CAA-C2A	2.44	121.06	113.79
20	c	5491	CLA	CAA-C2A-C3A	-2.44	106.40	113.00
20	D	354	CLA	C7-C6-C5	-2.44	106.76	113.26
20	c	5493	CLA	C2A-C3A-C4A	2.44	105.81	101.87
20	C	491	CLA	CMD-C2D-C1D	2.44	129.02	124.73
20	B	523	CLA	C2A-C3A-C4A	2.43	105.80	101.87
20	c	5492	CLA	C7-C6-C5	-2.43	106.78	113.26
20	B	515	CLA	C6-C5-C3	2.43	119.39	113.47
24	B	529	BCR	C32-C1-C6	2.43	114.05	110.24
20	b	5525	CLA	C3B-C4B-NB	-2.43	108.36	110.53
24	b	5528	BCR	C32-C1-C6	2.43	114.05	110.24
24	t	104	BCR	C8-C9-C10	-2.43	115.19	119.01
20	D	354	CLA	CED-O2D-CGD	2.43	121.42	115.92
24	H	107	BCR	C35-C13-C12	2.43	121.79	118.09
20	b	5514	CLA	C7-C6-C5	-2.42	106.80	113.26
20	a	5560	CLA	C2A-C3A-C4A	2.42	105.77	101.87
22	a	5564	PQ9	C14-C13-C15	2.42	119.42	115.23
22	A	564	PQ9	C14-C13-C15	2.42	119.42	115.23
20	c	5496	CLA	C3B-C4B-NB	-2.42	108.37	110.53
20	B	515	CLA	C12-C11-C10	-2.41	102.46	113.28
30	c	5507	DGD	O5D-C6D-C5D	2.41	114.86	109.42
20	b	5519	CLA	O2A-CGA-CBA	2.41	119.19	111.83
20	B	524	CLA	C1-C2-C3	2.41	130.15	126.20
24	t	104	BCR	C36-C18-C19	2.41	121.77	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	5503	CLA	O2A-CGA-CBA	2.41	119.18	111.83
24	t	104	BCR	C37-C22-C23	2.41	121.77	118.09
20	b	5522	CLA	C2A-C3A-C4A	2.41	105.76	101.87
20	C	492	CLA	CAA-C2A-C3A	-2.41	106.50	113.00
20	b	5523	CLA	C6-C5-C3	2.41	119.33	113.47
20	D	354	CLA	O2D-CGD-CBD	2.41	115.44	111.23
20	C	491	CLA	O2D-CGD-CBD	2.40	115.43	111.23
20	a	5559	CLA	C2A-C3A-C4A	2.40	105.75	101.87
24	t	104	BCR	C40-C30-C29	-2.40	99.73	108.95
28	B	530	MGE	O6D-C5D-C6D	2.40	112.39	106.44
20	c	5503	CLA	CAA-C2A-C3A	-2.40	106.51	113.00
24	h	5107	BCR	C37-C22-C23	2.40	121.75	118.09
28	d	5359	MGE	C3G-C2G-C1G	-2.40	106.20	111.78
20	C	492	CLA	C1-C2-C3	2.40	130.12	126.20
26	A	568	SQD	C3-C4-C5	-2.39	105.89	110.23
24	c	5504	BCR	C23-C22-C21	-2.39	115.25	119.01
20	C	493	CLA	O2D-CGD-CBD	2.39	115.41	111.23
20	c	5500	CLA	CAA-C2A-C3A	-2.39	106.54	113.00
20	D	355	CLA	C3B-C4B-NB	-2.39	108.40	110.53
28	B	530	MGE	O1G-C1G-C2G	-2.39	101.51	108.40
24	c	5505	BCR	C12-C13-C14	-2.39	115.25	119.01
24	c	5506	BCR	C36-C18-C19	2.39	121.74	118.09
30	h	5208	DGD	O5D-C1E-C2E	2.39	111.90	108.27
24	T	5104	BCR	C36-C18-C19	2.39	121.73	118.09
20	c	5499	CLA	C2A-C1A-CHA	2.39	128.01	123.87
20	c	5495	CLA	CED-O2D-CGD	2.38	121.32	115.92
24	B	527	BCR	C12-C13-C14	-2.38	115.26	119.01
24	c	5504	BCR	C12-C13-C14	-2.38	115.26	119.01
21	A	561	PHO	CMA-C3A-C4A	-2.38	109.48	114.61
28	B	530	MGE	C3G-C2G-C1G	-2.38	106.24	111.78
20	b	5518	CLA	O2D-CGD-CBD	2.38	115.39	111.23
20	b	5515	CLA	C2A-C3A-C4A	2.38	105.71	101.87
20	c	5495	CLA	C3B-C4B-NB	-2.37	108.41	110.53
26	t	213	SQD	C3-C4-C5	-2.37	105.93	110.23
26	d	5358	SQD	C3-C4-C5	-2.37	105.93	110.23
20	B	526	CLA	C2A-C3A-C4A	2.37	105.70	101.87
20	a	5560	CLA	C3B-C4B-NB	-2.37	108.41	110.53
20	C	501	CLA	C1-O2A-CGA	2.37	122.39	116.65
20	c	5500	CLA	CED-O2D-CGD	2.37	121.29	115.92
20	c	5496	CLA	C2A-C3A-C4A	2.37	105.69	101.87
24	c	5505	BCR	C36-C18-C19	2.37	121.70	118.09
32	F	51	HEM	CAB-C3B-C4B	2.37	134.84	124.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	514	CLA	CED-O2D-CGD	2.36	121.28	115.92
24	H	107	BCR	C36-C18-C19	2.36	121.70	118.09
24	a	5566	BCR	C35-C13-C12	2.36	121.69	118.09
26	A	568	SQD	C44-O6-C1	2.36	118.86	113.80
20	C	493	CLA	C2A-C3A-C4A	2.36	105.68	101.87
20	B	519	CLA	C3B-C4B-NB	-2.36	108.42	110.53
20	D	355	CLA	C1-O2A-CGA	2.36	122.35	116.65
32	f	5051	HEM	CBC-CAC-C3C	-2.35	115.76	127.53
24	c	5506	BCR	C12-C13-C14	-2.35	115.31	119.01
20	b	5514	CLA	CED-O2D-CGD	2.35	121.25	115.92
21	A	561	PHO	C2D-C1D-ND	2.35	111.13	109.43
20	b	5526	CLA	O2D-CGD-CBD	2.35	115.34	111.23
24	b	5529	BCR	C12-C13-C14	-2.35	115.31	119.01
20	c	5501	CLA	C12-C11-C10	-2.35	102.75	113.28
32	f	5051	HEM	CAB-C3B-C4B	2.35	134.76	124.39
20	B	523	CLA	CED-O2D-CGD	2.35	121.24	115.92
20	a	5563	CLA	O2D-CGD-CBD	2.34	115.33	111.23
24	B	529	BCR	C12-C13-C14	-2.34	115.32	119.01
24	D	357	BCR	C40-C30-C25	2.34	113.92	110.24
20	B	519	CLA	C2A-C3A-C4A	2.34	105.66	101.87
21	a	5561	PHO	C4A-C3A-C2A	2.34	105.07	102.84
20	C	499	CLA	C1-O2A-CGA	2.34	123.32	116.67
24	c	5504	BCR	C32-C1-C2	-2.34	99.96	108.95
20	A	559	CLA	CMD-C2D-C1D	2.34	128.85	124.73
20	B	513	CLA	O2D-CGD-CBD	2.34	115.32	111.23
24	t	104	BCR	C34-C9-C8	2.34	121.66	118.09
26	d	5358	SQD	O8-S-O7	2.34	117.25	111.40
20	B	524	CLA	C3B-C4B-NB	-2.34	108.44	110.53
20	B	521	CLA	O2A-CGA-CBA	2.34	118.96	111.83
20	c	5500	CLA	C2A-C3A-C4A	2.34	105.64	101.87
24	T	5104	BCR	C12-C13-C14	-2.34	115.33	119.01
20	C	503	CLA	C3B-C4B-NB	-2.34	108.44	110.53
20	B	519	CLA	C1-O2A-CGA	2.34	122.30	116.65
20	C	492	CLA	O2D-CGD-CBD	2.33	115.31	111.23
22	A	564	PQ9	C21-C22-C23	-2.33	122.28	127.62
20	C	492	CLA	C2A-C3A-C4A	2.33	105.64	101.87
24	B	529	BCR	C15-C14-C13	2.33	130.55	127.28
20	B	522	CLA	C2A-C3A-C4A	2.33	105.63	101.87
20	C	500	CLA	CMA-C3A-C2A	-2.33	104.98	113.98
24	C	504	BCR	C11-C10-C9	2.33	130.54	127.28
20	b	5513	CLA	C3B-C4B-NB	-2.33	108.45	110.53
24	h	5107	BCR	C34-C9-C8	2.33	121.64	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	5500	CLA	C3B-C4B-NB	-2.32	108.45	110.53
24	X	130	BCR	C8-C7-C6	2.32	133.19	127.00
20	d	5354	CLA	C2A-C3A-C4A	2.32	105.61	101.87
27	t	5217	LMT	O1B-C1B-C2B	2.32	113.79	108.09
27	T	217	LMT	C3'-C4'-C5'	-2.32	105.80	110.93
20	b	5521	CLA	O2D-CGD-CBD	2.31	115.27	111.23
24	A	566	BCR	C19-C18-C17	-2.31	115.37	119.01
22	D	356	PQ9	C11-C12-C13	-2.31	122.85	126.83
20	B	511	CLA	CED-O2D-CGD	2.31	121.16	115.92
26	L	5213	SQD	C15-C14-C13	2.31	126.05	114.37
20	C	501	CLA	C12-C11-C10	-2.31	102.92	113.28
20	b	5521	CLA	O2A-CGA-CBA	2.31	118.88	111.83
22	d	5356	PQ9	C19-C18-C20	2.31	119.23	115.23
20	C	493	CLA	C12-C11-C10	-2.31	102.94	113.28
20	a	5558	CLA	C3B-C4B-NB	-2.31	108.47	110.53
20	c	5501	CLA	C1-C2-C3	2.31	129.97	126.20
24	X	130	BCR	C36-C18-C19	2.30	121.61	118.09
20	B	525	CLA	C2A-C3A-C4A	2.30	105.59	101.87
20	b	5524	CLA	O2D-CGD-CBD	2.30	115.26	111.23
20	A	559	CLA	CAA-CBA-CGA	2.30	119.75	113.21
20	C	501	CLA	C2A-C1A-CHA	2.30	127.86	123.87
20	c	5497	CLA	C2A-C3A-C4A	2.30	105.59	101.87
20	b	5516	CLA	C3B-C4B-NB	-2.30	108.48	110.53
24	x	5130	BCR	C32-C1-C2	-2.30	100.12	108.95
20	A	560	CLA	CMD-C2D-C1D	2.30	128.78	124.73
20	B	519	CLA	C2A-C1A-CHA	2.30	127.86	123.87
20	b	5515	CLA	C1-C2-C3	2.30	129.96	126.20
21	A	562	PHO	CMA-C3A-C4A	-2.30	109.66	114.61
20	B	519	CLA	O2A-CGA-CBA	2.30	118.84	111.83
20	C	495	CLA	C2A-C3A-C4A	2.30	105.58	101.87
20	B	511	CLA	CMD-C2D-C1D	2.30	128.77	124.73
20	c	5497	CLA	C6-C5-C3	2.30	119.06	113.47
20	a	5560	CLA	O2A-CGA-CBA	2.30	118.83	111.83
20	A	563	CLA	C2A-C3A-C4A	2.29	105.58	101.87
20	c	5491	CLA	C2A-C3A-C4A	2.29	105.58	101.87
20	C	493	CLA	C3B-C4B-NB	-2.29	108.48	110.53
20	C	500	CLA	CED-O2D-CGD	2.29	121.12	115.92
24	x	5130	BCR	C37-C22-C23	2.29	121.59	118.09
24	x	5130	BCR	C8-C7-C6	2.29	133.12	127.00
26	d	5358	SQD	C44-O6-C1	2.29	118.70	113.80
20	C	493	CLA	C2A-C1A-CHA	2.29	127.84	123.87
20	a	5563	CLA	C2A-C3A-C4A	2.29	105.56	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	5506	BCR	C23-C22-C21	-2.29	115.41	119.01
24	x	5130	BCR	C36-C18-C19	2.29	121.58	118.09
20	c	5497	CLA	CAA-C2A-C3A	-2.29	106.82	113.00
24	C	506	BCR	C24-C23-C22	2.28	129.62	126.23
20	B	513	CLA	C6-C5-C3	2.28	119.03	113.47
28	i	5201	MGE	C3G-O3G-C1D	-2.28	108.90	113.80
20	b	5511	CLA	CED-O2D-CGD	2.28	121.09	115.92
20	B	512	CLA	C2A-C3A-C4A	2.28	105.55	101.87
20	C	495	CLA	C2A-C1A-CHA	2.28	127.82	123.87
20	B	514	CLA	CAA-C2A-C3A	-2.28	106.85	113.00
20	B	522	CLA	CMD-C2D-C1D	2.27	128.73	124.73
24	c	5504	BCR	C11-C10-C9	2.27	130.47	127.28
20	B	515	CLA	CMD-C2D-C1D	2.27	128.73	124.73
20	b	5511	CLA	CMD-C2D-C1D	2.27	128.73	124.73
24	C	504	BCR	C30-C25-C24	2.27	121.81	115.65
27	T	217	LMT	O1B-C1B-C2B	2.27	113.68	108.09
26	d	5358	SQD	C34-C33-C32	2.27	125.85	114.37
20	B	512	CLA	O2D-CGD-CBD	2.27	115.20	111.23
20	c	5494	CLA	C2A-C3A-C4A	2.27	105.54	101.87
20	C	497	CLA	C6-C5-C3	2.27	119.00	113.47
24	D	357	BCR	C23-C22-C21	-2.27	115.44	119.01
20	C	500	CLA	O2D-CGD-CBD	2.27	115.19	111.23
20	a	5558	CLA	CMD-C2D-C1D	2.27	128.72	124.73
20	b	5521	CLA	C1-C2-C3	2.27	129.91	126.20
20	B	521	CLA	C1-C2-C3	2.27	129.91	126.20
21	a	5561	PHO	O2A-CGA-CBA	2.26	118.73	111.83
24	H	107	BCR	C7-C8-C9	2.26	129.58	126.23
21	a	5561	PHO	CMA-C3A-C4A	-2.26	109.74	114.61
20	C	497	CLA	C12-C11-C10	-2.26	103.15	113.28
20	b	5512	CLA	O2D-CGD-CBD	2.26	115.18	111.23
22	a	5564	PQ9	C21-C22-C23	-2.26	122.45	127.62
24	a	5566	BCR	C34-C9-C8	2.26	121.54	118.09
20	A	563	CLA	CMA-C3A-C2A	-2.26	105.25	113.98
20	c	5491	CLA	CMD-C2D-C1D	2.26	128.70	124.73
20	d	5355	CLA	O2D-CGD-CBD	2.26	115.18	111.23
24	b	5529	BCR	C1-C6-C7	2.25	121.77	115.65
20	B	515	CLA	O2D-CGD-CBD	2.25	115.17	111.23
20	d	5354	CLA	CMD-C2D-C1D	2.25	128.69	124.73
20	b	5514	CLA	CAA-C2A-C3A	-2.25	106.91	113.00
26	d	5358	SQD	C17-C16-C15	2.25	125.75	114.37
26	t	213	SQD	C15-C14-C13	2.25	125.74	114.37
27	T	217	LMT	C1B-O1B-C4'	-2.25	112.65	117.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	D	357	BCR	C7-C8-C9	2.25	129.56	126.23
20	C	503	CLA	C1-C2-C3	2.25	130.40	126.76
24	X	130	BCR	C19-C18-C17	-2.25	115.48	119.01
28	b	5530	MGE	O1G-C1G-C2G	-2.25	101.92	108.40
20	b	5520	CLA	O2D-CGD-CBD	2.24	115.15	111.23
20	B	521	CLA	C12-C11-C10	-2.24	103.22	113.28
24	C	506	BCR	C23-C22-C21	-2.24	115.48	119.01
24	c	5505	BCR	C7-C8-C9	2.24	129.55	126.23
24	H	107	BCR	C37-C22-C23	2.24	121.51	118.09
20	C	502	CLA	O2D-CGD-CBD	2.24	115.14	111.23
20	B	515	CLA	C3B-C4B-NB	-2.24	108.53	110.53
20	b	5520	CLA	C12-C11-C10	-2.24	103.25	113.28
28	l	5210	MGE	O1G-C1G-C2G	-2.24	101.94	108.40
24	a	5566	BCR	C12-C13-C14	-2.24	115.49	119.01
20	c	5497	CLA	C3B-C4B-NB	-2.24	108.53	110.53
20	c	5498	CLA	C4D-CHA-C1A	2.24	123.91	121.24
24	c	5504	BCR	C7-C8-C9	2.24	129.54	126.23
20	B	520	CLA	CAA-C2A-C3A	-2.23	106.96	113.00
24	h	5107	BCR	C30-C25-C24	2.23	121.71	115.65
20	c	5497	CLA	C12-C11-C10	-2.23	103.28	113.28
20	B	521	CLA	C3B-C4B-NB	-2.23	108.54	110.53
20	b	5513	CLA	C7-C6-C5	-2.23	107.32	113.26
24	b	5528	BCR	C32-C1-C2	-2.23	100.39	108.95
20	A	558	CLA	CMA-C3A-C2A	-2.23	105.36	113.98
20	b	5515	CLA	CMA-C3A-C2A	-2.23	105.36	113.98
24	C	504	BCR	C12-C13-C14	-2.23	115.50	119.01
24	A	566	BCR	C12-C13-C14	-2.23	115.50	119.01
20	b	5526	CLA	C3B-C4B-NB	-2.23	108.54	110.53
24	C	506	BCR	C32-C1-C6	2.23	113.74	110.24
32	V	552	HEM	CAB-C3B-C2B	-2.23	121.19	128.43
21	A	561	PHO	OBD-CAD-C3D	2.23	131.37	127.89
20	b	5514	CLA	C2A-C1A-CHA	2.23	127.73	123.87
20	b	5523	CLA	O2D-CGD-CBD	2.23	115.12	111.23
20	c	5492	CLA	O2D-CGD-CBD	2.23	115.12	111.23
20	b	5517	CLA	C2A-C1A-CHA	2.23	127.73	123.87
20	A	563	CLA	C3B-C4B-NB	-2.22	108.55	110.53
20	A	563	CLA	O2D-CGD-CBD	2.22	115.11	111.23
24	B	528	BCR	C40-C30-C25	2.22	113.73	110.24
20	C	498	CLA	C12-C11-C10	-2.22	103.33	113.28
26	A	568	SQD	C34-C33-C32	2.22	125.59	114.37
20	B	514	CLA	C2A-C1A-CHA	2.22	127.72	123.87
26	A	5212	SQD	O8-S-O7	2.22	116.95	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	b	5528	BCR	C30-C25-C24	2.22	121.67	115.65
20	b	5526	CLA	C2A-C3A-C4A	2.22	105.45	101.87
24	H	107	BCR	C30-C25-C24	2.22	121.66	115.65
24	H	107	BCR	C28-C27-C26	2.21	118.00	114.06
24	T	5104	BCR	C34-C9-C8	2.21	121.47	118.09
20	c	5493	CLA	C3B-C4B-NB	-2.21	108.55	110.53
20	c	5493	CLA	O2D-CGD-CBD	2.21	115.10	111.23
20	c	5491	CLA	O2D-CGD-CBD	2.21	115.10	111.23
32	F	51	HEM	O1A-CGA-CBA	-2.21	116.08	123.09
20	B	517	CLA	C3B-C4B-NB	-2.21	108.56	110.53
20	C	492	CLA	C3B-C4B-NB	-2.21	108.56	110.53
20	b	5521	CLA	C12-C11-C10	-2.21	103.38	113.28
24	d	5357	BCR	C19-C18-C17	-2.21	115.53	119.01
20	A	563	CLA	CMD-C2D-C1D	2.21	128.62	124.73
20	c	5498	CLA	C2A-C3A-C4A	2.21	105.43	101.87
21	a	5562	PHO	C1-C2-C3	2.21	129.81	126.20
20	C	499	CLA	CAA-C2A-C3A	-2.20	107.04	113.00
24	b	5528	BCR	C7-C8-C9	2.20	129.50	126.23
21	A	561	PHO	C1-O2A-CGA	2.20	121.98	116.65
20	A	560	CLA	O2A-CGA-CBA	2.20	118.55	111.83
20	c	5493	CLA	C2A-C1A-CHA	2.20	127.69	123.87
24	c	5505	BCR	C34-C9-C8	2.20	121.45	118.09
26	a	212	SQD	O10-C23-C24	-2.20	116.98	124.77
20	b	5525	CLA	C2A-C3A-C4A	2.20	105.42	101.87
24	h	5107	BCR	C36-C18-C19	2.20	121.45	118.09
20	b	5519	CLA	C2A-C1A-CHA	2.20	127.69	123.87
26	A	5212	SQD	O47-C45-C44	2.20	116.23	108.34
24	d	5357	BCR	C32-C1-C6	2.20	113.69	110.24
30	H	208	DGD	C3G-C2G-C1G	-2.20	106.66	111.78
20	B	511	CLA	C3B-C4B-NB	-2.20	108.57	110.53
32	v	5552	HEM	CAB-C3B-C2B	-2.20	121.29	128.43
20	c	5496	CLA	CBA-CAA-C2A	2.20	120.33	113.79
24	A	566	BCR	C1-C6-C7	2.20	121.61	115.65
28	L	210	MGE	O1G-C1G-C2G	-2.20	102.07	108.40
20	b	5511	CLA	C3B-C4B-NB	-2.20	108.57	110.53
20	b	5518	CLA	CBA-CAA-C2A	2.19	120.32	113.79
21	A	562	PHO	O1D-CGD-CBD	-2.19	121.40	124.72
24	b	5528	BCR	C35-C13-C12	2.19	121.44	118.09
20	B	514	CLA	C1-O2A-CGA	2.19	121.96	116.65
20	b	5512	CLA	C2A-C3A-C4A	2.19	105.41	101.87
24	C	504	BCR	C16-C17-C18	2.19	130.35	127.28
20	C	491	CLA	CAA-C2A-C3A	-2.19	107.08	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	c	5500	CLA	CBA-CAA-C2A	2.19	120.31	113.79
28	D	360	MGE	O1G-C1A-C2A	2.19	118.50	111.83
20	b	5524	CLA	CMD-C2D-C1D	2.19	128.58	124.73
20	B	513	CLA	C2A-C3A-C4A	2.19	105.40	101.87
20	a	5559	CLA	CAA-CBA-CGA	2.19	119.41	113.21
20	c	5502	CLA	CBA-CAA-C2A	2.19	120.30	113.79
20	b	5513	CLA	CMA-C3A-C2A	-2.19	105.53	113.98
24	B	529	BCR	C36-C18-C19	2.19	121.43	118.09
24	b	5527	BCR	C12-C13-C14	-2.18	115.58	119.01
20	b	5520	CLA	C2A-C3A-C4A	2.18	105.39	101.87
24	t	104	BCR	C16-C17-C18	2.18	130.34	127.28
30	C	508	DGD	C6E-C5E-C4E	-2.18	107.67	113.02
20	b	5516	CLA	O2D-CGD-CBD	2.18	115.04	111.23
24	d	5357	BCR	C34-C9-C8	2.18	121.41	118.09
20	C	492	CLA	C7-C6-C5	-2.18	107.46	113.26
20	B	515	CLA	C2A-C1A-CHA	2.18	127.64	123.87
24	a	5566	BCR	C7-C8-C9	2.17	129.45	126.23
20	b	5515	CLA	CBA-CAA-C2A	2.17	120.25	113.79
20	B	516	CLA	C2A-C3A-C4A	2.17	105.38	101.87
20	C	498	CLA	C2A-C3A-C4A	2.17	105.37	101.87
24	C	505	BCR	C7-C8-C9	2.17	129.44	126.23
20	B	525	CLA	C2A-C1A-CHA	2.17	127.63	123.87
20	c	5492	CLA	C1-C2-C3	2.17	129.75	126.20
24	B	527	BCR	C19-C18-C17	-2.17	115.60	119.01
24	a	5566	BCR	C8-C9-C10	-2.17	115.60	119.01
24	A	566	BCR	C30-C25-C24	2.17	121.53	115.65
20	B	517	CLA	CBA-CAA-C2A	2.17	120.24	113.79
20	B	518	CLA	CBA-CAA-C2A	2.17	120.24	113.79
30	C	508	DGD	O3G-C3G-C2G	2.17	116.08	110.82
24	b	5529	BCR	C15-C14-C13	2.16	130.31	127.28
20	C	496	CLA	C1-O2A-CGA	2.16	121.89	116.65
20	B	517	CLA	CMD-C2D-C1D	2.16	128.53	124.73
22	D	356	PQ9	C14-C13-C15	2.16	118.98	115.23
24	d	5357	BCR	C23-C22-C21	-2.16	115.61	119.01
20	b	5518	CLA	C6-C5-C3	2.16	118.73	113.47
21	A	561	PHO	C3D-C4D-ND	2.16	110.47	107.71
20	B	511	CLA	C2A-C1A-CHA	2.16	127.60	123.86
20	b	5513	CLA	C6-C5-C3	2.16	118.73	113.47
20	d	5355	CLA	C2A-C3A-C4A	2.16	105.36	101.87
24	c	5504	BCR	C34-C9-C8	2.16	121.38	118.09
24	h	5107	BCR	C28-C27-C26	2.15	117.89	114.06
20	D	354	CLA	CMD-C2D-C1D	2.15	128.52	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	c	5505	BCR	C40-C30-C25	2.15	113.61	110.24
24	B	529	BCR	C11-C10-C9	2.15	130.29	127.28
20	c	5503	CLA	C1-O2A-CGA	2.14	121.84	116.65
20	b	5515	CLA	O2D-CGD-CBD	2.14	114.98	111.23
28	d	5360	MGE	O1G-C1A-C2A	2.14	118.37	111.83
20	B	517	CLA	O2D-CGD-CBD	2.14	114.98	111.23
24	B	529	BCR	C1-C6-C7	2.14	121.46	115.65
24	D	357	BCR	C34-C9-C8	2.14	121.36	118.09
20	c	5494	CLA	C2A-C1A-CHA	2.14	127.58	123.87
20	B	514	CLA	C3B-C4B-NB	-2.14	108.62	110.53
20	B	514	CLA	C1-C2-C3	2.14	129.71	126.20
20	c	5500	CLA	CMA-C3A-C2A	-2.14	105.71	113.98
20	a	5559	CLA	C1-C2-C3	2.14	129.70	126.20
20	B	515	CLA	CMA-C3A-C2A	-2.14	105.72	113.98
20	B	520	CLA	C2A-C3A-C4A	2.14	105.32	101.87
20	b	5511	CLA	C2A-C1A-CHA	2.14	127.56	123.86
20	B	518	CLA	C6-C7-C8	2.14	123.07	115.97
32	F	51	HEM	CAA-CBA-CGA	2.14	119.33	113.67
20	d	5355	CLA	C1-O2A-CGA	2.14	121.82	116.65
24	D	357	BCR	C36-C18-C19	2.14	121.35	118.09
20	c	5494	CLA	C3B-C4B-NB	-2.14	108.62	110.53
20	B	517	CLA	C2D-C1D-ND	2.13	112.24	110.13
24	H	107	BCR	C34-C9-C8	2.13	121.35	118.09
20	c	5496	CLA	CMD-C2D-C1D	2.13	128.49	124.73
21	a	5561	PHO	OBD-CAD-C3D	2.13	131.22	127.89
20	c	5499	CLA	C1-O2A-CGA	2.13	122.73	116.67
20	c	5495	CLA	C1-O2A-CGA	2.13	121.81	116.65
26	a	212	SQD	O47-C45-C44	2.13	115.99	108.34
26	a	212	SQD	O8-S-O7	2.13	116.73	111.40
30	c	5508	DGD	O1G-C1A-C2A	2.13	118.33	111.83
20	B	513	CLA	CMA-C3A-C2A	-2.13	105.75	113.98
20	A	560	CLA	O2D-CGD-CBD	2.13	114.95	111.23
26	A	568	SQD	C17-C16-C15	2.13	125.13	114.37
32	v	5552	HEM	CAA-C2A-C1A	2.13	129.10	124.94
20	b	5517	CLA	C2A-C3A-C4A	2.13	105.31	101.87
20	B	526	CLA	C6-C5-C3	2.13	118.65	113.47
24	A	566	BCR	C34-C9-C8	2.13	121.34	118.09
22	A	564	PQ9	C11-C2-C1	2.13	118.66	116.91
21	a	5561	PHO	C3D-C4D-ND	2.13	110.43	107.71
24	b	5529	BCR	C30-C25-C24	2.12	121.41	115.65
20	C	500	CLA	CAA-C2A-C3A	-2.12	107.26	113.00
28	I	201	MGE	C3G-O3G-C1D	-2.12	109.25	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	5517	CLA	CMD-C2D-C1D	2.12	128.47	124.73
20	b	5514	CLA	C1-O2A-CGA	2.12	121.79	116.65
20	c	5493	CLA	CBA-CAA-C2A	2.12	120.10	113.79
20	c	5491	CLA	C3B-C4B-NB	-2.12	108.64	110.53
20	b	5526	CLA	C6-C5-C3	2.12	118.63	113.47
20	c	5498	CLA	CMD-C2D-C1D	2.12	128.46	124.73
20	C	502	CLA	CBA-CAA-C2A	2.12	120.09	113.79
30	h	5208	DGD	C3G-C2G-C1G	-2.12	106.85	111.78
21	a	5562	PHO	CMA-C3A-C4A	-2.12	110.05	114.61
20	c	5495	CLA	C2A-C3A-C4A	2.11	105.28	101.87
24	B	528	BCR	C30-C25-C24	2.11	121.38	115.65
27	m	216	LMT	C1B-O1B-C4'	-2.11	112.97	117.98
20	b	5525	CLA	C2A-C1A-CHA	2.11	127.53	123.87
20	D	355	CLA	CBA-CAA-C2A	2.11	120.07	113.79
24	h	5107	BCR	C11-C12-C13	2.11	132.15	126.36
20	c	5500	CLA	O2D-CGD-CBD	2.11	114.92	111.23
20	c	5491	CLA	C2A-C1A-CHA	2.11	127.53	123.87
28	D	358	MGE	C3G-C2G-C1G	-2.11	106.87	111.78
24	T	5104	BCR	C8-C9-C10	-2.11	115.69	119.01
20	A	563	CLA	C7-C6-C5	-2.11	107.65	113.26
20	b	5517	CLA	C3B-C4B-NB	-2.10	108.66	110.53
20	b	5518	CLA	C2A-C3A-C4A	2.10	105.26	101.87
20	C	492	CLA	O1D-CGD-CBD	-2.10	120.38	124.52
32	V	552	HEM	C4B-C3B-C2B	-2.10	105.35	107.28
20	C	496	CLA	C2A-C3A-C4A	2.10	105.26	101.87
24	A	566	BCR	C32-C1-C6	2.10	113.53	110.24
20	a	5558	CLA	CMA-C3A-C2A	-2.10	105.88	113.98
32	V	552	HEM	CAA-C2A-C1A	2.10	129.03	124.94
30	C	508	DGD	O1G-C1A-C2A	2.10	118.22	111.83
20	c	5501	CLA	C2A-C1A-CHA	2.10	127.50	123.87
20	C	491	CLA	CBA-CAA-C2A	2.09	120.03	113.79
20	B	518	CLA	C2A-C3A-C4A	2.09	105.25	101.87
21	a	5562	PHO	CBC-CAC-C3C	-2.09	109.88	112.87
24	x	5130	BCR	C24-C23-C22	2.09	129.33	126.23
32	F	51	HEM	CMD-C2D-C1D	2.09	128.30	125.03
20	C	503	CLA	O2D-CGD-CBD	2.09	114.89	111.23
20	B	520	CLA	C12-C11-C10	-2.09	103.90	113.28
20	C	496	CLA	CMD-C2D-C1D	2.09	128.41	124.73
20	B	520	CLA	C2A-C1A-CHA	2.09	127.50	123.87
20	B	524	CLA	CMD-C2D-C1D	2.09	128.41	124.73
20	B	524	CLA	C2A-C3A-C4A	2.09	105.24	101.87
28	D	359	MGE	C3G-O3G-C1D	-2.09	109.32	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	523	CLA	CMA-C3A-C2A	-2.09	105.91	113.98
32	F	51	HEM	CAA-C2A-C1A	2.09	129.01	124.94
20	B	520	CLA	O2D-CGD-CBD	2.09	114.88	111.23
20	C	496	CLA	C2A-C1A-CHA	2.08	127.48	123.87
20	a	5563	CLA	CMD-C2D-C1D	2.08	128.40	124.73
20	B	515	CLA	CBA-CAA-C2A	2.08	119.99	113.79
20	B	522	CLA	CAA-C2A-C3A	-2.08	107.37	113.00
20	C	493	CLA	CBA-CAA-C2A	2.08	119.99	113.79
20	b	5525	CLA	CMD-C2D-C1D	2.08	128.39	124.73
20	d	5355	CLA	CMD-C2D-C1D	2.08	128.39	124.73
20	c	5496	CLA	O2D-CGD-CBD	2.08	114.86	111.23
24	c	5505	BCR	C19-C18-C17	-2.08	115.74	119.01
20	D	355	CLA	C2A-C3A-C4A	2.08	105.22	101.87
20	b	5523	CLA	CMA-C3A-C2A	-2.08	105.96	113.98
24	T	5104	BCR	C30-C25-C24	2.07	121.28	115.65
20	c	5502	CLA	CMD-C2D-C1D	2.07	128.38	124.73
32	f	5051	HEM	CAA-CBA-CGA	2.07	119.16	113.67
20	b	5518	CLA	C6-C7-C8	2.07	122.85	115.97
32	v	5552	HEM	C4B-C3B-C2B	-2.07	105.38	107.28
21	a	5561	PHO	CMA-C3A-C2A	-2.07	106.14	114.13
24	b	5529	BCR	C36-C18-C19	2.07	121.25	118.09
20	C	497	CLA	C2A-C3A-C4A	2.07	105.21	101.87
20	b	5513	CLA	C2A-C3A-C4A	2.07	105.21	101.87
20	B	525	CLA	CMD-C2D-C1D	2.06	128.36	124.73
20	b	5521	CLA	CMD-C2D-C1D	2.06	128.36	124.73
24	t	104	BCR	C30-C25-C24	2.06	121.24	115.65
24	B	528	BCR	C32-C1-C2	-2.06	101.03	108.95
24	C	505	BCR	C1-C6-C7	2.06	121.24	115.65
24	T	5104	BCR	C19-C18-C17	-2.06	115.77	119.01
28	D	360	MGE	O1G-C1G-C2G	-2.06	102.47	108.40
20	d	5354	CLA	C2A-C1A-CHA	2.06	127.44	123.87
20	D	355	CLA	CMD-C2D-C1D	2.06	128.35	124.73
20	a	5563	CLA	CMA-C3A-C2A	-2.05	106.04	113.98
27	M	5216	LMT	C1-O1'-C1'	-2.05	110.17	113.68
20	C	501	CLA	O2D-CGD-CBD	2.05	114.82	111.23
20	c	5498	CLA	C12-C11-C10	-2.05	104.08	113.28
26	t	213	SQD	O48-C23-O10	-2.05	118.49	123.63
20	c	5500	CLA	C12-C11-C10	-2.05	104.08	113.28
24	c	5505	BCR	C1-C6-C7	2.05	121.22	115.65
32	V	552	HEM	CAB-C3B-C4B	2.05	133.46	124.39
20	C	501	CLA	C2D-C1D-ND	2.05	112.16	110.13
28	b	5530	MGE	C3G-C2G-C1G	-2.05	107.01	111.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	b	5522	CLA	CMD-C2D-C1D	2.05	128.34	124.73
30	c	5508	DGD	O3G-C3G-C2G	2.05	115.80	110.82
20	b	5515	CLA	C3B-C4B-NB	-2.05	108.70	110.53
28	L	210	MGE	O1G-C1A-C2A	2.05	118.08	111.83
24	b	5527	BCR	C19-C18-C17	-2.05	115.79	119.01
21	a	5562	PHO	CMA-C3A-C2A	-2.04	106.23	114.13
28	b	5530	MGE	O1G-C1A-C2A	2.04	118.06	111.83
24	a	5566	BCR	C19-C18-C17	-2.04	115.80	119.01
24	c	5504	BCR	C8-C7-C6	2.04	132.45	127.00
27	M	5216	LMT	C1B-O1B-C4'	-2.04	113.14	117.98
20	c	5502	CLA	CMA-C3A-C2A	-2.04	106.10	113.98
24	T	5104	BCR	C16-C17-C18	2.04	130.13	127.28
20	b	5523	CLA	CBA-CAA-C2A	2.04	119.85	113.79
24	x	5130	BCR	C40-C30-C29	-2.04	101.13	108.95
20	C	496	CLA	O2D-CGD-CBD	2.04	114.79	111.23
20	B	512	CLA	C1-O2A-CGA	2.04	121.58	116.65
26	a	212	SQD	O5-C5-C4	2.04	113.37	109.70
20	b	5514	CLA	C3B-C4B-NB	-2.04	108.71	110.53
32	v	5552	HEM	C1B-NB-C4B	2.03	107.62	105.21
20	C	491	CLA	C3B-C4B-NB	-2.03	108.72	110.53
26	t	213	SQD	O8-S-O7	2.03	116.48	111.40
20	B	526	CLA	C3B-C4B-NB	-2.03	108.72	110.53
21	A	562	PHO	OBD-CAD-C3D	2.03	131.06	127.89
20	A	559	CLA	C3B-C4B-NB	-2.03	108.72	110.53
20	b	5512	CLA	C3B-C4B-NB	-2.03	108.72	110.53
20	b	5519	CLA	C6-C5-C3	2.03	118.42	113.47
20	B	523	CLA	CBA-CAA-C2A	2.03	119.83	113.79
20	a	5560	CLA	O2D-CGD-CBD	2.03	114.78	111.23
22	A	564	PQ9	C6-C5-C4	2.03	119.44	115.28
20	c	5498	CLA	C2D-C1D-ND	2.03	112.13	110.13
20	b	5520	CLA	CAA-C2A-C3A	-2.03	107.52	113.00
20	b	5513	CLA	CMD-C2D-C1D	2.03	128.30	124.73
22	D	356	PQ9	C30-C28-C29	2.03	119.26	114.59
24	a	5566	BCR	C1-C6-C7	2.03	121.15	115.65
24	b	5529	BCR	C37-C22-C23	2.03	121.19	118.09
20	B	517	CLA	C2A-C3A-C4A	2.03	105.14	101.87
20	c	5491	CLA	CMA-C3A-C2A	-2.03	106.15	113.98
24	b	5527	BCR	C37-C22-C23	2.03	121.18	118.09
24	h	5107	BCR	C8-C9-C10	-2.02	115.82	119.01
20	C	498	CLA	CMA-C3A-C2A	-2.02	106.16	113.98
32	v	5552	HEM	CAB-C3B-C4B	2.02	133.33	124.39
20	c	5492	CLA	C2A-C1A-CHA	2.02	127.38	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	496	CLA	CBA-CAA-C2A	2.02	119.81	113.79
20	B	512	CLA	C2A-C1A-CHA	2.02	127.38	123.87
30	h	5208	DGD	O3G-C3G-C2G	2.02	115.74	110.82
20	c	5501	CLA	C2A-C3A-C4A	2.02	105.13	101.87
20	B	520	CLA	C3B-C4B-NB	-2.02	108.73	110.53
28	l	5210	MGE	O1G-C1A-C2A	2.02	117.99	111.83
20	C	503	CLA	CMD-C2D-C1D	2.02	128.28	124.73
30	c	5509	DGD	O1G-C1A-C2A	2.02	117.99	111.83
20	C	502	CLA	CMD-C2D-C1D	2.02	128.28	124.73
20	D	355	CLA	CMA-C3A-C2A	-2.02	106.19	113.98
20	b	5515	CLA	C2A-C1A-CHA	2.01	127.36	123.87
20	B	512	CLA	C3B-C4B-NB	-2.01	108.73	110.53
24	B	528	BCR	C7-C8-C9	2.01	129.21	126.23
20	b	5519	CLA	O2D-CGD-CBD	2.01	114.75	111.23
24	C	505	BCR	C37-C22-C23	2.01	121.16	118.09
27	m	216	LMT	C4B-C3B-C2B	-2.01	107.30	110.83
32	F	51	HEM	C4C-C3C-C2C	-2.01	105.07	106.81
21	A	561	PHO	CMA-C3A-C2A	-2.01	106.36	114.13
20	C	500	CLA	C1-O2A-CGA	2.01	121.52	116.65
24	b	5529	BCR	C11-C10-C9	2.01	130.10	127.28
20	B	519	CLA	O2D-CGD-CBD	2.01	114.74	111.23
24	x	5130	BCR	C19-C18-C17	-2.01	115.85	119.01
20	C	500	CLA	C12-C11-C10	-2.01	104.28	113.28
20	C	497	CLA	C2A-C1A-CHA	2.01	127.35	123.87
24	B	529	BCR	C16-C17-C18	2.01	130.09	127.28
20	B	522	CLA	CBA-CAA-C2A	2.01	119.77	113.79
20	b	5519	CLA	C2A-C3A-C4A	2.01	105.11	101.87
28	D	359	MGE	O1G-C1A-C2A	2.01	117.95	111.83
20	a	5559	CLA	CHD-C1D-ND	-2.01	121.98	124.80
20	C	503	CLA	C2A-C3A-C4A	2.00	105.11	101.87
24	T	5104	BCR	C32-C1-C6	2.00	113.38	110.24
30	C	507	DGD	O6D-C1D-C2D	2.00	114.48	110.37
20	b	5513	CLA	C2A-C1A-CHA	2.00	127.34	123.87

All (24) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
30	C	507	DGD	C5D
30	C	507	DGD	C5E
30	C	507	DGD	C2D
30	C	508	DGD	C5D
30	C	508	DGD	C5E

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Mol	Chain	Res	Type	Atom
30	C	508	DGD	C2D
30	C	509	DGD	C5D
30	C	509	DGD	C5E
30	C	509	DGD	C2D
30	H	208	DGD	C5D
30	H	208	DGD	C5E
30	H	208	DGD	C2D
30	c	5507	DGD	C5D
30	c	5507	DGD	C5E
30	c	5507	DGD	C2D
30	c	5508	DGD	C5D
30	c	5508	DGD	C5E
30	c	5508	DGD	C2D
30	c	5509	DGD	C5D
30	c	5509	DGD	C5E
30	c	5509	DGD	C2D
30	h	5208	DGD	C5D
30	h	5208	DGD	C5E
30	h	5208	DGD	C2D

All (1538) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	558	CLA	C2B-C3B-CAB-CBB
20	A	558	CLA	C4B-C3B-CAB-CBB
20	A	559	CLA	C2B-C3B-CAB-CBB
20	A	559	CLA	C4B-C3B-CAB-CBB
20	A	560	CLA	C2B-C3B-CAB-CBB
20	A	560	CLA	C4B-C3B-CAB-CBB
20	A	563	CLA	C2B-C3B-CAB-CBB
20	A	563	CLA	C4B-C3B-CAB-CBB
20	B	511	CLA	C2B-C3B-CAB-CBB
20	B	511	CLA	C4B-C3B-CAB-CBB
20	B	511	CLA	CBD-CGD-O2D-CED
20	B	513	CLA	C2B-C3B-CAB-CBB
20	B	513	CLA	C4B-C3B-CAB-CBB
20	B	514	CLA	C2B-C3B-CAB-CBB
20	B	514	CLA	C4B-C3B-CAB-CBB
20	B	515	CLA	C2-C3-C5-C6
20	B	515	CLA	C4-C3-C5-C6
20	B	516	CLA	C1A-C2A-CAA-CBA
20	B	516	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	B	516	CLA	C2B-C3B-CAB-CBB
20	B	516	CLA	C4B-C3B-CAB-CBB
20	B	516	CLA	C1-C2-C3-C4
20	B	516	CLA	C1-C2-C3-C5
20	B	517	CLA	C1A-C2A-CAA-CBA
20	B	517	CLA	C3A-C2A-CAA-CBA
20	B	518	CLA	C1A-C2A-CAA-CBA
20	B	518	CLA	C3A-C2A-CAA-CBA
20	B	518	CLA	C2B-C3B-CAB-CBB
20	B	518	CLA	C4B-C3B-CAB-CBB
20	B	518	CLA	C1-C2-C3-C5
20	B	518	CLA	C6-C7-C8-C9
20	B	519	CLA	C4B-C3B-CAB-CBB
20	B	520	CLA	C2B-C3B-CAB-CBB
20	B	520	CLA	C4B-C3B-CAB-CBB
20	B	521	CLA	C2B-C3B-CAB-CBB
20	B	521	CLA	C4B-C3B-CAB-CBB
20	B	524	CLA	C4B-C3B-CAB-CBB
20	B	525	CLA	C2B-C3B-CAB-CBB
20	B	525	CLA	C4B-C3B-CAB-CBB
20	B	525	CLA	C1-C2-C3-C5
20	B	526	CLA	C1A-C2A-CAA-CBA
20	B	526	CLA	C2B-C3B-CAB-CBB
20	B	526	CLA	C4B-C3B-CAB-CBB
20	C	491	CLA	C2B-C3B-CAB-CBB
20	C	491	CLA	C4B-C3B-CAB-CBB
20	C	492	CLA	C2B-C3B-CAB-CBB
20	C	492	CLA	C4B-C3B-CAB-CBB
20	C	492	CLA	C1-C2-C3-C5
20	C	493	CLA	C2B-C3B-CAB-CBB
20	C	493	CLA	C4B-C3B-CAB-CBB
20	C	494	CLA	C1A-C2A-CAA-CBA
20	C	495	CLA	C1A-C2A-CAA-CBA
20	C	495	CLA	CBD-CGD-O2D-CED
20	C	495	CLA	C1-C2-C3-C5
20	C	495	CLA	C2-C3-C5-C6
20	C	495	CLA	C4-C3-C5-C6
20	C	496	CLA	C1A-C2A-CAA-CBA
20	C	496	CLA	C2B-C3B-CAB-CBB
20	C	496	CLA	C4B-C3B-CAB-CBB
20	C	496	CLA	CBD-CGD-O2D-CED
20	C	497	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	C	497	CLA	C4B-C3B-CAB-CBB
20	C	499	CLA	C4B-C3B-CAB-CBB
20	C	500	CLA	C2B-C3B-CAB-CBB
20	C	500	CLA	C4B-C3B-CAB-CBB
20	C	500	CLA	C1-C2-C3-C5
20	C	501	CLA	C2B-C3B-CAB-CBB
20	C	501	CLA	C4B-C3B-CAB-CBB
20	C	501	CLA	C1-C2-C3-C5
20	C	502	CLA	C1A-C2A-CAA-CBA
20	C	503	CLA	C1A-C2A-CAA-CBA
20	C	503	CLA	C4B-C3B-CAB-CBB
20	C	503	CLA	C1-C2-C3-C4
20	C	503	CLA	C1-C2-C3-C5
20	D	354	CLA	C1-C2-C3-C4
20	D	354	CLA	C1-C2-C3-C5
20	D	355	CLA	C1A-C2A-CAA-CBA
20	D	355	CLA	C3A-C2A-CAA-CBA
20	D	355	CLA	C2B-C3B-CAB-CBB
20	D	355	CLA	C4B-C3B-CAB-CBB
20	D	355	CLA	C1-C2-C3-C4
20	D	355	CLA	C1-C2-C3-C5
20	a	5558	CLA	C2B-C3B-CAB-CBB
20	a	5558	CLA	C4B-C3B-CAB-CBB
20	a	5558	CLA	CBD-CGD-O2D-CED
20	a	5559	CLA	C2B-C3B-CAB-CBB
20	a	5559	CLA	C4B-C3B-CAB-CBB
20	a	5560	CLA	C2B-C3B-CAB-CBB
20	a	5560	CLA	C4B-C3B-CAB-CBB
20	a	5563	CLA	C2B-C3B-CAB-CBB
20	a	5563	CLA	C4B-C3B-CAB-CBB
20	b	5511	CLA	C2B-C3B-CAB-CBB
20	b	5511	CLA	C4B-C3B-CAB-CBB
20	b	5511	CLA	CBD-CGD-O2D-CED
20	b	5513	CLA	C2B-C3B-CAB-CBB
20	b	5513	CLA	C4B-C3B-CAB-CBB
20	b	5514	CLA	C2B-C3B-CAB-CBB
20	b	5514	CLA	C4B-C3B-CAB-CBB
20	b	5515	CLA	C2-C3-C5-C6
20	b	5515	CLA	C4-C3-C5-C6
20	b	5516	CLA	C1A-C2A-CAA-CBA
20	b	5516	CLA	C3A-C2A-CAA-CBA
20	b	5516	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	b	5516	CLA	C4B-C3B-CAB-CBB
20	b	5516	CLA	C1-C2-C3-C4
20	b	5516	CLA	C1-C2-C3-C5
20	b	5517	CLA	C1A-C2A-CAA-CBA
20	b	5517	CLA	C3A-C2A-CAA-CBA
20	b	5518	CLA	C1A-C2A-CAA-CBA
20	b	5518	CLA	C3A-C2A-CAA-CBA
20	b	5518	CLA	C2B-C3B-CAB-CBB
20	b	5518	CLA	C4B-C3B-CAB-CBB
20	b	5518	CLA	C1-C2-C3-C5
20	b	5518	CLA	C6-C7-C8-C9
20	b	5519	CLA	C4B-C3B-CAB-CBB
20	b	5520	CLA	C2B-C3B-CAB-CBB
20	b	5520	CLA	C4B-C3B-CAB-CBB
20	b	5520	CLA	C1-C2-C3-C4
20	b	5521	CLA	C2B-C3B-CAB-CBB
20	b	5521	CLA	C4B-C3B-CAB-CBB
20	b	5524	CLA	C4B-C3B-CAB-CBB
20	b	5525	CLA	C2B-C3B-CAB-CBB
20	b	5525	CLA	C4B-C3B-CAB-CBB
20	b	5525	CLA	C1-C2-C3-C5
20	b	5526	CLA	C1A-C2A-CAA-CBA
20	b	5526	CLA	C4B-C3B-CAB-CBB
20	c	5491	CLA	C1A-C2A-CAA-CBA
20	c	5491	CLA	C2B-C3B-CAB-CBB
20	c	5491	CLA	C4B-C3B-CAB-CBB
20	c	5492	CLA	C2B-C3B-CAB-CBB
20	c	5492	CLA	C4B-C3B-CAB-CBB
20	c	5492	CLA	C1-C2-C3-C5
20	c	5493	CLA	C2B-C3B-CAB-CBB
20	c	5493	CLA	C4B-C3B-CAB-CBB
20	c	5494	CLA	C1A-C2A-CAA-CBA
20	c	5495	CLA	C1A-C2A-CAA-CBA
20	c	5495	CLA	CBD-CGD-O2D-CED
20	c	5495	CLA	C1-C2-C3-C5
20	c	5495	CLA	C2-C3-C5-C6
20	c	5495	CLA	C4-C3-C5-C6
20	c	5496	CLA	C1A-C2A-CAA-CBA
20	c	5496	CLA	C2B-C3B-CAB-CBB
20	c	5496	CLA	C4B-C3B-CAB-CBB
20	c	5496	CLA	CBD-CGD-O2D-CED
20	c	5497	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	c	5497	CLA	C4B-C3B-CAB-CBB
20	c	5499	CLA	C4B-C3B-CAB-CBB
20	c	5500	CLA	C2B-C3B-CAB-CBB
20	c	5500	CLA	C4B-C3B-CAB-CBB
20	c	5500	CLA	CBD-CGD-O2D-CED
20	c	5500	CLA	C1-C2-C3-C5
20	c	5501	CLA	C2B-C3B-CAB-CBB
20	c	5501	CLA	C4B-C3B-CAB-CBB
20	c	5501	CLA	C1-C2-C3-C5
20	c	5502	CLA	C1A-C2A-CAA-CBA
20	c	5503	CLA	C1A-C2A-CAA-CBA
20	c	5503	CLA	C1-C2-C3-C4
20	c	5503	CLA	C1-C2-C3-C5
20	d	5354	CLA	C1-C2-C3-C4
20	d	5354	CLA	C1-C2-C3-C5
20	d	5355	CLA	C1A-C2A-CAA-CBA
20	d	5355	CLA	C3A-C2A-CAA-CBA
20	d	5355	CLA	C2B-C3B-CAB-CBB
20	d	5355	CLA	C4B-C3B-CAB-CBB
20	d	5355	CLA	C1-C2-C3-C4
21	A	561	PHO	C4C-C3C-CAC-CBC
21	a	5561	PHO	C4C-C3C-CAC-CBC
22	A	564	PQ9	C11-C12-C13-C14
22	A	564	PQ9	C11-C12-C13-C15
22	A	564	PQ9	C16-C17-C18-C19
22	A	564	PQ9	C16-C17-C18-C20
22	D	356	PQ9	C16-C17-C18-C19
22	D	356	PQ9	C16-C17-C18-C20
22	D	356	PQ9	C21-C22-C23-C25
22	a	5564	PQ9	C11-C12-C13-C14
22	a	5564	PQ9	C11-C12-C13-C15
22	a	5564	PQ9	C16-C17-C18-C19
22	a	5564	PQ9	C16-C17-C18-C20
22	d	5356	PQ9	C16-C17-C18-C19
22	d	5356	PQ9	C16-C17-C18-C20
22	d	5356	PQ9	C21-C22-C23-C25
24	A	566	BCR	C5-C6-C7-C8
24	B	527	BCR	C6-C7-C8-C9
24	B	528	BCR	C6-C7-C8-C9
24	B	529	BCR	C6-C7-C8-C9
24	B	529	BCR	C23-C24-C25-C26
24	C	504	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
24	C	504	BCR	C5-C6-C7-C8
24	C	504	BCR	C6-C7-C8-C9
24	C	505	BCR	C6-C7-C8-C9
24	C	506	BCR	C22-C23-C24-C25
24	C	506	BCR	C23-C24-C25-C26
24	D	357	BCR	C6-C7-C8-C9
24	T	5104	BCR	C6-C7-C8-C9
24	b	5527	BCR	C6-C7-C8-C9
24	b	5528	BCR	C6-C7-C8-C9
24	b	5529	BCR	C6-C7-C8-C9
24	b	5529	BCR	C23-C24-C25-C26
24	c	5504	BCR	C1-C6-C7-C8
24	c	5504	BCR	C5-C6-C7-C8
24	c	5504	BCR	C6-C7-C8-C9
24	c	5505	BCR	C6-C7-C8-C9
24	c	5506	BCR	C22-C23-C24-C25
24	c	5506	BCR	C23-C24-C25-C26
24	d	5357	BCR	C6-C7-C8-C9
24	t	104	BCR	C6-C7-C8-C9
26	A	568	SQD	O5-C1-O6-C44
26	A	568	SQD	C5-C6-S-O7
26	A	568	SQD	C5-C6-S-O8
26	A	568	SQD	C5-C6-S-O9
26	A	5212	SQD	O5-C1-O6-C44
26	A	5212	SQD	O6-C44-C45-O47
26	L	5213	SQD	O5-C1-O6-C44
26	L	5213	SQD	O10-C23-O48-C46
26	L	5213	SQD	O5-C5-C6-S
26	a	212	SQD	O5-C1-O6-C44
26	a	212	SQD	O6-C44-C45-O47
26	d	5358	SQD	O5-C1-O6-C44
26	d	5358	SQD	C5-C6-S-O7
26	d	5358	SQD	C5-C6-S-O8
26	d	5358	SQD	C5-C6-S-O9
26	t	213	SQD	O5-C1-O6-C44
26	t	213	SQD	O5-C5-C6-S
28	B	530	MGE	C2B-C1B-O2G-C2G
28	B	530	MGE	C2D-C1D-O3G-C3G
28	B	530	MGE	O6D-C1D-O3G-C3G
28	D	358	MGE	C2B-C1B-O2G-C2G
28	D	359	MGE	C2B-C1B-O2G-C2G
28	D	360	MGE	C2B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
28	I	201	MGE	O1A-C1A-O1G-C1G
28	I	201	MGE	C2B-C1B-O2G-C2G
28	b	5530	MGE	C2B-C1B-O2G-C2G
28	b	5530	MGE	C2D-C1D-O3G-C3G
28	b	5530	MGE	O6D-C1D-O3G-C3G
28	d	5359	MGE	C2B-C1B-O2G-C2G
28	d	5360	MGE	C2B-C1B-O2G-C2G
28	d	5361	MGE	C2B-C1B-O2G-C2G
28	i	5201	MGE	C2B-C1B-O2G-C2G
30	C	507	DGD	C2D-C1D-O3G-C3G
30	C	507	DGD	C2E-C1E-O5D-C6D
30	C	508	DGD	C2B-C1B-O2G-C2G
30	C	508	DGD	O6E-C1E-O5D-C6D
30	H	208	DGD	O6D-C1D-O3G-C3G
30	H	208	DGD	C2E-C1E-O5D-C6D
30	c	5507	DGD	C2E-C1E-O5D-C6D
30	c	5508	DGD	C2B-C1B-O2G-C2G
30	c	5508	DGD	O1B-C1B-O2G-C2G
30	c	5508	DGD	O6E-C1E-O5D-C6D
30	h	5208	DGD	O6D-C1D-O3G-C3G
30	h	5208	DGD	C2E-C1E-O5D-C6D
32	F	51	HEM	C2B-C3B-CAB-CBB
32	F	51	HEM	C4B-C3B-CAB-CBB
32	V	552	HEM	C2B-C3B-CAB-CBB
32	V	552	HEM	C2C-C3C-CAC-CBC
32	V	552	HEM	C4C-C3C-CAC-CBC
32	f	5051	HEM	C2B-C3B-CAB-CBB
32	f	5051	HEM	C4B-C3B-CAB-CBB
32	v	5552	HEM	C2B-C3B-CAB-CBB
32	v	5552	HEM	C2C-C3C-CAC-CBC
32	v	5552	HEM	C4C-C3C-CAC-CBC
20	A	558	CLA	O1D-CGD-O2D-CED
20	a	5558	CLA	O1D-CGD-O2D-CED
20	C	494	CLA	O1D-CGD-O2D-CED
26	A	5212	SQD	C24-C23-O48-C46
26	a	212	SQD	C24-C23-O48-C46
20	A	558	CLA	CBD-CGD-O2D-CED
20	B	513	CLA	CBD-CGD-O2D-CED
20	B	514	CLA	CBD-CGD-O2D-CED
20	B	517	CLA	CBD-CGD-O2D-CED
20	B	526	CLA	CBD-CGD-O2D-CED
20	C	493	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	C	494	CLA	CBD-CGD-O2D-CED
20	C	499	CLA	CBD-CGD-O2D-CED
20	C	500	CLA	CBD-CGD-O2D-CED
20	C	502	CLA	CBD-CGD-O2D-CED
20	D	355	CLA	CBD-CGD-O2D-CED
20	b	5513	CLA	CBD-CGD-O2D-CED
20	b	5514	CLA	CBD-CGD-O2D-CED
20	b	5517	CLA	CBD-CGD-O2D-CED
20	b	5524	CLA	CBD-CGD-O2D-CED
20	b	5526	CLA	CBD-CGD-O2D-CED
20	c	5493	CLA	CBD-CGD-O2D-CED
20	c	5494	CLA	CBD-CGD-O2D-CED
20	c	5499	CLA	CBD-CGD-O2D-CED
20	d	5355	CLA	CBD-CGD-O2D-CED
21	A	562	PHO	CBD-CGD-O2D-CED
21	a	5562	PHO	CBD-CGD-O2D-CED
28	D	360	MGE	O1A-C1A-O1G-C1G
28	i	5201	MGE	O1A-C1A-O1G-C1G
20	C	495	CLA	O1D-CGD-O2D-CED
20	c	5494	CLA	O1D-CGD-O2D-CED
20	c	5495	CLA	O1D-CGD-O2D-CED
22	A	564	PQ9	C26-C27-C28-C29
22	d	5356	PQ9	C26-C27-C28-C30
20	B	526	CLA	O1D-CGD-O2D-CED
20	b	5526	CLA	O1D-CGD-O2D-CED
20	c	5499	CLA	O1D-CGD-O2D-CED
26	L	5213	SQD	C24-C23-O48-C46
26	t	213	SQD	C24-C23-O48-C46
28	I	201	MGE	C2A-C1A-O1G-C1G
20	B	515	CLA	CBD-CGD-O2D-CED
20	b	5515	CLA	CBD-CGD-O2D-CED
26	t	213	SQD	O10-C23-O48-C46
28	D	359	MGE	O1A-C1A-O1G-C1G
28	L	210	MGE	O1A-C1A-O1G-C1G
28	d	5360	MGE	O1A-C1A-O1G-C1G
28	d	5361	MGE	O1A-C1A-O1G-C1G
28	l	5210	MGE	O1A-C1A-O1G-C1G
20	B	511	CLA	O1D-CGD-O2D-CED
20	C	493	CLA	O1D-CGD-O2D-CED
20	C	499	CLA	O1D-CGD-O2D-CED
20	C	500	CLA	O1D-CGD-O2D-CED
20	c	5493	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	c	5496	CLA	O1D-CGD-O2D-CED
20	c	5500	CLA	O1D-CGD-O2D-CED
20	C	496	CLA	O1D-CGD-O2D-CED
26	A	5212	SQD	O10-C23-O48-C46
20	B	524	CLA	CBD-CGD-O2D-CED
20	c	5502	CLA	CBD-CGD-O2D-CED
28	B	530	MGE	O1B-C1B-O2G-C2G
28	D	358	MGE	O1B-C1B-O2G-C2G
28	D	359	MGE	O1B-C1B-O2G-C2G
28	I	201	MGE	O1B-C1B-O2G-C2G
28	b	5530	MGE	O1B-C1B-O2G-C2G
28	d	5359	MGE	O1B-C1B-O2G-C2G
28	d	5360	MGE	O1B-C1B-O2G-C2G
28	i	5201	MGE	O1B-C1B-O2G-C2G
30	C	508	DGD	O1B-C1B-O2G-C2G
22	D	356	PQ9	C26-C27-C28-C29
22	a	5564	PQ9	C26-C27-C28-C29
22	d	5356	PQ9	C26-C27-C28-C29
20	B	512	CLA	C3-C5-C6-C7
20	B	523	CLA	C3-C5-C6-C7
20	b	5512	CLA	C3-C5-C6-C7
20	b	5523	CLA	C3-C5-C6-C7
21	A	562	PHO	C3-C5-C6-C7
21	a	5562	PHO	C3-C5-C6-C7
21	A	562	PHO	O1D-CGD-O2D-CED
28	D	359	MGE	C2A-C1A-O1G-C1G
28	D	360	MGE	C2A-C1A-O1G-C1G
28	L	210	MGE	C2A-C1A-O1G-C1G
28	d	5360	MGE	C2A-C1A-O1G-C1G
28	i	5201	MGE	C2A-C1A-O1G-C1G
28	l	5210	MGE	C2A-C1A-O1G-C1G
20	A	563	CLA	CBD-CGD-O2D-CED
20	B	519	CLA	CBD-CGD-O2D-CED
20	B	525	CLA	CBD-CGD-O2D-CED
20	C	498	CLA	CBD-CGD-O2D-CED
20	b	5519	CLA	CBD-CGD-O2D-CED
20	b	5523	CLA	CBD-CGD-O2D-CED
20	b	5525	CLA	CBD-CGD-O2D-CED
20	c	5498	CLA	CBD-CGD-O2D-CED
20	B	513	CLA	O1D-CGD-O2D-CED
20	b	5511	CLA	O1D-CGD-O2D-CED
21	a	5562	PHO	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	a	212	SQD	O10-C23-O48-C46
20	d	5355	CLA	C2A-CAA-CBA-CGA
22	A	564	PQ9	C26-C27-C28-C30
22	D	356	PQ9	C26-C27-C28-C30
22	a	5564	PQ9	C26-C27-C28-C30
20	B	518	CLA	C3-C5-C6-C7
20	b	5518	CLA	C3-C5-C6-C7
28	d	5361	MGE	C2A-C1A-O1G-C1G
22	D	356	PQ9	C21-C22-C23-C24
22	d	5356	PQ9	C21-C22-C23-C24
30	c	5508	DGD	C4D-C5D-C6D-O5D
28	D	360	MGE	O1B-C1B-O2G-C2G
28	d	5361	MGE	O1B-C1B-O2G-C2G
20	b	5513	CLA	O1D-CGD-O2D-CED
20	B	523	CLA	CBD-CGD-O2D-CED
20	a	5563	CLA	CBD-CGD-O2D-CED
20	B	517	CLA	O1D-CGD-O2D-CED
20	d	5355	CLA	O1D-CGD-O2D-CED
28	D	360	MGE	O6D-C5D-C6D-O5D
30	C	508	DGD	C4D-C5D-C6D-O5D
30	C	507	DGD	C4E-C5E-C6E-O5E
30	c	5507	DGD	C4E-C5E-C6E-O5E
20	D	355	CLA	O1D-CGD-O2D-CED
20	b	5517	CLA	O1D-CGD-O2D-CED
30	C	508	DGD	O6D-C5D-C6D-O5D
30	c	5508	DGD	O6D-C5D-C6D-O5D
20	B	515	CLA	C3-C5-C6-C7
28	b	5530	MGE	C2A-C1A-O1G-C1G
28	d	5361	MGE	O6D-C5D-C6D-O5D
20	C	502	CLA	O1D-CGD-O2D-CED
28	I	201	MGE	O6D-C5D-C6D-O5D
20	C	498	CLA	C2A-CAA-CBA-CGA
20	D	355	CLA	C2A-CAA-CBA-CGA
20	b	5520	CLA	C2A-CAA-CBA-CGA
20	c	5498	CLA	C2A-CAA-CBA-CGA
20	c	5501	CLA	C2A-CAA-CBA-CGA
20	B	514	CLA	O1D-CGD-O2D-CED
20	b	5524	CLA	O1D-CGD-O2D-CED
28	I	201	MGE	O6D-C1D-O3G-C3G
28	i	5201	MGE	O6D-C1D-O3G-C3G
30	C	507	DGD	O6D-C1D-O3G-C3G
30	C	507	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
30	H	208	DGD	O6E-C1E-O5D-C6D
30	c	5507	DGD	O6D-C1D-O3G-C3G
30	h	5208	DGD	O6E-C1E-O5D-C6D
28	B	530	MGE	C2A-C1A-O1G-C1G
20	B	522	CLA	CBD-CGD-O2D-CED
20	b	5522	CLA	CBD-CGD-O2D-CED
28	b	5530	MGE	O1A-C1A-O1G-C1G
30	C	507	DGD	C4D-C5D-C6D-O5D
28	D	359	MGE	O6D-C5D-C6D-O5D
28	d	5360	MGE	O6D-C5D-C6D-O5D
20	b	5514	CLA	O1D-CGD-O2D-CED
28	D	359	MGE	C4D-C5D-C6D-O5D
20	C	491	CLA	CBD-CGD-O2D-CED
20	c	5491	CLA	CBD-CGD-O2D-CED
28	B	530	MGE	O1A-C1A-O1G-C1G
20	c	5502	CLA	O1D-CGD-O2D-CED
25	a	5567	LHG	C24-C23-O8-C6
26	A	568	SQD	C24-C23-O48-C46
26	d	5358	SQD	C24-C23-O48-C46
28	i	5201	MGE	O6D-C5D-C6D-O5D
20	C	501	CLA	CBD-CGD-O2D-CED
20	b	5518	CLA	CBD-CGD-O2D-CED
30	C	507	DGD	O6D-C5D-C6D-O5D
30	c	5507	DGD	O6D-C5D-C6D-O5D
30	c	5507	DGD	C4D-C5D-C6D-O5D
20	B	515	CLA	O1D-CGD-O2D-CED
20	B	524	CLA	O1D-CGD-O2D-CED
20	b	5515	CLA	O1D-CGD-O2D-CED
28	d	5360	MGE	C4D-C5D-C6D-O5D
22	D	356	PQ9	C24-C23-C25-C26
22	d	5356	PQ9	C24-C23-C25-C26
22	D	356	PQ9	C22-C23-C25-C26
22	d	5356	PQ9	C22-C23-C25-C26
20	A	558	CLA	C14-C13-C15-C16
20	B	514	CLA	C6-C7-C8-C9
20	B	518	CLA	C14-C13-C15-C16
20	B	522	CLA	C6-C7-C8-C9
20	C	501	CLA	C6-C7-C8-C9
20	a	5558	CLA	C14-C13-C15-C16
20	b	5514	CLA	C6-C7-C8-C9
20	b	5518	CLA	C14-C13-C15-C16
20	b	5522	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	c	5501	CLA	C6-C7-C8-C9
28	I	201	MGE	C2D-C1D-O3G-C3G
28	i	5201	MGE	C2D-C1D-O3G-C3G
30	H	208	DGD	C2D-C1D-O3G-C3G
30	c	5507	DGD	C2D-C1D-O3G-C3G
30	h	5208	DGD	C2D-C1D-O3G-C3G
30	h	5208	DGD	O6D-C5D-C6D-O5D
25	A	567	LHG	C24-C23-O8-C6
26	d	5358	SQD	O10-C23-O48-C46
20	b	5525	CLA	O1D-CGD-O2D-CED
20	B	520	CLA	C2A-CAA-CBA-CGA
20	C	501	CLA	C2A-CAA-CBA-CGA
30	H	208	DGD	O6D-C5D-C6D-O5D
20	b	5523	CLA	O1D-CGD-O2D-CED
20	B	525	CLA	O1D-CGD-O2D-CED
20	c	5498	CLA	O1D-CGD-O2D-CED
22	A	564	PQ9	C21-C22-C23-C24
20	C	491	CLA	C15-C16-C17-C18
20	C	498	CLA	O1D-CGD-O2D-CED
28	B	530	MGE	C1B-C2B-C3B-C4B
20	C	493	CLA	C13-C15-C16-C17
20	B	520	CLA	C6-C7-C8-C10
20	b	5520	CLA	C6-C7-C8-C10
20	b	5519	CLA	O1D-CGD-O2D-CED
22	D	356	PQ9	C18-C20-C21-C22
22	d	5356	PQ9	C18-C20-C21-C22
20	b	5515	CLA	C3-C5-C6-C7
20	b	5517	CLA	C10-C11-C12-C13
20	c	5491	CLA	C15-C16-C17-C18
20	c	5493	CLA	C13-C15-C16-C17
28	D	358	MGE	C1B-C2B-C3B-C4B
28	d	5359	MGE	C1B-C2B-C3B-C4B
30	c	5507	DGD	C1A-C2A-C3A-C4A
25	A	567	LHG	O10-C23-O8-C6
25	a	5567	LHG	O10-C23-O8-C6
26	A	568	SQD	O10-C23-O48-C46
20	A	558	CLA	C10-C11-C12-C13
20	B	517	CLA	C10-C11-C12-C13
20	b	5513	CLA	C5-C6-C7-C8
20	c	5497	CLA	C15-C16-C17-C18
21	A	562	PHO	C10-C11-C12-C13
21	A	562	PHO	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
21	a	5562	PHO	C13-C15-C16-C17
28	d	5361	MGE	C4D-C5D-C6D-O5D
20	C	494	CLA	C2A-CAA-CBA-CGA
20	C	496	CLA	C2A-CAA-CBA-CGA
20	c	5494	CLA	C2A-CAA-CBA-CGA
20	c	5502	CLA	C2A-CAA-CBA-CGA
20	A	563	CLA	C5-C6-C7-C8
20	C	500	CLA	C5-C6-C7-C8
20	c	5493	CLA	C10-C11-C12-C13
21	a	5562	PHO	C10-C11-C12-C13
30	c	5508	DGD	C4E-C5E-C6E-O5E
28	b	5530	MGE	C1B-C2B-C3B-C4B
30	C	507	DGD	C1A-C2A-C3A-C4A
30	c	5507	DGD	O6E-C1E-O5D-C6D
30	C	508	DGD	C4E-C5E-C6E-O5E
20	A	559	CLA	C15-C16-C17-C18
20	B	513	CLA	C5-C6-C7-C8
20	B	519	CLA	C15-C16-C17-C18
20	B	523	CLA	C10-C11-C12-C13
20	C	497	CLA	C15-C16-C17-C18
20	a	5558	CLA	C10-C11-C12-C13
20	a	5563	CLA	C5-C6-C7-C8
20	b	5519	CLA	C15-C16-C17-C18
20	b	5522	CLA	C10-C11-C12-C13
30	C	509	DGD	C2A-C1A-O1G-C1G
20	b	5516	CLA	CBD-CGD-O2D-CED
28	D	360	MGE	C4D-C5D-C6D-O5D
28	d	5360	MGE	C1B-C2B-C3B-C4B
20	b	5516	CLA	C13-C15-C16-C17
20	c	5500	CLA	C5-C6-C7-C8
22	a	5564	PQ9	C21-C22-C23-C24
20	A	563	CLA	O1D-CGD-O2D-CED
20	B	522	CLA	C10-C11-C12-C13
20	a	5559	CLA	C15-C16-C17-C18
20	b	5523	CLA	C10-C11-C12-C13
30	c	5507	DGD	O6E-C5E-C6E-O5E
28	D	358	MGE	C1A-C2A-C3A-C4A
28	D	359	MGE	C1B-C2B-C3B-C4B
28	d	5359	MGE	C1A-C2A-C3A-C4A
20	B	519	CLA	O1D-CGD-O2D-CED
20	B	523	CLA	O1D-CGD-O2D-CED
20	B	519	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
20	B	516	CLA	CBD-CGD-O2D-CED
20	B	520	CLA	CBD-CGD-O2D-CED
28	L	210	MGE	C2B-C1B-O2G-C2G
20	B	516	CLA	C13-C15-C16-C17
20	c	5493	CLA	C5-C6-C7-C8
20	B	526	CLA	C13-C15-C16-C17
20	C	493	CLA	C10-C11-C12-C13
20	b	5516	CLA	C10-C11-C12-C13
20	b	5517	CLA	C5-C6-C7-C8
30	C	507	DGD	O6E-C5E-C6E-O5E
30	c	5507	DGD	O1B-C1B-O2G-C2G
20	C	502	CLA	C2A-CAA-CBA-CGA
20	c	5496	CLA	C2A-CAA-CBA-CGA
30	c	5509	DGD	C2A-C1A-O1G-C1G
20	C	493	CLA	C5-C6-C7-C8
20	b	5512	CLA	C15-C16-C17-C18
20	b	5515	CLA	C13-C15-C16-C17
20	b	5526	CLA	C13-C15-C16-C17
20	c	5500	CLA	C15-C16-C17-C18
20	a	5563	CLA	O1D-CGD-O2D-CED
20	B	512	CLA	C15-C16-C17-C18
20	B	522	CLA	C13-C15-C16-C17
20	b	5522	CLA	C13-C15-C16-C17
20	c	5495	CLA	C15-C16-C17-C18
20	B	515	CLA	C13-C15-C16-C17
20	B	516	CLA	C10-C11-C12-C13
20	B	517	CLA	C5-C6-C7-C8
20	B	523	CLA	C5-C6-C7-C8
20	C	495	CLA	C10-C11-C12-C13
20	C	495	CLA	C15-C16-C17-C18
20	a	5560	CLA	C10-C11-C12-C13
20	b	5519	CLA	C10-C11-C12-C13
20	b	5523	CLA	C5-C6-C7-C8
20	c	5498	CLA	C13-C15-C16-C17
20	A	560	CLA	C10-C11-C12-C13
20	B	517	CLA	C8-C10-C11-C12
20	c	5495	CLA	C10-C11-C12-C13
20	d	5355	CLA	C1-C2-C3-C5
20	c	5501	CLA	CBD-CGD-O2D-CED
28	l	5210	MGE	C2B-C1B-O2G-C2G
30	c	5507	DGD	C2B-C1B-O2G-C2G
28	L	210	MGE	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
28	l	5210	MGE	O1B-C1B-O2G-C2G
30	C	507	DGD	O1B-C1B-O2G-C2G
30	c	5509	DGD	O1B-C1B-O2G-C2G
28	L	210	MGE	C2D-C1D-O3G-C3G
28	l	5210	MGE	C2D-C1D-O3G-C3G
30	C	508	DGD	C2E-C1E-O5D-C6D
30	c	5508	DGD	C2E-C1E-O5D-C6D
20	C	498	CLA	C13-C15-C16-C17
20	b	5517	CLA	C8-C10-C11-C12
30	C	509	DGD	O1A-C1A-O1G-C1G
20	B	517	CLA	C2A-CAA-CBA-CGA
20	b	5517	CLA	C2A-CAA-CBA-CGA
20	A	559	CLA	C5-C6-C7-C8
20	C	500	CLA	C15-C16-C17-C18
20	a	5559	CLA	C5-C6-C7-C8
25	A	567	LHG	O1-C1-C2-C3
30	c	5509	DGD	O1A-C1A-O1G-C1G
28	L	210	MGE	O6D-C1D-O3G-C3G
28	l	5210	MGE	O6D-C1D-O3G-C3G
30	C	507	DGD	C2B-C1B-O2G-C2G
30	c	5509	DGD	C2B-C1B-O2G-C2G
30	H	208	DGD	C4D-C5D-C6D-O5D
20	b	5520	CLA	C5-C6-C7-C8
20	c	5492	CLA	C11-C12-C13-C14
20	B	520	CLA	C5-C6-C7-C8
30	h	5208	DGD	C4D-C5D-C6D-O5D
26	L	5213	SQD	C11-C12-C13-C14
28	B	530	MGE	C9A-CAA-CBA-CCA
28	D	359	MGE	C3B-C4B-C5B-C6B
28	L	210	MGE	CCB-CDB-CEB-CFB
28	i	5201	MGE	C9A-CAA-CBA-CCA
30	H	208	DGD	C5B-C6B-C7B-C8B
25	a	5567	LHG	C30-C31-C32-C33
26	t	213	SQD	C9-C10-C11-C12
28	b	5530	MGE	C9A-CAA-CBA-CCA
26	t	213	SQD	C11-C12-C13-C14
28	l	5210	MGE	C5B-C6B-C7B-C8B
30	h	5208	DGD	C5B-C6B-C7B-C8B
30	h	5208	DGD	C2A-C1A-O1G-C1G
28	d	5360	MGE	C3B-C4B-C5B-C6B
28	l	5210	MGE	CCB-CDB-CEB-CFB
30	H	208	DGD	C5A-C6A-C7A-C8A

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Mol	Chain	Res	Type	Atoms
30	h	5208	DGD	C5A-C6A-C7A-C8A
25	A	567	LHG	C30-C31-C32-C33
28	D	359	MGE	C8B-C9B-CAB-CBB
28	L	210	MGE	C3B-C4B-C5B-C6B
28	L	210	MGE	C5B-C6B-C7B-C8B
28	d	5360	MGE	C8B-C9B-CAB-CBB
28	l	5210	MGE	C3B-C4B-C5B-C6B
30	C	507	DGD	C9A-CAA-CBA-CCA
20	B	512	CLA	C4B-C3B-CAB-CBB
20	B	517	CLA	C4B-C3B-CAB-CBB
20	C	494	CLA	C4B-C3B-CAB-CBB
20	C	495	CLA	C4B-C3B-CAB-CBB
20	b	5512	CLA	C4B-C3B-CAB-CBB
20	b	5517	CLA	C4B-C3B-CAB-CBB
20	c	5494	CLA	C4B-C3B-CAB-CBB
20	c	5495	CLA	C4B-C3B-CAB-CBB
20	c	5503	CLA	C4B-C3B-CAB-CBB
20	C	492	CLA	C11-C12-C13-C14
20	C	492	CLA	C11-C12-C13-C15
20	c	5492	CLA	C11-C12-C13-C15
30	C	509	DGD	C8B-C9B-CAB-CBB
26	A	568	SQD	C8-C7-O47-C45
26	d	5358	SQD	C8-C7-O47-C45
20	A	560	CLA	C11-C12-C13-C15
20	a	5560	CLA	C11-C12-C13-C15
26	d	5358	SQD	C32-C33-C34-C35
28	I	201	MGE	C9A-CAA-CBA-CCA
20	C	495	CLA	C5-C6-C7-C8
28	B	530	MGE	C3B-C4B-C5B-C6B
30	C	509	DGD	C7A-C8A-C9A-CAA
30	C	509	DGD	C9B-CAB-CBB-CCB
30	c	5507	DGD	C9A-CAA-CBA-CCA
30	c	5509	DGD	C8B-C9B-CAB-CBB
30	c	5509	DGD	C9B-CAB-CBB-CCB
20	B	512	CLA	C3A-C2A-CAA-CBA
20	B	515	CLA	C3A-C2A-CAA-CBA
20	C	494	CLA	C3A-C2A-CAA-CBA
20	C	495	CLA	C3A-C2A-CAA-CBA
20	C	496	CLA	C3A-C2A-CAA-CBA
20	D	354	CLA	C3A-C2A-CAA-CBA
20	b	5515	CLA	C3A-C2A-CAA-CBA
20	c	5494	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	c	5495	CLA	C3A-C2A-CAA-CBA
20	c	5496	CLA	C3A-C2A-CAA-CBA
20	d	5354	CLA	C3A-C2A-CAA-CBA
20	B	522	CLA	O1D-CGD-O2D-CED
26	A	568	SQD	C32-C33-C34-C35
26	L	5213	SQD	C9-C10-C11-C12
28	L	210	MGE	C4B-C5B-C6B-C7B
30	c	5509	DGD	C7A-C8A-C9A-CAA
20	c	5495	CLA	C5-C6-C7-C8
20	b	5522	CLA	O1D-CGD-O2D-CED
28	L	210	MGE	CAB-CBB-CCB-CDB
28	b	5530	MGE	C4A-C5A-C6A-C7A
28	b	5530	MGE	C3B-C4B-C5B-C6B
28	B	530	MGE	C4A-C5A-C6A-C7A
28	D	358	MGE	C7A-C8A-C9A-CAA
28	d	5359	MGE	C7A-C8A-C9A-CAA
28	d	5361	MGE	C4B-C5B-C6B-C7B
28	D	358	MGE	C7B-C8B-C9B-CAB
28	D	360	MGE	C6B-C7B-C8B-C9B
28	l	5210	MGE	C4B-C5B-C6B-C7B
28	l	5210	MGE	C9B-CAB-CBB-CCB
20	A	560	CLA	C13-C15-C16-C17
28	D	360	MGE	C4B-C5B-C6B-C7B
28	L	210	MGE	C9B-CAB-CBB-CCB
28	d	5359	MGE	C7B-C8B-C9B-CAB
28	d	5361	MGE	C6B-C7B-C8B-C9B
30	H	208	DGD	C3B-C4B-C5B-C6B
26	L	5213	SQD	C12-C13-C14-C15
28	d	5359	MGE	C4B-C5B-C6B-C7B
28	l	5210	MGE	CAB-CBB-CCB-CDB
30	C	507	DGD	C3B-C4B-C5B-C6B
30	h	5208	DGD	C3B-C4B-C5B-C6B
20	c	5491	CLA	O1D-CGD-O2D-CED
26	t	213	SQD	C12-C13-C14-C15
28	D	358	MGE	C4B-C5B-C6B-C7B
20	C	491	CLA	O1D-CGD-O2D-CED
30	h	5208	DGD	O1A-C1A-O1G-C1G
20	B	519	CLA	C2B-C3B-CAB-CBB
20	B	524	CLA	C2B-C3B-CAB-CBB
20	C	495	CLA	C2B-C3B-CAB-CBB
20	C	499	CLA	C2B-C3B-CAB-CBB
20	C	503	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	b	5519	CLA	C2B-C3B-CAB-CBB
20	b	5524	CLA	C2B-C3B-CAB-CBB
20	b	5526	CLA	C2B-C3B-CAB-CBB
20	c	5494	CLA	C2B-C3B-CAB-CBB
20	c	5495	CLA	C2B-C3B-CAB-CBB
20	c	5499	CLA	C2B-C3B-CAB-CBB
20	c	5503	CLA	C2B-C3B-CAB-CBB
24	A	566	BCR	C1-C6-C7-C8
24	A	566	BCR	C23-C24-C25-C26
24	A	566	BCR	C23-C24-C25-C30
24	B	529	BCR	C23-C24-C25-C30
24	C	506	BCR	C23-C24-C25-C30
24	D	357	BCR	C5-C6-C7-C8
24	T	5104	BCR	C23-C24-C25-C26
24	T	5104	BCR	C23-C24-C25-C30
24	X	130	BCR	C23-C24-C25-C26
24	X	130	BCR	C23-C24-C25-C30
24	a	5566	BCR	C1-C6-C7-C8
24	a	5566	BCR	C5-C6-C7-C8
24	a	5566	BCR	C23-C24-C25-C26
24	a	5566	BCR	C23-C24-C25-C30
24	b	5529	BCR	C23-C24-C25-C30
24	c	5504	BCR	C23-C24-C25-C30
24	c	5506	BCR	C23-C24-C25-C30
24	d	5357	BCR	C5-C6-C7-C8
24	h	5107	BCR	C1-C6-C7-C8
24	t	104	BCR	C23-C24-C25-C26
24	t	104	BCR	C23-C24-C25-C30
24	x	5130	BCR	C23-C24-C25-C26
24	x	5130	BCR	C23-C24-C25-C30
28	I	201	MGE	C9B-CAB-CBB-CCB
30	C	509	DGD	C2B-C1B-O2G-C2G
30	H	208	DGD	C2B-C1B-O2G-C2G
30	H	208	DGD	C2A-C1A-O1G-C1G
20	B	514	CLA	C3-C5-C6-C7
20	C	498	CLA	C3-C5-C6-C7
28	D	358	MGE	C4A-C5A-C6A-C7A
28	D	358	MGE	C8B-C9B-CAB-CBB
28	d	5359	MGE	C8B-C9B-CAB-CBB
28	i	5201	MGE	C9B-CAB-CBB-CCB
26	A	568	SQD	C12-C13-C14-C15
28	B	530	MGE	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
30	c	5507	DGD	C4A-C5A-C6A-C7A
30	c	5507	DGD	C3B-C4B-C5B-C6B
28	b	5530	MGE	CBB-CCB-CDB-CEB
28	d	5359	MGE	C4A-C5A-C6A-C7A
30	H	208	DGD	C4B-C5B-C6B-C7B
30	h	5208	DGD	C4B-C5B-C6B-C7B
28	b	5530	MGE	C7B-C8B-C9B-CAB
28	i	5201	MGE	C3B-C4B-C5B-C6B
26	A	568	SQD	O49-C7-O47-C45
26	d	5358	SQD	O49-C7-O47-C45
30	C	509	DGD	O1B-C1B-O2G-C2G
20	B	523	CLA	C4-C3-C5-C6
28	B	530	MGE	C7B-C8B-C9B-CAB
30	H	208	DGD	CBA-CCA-CDA-CEA
28	I	201	MGE	C3B-C4B-C5B-C6B
28	d	5359	MGE	C5A-C6A-C7A-C8A
30	C	507	DGD	C4A-C5A-C6A-C7A
20	A	559	CLA	C6-C7-C8-C9
20	a	5559	CLA	C6-C7-C8-C9
21	a	5561	PHO	C11-C10-C8-C9
26	d	5358	SQD	C12-C13-C14-C15
30	h	5208	DGD	CBA-CCA-CDA-CEA
20	D	354	CLA	C13-C15-C16-C17
28	D	358	MGE	C5A-C6A-C7A-C8A
28	i	5201	MGE	C7A-C8A-C9A-CAA
28	I	201	MGE	C2A-C3A-C4A-C5A
30	C	509	DGD	CBB-CCB-CDB-CEB
28	l	5210	MGE	C6B-C7B-C8B-C9B
30	c	5509	DGD	CBB-CCB-CDB-CEB
20	b	5514	CLA	C3-C5-C6-C7
20	c	5498	CLA	C3-C5-C6-C7
25	A	567	LHG	C8-C7-O7-C5
25	a	5567	LHG	C8-C7-O7-C5
26	L	5213	SQD	C8-C7-O47-C45
26	t	213	SQD	C8-C7-O47-C45
30	h	5208	DGD	C2B-C1B-O2G-C2G
20	a	5560	CLA	C13-C15-C16-C17
20	b	5516	CLA	C5-C6-C7-C8
21	A	561	PHO	C8-C10-C11-C12
25	A	567	LHG	O9-C7-O7-C5
28	I	201	MGE	C3A-C4A-C5A-C6A
28	l	5210	MGE	C7A-C8A-C9A-CAA

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Mol	Chain	Res	Type	Atoms
20	b	5520	CLA	CBD-CGD-O2D-CED
20	B	516	CLA	C5-C6-C7-C8
20	b	5526	CLA	C15-C16-C17-C18
28	L	210	MGE	C7A-C8A-C9A-CAA
30	C	508	DGD	C5D-C6D-O5D-C1E
30	c	5508	DGD	C5D-C6D-O5D-C1E
28	i	5201	MGE	C2A-C3A-C4A-C5A
21	A	561	PHO	C16-C17-C18-C20
21	a	5561	PHO	C16-C17-C18-C20
20	B	518	CLA	CBD-CGD-O2D-CED
28	I	201	MGE	C7A-C8A-C9A-CAA
28	L	210	MGE	C6B-C7B-C8B-C9B
20	b	5523	CLA	C4-C3-C5-C6
20	B	526	CLA	C15-C16-C17-C18
20	C	497	CLA	C5-C6-C7-C8
20	c	5495	CLA	C13-C15-C16-C17
20	d	5354	CLA	C13-C15-C16-C17
21	a	5561	PHO	C8-C10-C11-C12
28	i	5201	MGE	C3A-C4A-C5A-C6A
28	d	5361	MGE	C1B-C2B-C3B-C4B
30	h	5208	DGD	C1B-C2B-C3B-C4B
30	C	509	DGD	C2A-C3A-C4A-C5A
30	c	5509	DGD	CCB-CDB-CEB-CFB
20	C	495	CLA	C13-C15-C16-C17
32	V	552	HEM	C4B-C3B-CAB-CBB
32	v	5552	HEM	C4B-C3B-CAB-CBB
30	H	208	DGD	O1A-C1A-O1G-C1G
20	C	501	CLA	O1D-CGD-O2D-CED
30	H	208	DGD	C1B-C2B-C3B-C4B
28	D	360	MGE	O2G-C2G-C3G-O3G
28	d	5361	MGE	O2G-C2G-C3G-O3G
28	D	360	MGE	C7A-C8A-C9A-CAA
30	C	509	DGD	CCB-CDB-CEB-CFB
26	d	5358	SQD	C25-C26-C27-C28
28	D	360	MGE	C5B-C6B-C7B-C8B
28	d	5361	MGE	C8B-C9B-CAB-CBB
30	c	5509	DGD	C2A-C3A-C4A-C5A
28	D	359	MGE	CAB-CBB-CCB-CDB
28	B	530	MGE	C8B-C9B-CAB-CBB
28	d	5361	MGE	C5B-C6B-C7B-C8B
30	C	508	DGD	C5A-C6A-C7A-C8A
26	A	568	SQD	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
28	d	5360	MGE	CBB-CCB-CDB-CEB
28	d	5361	MGE	C7A-C8A-C9A-CAA
30	H	208	DGD	O1B-C1B-O2G-C2G
30	h	5208	DGD	O1B-C1B-O2G-C2G
20	C	503	CLA	C2A-CAA-CBA-CGA
25	A	567	LHG	C28-C29-C30-C31
28	D	359	MGE	CBB-CCB-CDB-CEB
28	D	360	MGE	C7B-C8B-C9B-CAB
21	a	5561	PHO	C16-C17-C18-C19
28	D	360	MGE	C8B-C9B-CAB-CBB
20	B	515	CLA	C1A-C2A-CAA-CBA
20	C	491	CLA	C1A-C2A-CAA-CBA
20	D	354	CLA	C1A-C2A-CAA-CBA
20	b	5515	CLA	C1A-C2A-CAA-CBA
20	d	5354	CLA	C1A-C2A-CAA-CBA
20	c	5497	CLA	C5-C6-C7-C8
28	d	5360	MGE	CAB-CBB-CCB-CDB
20	d	5355	CLA	C2C-C3C-CAC-CBC
26	A	568	SQD	C17-C18-C19-C20
28	d	5361	MGE	C7B-C8B-C9B-CAB
30	c	5508	DGD	C5A-C6A-C7A-C8A
21	a	5561	PHO	C5-C6-C7-C8
25	a	5567	LHG	O9-C7-O7-C5
26	L	5213	SQD	O49-C7-O47-C45
20	A	558	CLA	C11-C10-C8-C7
20	A	558	CLA	C12-C13-C15-C16
20	A	559	CLA	C12-C13-C15-C16
20	B	514	CLA	C11-C10-C8-C7
20	B	522	CLA	C11-C10-C8-C7
20	B	525	CLA	C11-C10-C8-C7
20	C	493	CLA	C11-C12-C13-C15
20	C	495	CLA	C11-C10-C8-C7
20	C	496	CLA	C11-C10-C8-C7
20	C	496	CLA	C12-C13-C15-C16
20	C	500	CLA	C11-C10-C8-C7
20	a	5558	CLA	C11-C10-C8-C7
20	a	5558	CLA	C12-C13-C15-C16
20	a	5559	CLA	C12-C13-C15-C16
20	b	5514	CLA	C11-C10-C8-C7
20	b	5522	CLA	C11-C10-C8-C7
20	b	5525	CLA	C11-C10-C8-C7
20	c	5493	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
20	c	5495	CLA	C11-C10-C8-C7
20	c	5496	CLA	C11-C10-C8-C7
20	c	5496	CLA	C12-C13-C15-C16
20	c	5500	CLA	C11-C10-C8-C7
20	c	5501	CLA	C11-C10-C8-C7
21	A	562	PHO	C11-C10-C8-C7
21	A	561	PHO	C16-C17-C18-C19
20	b	5515	CLA	C15-C16-C17-C18
21	A	562	PHO	C15-C16-C17-C18
25	a	5567	LHG	C28-C29-C30-C31
20	A	558	CLA	C2A-CAA-CBA-CGA
20	a	5558	CLA	C2A-CAA-CBA-CGA
20	B	513	CLA	C14-C13-C15-C16
20	B	514	CLA	C11-C10-C8-C9
20	B	525	CLA	C6-C7-C8-C9
20	B	525	CLA	C11-C10-C8-C9
20	C	493	CLA	C6-C7-C8-C9
20	C	493	CLA	C11-C12-C13-C14
20	C	500	CLA	C11-C10-C8-C9
20	C	501	CLA	C11-C10-C8-C9
20	a	5559	CLA	C14-C13-C15-C16
20	b	5513	CLA	C14-C13-C15-C16
20	b	5514	CLA	C11-C10-C8-C9
20	b	5519	CLA	C14-C13-C15-C16
20	b	5520	CLA	C6-C7-C8-C9
20	b	5525	CLA	C6-C7-C8-C9
20	b	5525	CLA	C11-C10-C8-C9
20	c	5493	CLA	C11-C12-C13-C14
20	c	5500	CLA	C11-C10-C8-C9
21	A	562	PHO	C11-C10-C8-C9
21	a	5562	PHO	C11-C10-C8-C9
28	D	359	MGE	C9B-CAB-CBB-CCB
28	i	5201	MGE	C4A-C5A-C6A-C7A
21	A	561	PHO	C5-C6-C7-C8
20	b	5521	CLA	C15-C16-C17-C18
20	b	5518	CLA	O1D-CGD-O2D-CED
28	D	359	MGE	C1G-C2G-C3G-O3G
28	d	5360	MGE	C1G-C2G-C3G-O3G
26	L	5213	SQD	C25-C26-C27-C28
20	B	515	CLA	C15-C16-C17-C18
20	C	491	CLA	C13-C15-C16-C17
28	b	5530	MGE	C8B-C9B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	C	509	DGD	C7B-C8B-C9B-CAB
30	h	5208	DGD	C7A-C8A-C9A-CAA
26	d	5358	SQD	C17-C18-C19-C20
20	D	355	CLA	C2C-C3C-CAC-CBC
27	A	569	LMT	C3-C4-C5-C6
30	H	208	DGD	CAA-CBA-CCA-CDA
30	c	5509	DGD	C7B-C8B-C9B-CAB
28	I	201	MGE	C4A-C5A-C6A-C7A
30	H	208	DGD	C7A-C8A-C9A-CAA
28	D	358	MGE	O6D-C5D-C6D-O5D
30	c	5508	DGD	C4A-C5A-C6A-C7A
28	d	5359	MGE	O6D-C5D-C6D-O5D
26	t	213	SQD	C25-C26-C27-C28
26	L	5213	SQD	C17-C18-C19-C20
30	C	508	DGD	C4A-C5A-C6A-C7A
25	A	567	LHG	C26-C27-C28-C29
28	B	530	MGE	C5A-C6A-C7A-C8A
28	i	5201	MGE	C6A-C7A-C8A-C9A
28	d	5360	MGE	C9B-CAB-CBB-CCB
30	h	5208	DGD	CAA-CBA-CCA-CDA
30	C	507	DGD	CBA-CCA-CDA-CEA
28	l	5210	MGE	CDB-CEB-CFB-CGB
28	b	5530	MGE	C5A-C6A-C7A-C8A
28	L	210	MGE	CDB-CEB-CFB-CGB
27	a	5568	LMT	C3-C4-C5-C6
28	d	5361	MGE	C2A-C3A-C4A-C5A
25	a	5567	LHG	C35-C36-C37-C38
28	I	201	MGE	C6A-C7A-C8A-C9A
28	l	5210	MGE	CBB-CCB-CDB-CEB
25	A	567	LHG	C35-C36-C37-C38
30	c	5507	DGD	CBA-CCA-CDA-CEA
26	t	213	SQD	O49-C7-O47-C45
25	a	5567	LHG	C26-C27-C28-C29
30	c	5509	DGD	CDB-CEB-CFB-CGB
25	a	5567	LHG	C27-C28-C29-C30
26	t	213	SQD	C17-C18-C19-C20
28	d	5361	MGE	C5A-C6A-C7A-C8A
26	A	568	SQD	C27-C28-C29-C30
28	D	360	MGE	C5A-C6A-C7A-C8A
20	B	521	CLA	C15-C16-C17-C18
20	b	5522	CLA	C5-C6-C7-C8
20	c	5491	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
20	B	520	CLA	O1D-CGD-O2D-CED
20	A	563	CLA	C4-C3-C5-C6
20	b	5513	CLA	C4-C3-C5-C6
30	C	509	DGD	CDB-CEB-CFB-CGB
28	D	360	MGE	C1B-C2B-C3B-C4B
26	d	5358	SQD	C28-C29-C30-C31
26	d	5358	SQD	C27-C28-C29-C30
20	A	558	CLA	C11-C10-C8-C9
20	A	559	CLA	C14-C13-C15-C16
20	B	512	CLA	C11-C10-C8-C9
20	B	515	CLA	C14-C13-C15-C16
20	B	519	CLA	C14-C13-C15-C16
20	B	520	CLA	C6-C7-C8-C9
20	B	522	CLA	C11-C10-C8-C9
20	C	495	CLA	C11-C10-C8-C9
20	C	496	CLA	C11-C10-C8-C9
20	C	496	CLA	C14-C13-C15-C16
20	D	354	CLA	C14-C13-C15-C16
20	a	5558	CLA	C11-C10-C8-C9
20	b	5512	CLA	C11-C10-C8-C9
20	b	5515	CLA	C14-C13-C15-C16
20	b	5522	CLA	C11-C10-C8-C9
20	b	5524	CLA	C6-C7-C8-C9
20	c	5493	CLA	C6-C7-C8-C9
20	c	5495	CLA	C11-C10-C8-C9
20	c	5496	CLA	C11-C10-C8-C9
20	c	5496	CLA	C14-C13-C15-C16
20	c	5501	CLA	C11-C10-C8-C9
20	d	5354	CLA	C14-C13-C15-C16
21	A	561	PHO	C6-C7-C8-C9
21	A	561	PHO	C11-C10-C8-C9
21	a	5561	PHO	C6-C7-C8-C9
20	c	5501	CLA	O1D-CGD-O2D-CED
20	B	515	CLA	C4B-C3B-CAB-CBB
20	b	5515	CLA	C4B-C3B-CAB-CBB
20	B	525	CLA	C5-C6-C7-C8
21	a	5562	PHO	C15-C16-C17-C18
20	b	5516	CLA	C2A-CAA-CBA-CGA
20	A	560	CLA	C11-C10-C8-C7
20	B	512	CLA	C11-C10-C8-C7
20	B	513	CLA	C11-C10-C8-C7
20	B	513	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
20	B	518	CLA	C6-C7-C8-C10
20	B	519	CLA	C12-C13-C15-C16
20	B	524	CLA	C6-C7-C8-C10
20	B	525	CLA	C6-C7-C8-C10
20	C	493	CLA	C6-C7-C8-C10
20	C	501	CLA	C11-C10-C8-C7
20	D	354	CLA	C12-C13-C15-C16
20	a	5559	CLA	C11-C10-C8-C7
20	a	5560	CLA	C11-C10-C8-C7
20	b	5512	CLA	C11-C10-C8-C7
20	b	5513	CLA	C12-C13-C15-C16
20	b	5518	CLA	C6-C7-C8-C10
20	b	5524	CLA	C6-C7-C8-C10
20	b	5525	CLA	C6-C7-C8-C10
20	c	5493	CLA	C6-C7-C8-C10
20	c	5501	CLA	C6-C7-C8-C10
20	d	5354	CLA	C12-C13-C15-C16
21	A	561	PHO	C6-C7-C8-C10
21	a	5561	PHO	C6-C7-C8-C10
21	a	5562	PHO	C11-C10-C8-C7
20	B	522	CLA	C8-C10-C11-C12
20	b	5518	CLA	C5-C6-C7-C8
20	b	5521	CLA	C8-C10-C11-C12
20	c	5501	CLA	C10-C11-C12-C13
30	H	208	DGD	CCA-CDA-CEA-CFA
30	c	5509	DGD	C4A-C5A-C6A-C7A
20	B	519	CLA	C4-C3-C5-C6
20	B	526	CLA	C3A-C2A-CAA-CBA
20	a	5563	CLA	C4-C3-C5-C6
20	b	5512	CLA	C3A-C2A-CAA-CBA
20	b	5519	CLA	C4-C3-C5-C6
20	b	5526	CLA	C3A-C2A-CAA-CBA
20	B	522	CLA	C5-C6-C7-C8
20	b	5525	CLA	C5-C6-C7-C8
30	C	509	DGD	C4A-C5A-C6A-C7A
30	h	5208	DGD	CCA-CDA-CEA-CFA
20	C	501	CLA	C5-C6-C7-C8
28	L	210	MGE	CBB-CCB-CDB-CEB
26	A	568	SQD	O6-C44-C45-C46
26	A	5212	SQD	O6-C44-C45-C46
26	L	5213	SQD	C44-C45-C46-O48
26	a	212	SQD	O6-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
26	d	5358	SQD	O6-C44-C45-C46
26	t	213	SQD	C44-C45-C46-O48
28	D	360	MGE	C1G-C2G-C3G-O3G
28	d	5361	MGE	C1G-C2G-C3G-O3G
28	d	5360	MGE	C6B-C7B-C8B-C9B
20	b	5522	CLA	C8-C10-C11-C12
20	B	515	CLA	C1-C2-C3-C4
20	B	518	CLA	C1-C2-C3-C4
20	B	522	CLA	C1-C2-C3-C4
20	B	525	CLA	C1-C2-C3-C4
20	B	526	CLA	C1-C2-C3-C4
20	C	492	CLA	C1-C2-C3-C4
20	C	495	CLA	C1-C2-C3-C4
20	C	500	CLA	C1-C2-C3-C4
20	C	501	CLA	C1-C2-C3-C4
20	b	5515	CLA	C1-C2-C3-C4
20	b	5517	CLA	C1-C2-C3-C4
20	b	5518	CLA	C1-C2-C3-C4
20	b	5522	CLA	C1-C2-C3-C4
20	b	5523	CLA	C1-C2-C3-C4
20	b	5525	CLA	C1-C2-C3-C4
20	b	5526	CLA	C1-C2-C3-C4
20	c	5492	CLA	C1-C2-C3-C4
20	c	5495	CLA	C1-C2-C3-C4
20	c	5500	CLA	C1-C2-C3-C4
20	c	5501	CLA	C1-C2-C3-C4
20	B	513	CLA	C4-C3-C5-C6
26	A	568	SQD	C10-C11-C12-C13
20	a	5563	CLA	C2-C3-C5-C6
20	b	5519	CLA	C2-C3-C5-C6
20	B	518	CLA	C5-C6-C7-C8
21	A	561	PHO	C15-C16-C17-C18
25	A	567	LHG	C27-C28-C29-C30
30	c	5509	DGD	C4E-C5E-C6E-O5E
24	C	504	BCR	C23-C24-C25-C30
24	C	505	BCR	C1-C6-C7-C8
24	H	107	BCR	C1-C6-C7-C8
24	H	107	BCR	C23-C24-C25-C30
24	X	130	BCR	C5-C6-C7-C8
24	c	5505	BCR	C1-C6-C7-C8
24	d	5357	BCR	C1-C6-C7-C8
24	h	5107	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
24	x	5130	BCR	C5-C6-C7-C8
20	c	5501	CLA	C5-C6-C7-C8
20	b	5524	CLA	C11-C10-C8-C9
26	d	5358	SQD	C10-C11-C12-C13
20	b	5515	CLA	C2A-CAA-CBA-CGA
20	b	5514	CLA	C13-C15-C16-C17
26	A	568	SQD	O6-C44-C45-O47
26	d	5358	SQD	O6-C44-C45-O47
28	D	359	MGE	O2G-C2G-C3G-O3G
28	d	5360	MGE	O2G-C2G-C3G-O3G
28	d	5359	MGE	C2A-C3A-C4A-C5A
28	d	5361	MGE	C4A-C5A-C6A-C7A
20	b	5516	CLA	O1D-CGD-O2D-CED
28	i	5201	MGE	C6B-C7B-C8B-C9B
20	B	514	CLA	C13-C15-C16-C17
21	a	5561	PHO	C15-C16-C17-C18
20	A	563	CLA	C2-C3-C5-C6
20	B	519	CLA	C2-C3-C5-C6
30	C	508	DGD	C7A-C8A-C9A-CAA
20	A	559	CLA	C1-C2-C3-C5
20	B	515	CLA	C1-C2-C3-C5
20	B	517	CLA	C1-C2-C3-C5
20	B	519	CLA	C1-C2-C3-C5
20	B	520	CLA	C1-C2-C3-C5
20	B	523	CLA	C1-C2-C3-C5
20	B	526	CLA	C1-C2-C3-C5
20	C	498	CLA	C1-C2-C3-C5
20	a	5559	CLA	C1-C2-C3-C5
20	b	5515	CLA	C1-C2-C3-C5
20	b	5517	CLA	C1-C2-C3-C5
20	b	5519	CLA	C1-C2-C3-C5
20	b	5520	CLA	C1-C2-C3-C5
20	b	5523	CLA	C1-C2-C3-C5
20	b	5526	CLA	C1-C2-C3-C5
20	c	5497	CLA	C1-C2-C3-C5
20	c	5498	CLA	C1-C2-C3-C5
21	A	561	PHO	C1-C2-C3-C5
21	a	5561	PHO	C1-C2-C3-C5
20	A	560	CLA	C11-C10-C8-C9
20	B	516	CLA	C11-C12-C13-C14
20	a	5560	CLA	C11-C10-C8-C9
20	b	5516	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
30	H	208	DGD	C2A-C3A-C4A-C5A
28	B	530	MGE	C2A-C3A-C4A-C5A
30	h	5208	DGD	C2A-C3A-C4A-C5A
28	I	201	MGE	C6B-C7B-C8B-C9B
28	D	360	MGE	C9A-CAA-CBA-CCA
20	B	516	CLA	O1D-CGD-O2D-CED
20	C	492	CLA	CBD-CGD-O2D-CED
20	B	521	CLA	C8-C10-C11-C12
28	l	5210	MGE	C2A-C3A-C4A-C5A
20	C	496	CLA	C5-C6-C7-C8
28	D	358	MGE	C2A-C3A-C4A-C5A
20	b	5520	CLA	O1D-CGD-O2D-CED
30	c	5507	DGD	C5A-C6A-C7A-C8A
30	c	5508	DGD	C8A-C9A-CAA-CBA
20	B	516	CLA	C11-C12-C13-C15
20	C	498	CLA	C11-C10-C8-C7
20	C	501	CLA	C6-C7-C8-C10
20	b	5513	CLA	C11-C10-C8-C7
20	b	5516	CLA	C11-C12-C13-C15
20	b	5519	CLA	C12-C13-C15-C16
20	B	514	CLA	C15-C16-C17-C18
20	b	5514	CLA	C15-C16-C17-C18
20	c	5496	CLA	C5-C6-C7-C8
30	C	507	DGD	C5A-C6A-C7A-C8A
30	c	5508	DGD	C7A-C8A-C9A-CAA
28	D	359	MGE	CDB-CEB-CFB-CGB
26	L	5213	SQD	C5-C6-S-O8
26	t	213	SQD	C5-C6-S-O8
30	C	507	DGD	C5D-C6D-O5D-C1E
30	c	5507	DGD	C5D-C6D-O5D-C1E
28	D	360	MGE	C2A-C3A-C4A-C5A
20	c	5503	CLA	C2A-CAA-CBA-CGA
20	B	524	CLA	C11-C10-C8-C9
28	L	210	MGE	C2A-C3A-C4A-C5A
28	L	210	MGE	C4A-C5A-C6A-C7A
20	B	521	CLA	C4-C3-C5-C6
28	i	5201	MGE	CDB-CEB-CFB-CGB
20	B	521	CLA	CBD-CGD-O2D-CED
28	d	5360	MGE	CDB-CEB-CFB-CGB
20	c	5492	CLA	CBD-CGD-O2D-CED
28	d	5361	MGE	C9A-CAA-CBA-CCA
25	a	5567	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
28	D	359	MGE	C6B-C7B-C8B-C9B
30	C	509	DGD	C4E-C5E-C6E-O5E
28	i	5201	MGE	C5A-C6A-C7A-C8A
28	l	5210	MGE	C4A-C5A-C6A-C7A
26	d	5358	SQD	C9-C10-C11-C12
20	b	5521	CLA	C4-C3-C5-C6
20	c	5491	CLA	C2A-CAA-CBA-CGA
20	B	523	CLA	C2-C3-C5-C6
20	B	514	CLA	C5-C6-C7-C8
20	b	5525	CLA	C10-C11-C12-C13
28	d	5360	MGE	C7B-C8B-C9B-CAB
26	L	5213	SQD	O47-C45-C46-O48
26	t	213	SQD	O47-C45-C46-O48
28	i	5201	MGE	O1G-C1G-C2G-O2G
20	B	512	CLA	C10-C11-C12-C13
20	B	524	CLA	C6-C7-C8-C9
26	A	568	SQD	C9-C10-C11-C12
30	c	5507	DGD	C5B-C6B-C7B-C8B
30	c	5509	DGD	C6B-C7B-C8B-C9B
20	B	517	CLA	C13-C15-C16-C17
30	C	509	DGD	C6B-C7B-C8B-C9B
26	d	5358	SQD	C24-C25-C26-C27
20	d	5355	CLA	C4C-C3C-CAC-CBC
28	D	359	MGE	C7B-C8B-C9B-CAB
30	C	508	DGD	C8A-C9A-CAA-CBA
25	A	567	LHG	C9-C10-C11-C12
20	C	501	CLA	C10-C11-C12-C13
28	b	5530	MGE	C5B-C6B-C7B-C8B
25	a	5567	LHG	C23-C24-C25-C26
20	b	5514	CLA	C5-C6-C7-C8
20	D	355	CLA	C4C-C3C-CAC-CBC
26	A	568	SQD	C24-C25-C26-C27
20	C	498	CLA	C4B-C3B-CAB-CBB
20	C	502	CLA	C4B-C3B-CAB-CBB
20	a	5559	CLA	C1A-C2A-CAA-CBA
20	c	5498	CLA	C4B-C3B-CAB-CBB
30	c	5509	DGD	C4B-C5B-C6B-C7B
28	I	201	MGE	CDB-CEB-CFB-CGB
24	C	506	BCR	C6-C7-C8-C9
30	C	507	DGD	C5B-C6B-C7B-C8B
20	A	559	CLA	C11-C10-C8-C7
20	B	518	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
20	B	520	CLA	C11-C10-C8-C7
20	B	526	CLA	C11-C12-C13-C15
20	C	492	CLA	C11-C10-C8-C7
20	b	5518	CLA	C11-C10-C8-C7
20	b	5526	CLA	C11-C12-C13-C15
20	c	5498	CLA	C11-C10-C8-C7
28	D	360	MGE	C4A-C5A-C6A-C7A
28	I	201	MGE	C5A-C6A-C7A-C8A
28	b	5530	MGE	C2A-C3A-C4A-C5A
25	A	567	LHG	C23-C24-C25-C26
28	B	530	MGE	C9B-CAB-CBB-CCB
28	I	201	MGE	O1G-C1G-C2G-O2G
30	c	5508	DGD	C9A-CAA-CBA-CCA
20	b	5512	CLA	C10-C11-C12-C13
20	C	496	CLA	C13-C15-C16-C17
20	B	521	CLA	C2-C3-C5-C6
30	C	508	DGD	C9A-CAA-CBA-CCA
26	L	5213	SQD	C19-C20-C21-C22
20	C	499	CLA	CAD-CBD-CGD-O2D
20	C	500	CLA	CAD-CBD-CGD-O2D
20	c	5499	CLA	CAD-CBD-CGD-O2D
20	c	5500	CLA	CAD-CBD-CGD-O2D
20	C	492	CLA	O1D-CGD-O2D-CED
20	B	516	CLA	C2A-CAA-CBA-CGA
26	t	213	SQD	C19-C20-C21-C22
20	B	525	CLA	C10-C11-C12-C13
30	c	5509	DGD	CAB-CBB-CCB-CDB
20	C	499	CLA	CAD-CBD-CGD-O1D
20	C	500	CLA	CAD-CBD-CGD-O1D
20	c	5499	CLA	CAD-CBD-CGD-O1D
20	c	5500	CLA	CAD-CBD-CGD-O1D
20	a	5559	CLA	C3-C5-C6-C7
20	B	512	CLA	C2B-C3B-CAB-CBB
20	B	515	CLA	C2B-C3B-CAB-CBB
20	B	517	CLA	C2B-C3B-CAB-CBB
20	C	494	CLA	C2B-C3B-CAB-CBB
20	b	5512	CLA	C2B-C3B-CAB-CBB
20	b	5515	CLA	C2B-C3B-CAB-CBB
20	b	5517	CLA	C2B-C3B-CAB-CBB
20	c	5502	CLA	C2B-C3B-CAB-CBB
24	D	357	BCR	C1-C6-C7-C8
28	B	530	MGE	C5B-C6B-C7B-C8B

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Mol	Chain	Res	Type	Atoms
30	C	509	DGD	CAB-CBB-CCB-CDB
26	A	568	SQD	C28-C29-C30-C31
30	C	509	DGD	C4B-C5B-C6B-C7B
28	B	530	MGE	C6B-C7B-C8B-C9B
20	A	559	CLA	C3-C5-C6-C7
22	A	564	PQ9	C12-C11-C2-C1
22	a	5564	PQ9	C12-C11-C2-C1
20	c	5496	CLA	C13-C15-C16-C17
25	A	567	LHG	C25-C26-C27-C28
25	A	567	LHG	C6-C5-O7-C7
25	a	5567	LHG	C6-C5-O7-C7
20	B	513	CLA	C2-C3-C5-C6
20	b	5521	CLA	C2-C3-C5-C6
28	L	210	MGE	C3A-C4A-C5A-C6A
28	b	5530	MGE	C9B-CAB-CBB-CCB
28	d	5359	MGE	CAB-CBB-CCB-CDB
20	B	518	CLA	O1D-CGD-O2D-CED
20	b	5515	CLA	C11-C10-C8-C9
20	B	521	CLA	O1D-CGD-O2D-CED
20	B	514	CLA	C6-C7-C8-C10
20	b	5520	CLA	C11-C10-C8-C7
20	b	5523	CLA	C12-C13-C15-C16
20	b	5513	CLA	C2-C3-C5-C6
27	m	216	LMT	C1-C2-C3-C4
30	h	5208	DGD	O2G-C2G-C3G-O3G
28	L	210	MGE	C9A-CAA-CBA-CCA
20	B	515	CLA	C2A-CAA-CBA-CGA
28	B	530	MGE	CAB-CBB-CCB-CDB
25	a	5567	LHG	C25-C26-C27-C28
28	i	5201	MGE	C2G-C3G-O3G-C1D
20	B	519	CLA	C5-C6-C7-C8
20	C	491	CLA	C2A-CAA-CBA-CGA
21	a	5561	PHO	C2A-CAA-CBA-CGA
28	l	5210	MGE	C9A-CAA-CBA-CCA
26	d	5358	SQD	C19-C20-C21-C22
20	B	513	CLA	C11-C10-C8-C9
20	B	515	CLA	C11-C10-C8-C9
20	B	526	CLA	C11-C12-C13-C14
20	a	5559	CLA	C11-C10-C8-C9
20	b	5513	CLA	C11-C10-C8-C9
20	B	523	CLA	C4B-C3B-CAB-CBB
20	b	5523	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
20	c	5502	CLA	C4B-C3B-CAB-CBB
28	i	5201	MGE	CBB-CCB-CDB-CEB
30	C	509	DGD	C1B-C2B-C3B-C4B
28	B	530	MGE	CAA-CBA-CCA-CDA
28	D	360	MGE	CDB-CEB-CFB-CGB
20	B	515	CLA	C11-C10-C8-C7
20	b	5518	CLA	C12-C13-C15-C16
20	b	5522	CLA	C6-C7-C8-C10
26	L	5213	SQD	C27-C28-C29-C30
20	b	5517	CLA	C13-C15-C16-C17
20	C	502	CLA	C3A-C2A-CAA-CBA
20	C	503	CLA	C3A-C2A-CAA-CBA
27	M	5216	LMT	C1-C2-C3-C4
20	B	514	CLA	C10-C11-C12-C13
20	b	5525	CLA	C13-C15-C16-C17
20	c	5492	CLA	O1D-CGD-O2D-CED
20	B	516	CLA	C15-C16-C17-C18
20	a	5559	CLA	C2-C1-O2A-CGA
20	b	5514	CLA	C10-C11-C12-C13
28	b	5530	MGE	CAB-CBB-CCB-CDB
26	t	213	SQD	C24-C25-C26-C27
22	d	5356	PQ9	C19-C18-C20-C21
26	L	5213	SQD	C24-C25-C26-C27
20	b	5521	CLA	CBD-CGD-O2D-CED
20	b	5526	CLA	C11-C12-C13-C14
28	b	5530	MGE	C6B-C7B-C8B-C9B
20	B	525	CLA	C13-C15-C16-C17
25	A	567	LHG	C4-C5-O7-C7
25	a	5567	LHG	C4-C5-O7-C7
20	A	559	CLA	C1-C2-C3-C4
20	B	517	CLA	C1-C2-C3-C4
20	B	519	CLA	C1-C2-C3-C4
20	B	520	CLA	C1-C2-C3-C4
20	B	523	CLA	C1-C2-C3-C4
20	C	498	CLA	C1-C2-C3-C4
20	a	5559	CLA	C1-C2-C3-C4
20	b	5519	CLA	C1-C2-C3-C4
20	c	5498	CLA	C1-C2-C3-C4
21	A	561	PHO	C1-C2-C3-C4
21	a	5561	PHO	C1-C2-C3-C4
20	b	5523	CLA	C2-C3-C5-C6
20	C	498	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
20	c	5498	CLA	C15-C16-C17-C18
26	A	568	SQD	C19-C20-C21-C22
20	b	5512	CLA	C2A-CAA-CBA-CGA
20	A	559	CLA	C1A-C2A-CAA-CBA
20	A	560	CLA	C1A-C2A-CAA-CBA
20	B	512	CLA	C1A-C2A-CAA-CBA
20	b	5512	CLA	C1A-C2A-CAA-CBA
20	C	498	CLA	C2B-C3B-CAB-CBB
20	C	502	CLA	C2B-C3B-CAB-CBB
20	c	5498	CLA	C2B-C3B-CAB-CBB
24	C	504	BCR	C23-C24-C25-C26
24	H	107	BCR	C5-C6-C7-C8
24	H	107	BCR	C23-C24-C25-C26
24	c	5504	BCR	C23-C24-C25-C26
24	h	5107	BCR	C5-C6-C7-C8
24	h	5107	BCR	C23-C24-C25-C26
30	c	5509	DGD	C1B-C2B-C3B-C4B
20	c	5500	CLA	C4-C3-C5-C6
22	D	356	PQ9	C19-C18-C20-C21
22	d	5356	PQ9	C17-C18-C20-C21
20	B	522	CLA	C6-C7-C8-C10
20	B	523	CLA	C12-C13-C15-C16
20	b	5514	CLA	C6-C7-C8-C10
20	b	5515	CLA	C11-C10-C8-C7
20	c	5492	CLA	C11-C10-C8-C7
20	B	512	CLA	C2A-CAA-CBA-CGA
27	M	5216	LMT	O1'-C1-C2-C3
30	H	208	DGD	O2G-C2G-C3G-O3G
27	T	217	LMT	C4-C5-C6-C7
30	h	5208	DGD	C6B-C7B-C8B-C9B
28	l	5210	MGE	C3A-C4A-C5A-C6A
26	t	213	SQD	C27-C28-C29-C30
20	B	524	CLA	C11-C10-C8-C7
20	C	498	CLA	C4-C3-C5-C6
20	c	5498	CLA	C2-C3-C5-C6
22	D	356	PQ9	C17-C18-C20-C21
30	C	508	DGD	O6E-C5E-C6E-O5E
20	B	522	CLA	C1-C2-C3-C5
20	b	5522	CLA	C1-C2-C3-C5
28	I	201	MGE	CBB-CCB-CDB-CEB
30	c	5509	DGD	C3A-C4A-C5A-C6A
20	C	498	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
21	a	5561	PHO	C2C-C3C-CAC-CBC
28	D	358	MGE	CAB-CBB-CCB-CDB
20	c	5498	CLA	C10-C11-C12-C13
24	T	5104	BCR	C22-C23-C24-C25
24	c	5506	BCR	C6-C7-C8-C9
20	c	5498	CLA	C4-C3-C5-C6
20	C	492	CLA	C10-C11-C12-C13
20	b	5519	CLA	C5-C6-C7-C8
28	D	360	MGE	O1G-C1G-C2G-C3G
28	d	5361	MGE	O1G-C1G-C2G-C3G
20	c	5498	CLA	C8-C10-C11-C12
32	V	552	HEM	CAD-CBD-CGD-O2D
25	A	567	LHG	O1-C1-C2-O2
20	C	500	CLA	C4-C3-C5-C6
32	v	5552	HEM	CAD-CBD-CGD-O2D
28	d	5361	MGE	CDB-CEB-CFB-CGB
30	C	509	DGD	C3A-C4A-C5A-C6A
28	B	530	MGE	C1A-C2A-C3A-C4A
20	b	5520	CLA	C13-C15-C16-C17
20	C	498	CLA	C2-C3-C5-C6
20	B	520	CLA	C13-C15-C16-C17
20	C	498	CLA	C10-C11-C12-C13
20	A	559	CLA	C11-C10-C8-C9
20	a	5560	CLA	C11-C12-C13-C14
26	a	212	SQD	C5-C6-S-O8
28	D	359	MGE	C2G-C3G-O3G-C1D
28	I	201	MGE	C2G-C3G-O3G-C1D
28	d	5360	MGE	C2G-C3G-O3G-C1D
20	A	559	CLA	C2-C1-O2A-CGA
20	B	517	CLA	C2-C1-O2A-CGA
20	b	5517	CLA	C2-C1-O2A-CGA
30	H	208	DGD	C6B-C7B-C8B-C9B
20	c	5502	CLA	C3A-C2A-CAA-CBA
20	c	5503	CLA	C3A-C2A-CAA-CBA
20	C	497	CLA	O2A-C1-C2-C3
20	c	5497	CLA	O2A-C1-C2-C3
32	v	5552	HEM	CAD-CBD-CGD-O1D
21	A	561	PHO	C2A-CAA-CBA-CGA
32	V	552	HEM	CAD-CBD-CGD-O1D
20	b	5521	CLA	O1D-CGD-O2D-CED
27	m	216	LMT	O1'-C1-C2-C3
24	t	104	BCR	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
30	c	5508	DGD	C2A-C1A-O1G-C1G
26	t	213	SQD	O6-C44-C45-C46
28	b	5530	MGE	CAA-CBA-CCA-CDA
20	a	5560	CLA	CBD-CGD-O2D-CED
30	c	5508	DGD	O1A-C1A-O1G-C1G
20	c	5497	CLA	CAA-CBA-CGA-O2A
28	L	210	MGE	O2G-C1B-C2B-C3B
28	d	5361	MGE	O2G-C1B-C2B-C3B
21	A	561	PHO	C2C-C3C-CAC-CBC
20	A	560	CLA	C11-C12-C13-C14
20	B	520	CLA	C11-C10-C8-C9
20	C	498	CLA	C11-C10-C8-C9
20	b	5520	CLA	C11-C10-C8-C9
20	b	5523	CLA	C14-C13-C15-C16
20	c	5498	CLA	C11-C10-C8-C9
28	l	5210	MGE	O2G-C1B-C2B-C3B
27	a	5568	LMT	C1-C2-C3-C4
30	H	208	DGD	C9A-CAA-CBA-CCA
26	A	568	SQD	O47-C7-C8-C9
26	d	5358	SQD	O47-C7-C8-C9
28	D	360	MGE	O2G-C1B-C2B-C3B
20	B	518	CLA	C12-C13-C15-C16
20	C	501	CLA	C12-C13-C15-C16
20	b	5523	CLA	C11-C12-C13-C15
20	B	512	CLA	C5-C6-C7-C8
20	B	523	CLA	C2B-C3B-CAB-CBB
20	b	5523	CLA	C2B-C3B-CAB-CBB
24	C	505	BCR	C5-C6-C7-C8
24	X	130	BCR	C1-C6-C7-C8
24	c	5505	BCR	C5-C6-C7-C8
30	h	5208	DGD	C9A-CAA-CBA-CCA
20	c	5498	CLA	C2-C1-O2A-CGA
20	C	494	CLA	CAA-CBA-CGA-O2A
20	c	5494	CLA	CAA-CBA-CGA-O2A
26	A	568	SQD	C13-C14-C15-C16
26	L	5213	SQD	C45-C46-O48-C23
20	b	5516	CLA	C15-C16-C17-C18
20	B	515	CLA	CAA-CBA-CGA-O2A
20	C	497	CLA	CAA-CBA-CGA-O2A
20	b	5515	CLA	CAA-CBA-CGA-O2A
20	b	5524	CLA	C11-C10-C8-C7
30	C	507	DGD	O2G-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
20	C	495	CLA	CAA-CBA-CGA-O2A
20	c	5495	CLA	CAA-CBA-CGA-O2A
20	B	523	CLA	C14-C13-C15-C16
20	c	5492	CLA	C11-C10-C8-C9
26	L	5213	SQD	O6-C44-C45-C46
28	I	201	MGE	O1G-C1G-C2G-C3G
28	i	5201	MGE	O1G-C1G-C2G-C3G
20	c	5492	CLA	C1A-C2A-CAA-CBA
20	b	5525	CLA	C4-C3-C5-C6
24	X	130	BCR	C6-C7-C8-C9
24	x	5130	BCR	C6-C7-C8-C9
20	C	499	CLA	CAA-CBA-CGA-O2A
20	c	5499	CLA	CAA-CBA-CGA-O2A
30	c	5507	DGD	O2G-C1B-C2B-C3B
28	D	358	MGE	C3B-C4B-C5B-C6B
20	B	520	CLA	C15-C16-C17-C18
28	I	201	MGE	C4B-C5B-C6B-C7B
26	L	5213	SQD	C5-C6-S-O7
26	L	5213	SQD	C5-C6-S-O9
26	t	213	SQD	C5-C6-S-O7
26	t	213	SQD	C5-C6-S-O9
20	B	525	CLA	C4-C3-C5-C6
20	B	521	CLA	C2-C1-O2A-CGA
20	C	498	CLA	C2-C1-O2A-CGA
20	C	502	CLA	C2-C1-O2A-CGA
20	D	354	CLA	C2-C1-O2A-CGA
20	b	5521	CLA	C2-C1-O2A-CGA
20	d	5354	CLA	C2-C1-O2A-CGA
20	B	520	CLA	C12-C13-C15-C16
20	B	523	CLA	C11-C12-C13-C15
20	D	354	CLA	C11-C12-C13-C15
20	a	5558	CLA	C11-C12-C13-C15
27	a	5568	LMT	C7-C8-C9-C10
21	A	562	PHO	O2A-C1-C2-C3
30	c	5508	DGD	O6E-C5E-C6E-O5E
28	L	210	MGE	O1B-C1B-C2B-C3B
20	C	493	CLA	C3A-C2A-CAA-CBA
20	c	5491	CLA	C3A-C2A-CAA-CBA
20	c	5493	CLA	C3A-C2A-CAA-CBA
21	a	5562	PHO	C4-C3-C5-C6
20	B	515	CLA	CAA-CBA-CGA-O1A
28	d	5361	MGE	O1B-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
28	l	5210	MGE	O1B-C1B-C2B-C3B
26	d	5358	SQD	C13-C14-C15-C16
28	D	360	MGE	O1B-C1B-C2B-C3B
20	c	5494	CLA	CAA-CBA-CGA-O1A
20	B	518	CLA	C11-C10-C8-C9
20	C	492	CLA	C11-C10-C8-C9
20	C	498	CLA	C6-C7-C8-C9
20	C	501	CLA	C14-C13-C15-C16
20	D	354	CLA	C11-C12-C13-C14
20	b	5518	CLA	C11-C10-C8-C9
20	b	5523	CLA	C11-C12-C13-C14
28	I	201	MGE	C4D-C5D-C6D-O5D
20	c	5495	CLA	CAA-CBA-CGA-O1A
20	b	5512	CLA	C13-C15-C16-C17
30	c	5507	DGD	O1B-C1B-C2B-C3B
20	c	5491	CLA	CAA-CBA-CGA-O2A
20	B	512	CLA	C13-C15-C16-C17
20	C	494	CLA	CAA-CBA-CGA-O1A
20	C	495	CLA	CAA-CBA-CGA-O1A
20	C	497	CLA	CAA-CBA-CGA-O1A
20	C	499	CLA	CAA-CBA-CGA-O1A
20	c	5497	CLA	CAA-CBA-CGA-O1A
26	A	568	SQD	O49-C7-C8-C9
26	d	5358	SQD	O49-C7-C8-C9
20	b	5512	CLA	C5-C6-C7-C8
20	b	5515	CLA	CAA-CBA-CGA-O1A
30	C	507	DGD	O1B-C1B-C2B-C3B
20	B	513	CLA	C2A-CAA-CBA-CGA
20	B	513	CLA	CAD-CBD-CGD-O2D
20	B	523	CLA	CAD-CBD-CGD-O2D
20	C	497	CLA	CAD-CBD-CGD-O2D
20	b	5513	CLA	CAD-CBD-CGD-O2D
20	c	5497	CLA	CAD-CBD-CGD-O2D
20	c	5498	CLA	CAD-CBD-CGD-O2D
28	l	5210	MGE	O1G-C1A-C2A-C3A
28	b	5530	MGE	C1A-C2A-C3A-C4A
20	b	5524	CLA	CAA-CBA-CGA-O2A
20	C	491	CLA	C1-C2-C3-C4
20	C	497	CLA	C1-C2-C3-C4
20	C	502	CLA	C1-C2-C3-C4
20	b	5514	CLA	C1-C2-C3-C4
20	c	5497	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
20	c	5502	CLA	C1-C2-C3-C4
20	B	513	CLA	C13-C15-C16-C17
28	L	210	MGE	O1G-C1A-C2A-C3A
20	B	524	CLA	CAA-CBA-CGA-O2A
30	C	509	DGD	O1G-C1A-C2A-C3A
20	c	5491	CLA	CAA-CBA-CGA-O1A
20	c	5499	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

126 monomers are involved in 476 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	B	524	CLA	4	0
28	D	358	MGE	2	0
27	T	217	LMT	6	0
30	C	507	DGD	6	0
20	C	497	CLA	5	0
20	B	521	CLA	3	0
24	H	107	BCR	2	0
20	b	5522	CLA	4	0
20	C	491	CLA	2	0
20	b	5511	CLA	1	0
20	d	5354	CLA	6	0
30	h	5208	DGD	3	0
20	C	503	CLA	1	0
30	C	508	DGD	2	0
21	A	561	PHO	6	0
27	t	5217	LMT	5	0
20	c	5493	CLA	6	0
28	I	201	MGE	1	0
26	t	213	SQD	1	0
28	D	359	MGE	1	0
20	B	526	CLA	1	0
20	b	5519	CLA	3	0
20	a	5560	CLA	1	0
24	b	5528	BCR	2	0
24	c	5506	BCR	6	0
30	H	208	DGD	3	0
20	B	517	CLA	9	0
20	c	5491	CLA	2	0
20	B	519	CLA	3	0
20	B	512	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	b	5530	MGE	1	0
32	v	5552	HEM	1	0
20	b	5512	CLA	3	0
20	b	5516	CLA	1	0
20	b	5518	CLA	9	0
28	B	530	MGE	1	0
20	C	500	CLA	2	0
20	b	5517	CLA	9	0
20	A	558	CLA	9	0
28	D	360	MGE	7	0
20	B	520	CLA	7	0
20	b	5520	CLA	6	0
21	A	562	PHO	6	0
20	C	501	CLA	9	0
20	B	522	CLA	3	0
20	c	5503	CLA	1	0
20	c	5495	CLA	10	0
20	B	513	CLA	8	0
20	b	5514	CLA	6	0
27	a	5568	LMT	1	0
30	c	5508	DGD	4	0
20	B	518	CLA	9	0
24	C	506	BCR	6	0
20	D	354	CLA	6	0
24	C	504	BCR	7	0
22	A	564	PQ9	1	0
24	A	566	BCR	1	0
20	c	5498	CLA	5	0
22	D	356	PQ9	5	0
20	b	5525	CLA	2	0
24	d	5357	BCR	6	0
24	x	5130	BCR	10	0
20	B	511	CLA	1	0
20	C	499	CLA	2	0
20	b	5513	CLA	8	0
20	c	5501	CLA	9	0
20	B	516	CLA	3	0
20	b	5515	CLA	10	0
20	b	5526	CLA	1	0
20	C	493	CLA	7	0
21	a	5561	PHO	5	0
20	C	498	CLA	6	0

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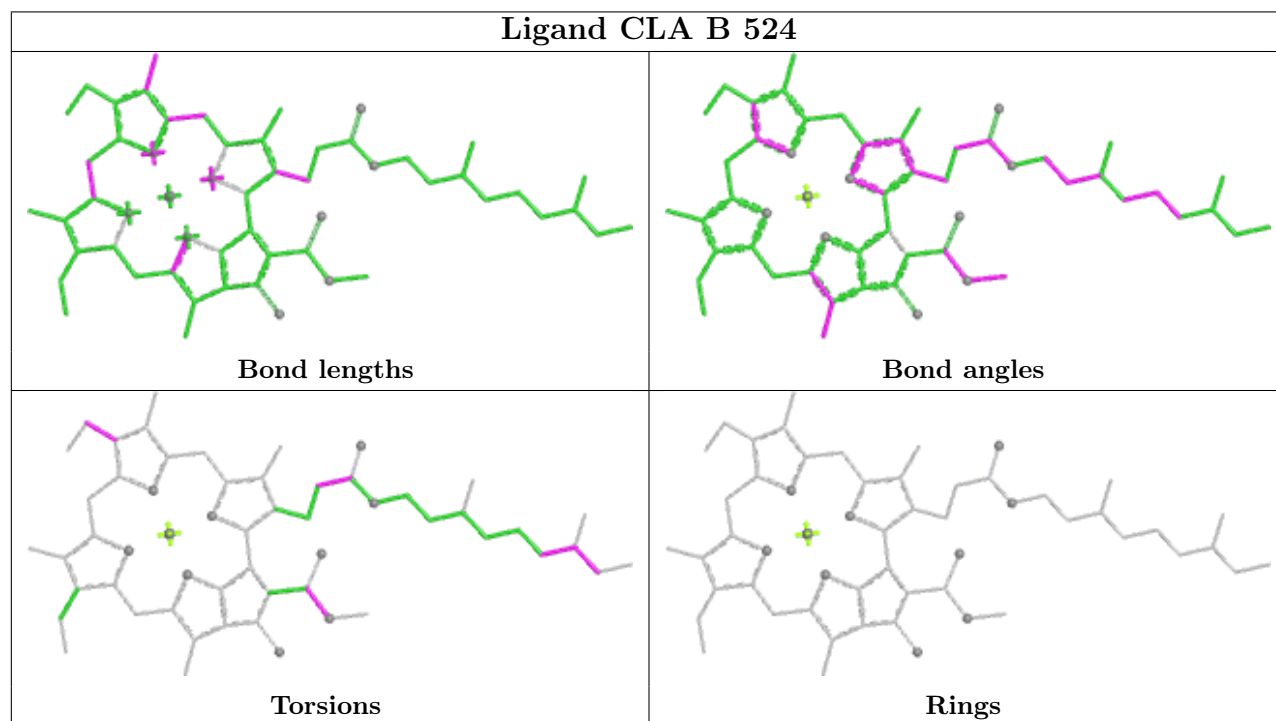
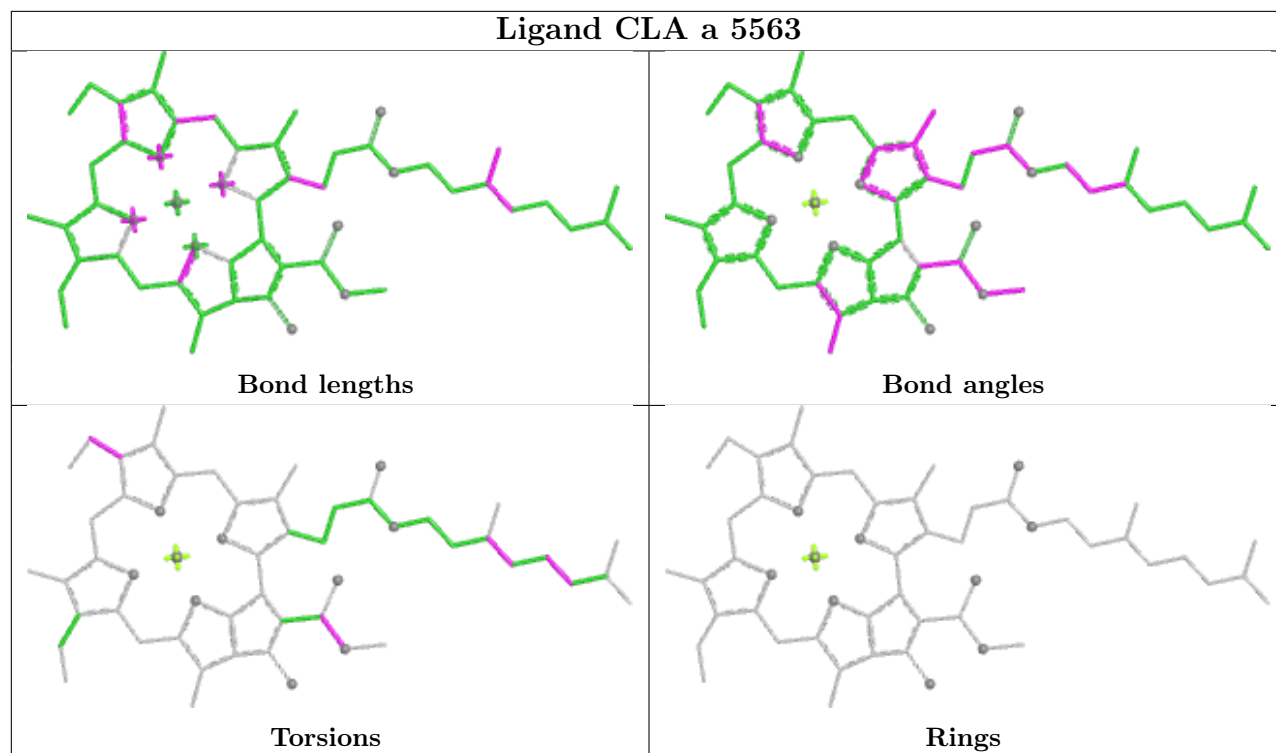
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24	t	104	BCR	9	0
20	C	496	CLA	2	0
24	c	5504	BCR	9	0
24	b	5529	BCR	1	0
20	b	5523	CLA	1	0
20	a	5559	CLA	5	0
26	L	5213	SQD	1	0
20	b	5524	CLA	2	0
20	A	560	CLA	1	0
28	d	5361	MGE	7	0
28	d	5359	MGE	2	0
24	a	5566	BCR	3	0
20	B	515	CLA	11	0
20	C	494	CLA	2	0
24	b	5527	BCR	3	0
20	C	502	CLA	2	0
24	D	357	BCR	4	0
28	i	5201	MGE	2	0
24	B	528	BCR	2	0
20	D	355	CLA	3	0
25	A	567	LHG	4	0
30	c	5507	DGD	5	0
21	a	5562	PHO	7	0
20	b	5521	CLA	1	0
20	C	495	CLA	9	0
32	F	51	HEM	3	0
32	f	5051	HEM	3	0
20	c	5502	CLA	1	0
24	X	130	BCR	9	0
24	T	5104	BCR	8	0
24	B	529	BCR	2	0
28	d	5360	MGE	2	0
20	B	514	CLA	5	0
20	c	5492	CLA	1	0
25	a	5567	LHG	4	0
32	V	552	HEM	2	0
20	c	5496	CLA	2	0
20	c	5499	CLA	1	0
22	d	5356	PQ9	5	0
28	l	5210	MGE	4	0

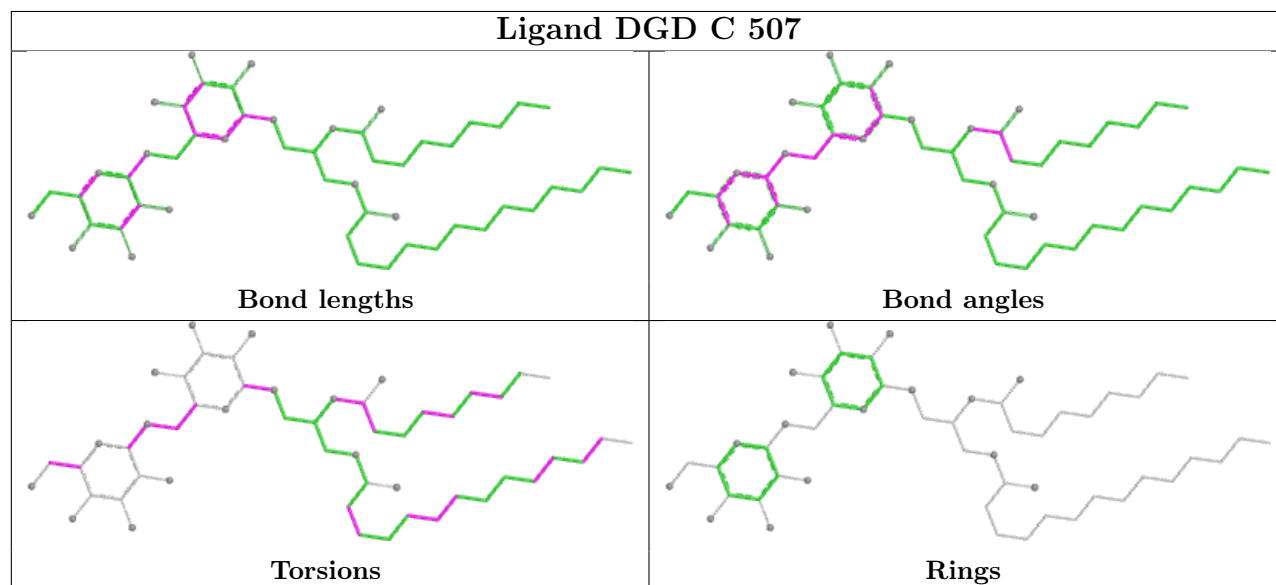
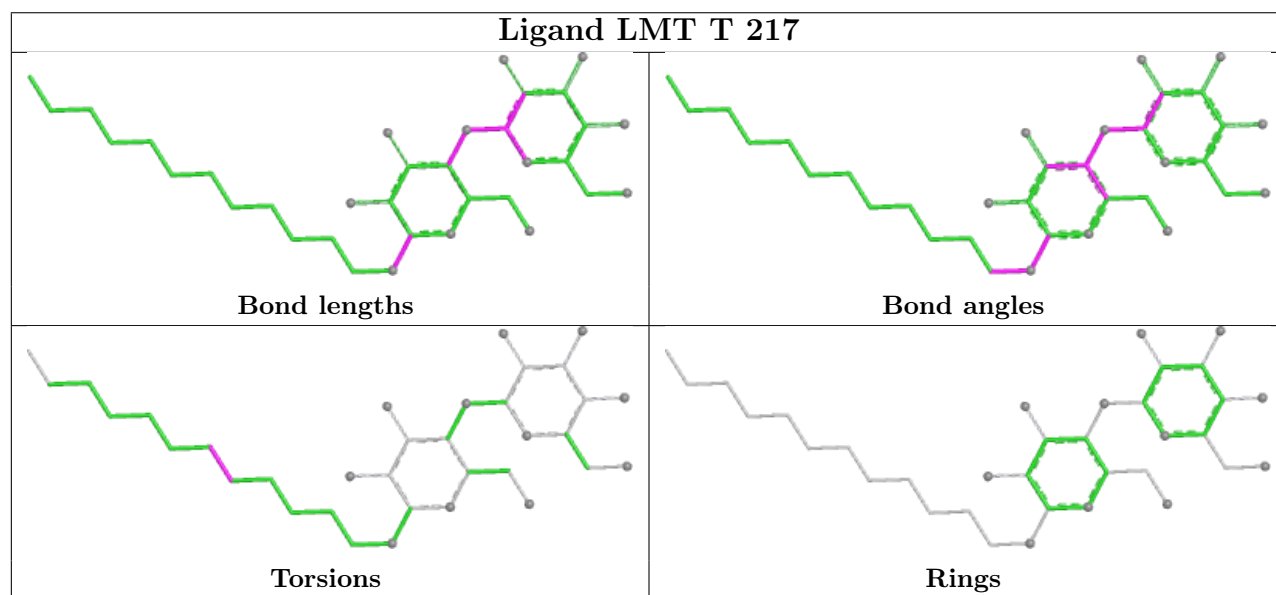
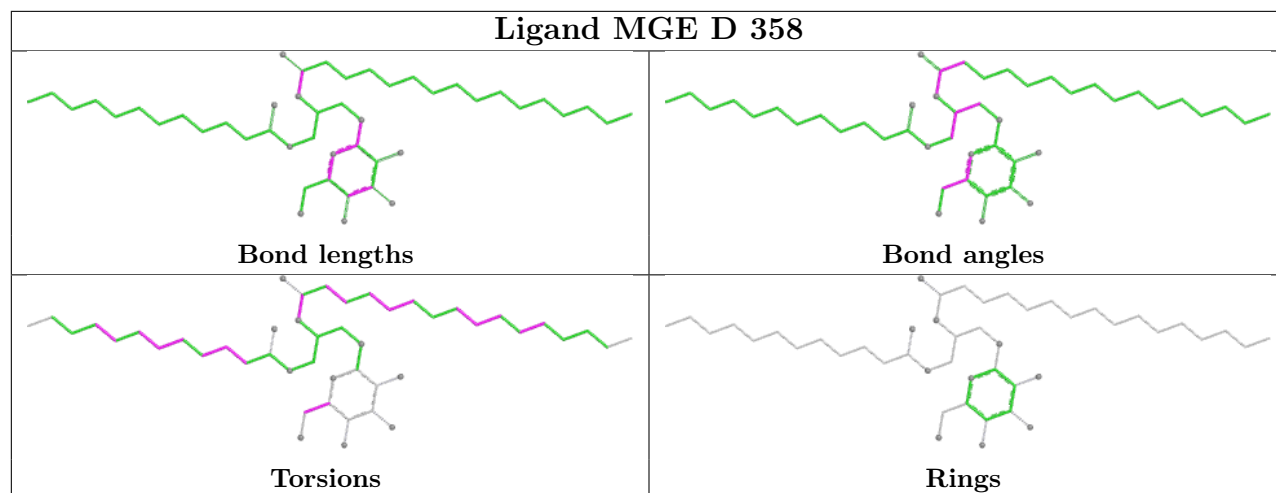
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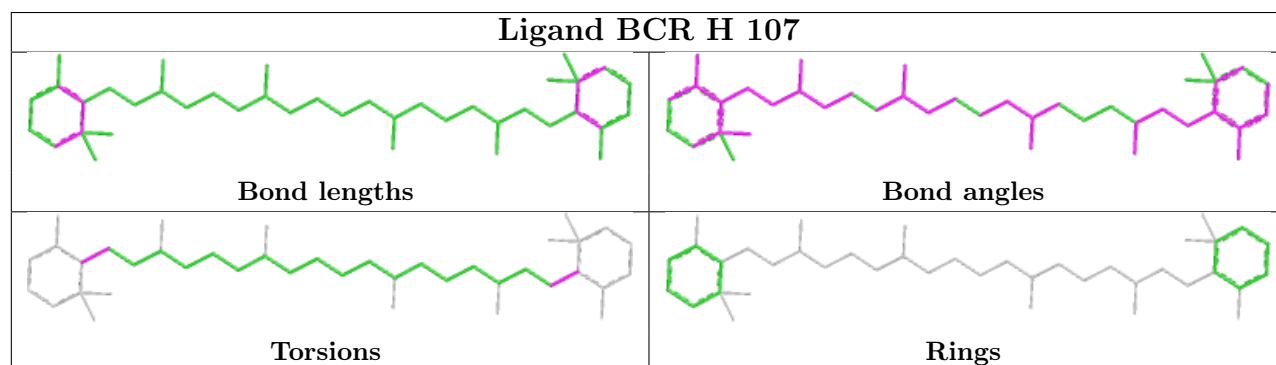
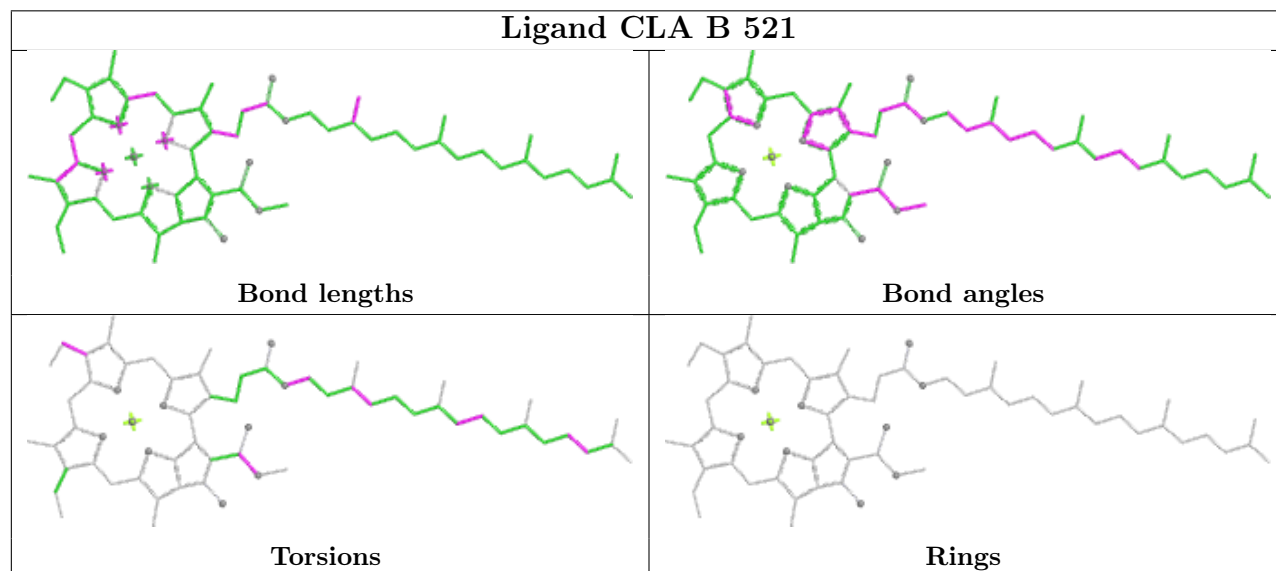
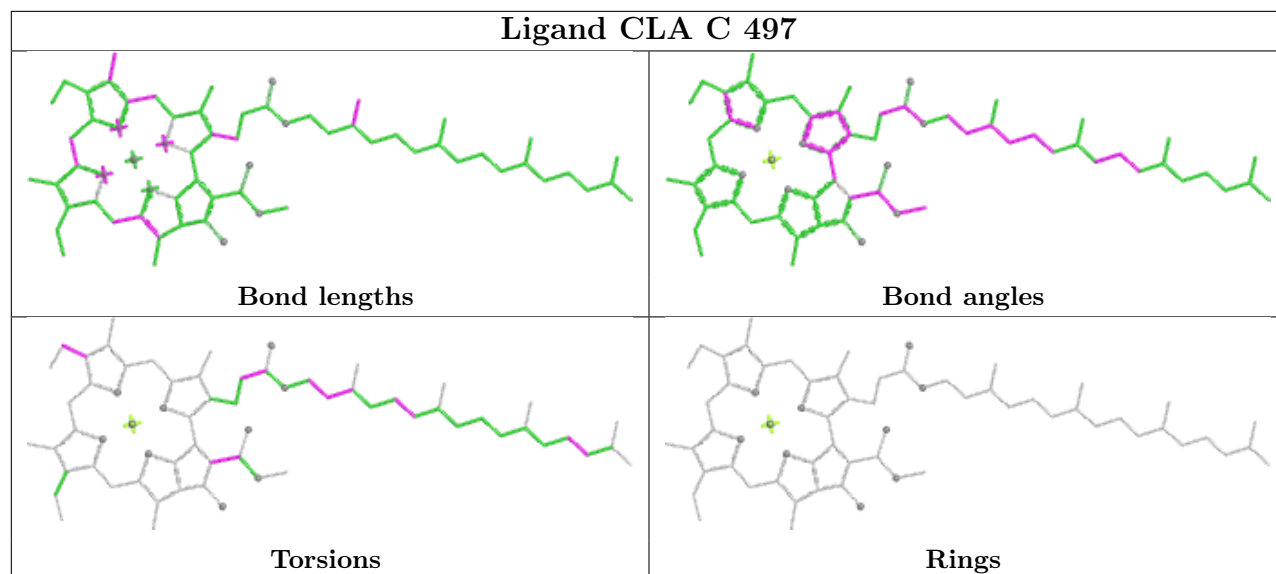
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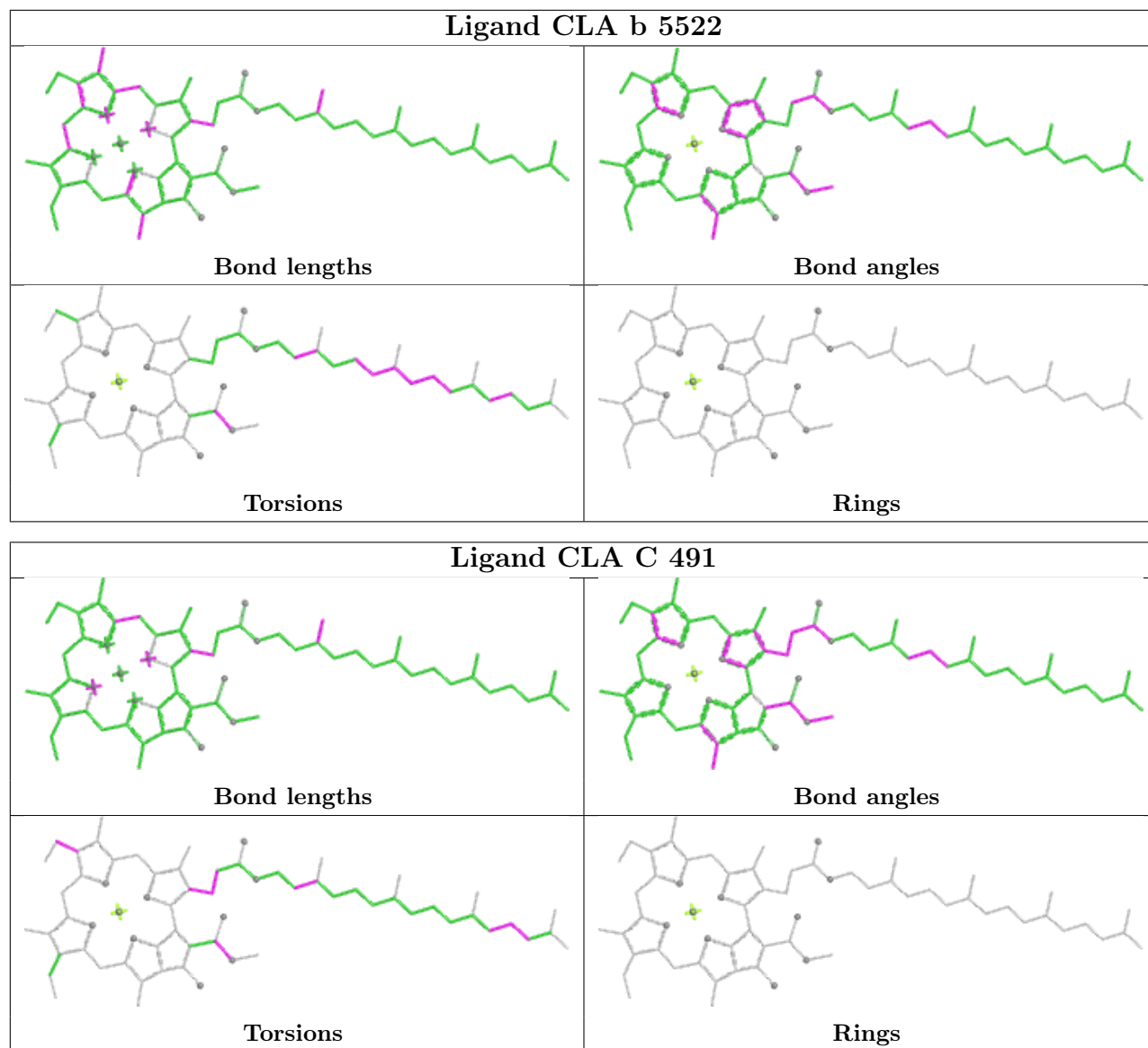
Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	L	210	MGE	2	0
24	C	505	BCR	6	0
20	B	525	CLA	2	0
20	c	5497	CLA	5	0
20	a	5558	CLA	10	0
20	c	5494	CLA	2	0
30	c	5509	DGD	9	0
30	C	509	DGD	10	0
24	B	527	BCR	3	0
20	d	5355	CLA	4	0
24	c	5505	BCR	6	0
20	A	559	CLA	4	0

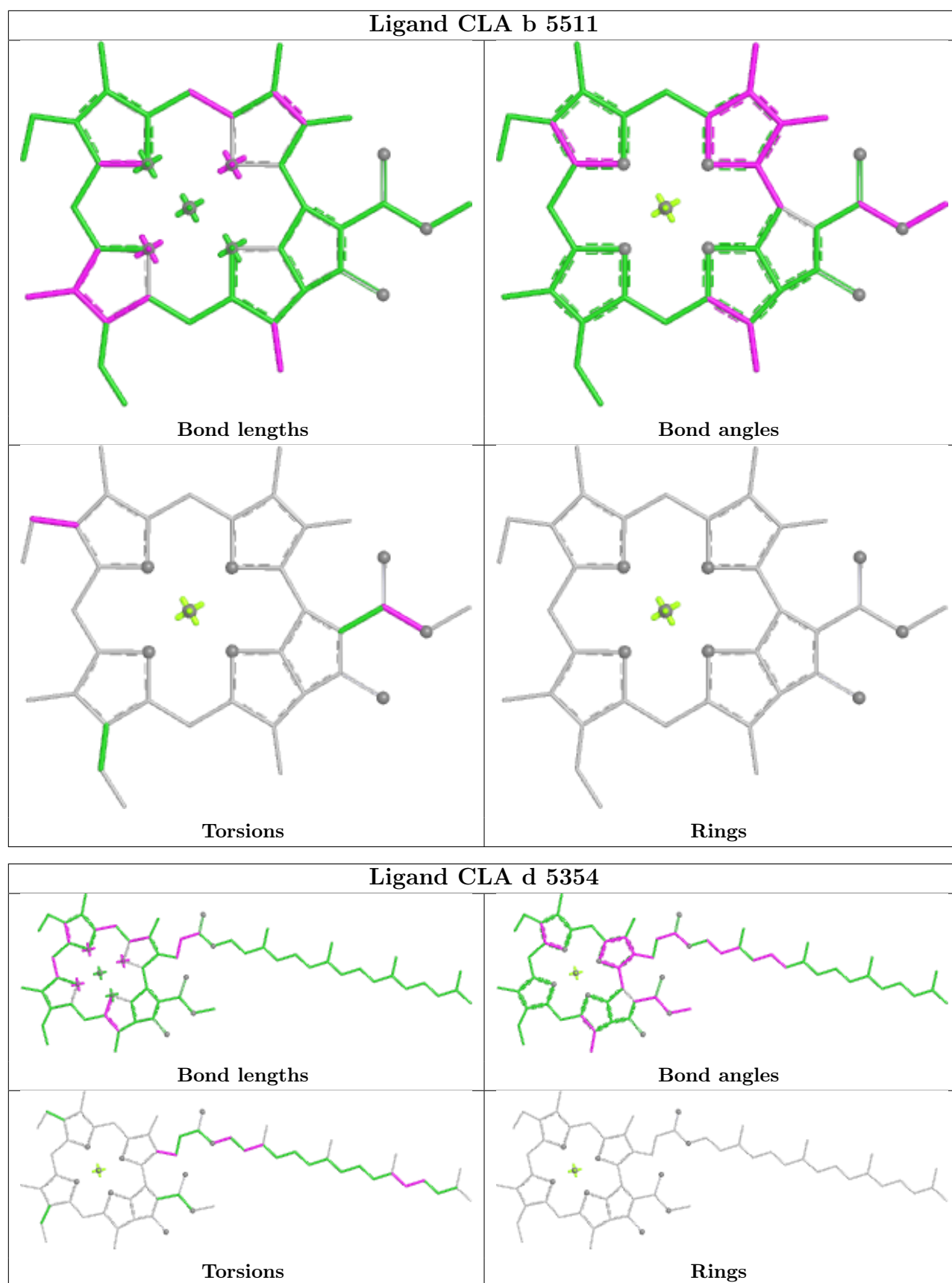
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



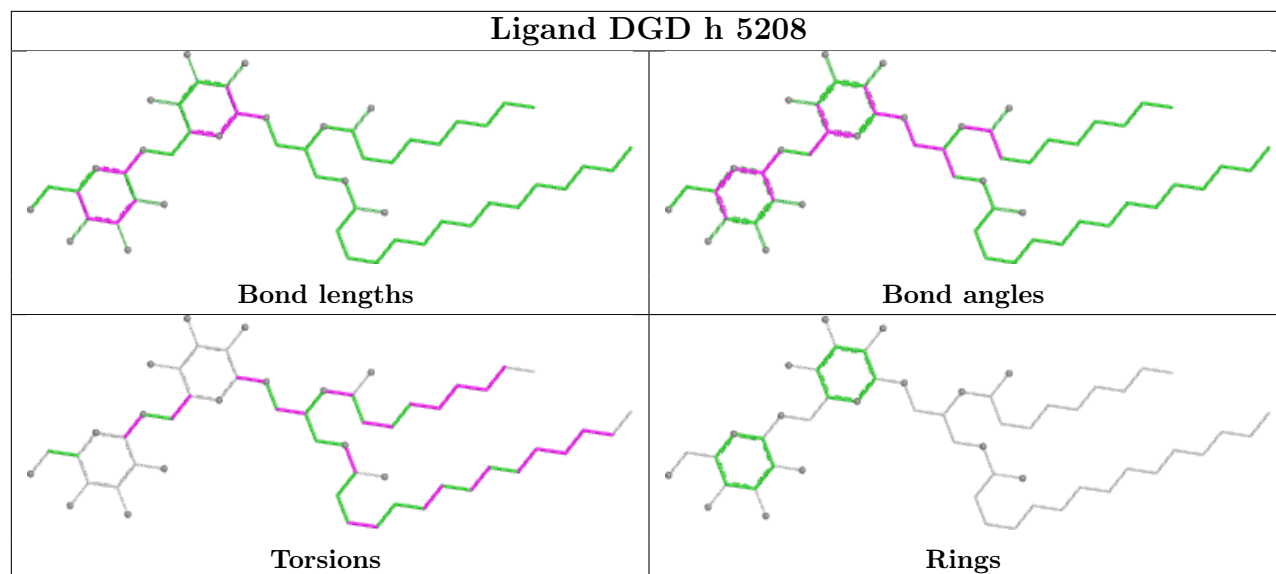




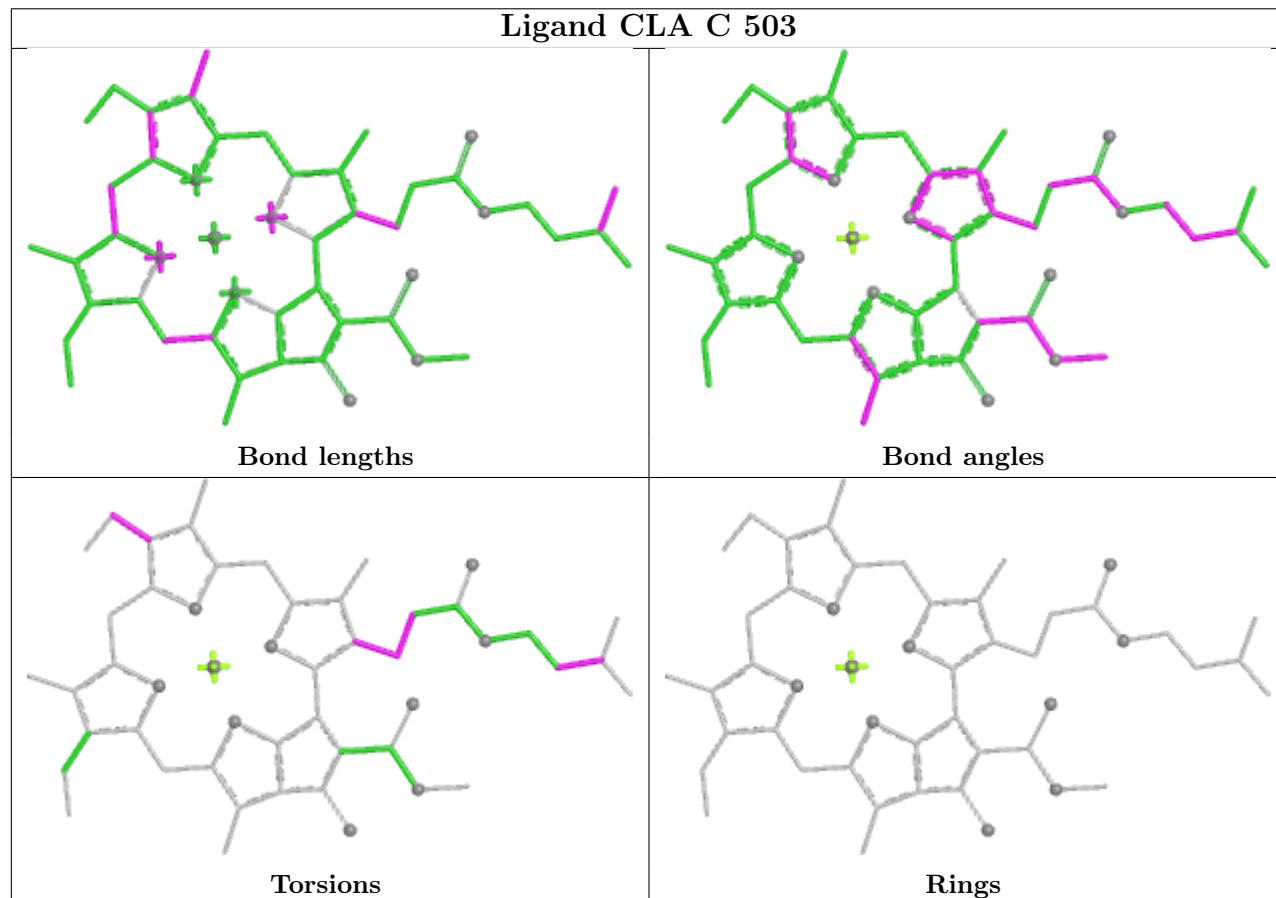


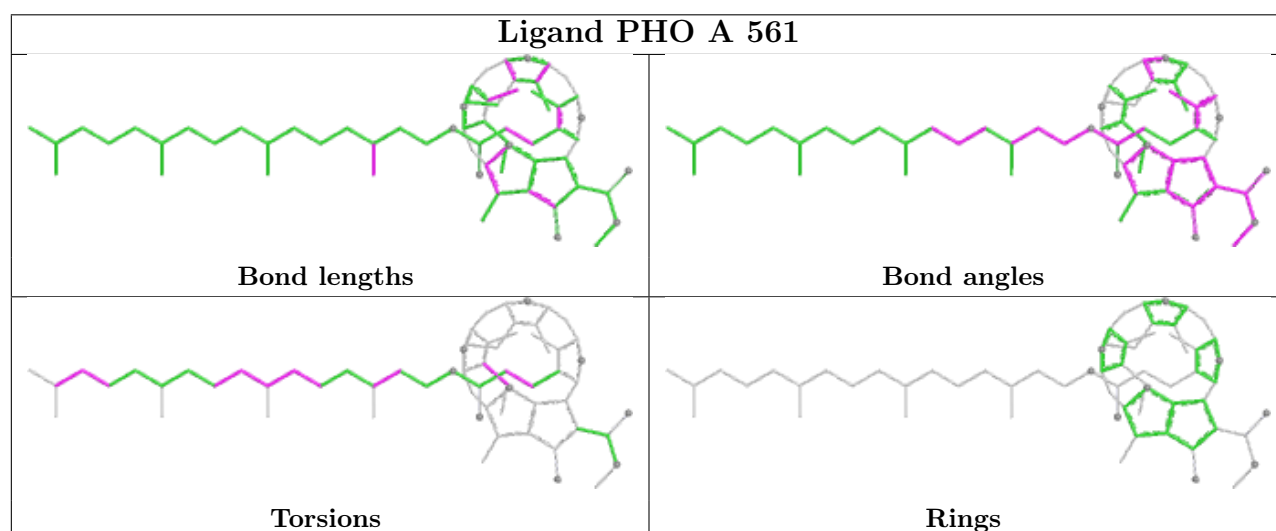
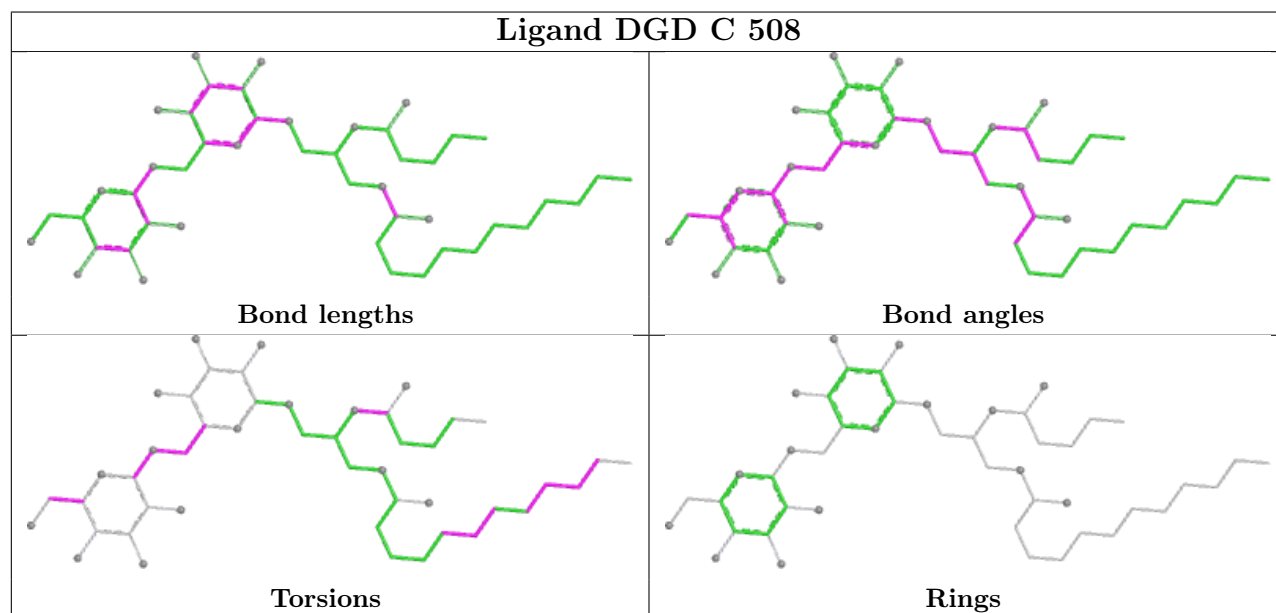
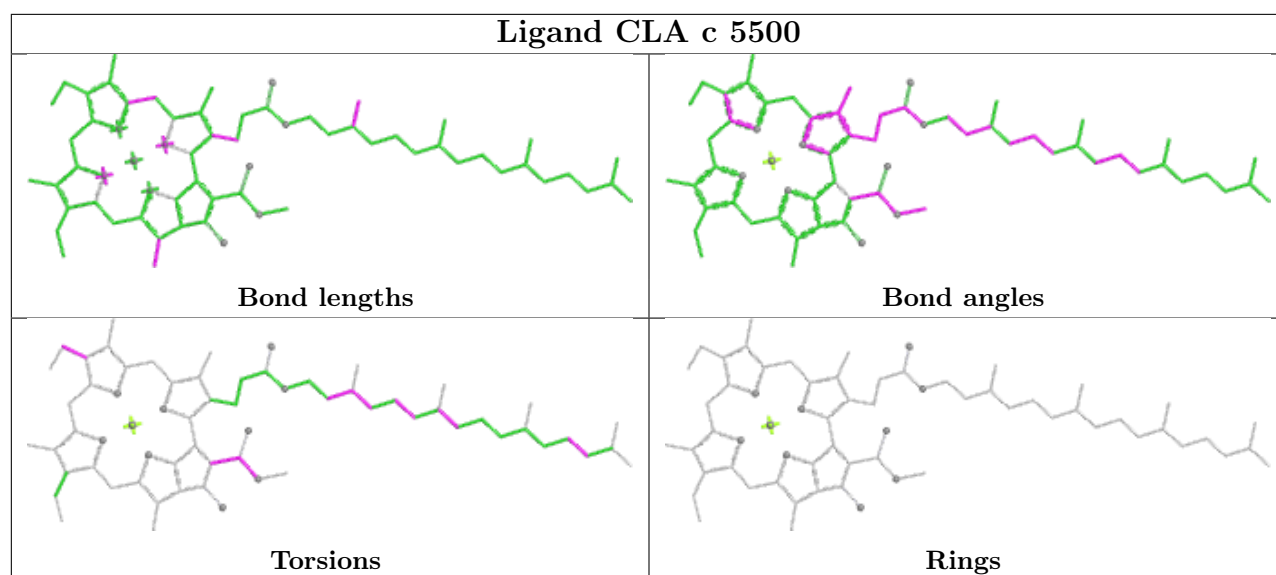


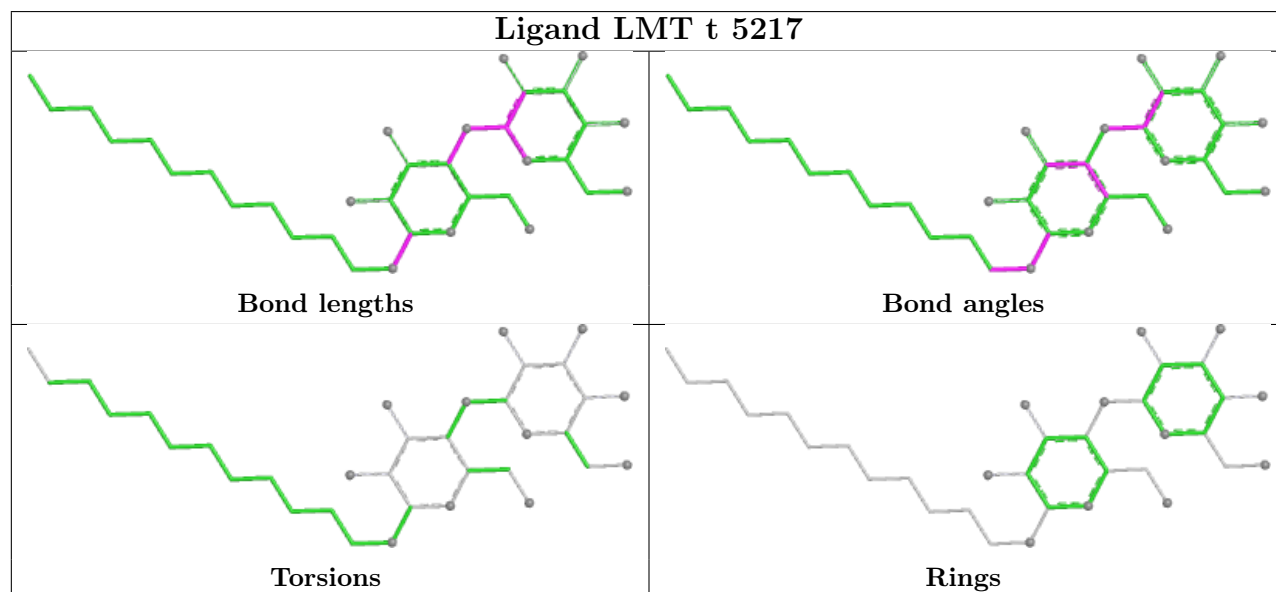
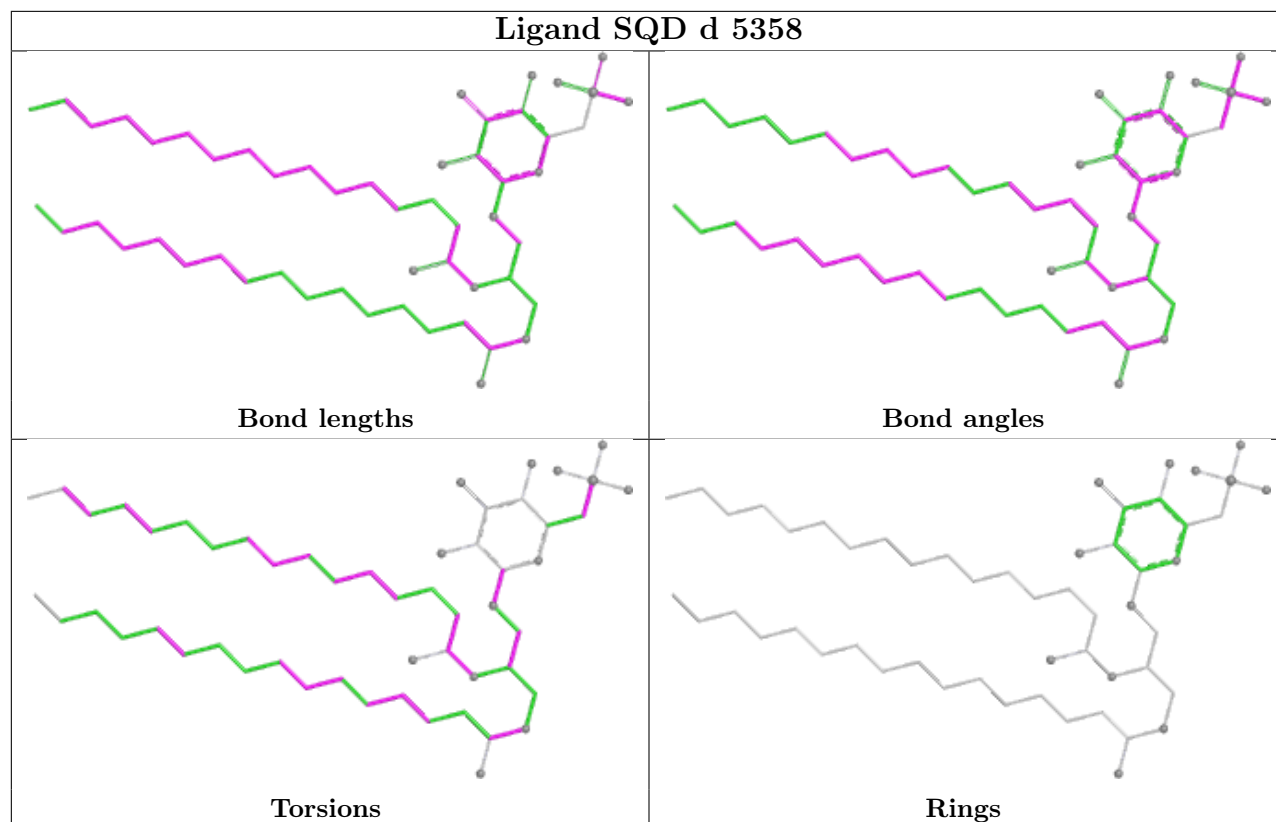
Ligand DGD h 5208

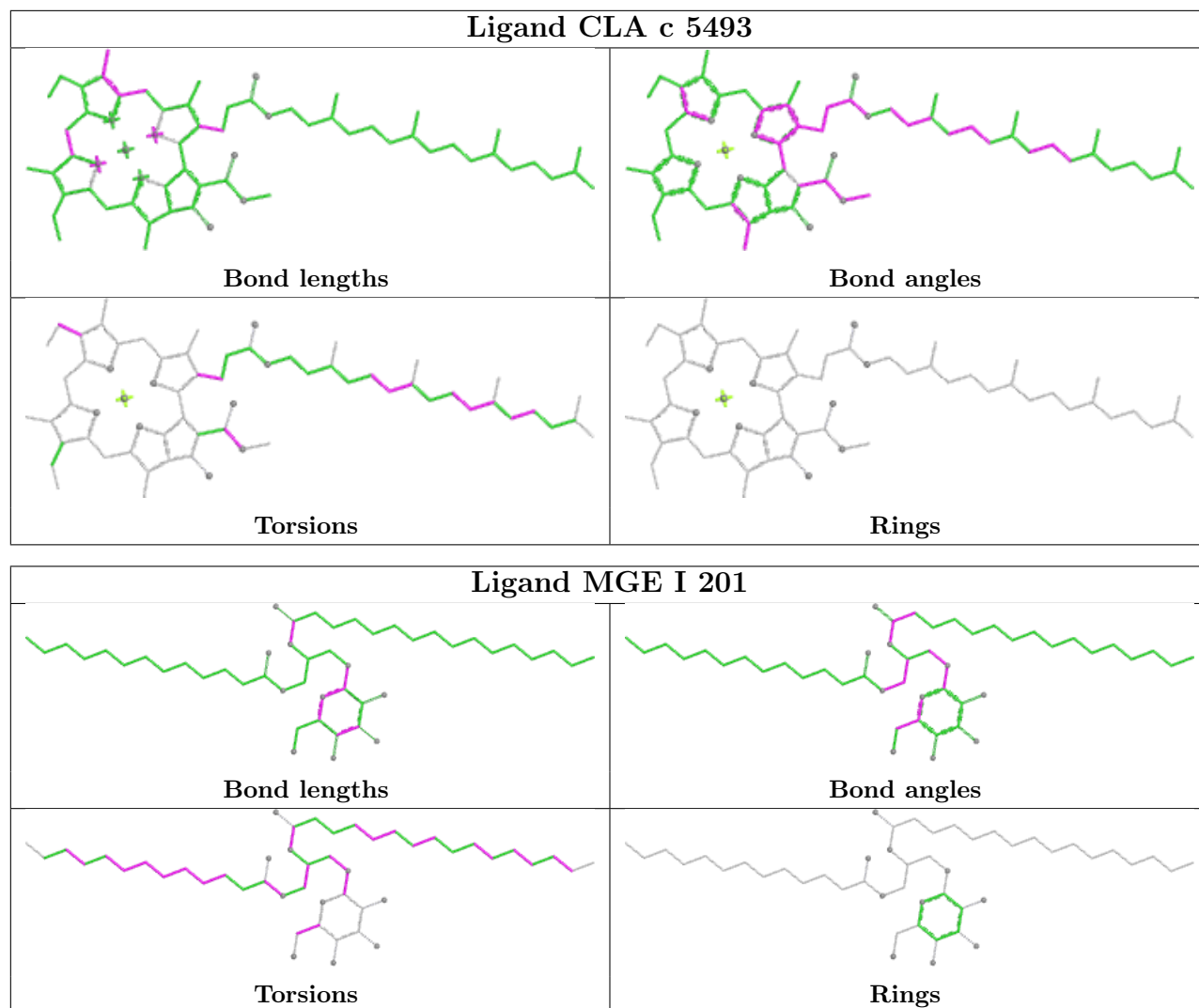


Ligand CLA C 503

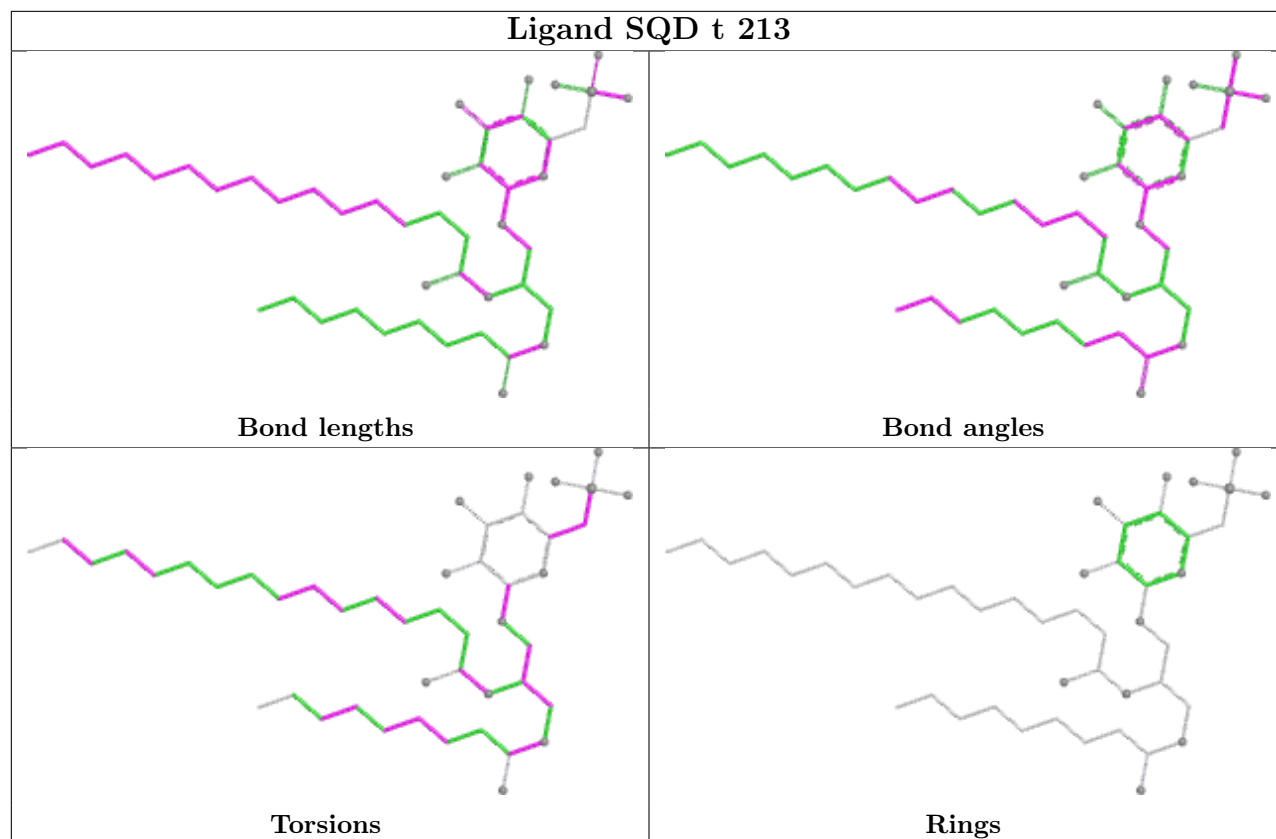




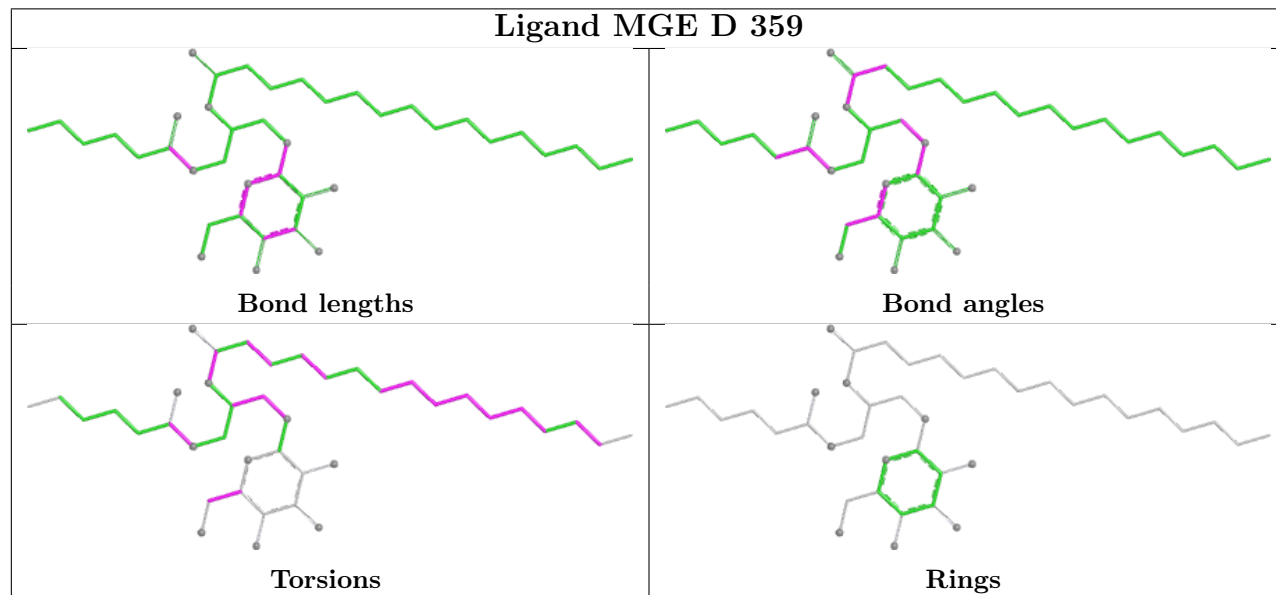




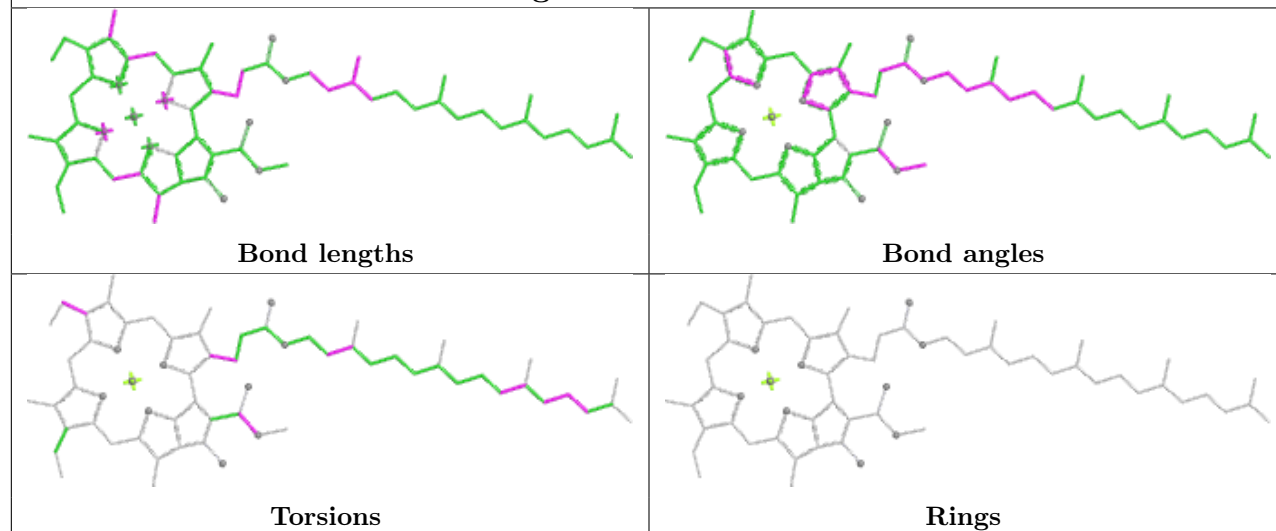
Ligand SQD t 213



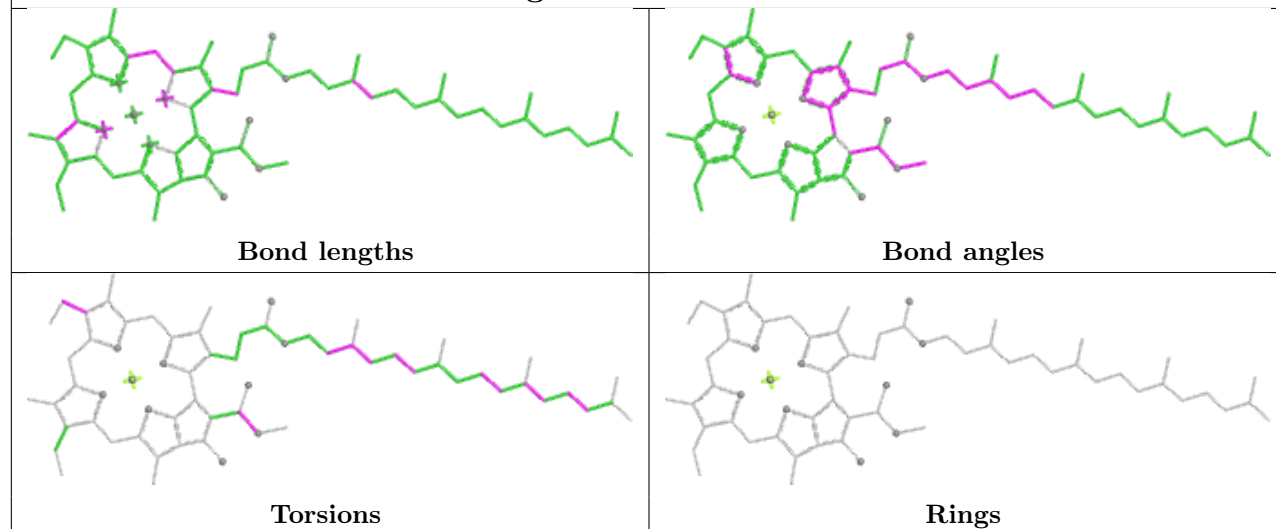
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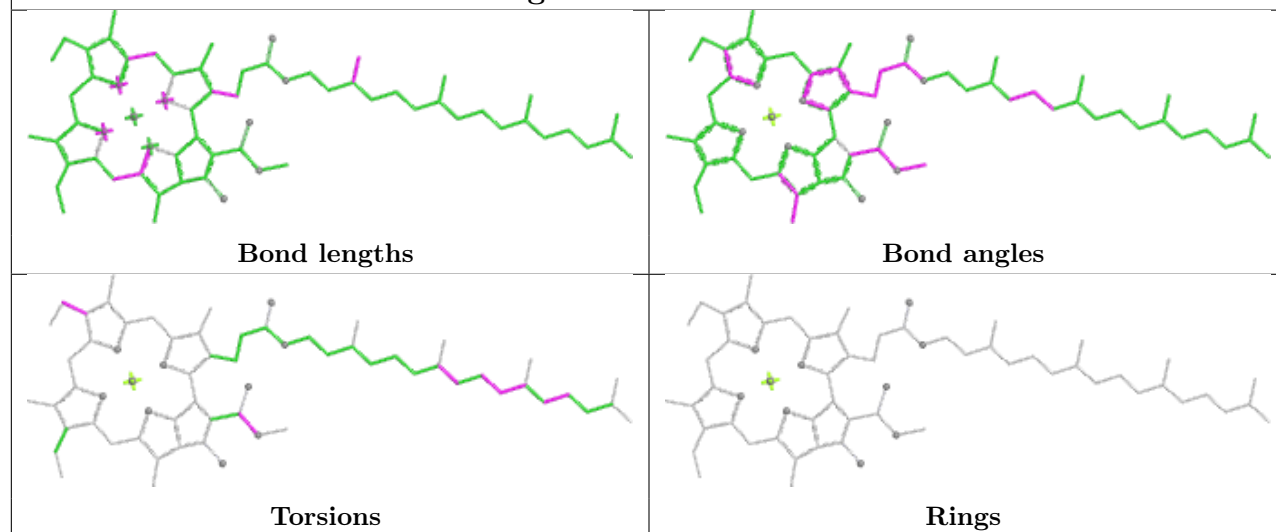
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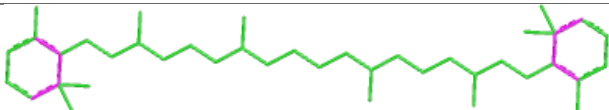
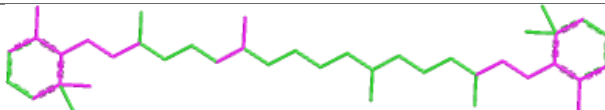
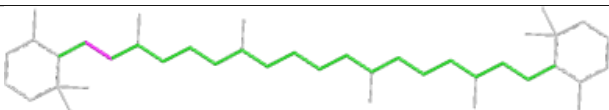
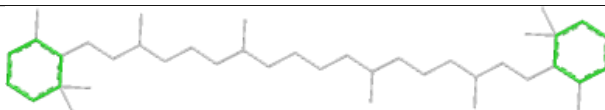


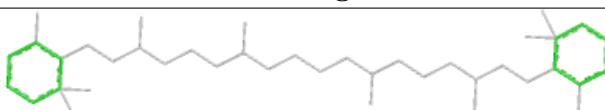
Ligand CLA b 5519

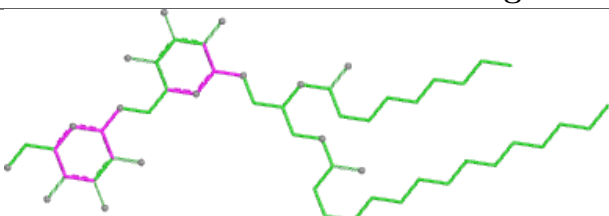
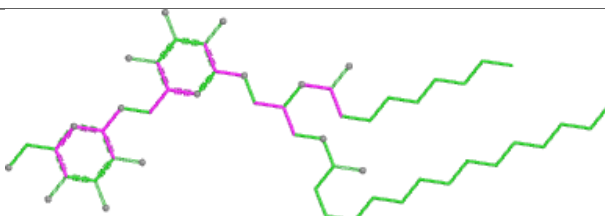
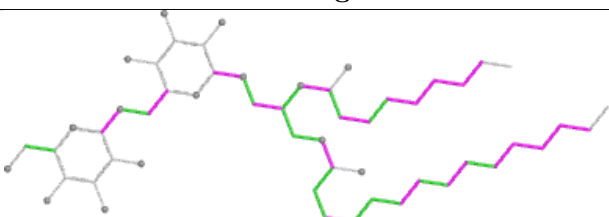
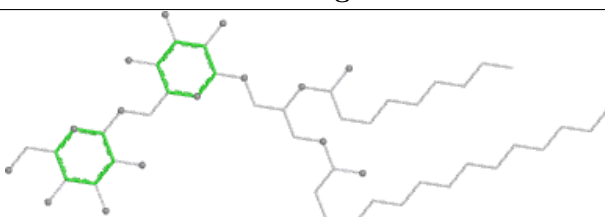


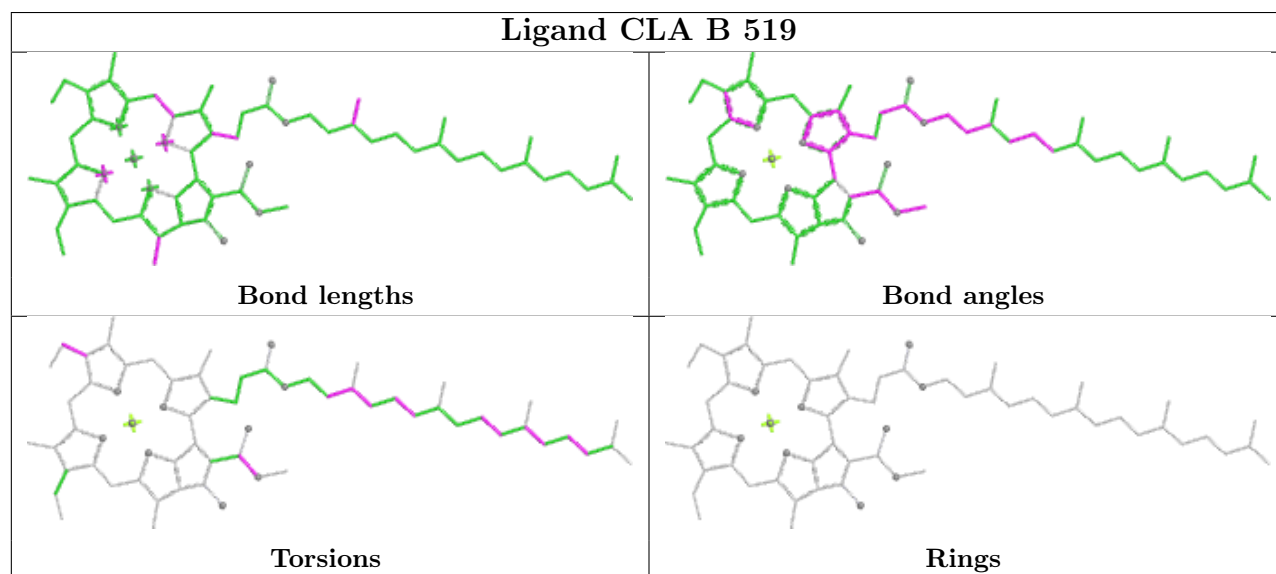
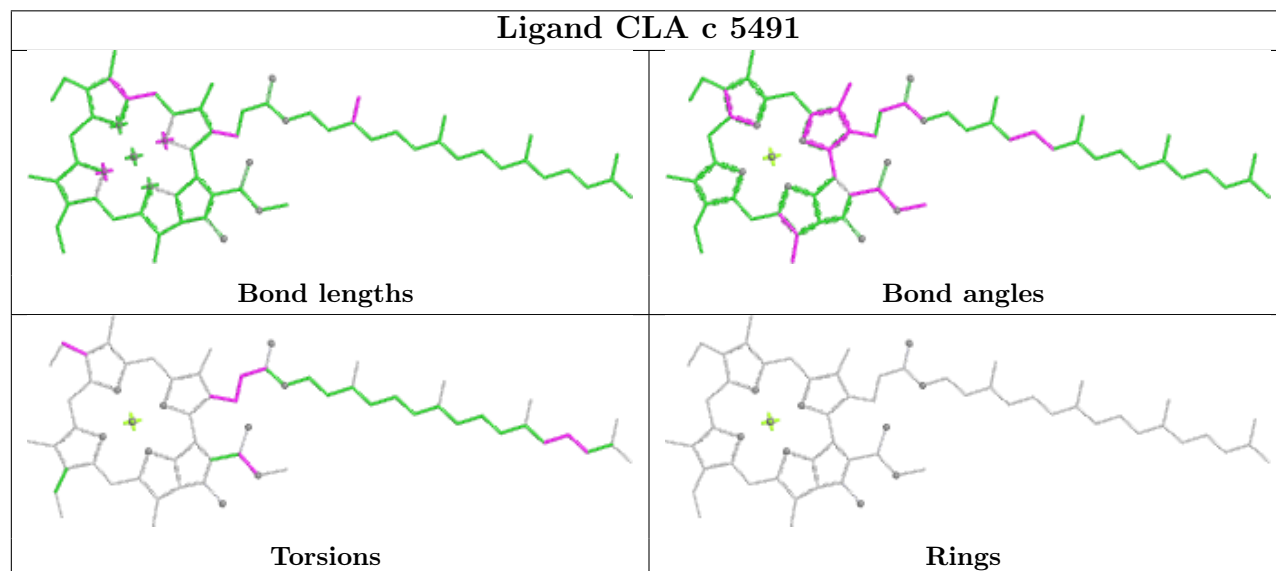
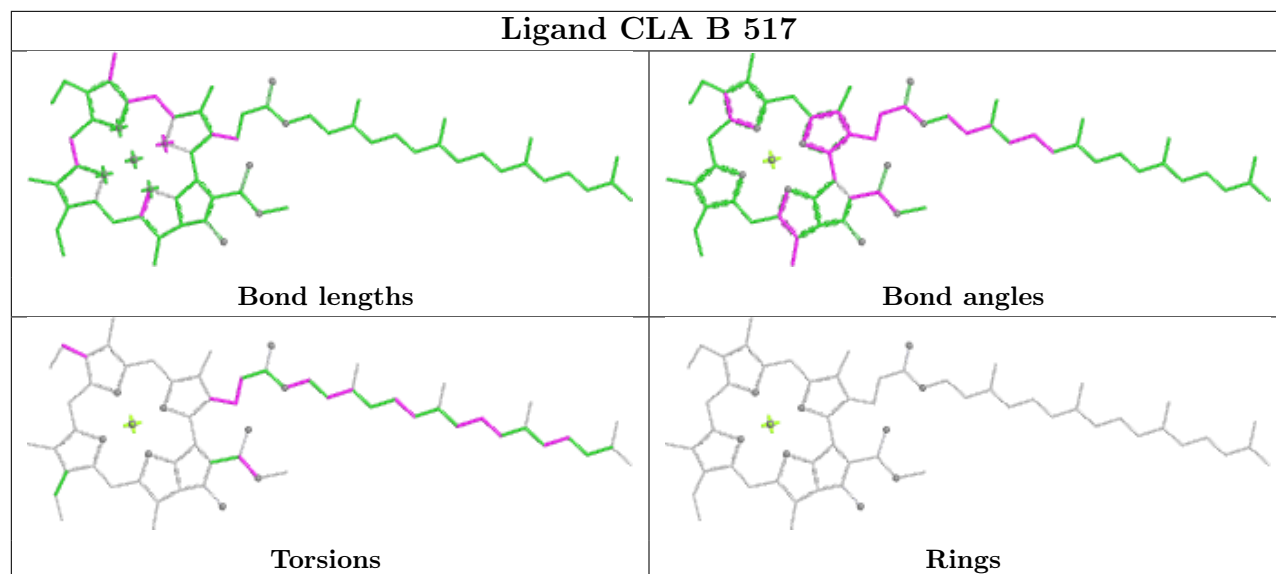
Ligand CLA a 5560



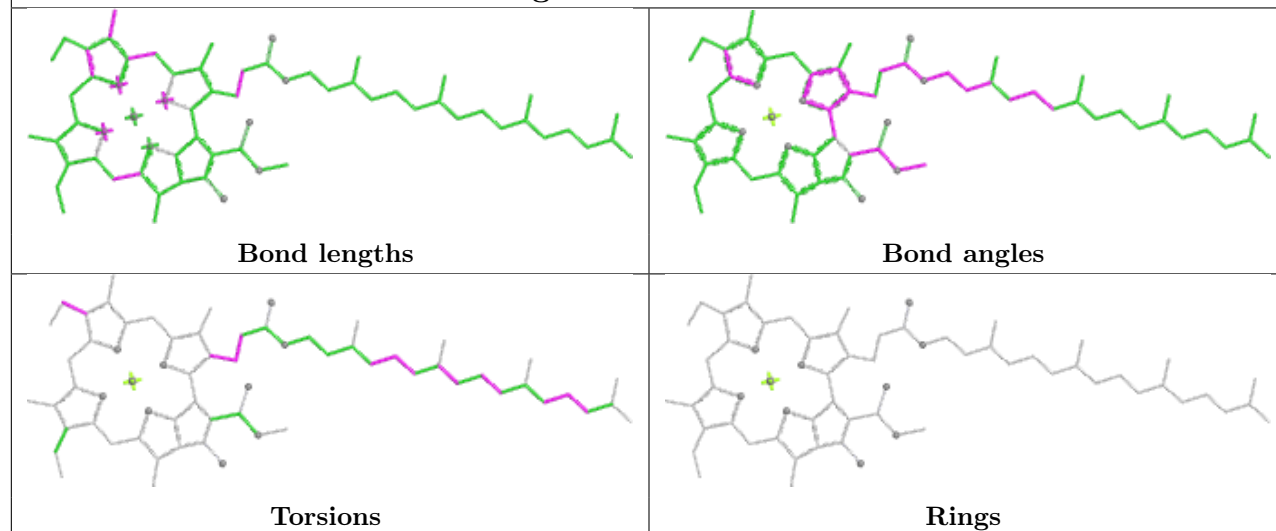
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Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR c 5506	
	
Bond lengths	Bond angles
	
Torsions	Rings

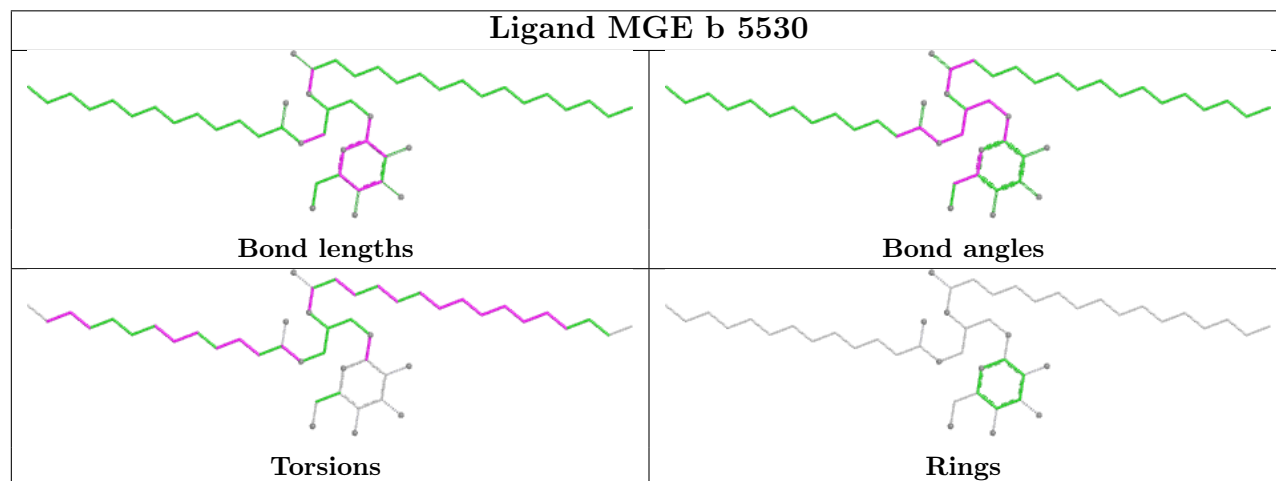
Ligand DGD H 208	
	
Bond lengths	Bond angles
	
Torsions	Rings



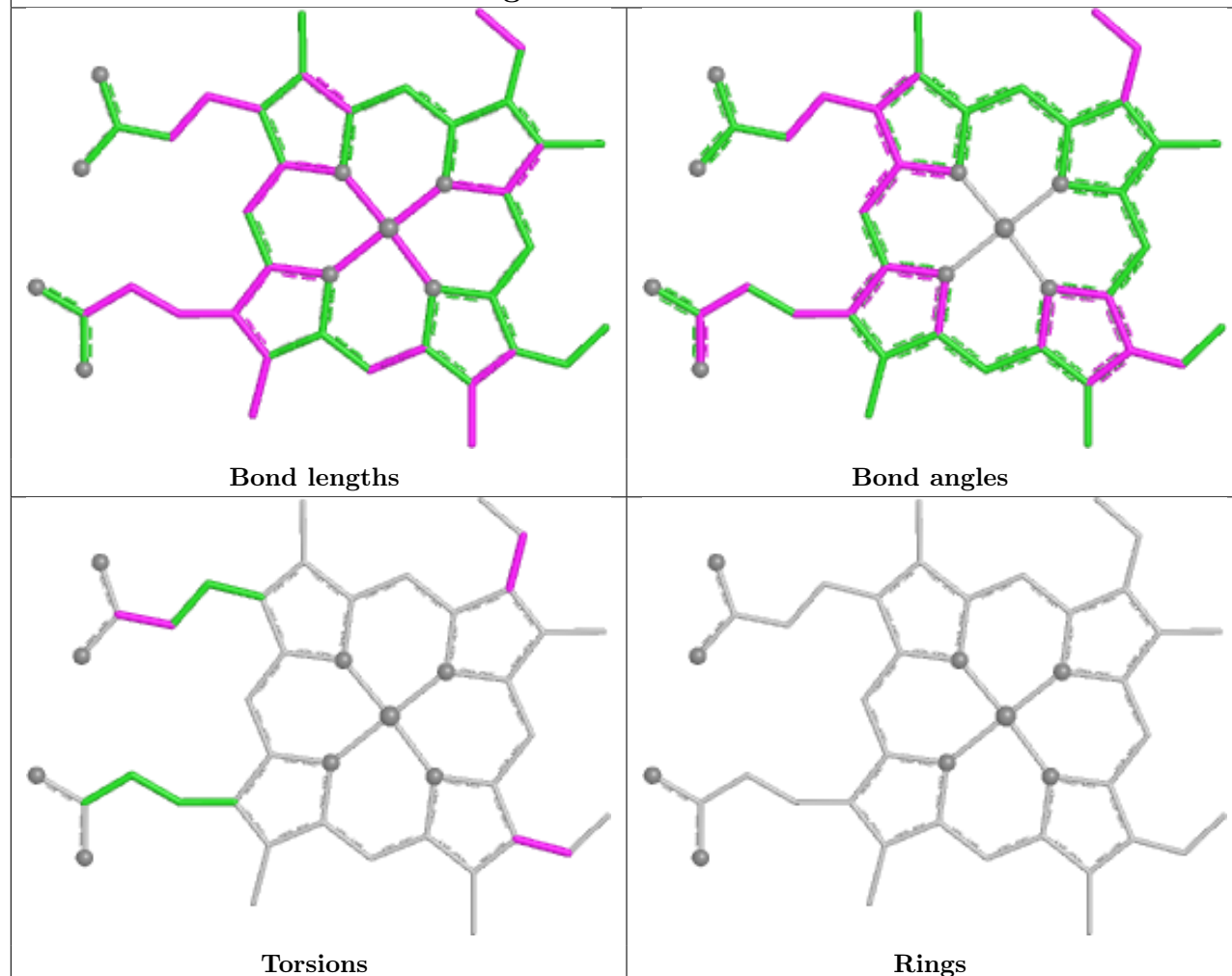
Ligand CLA B 512



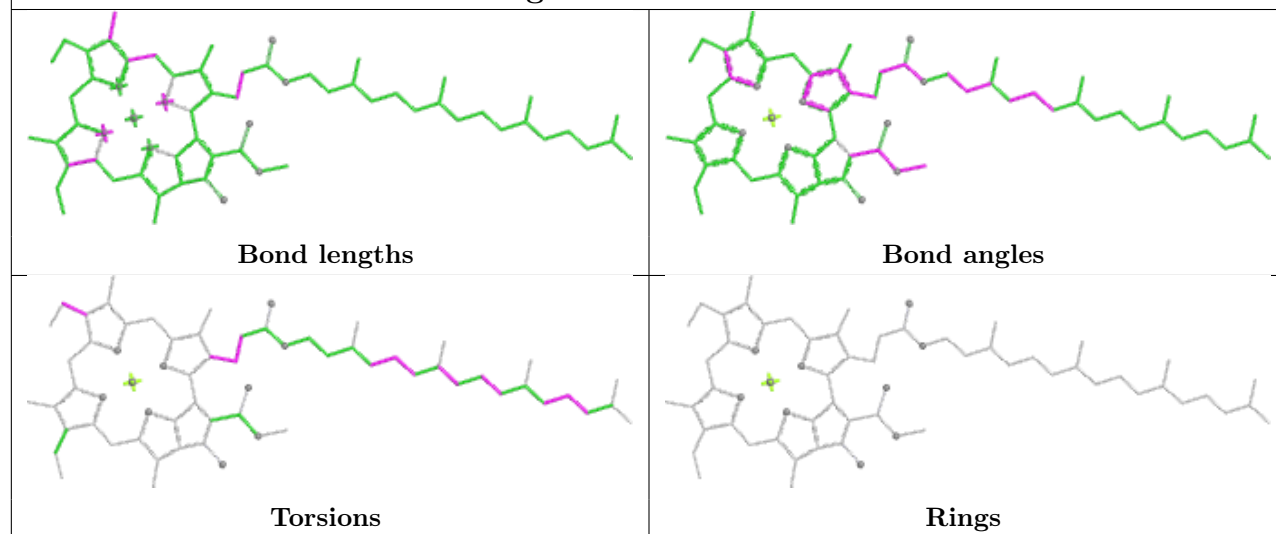
Ligand MGE b 5530

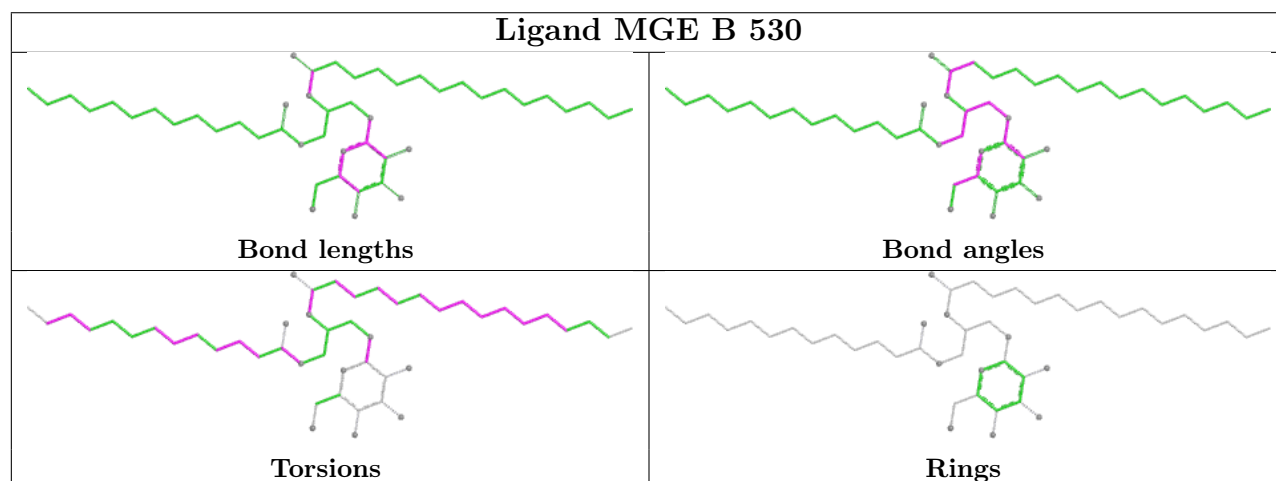
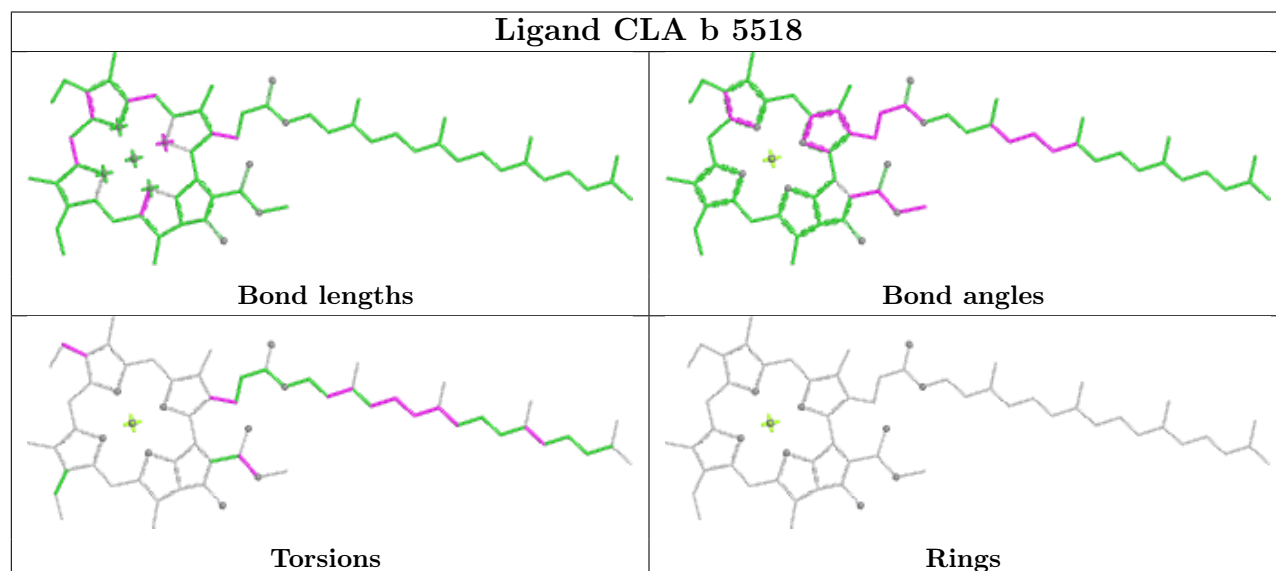
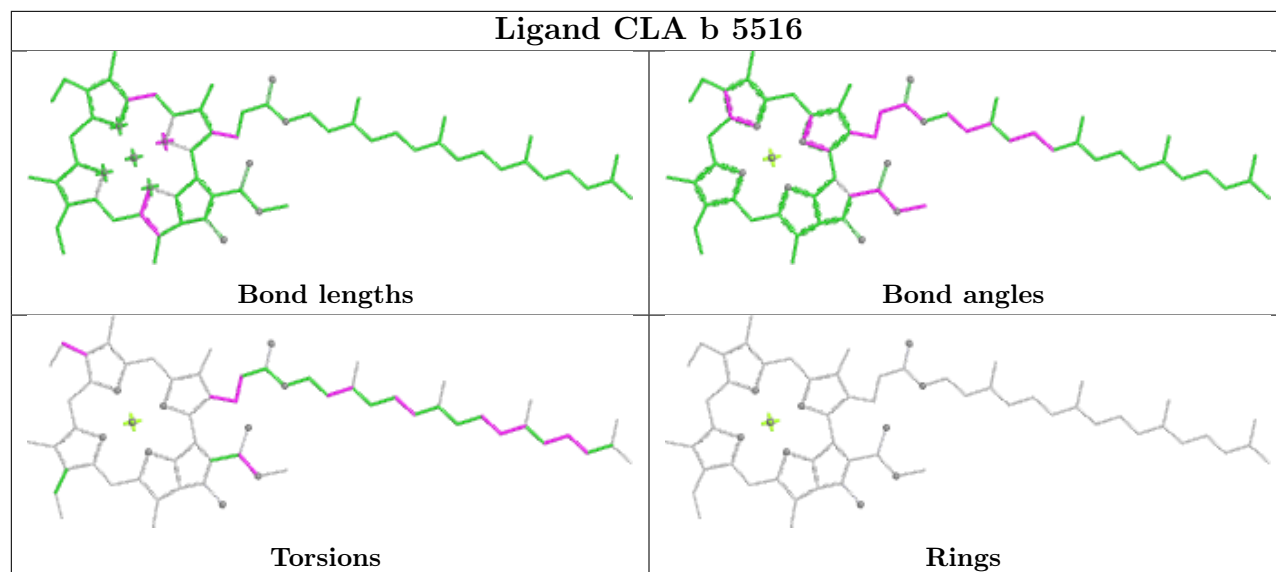


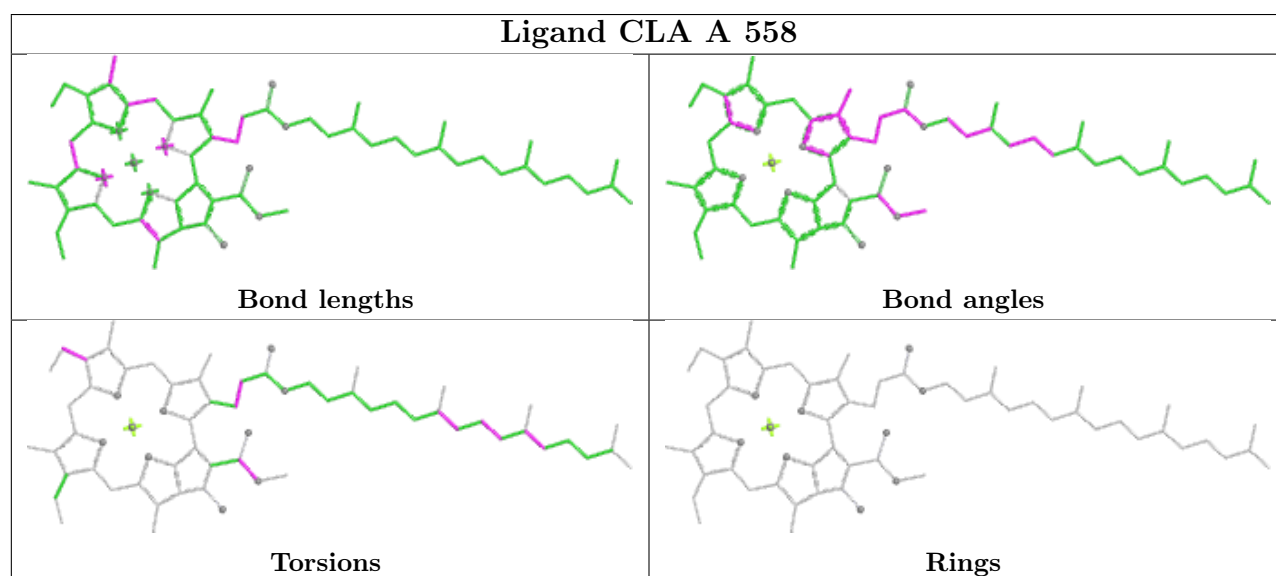
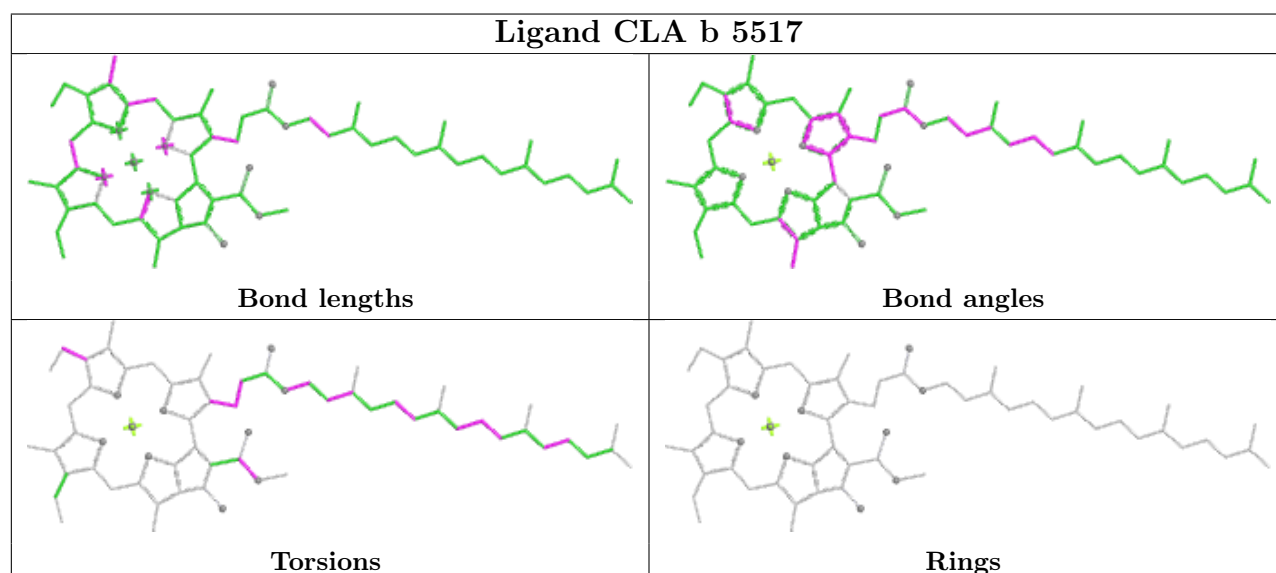
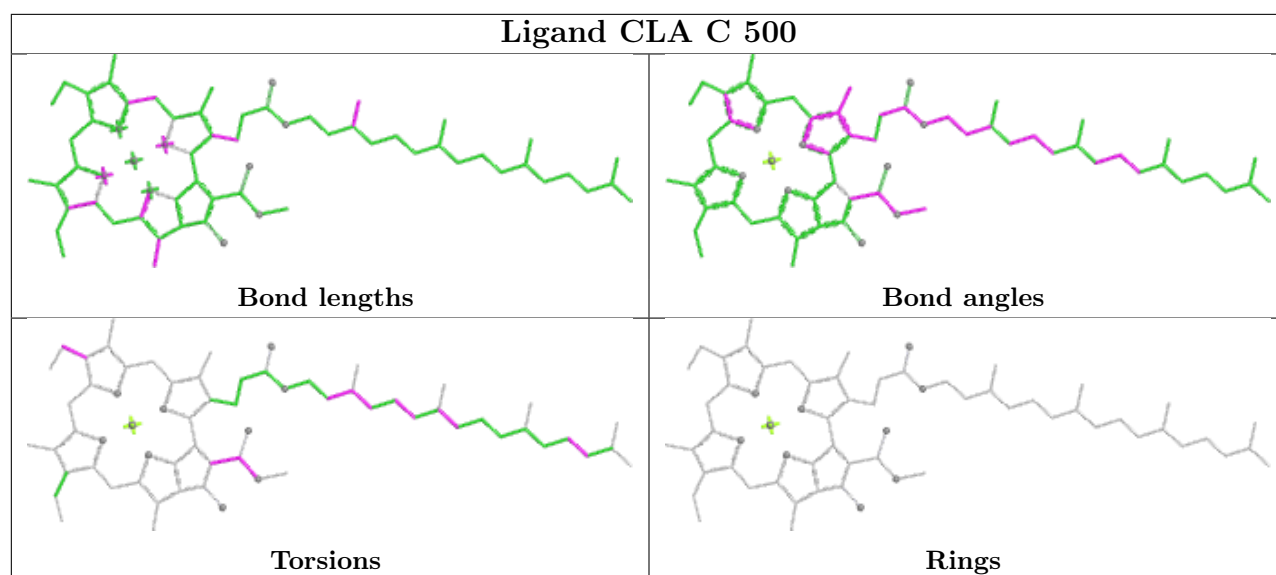
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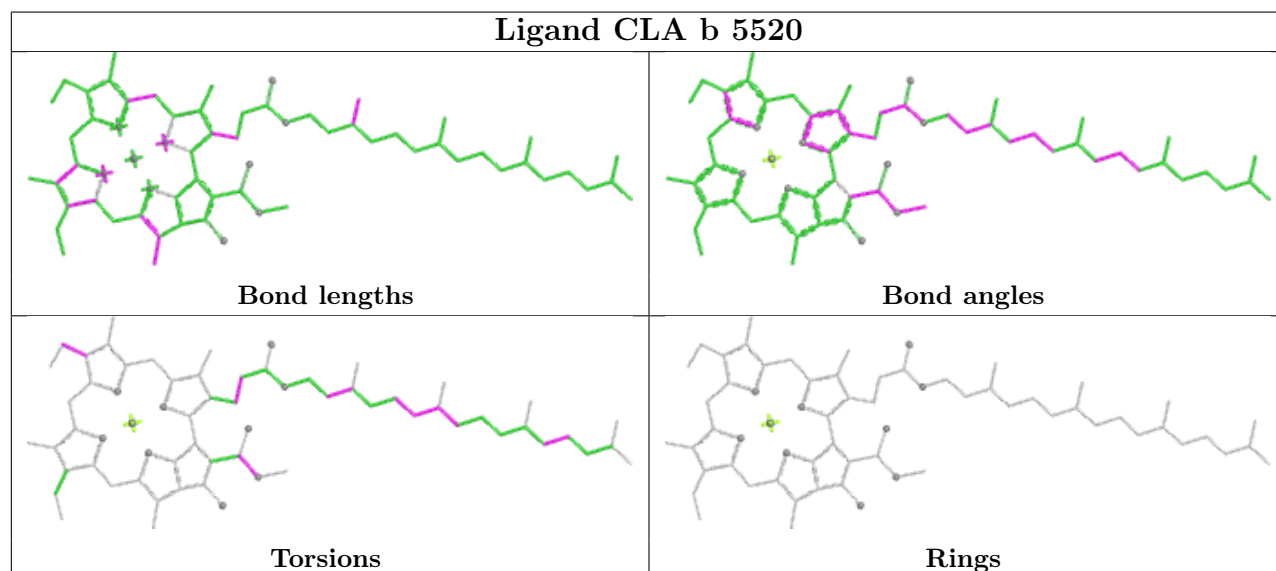
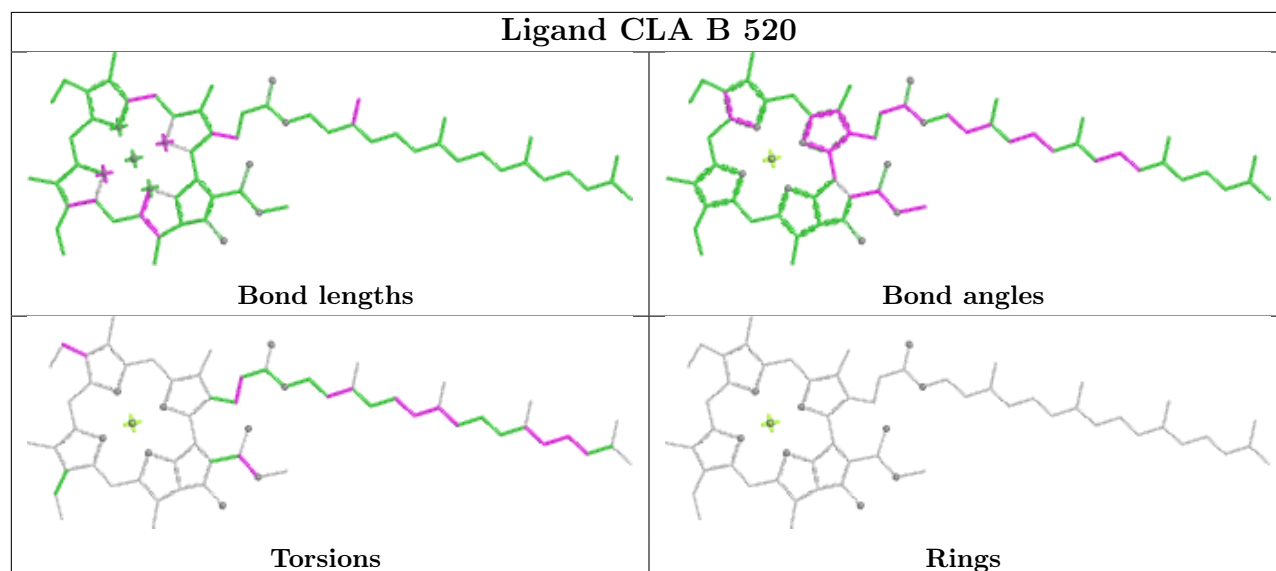
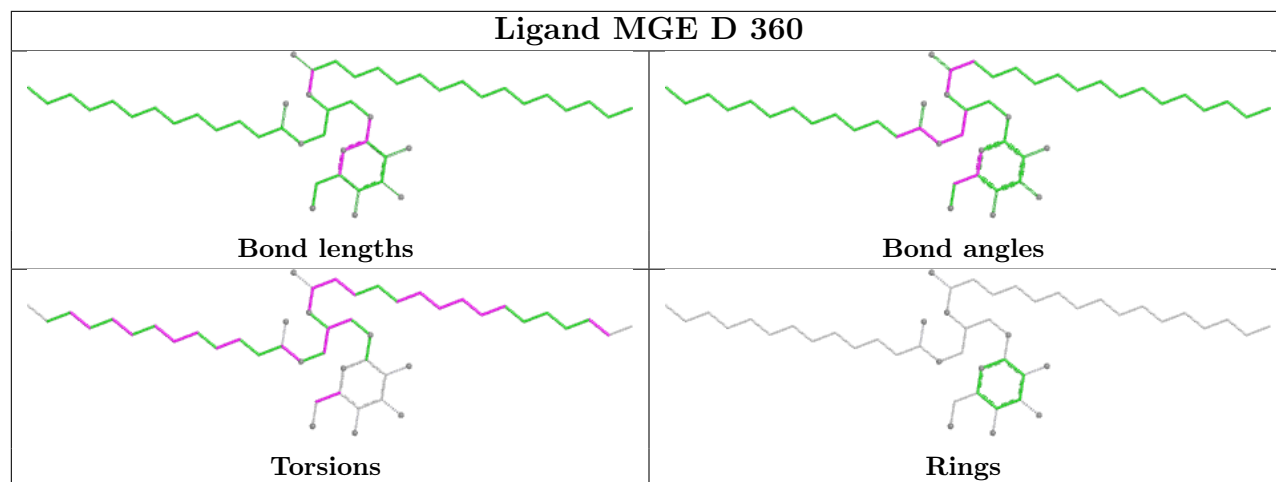


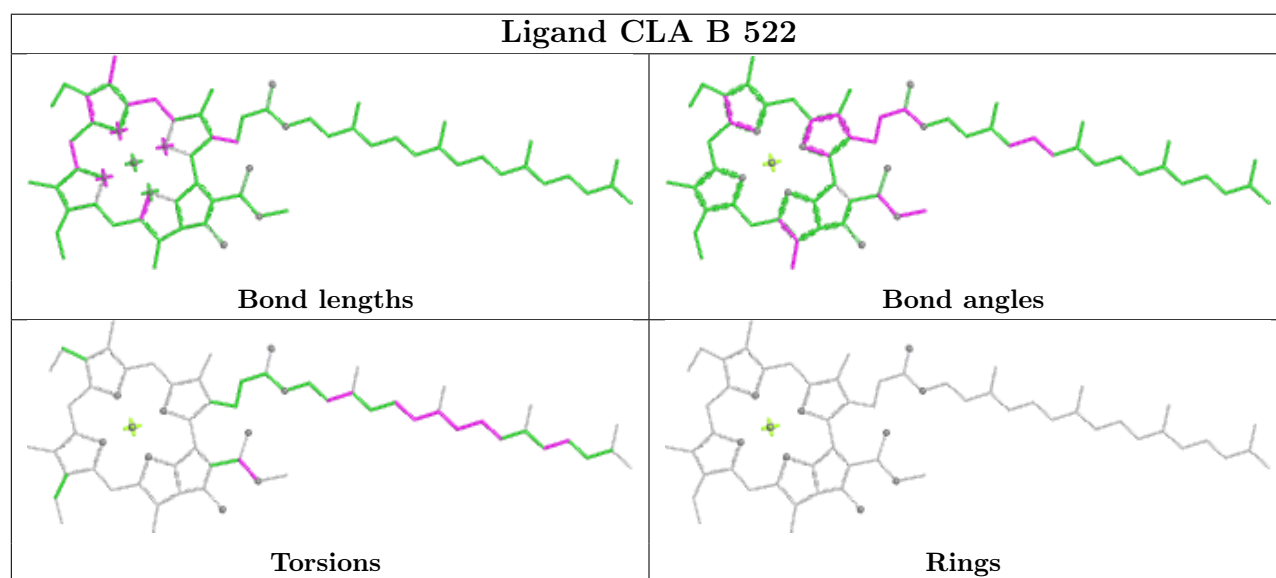
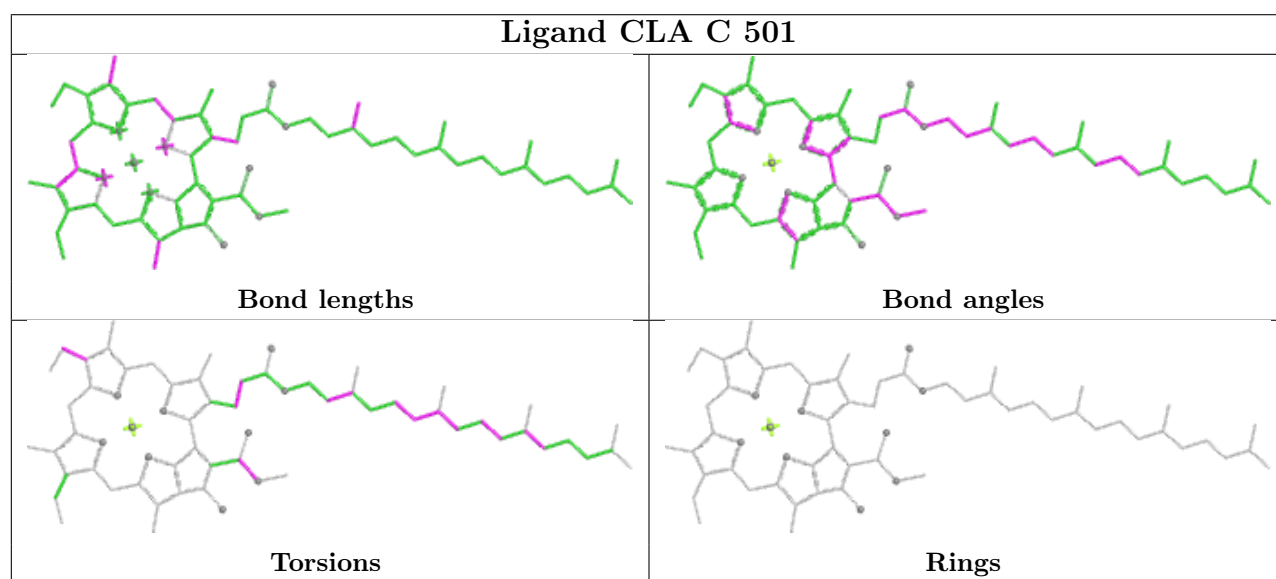
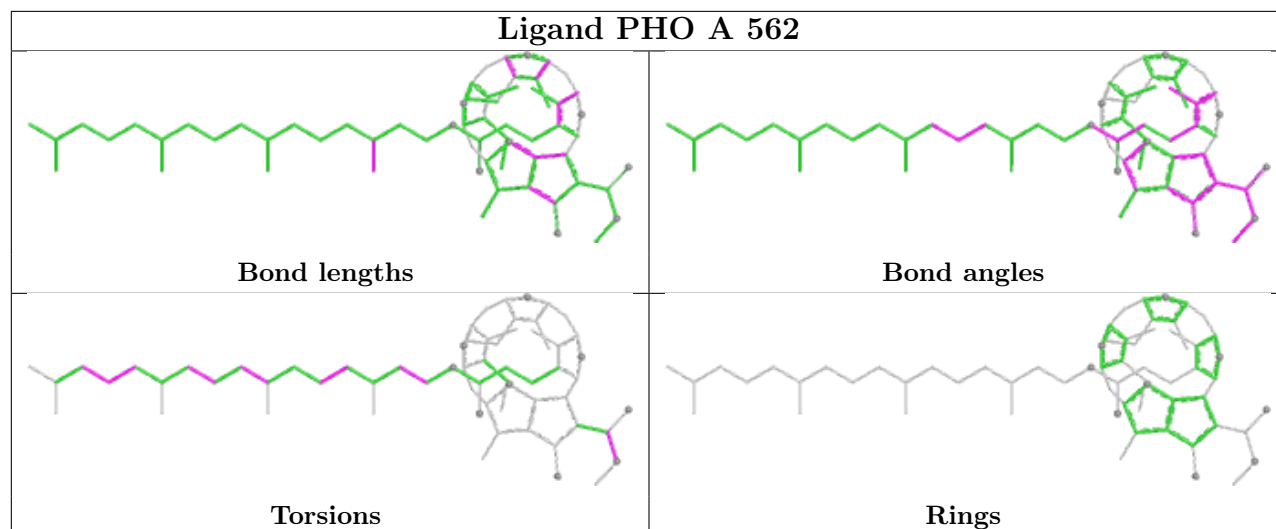
Ligand CLA b 5512

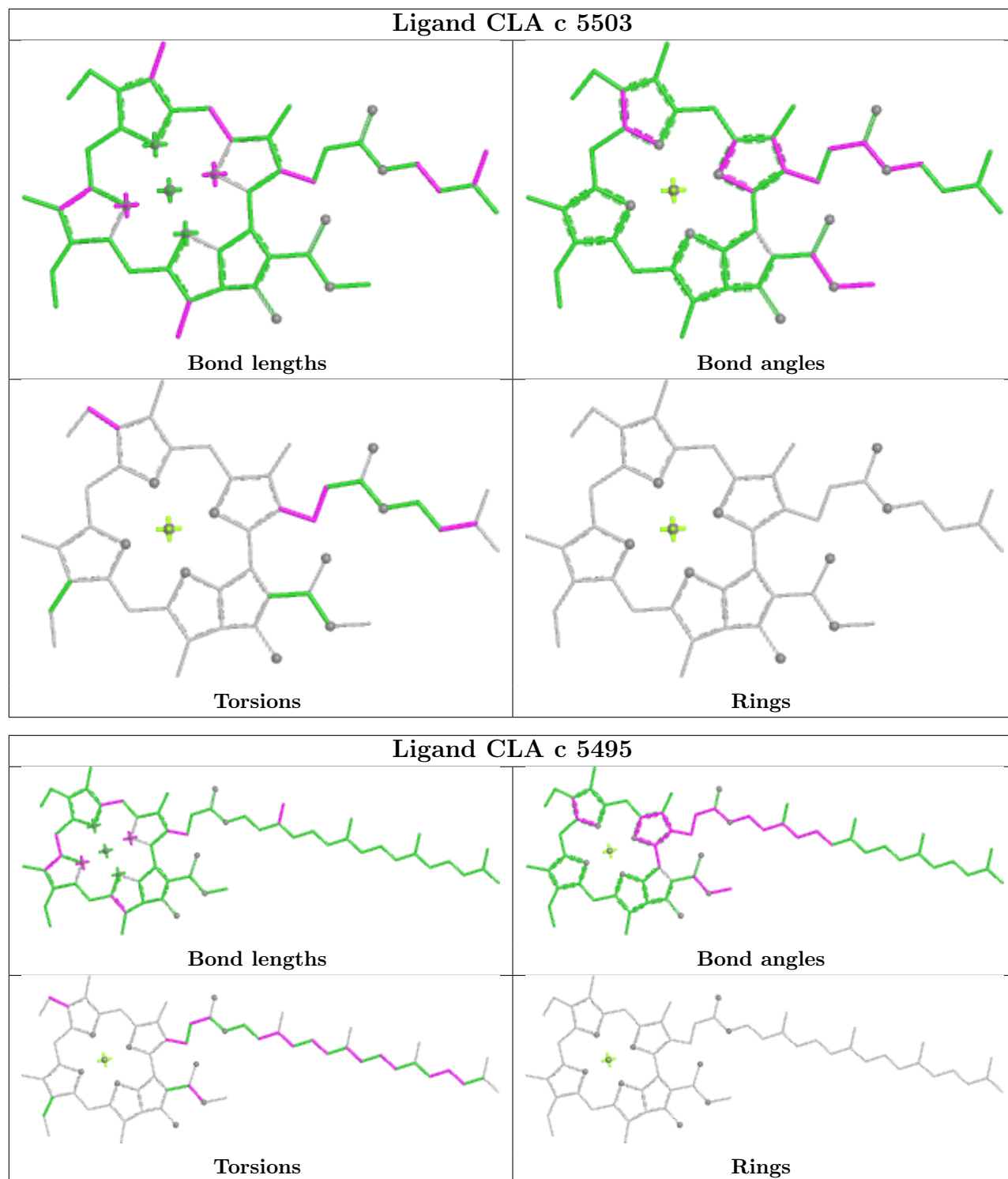




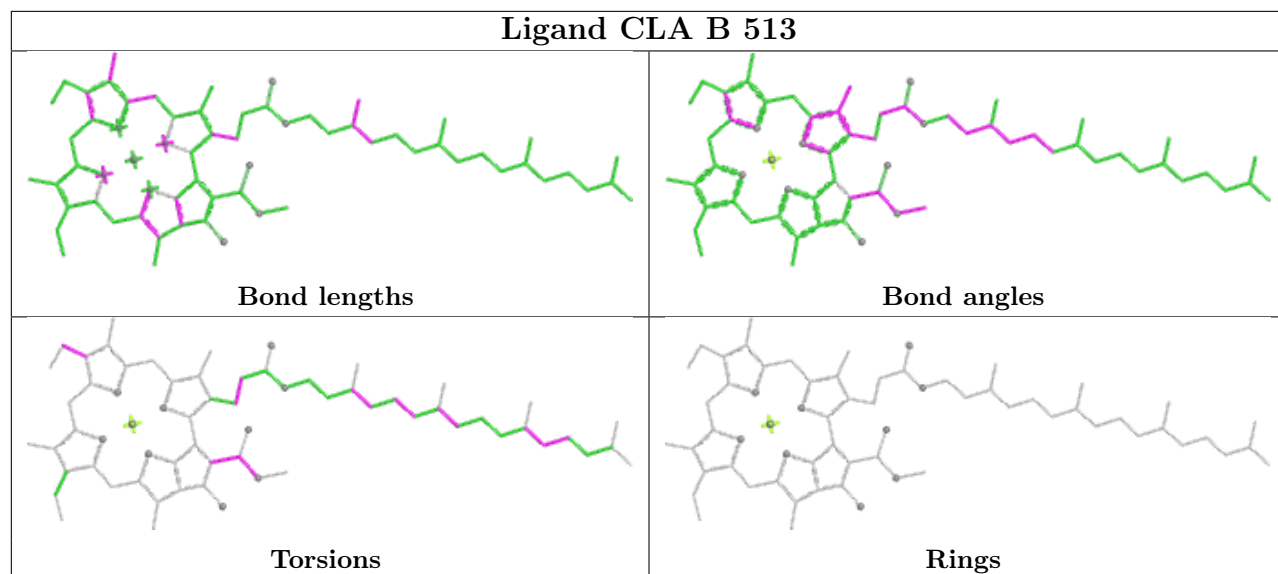




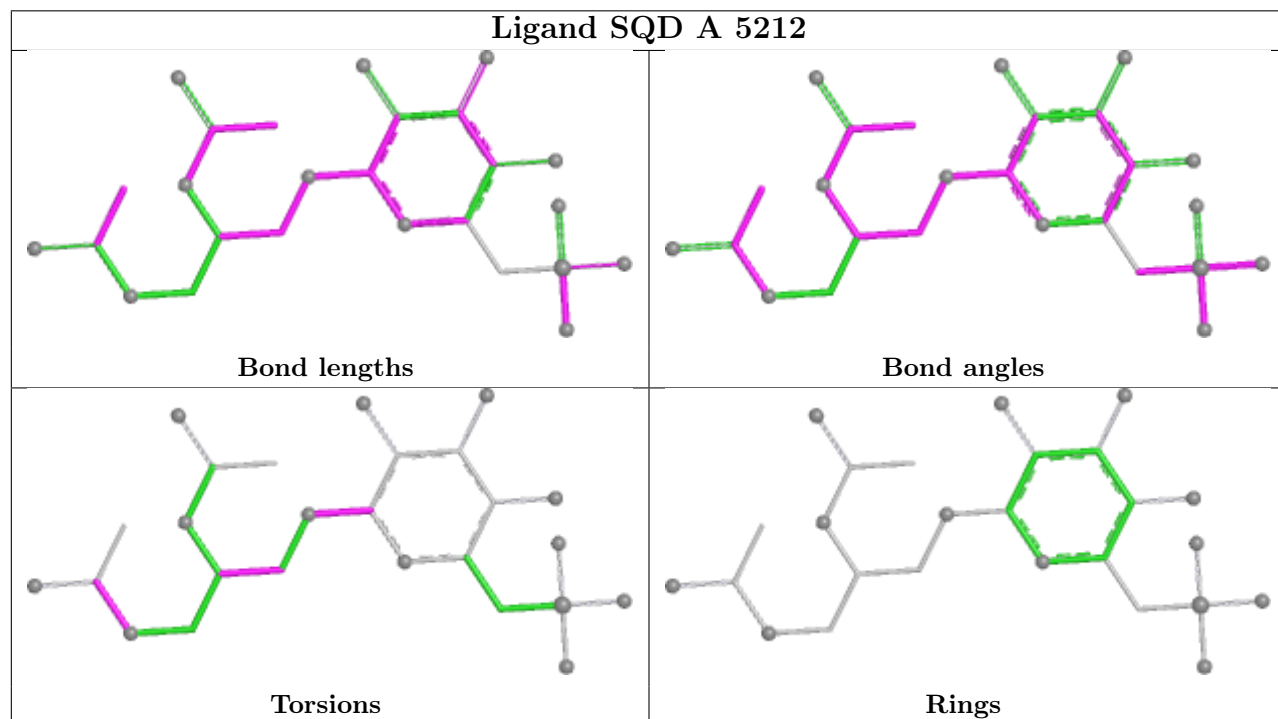


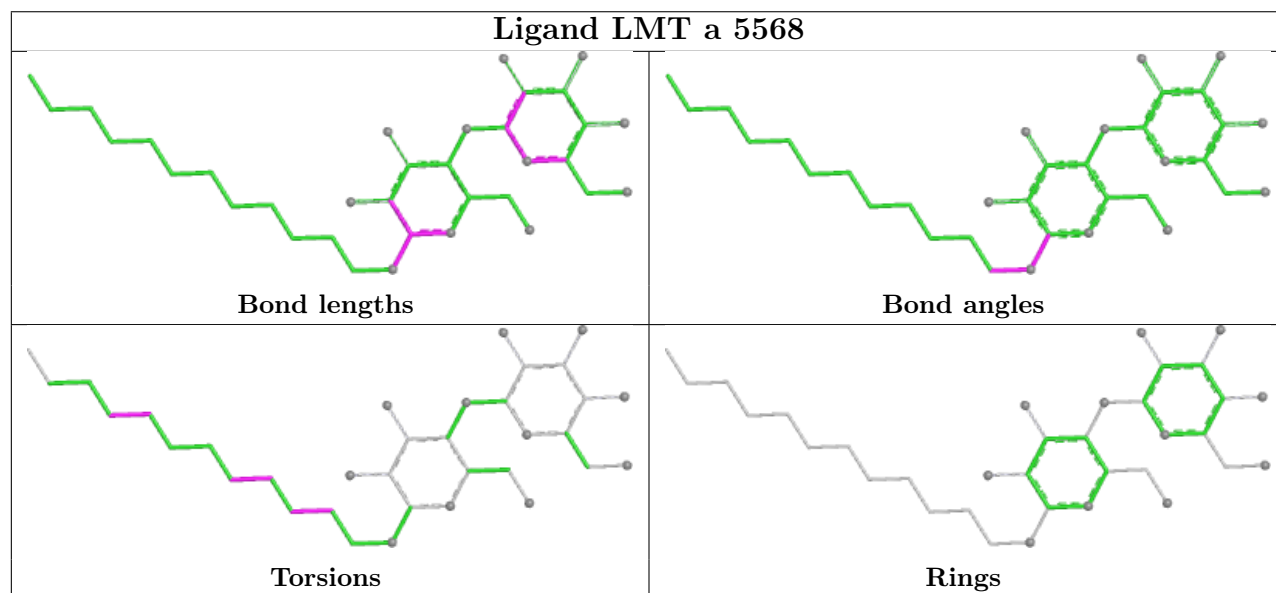
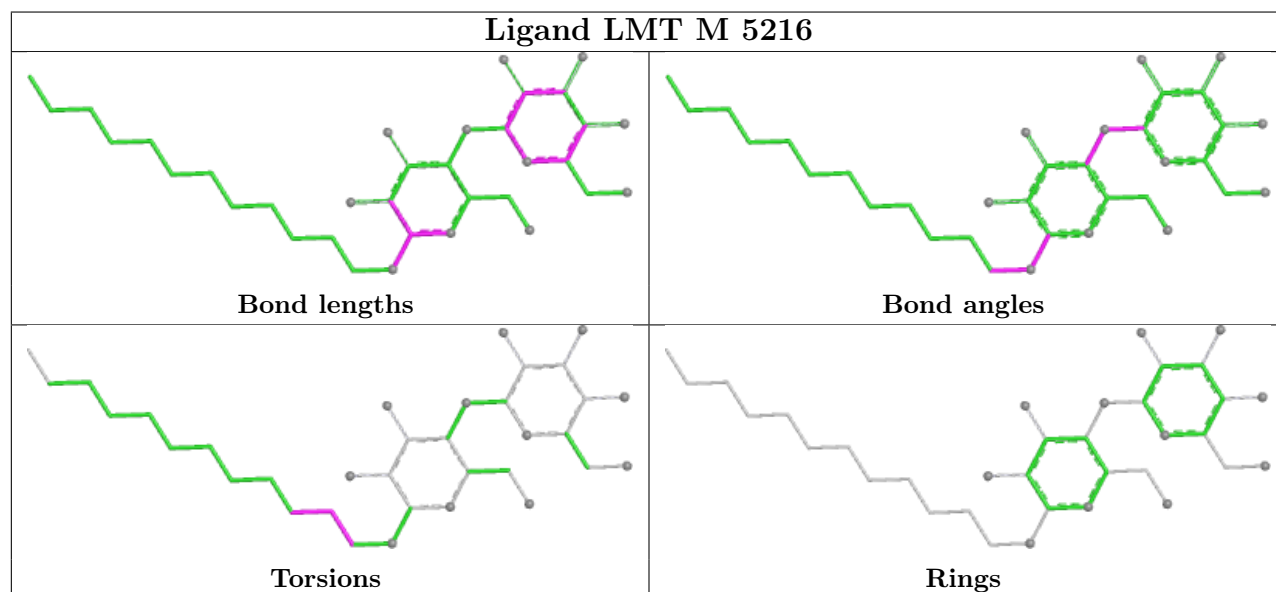
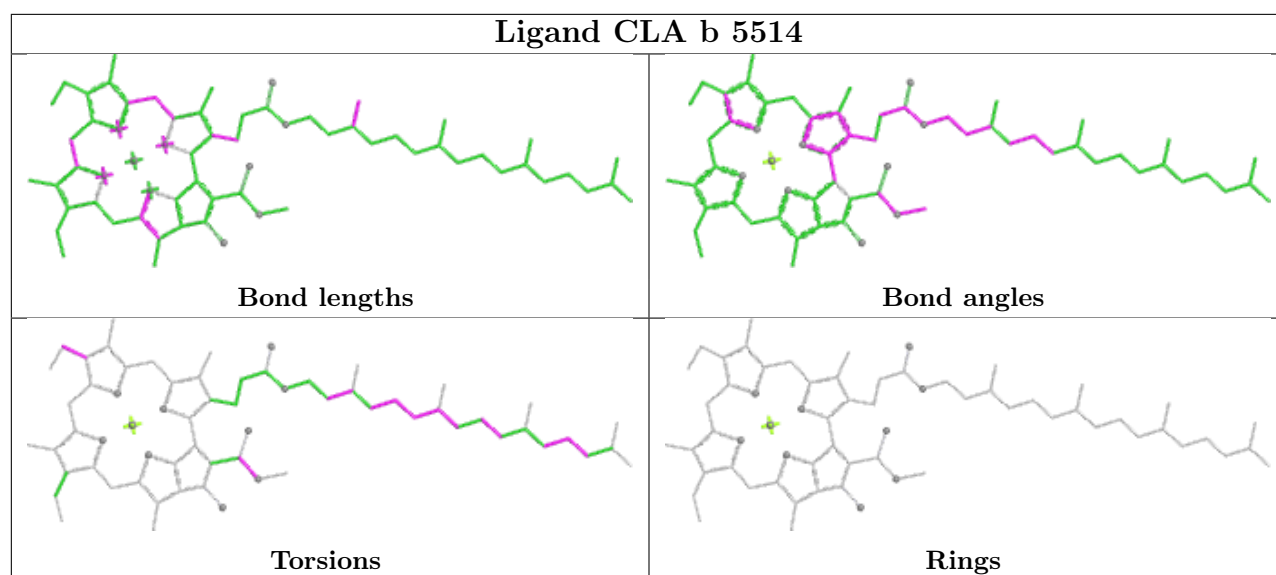


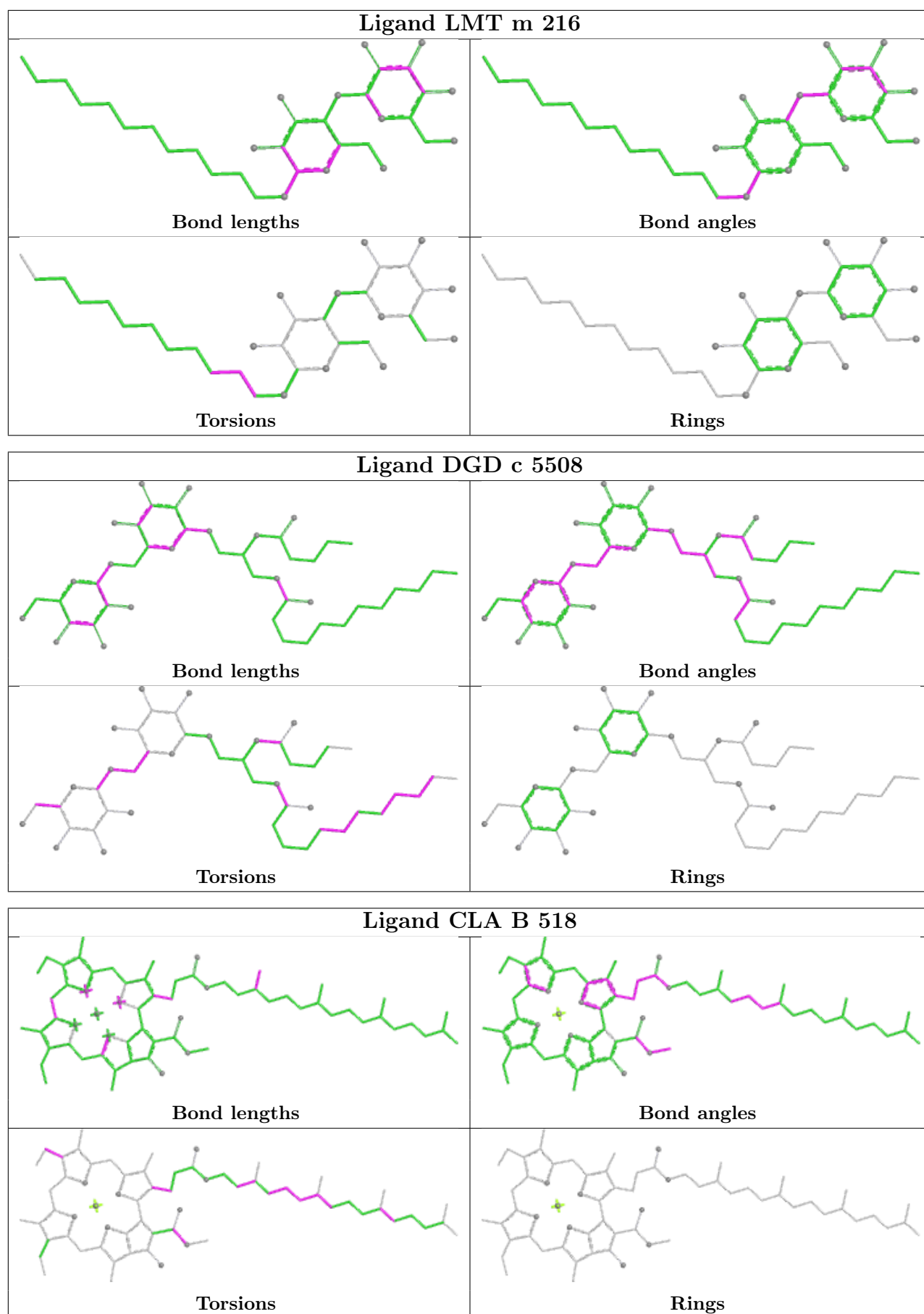
Ligand CLA B 513

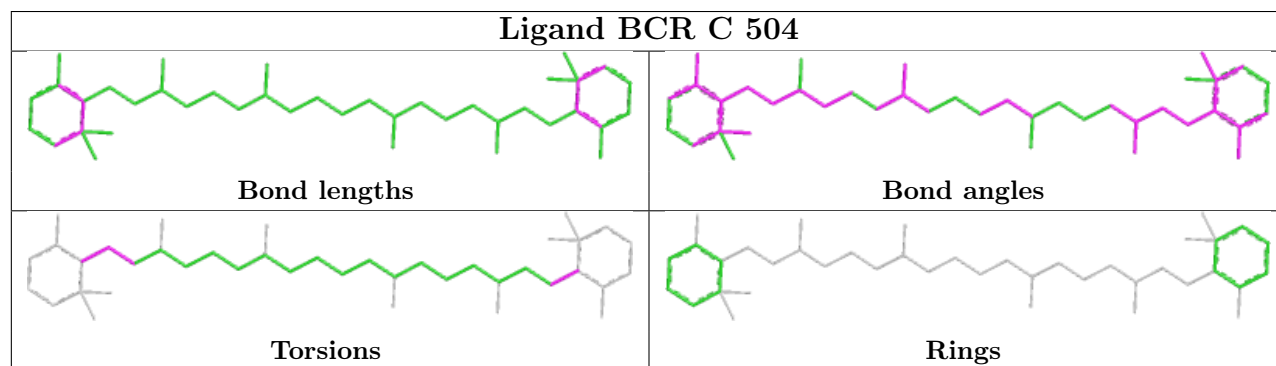
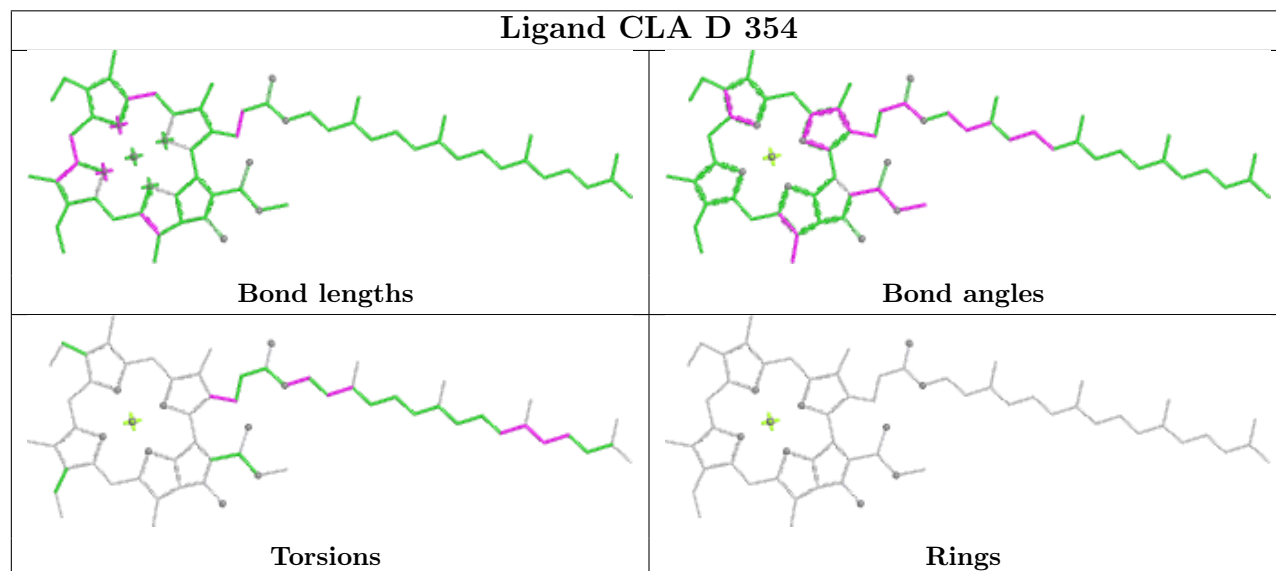
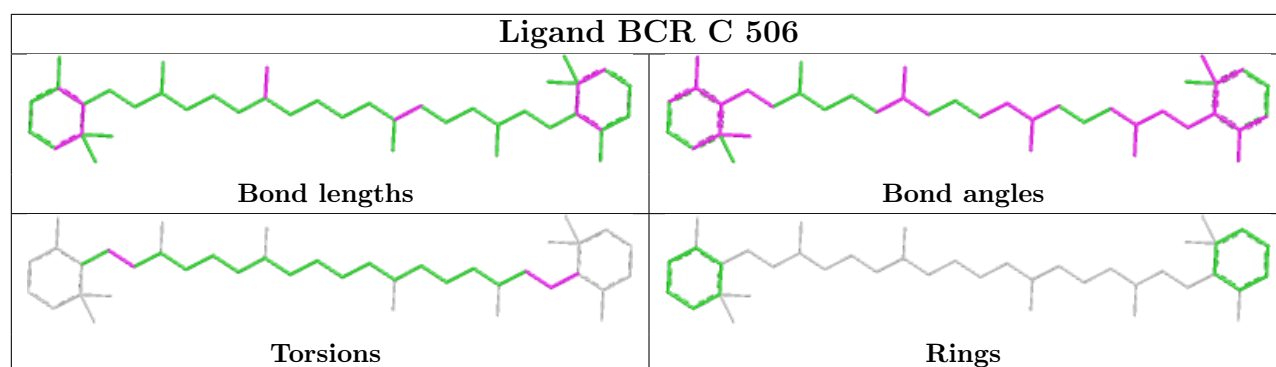


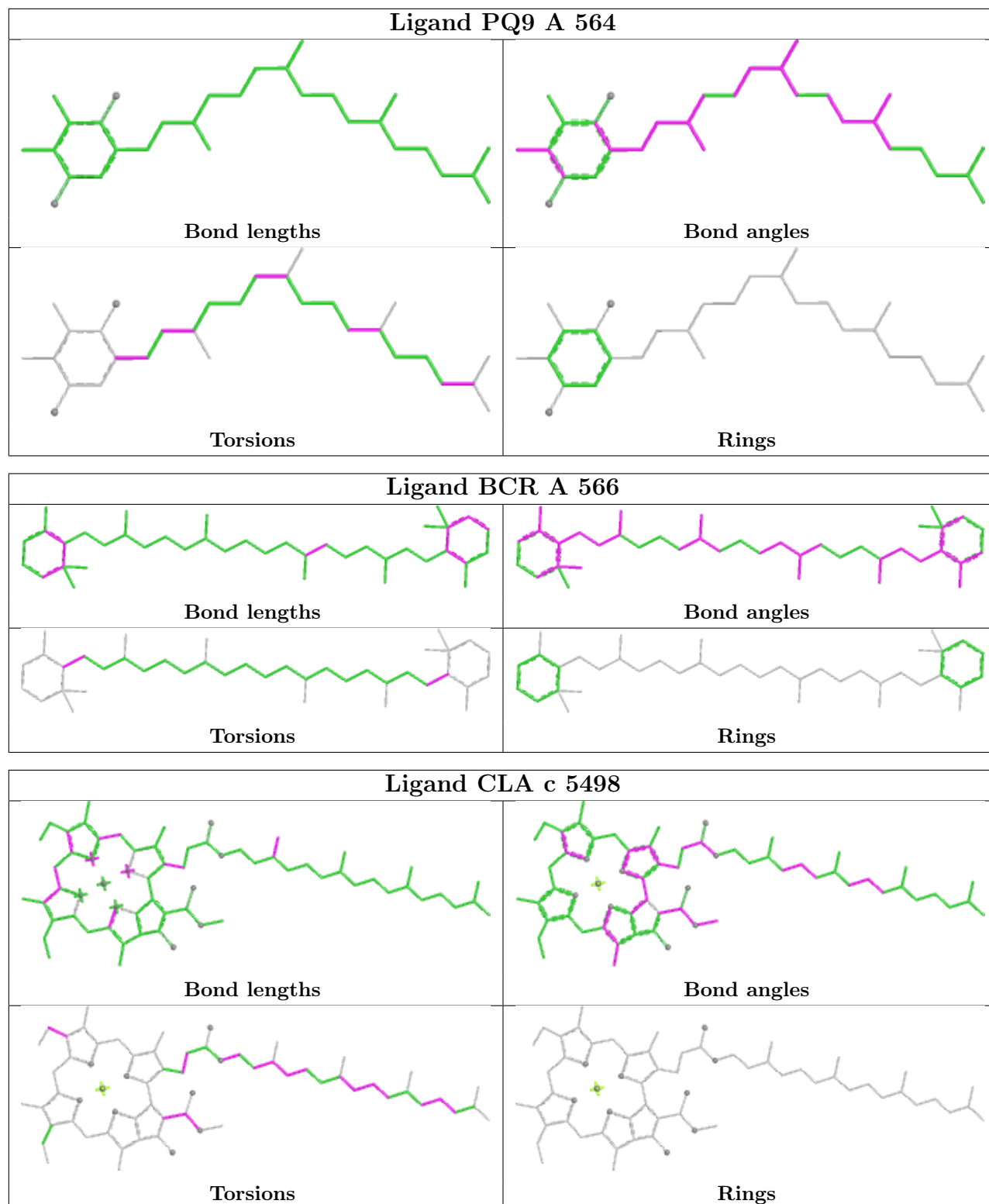
Ligand SQD A 5212



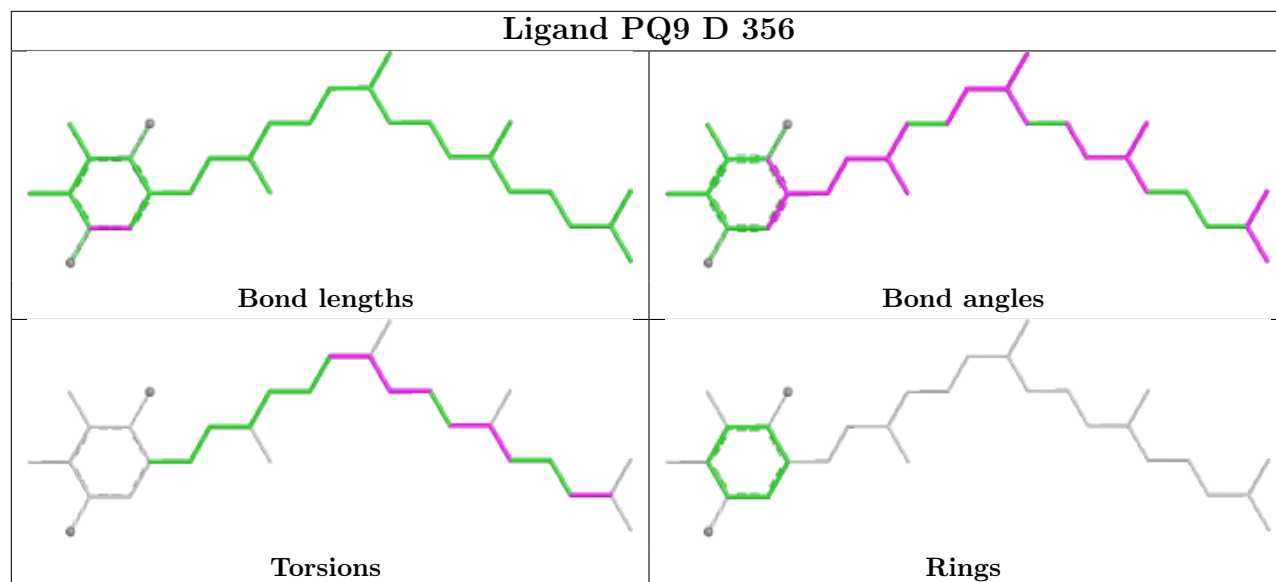




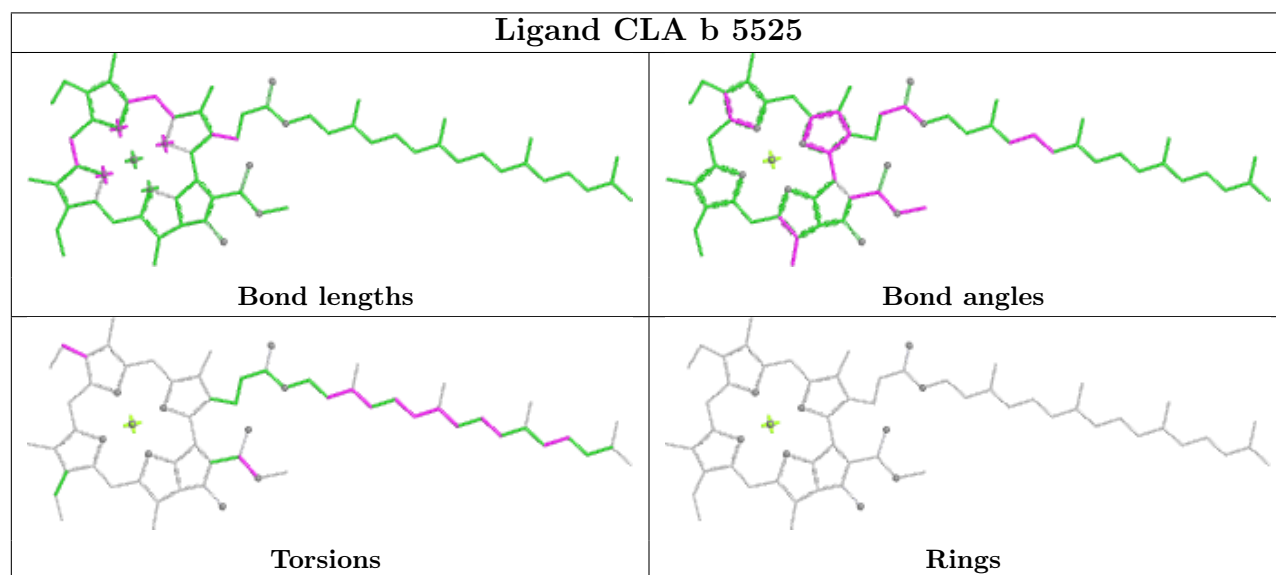




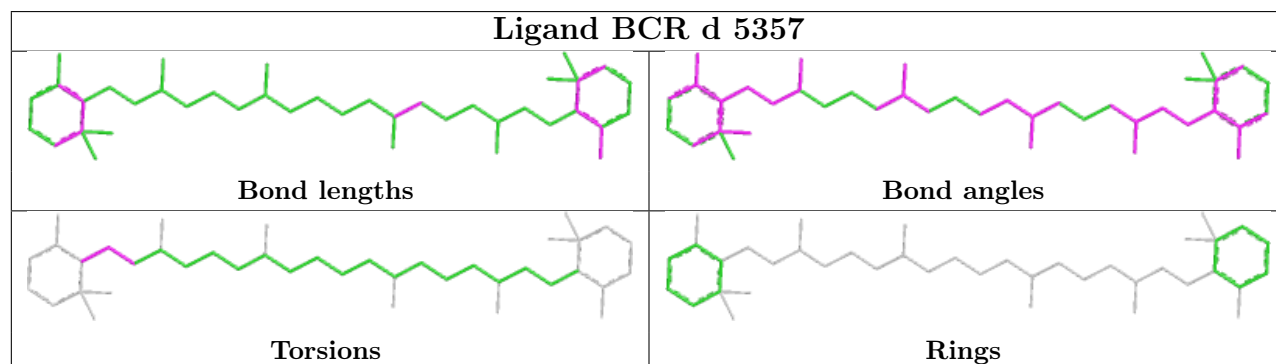
Ligand PQ9 D 356

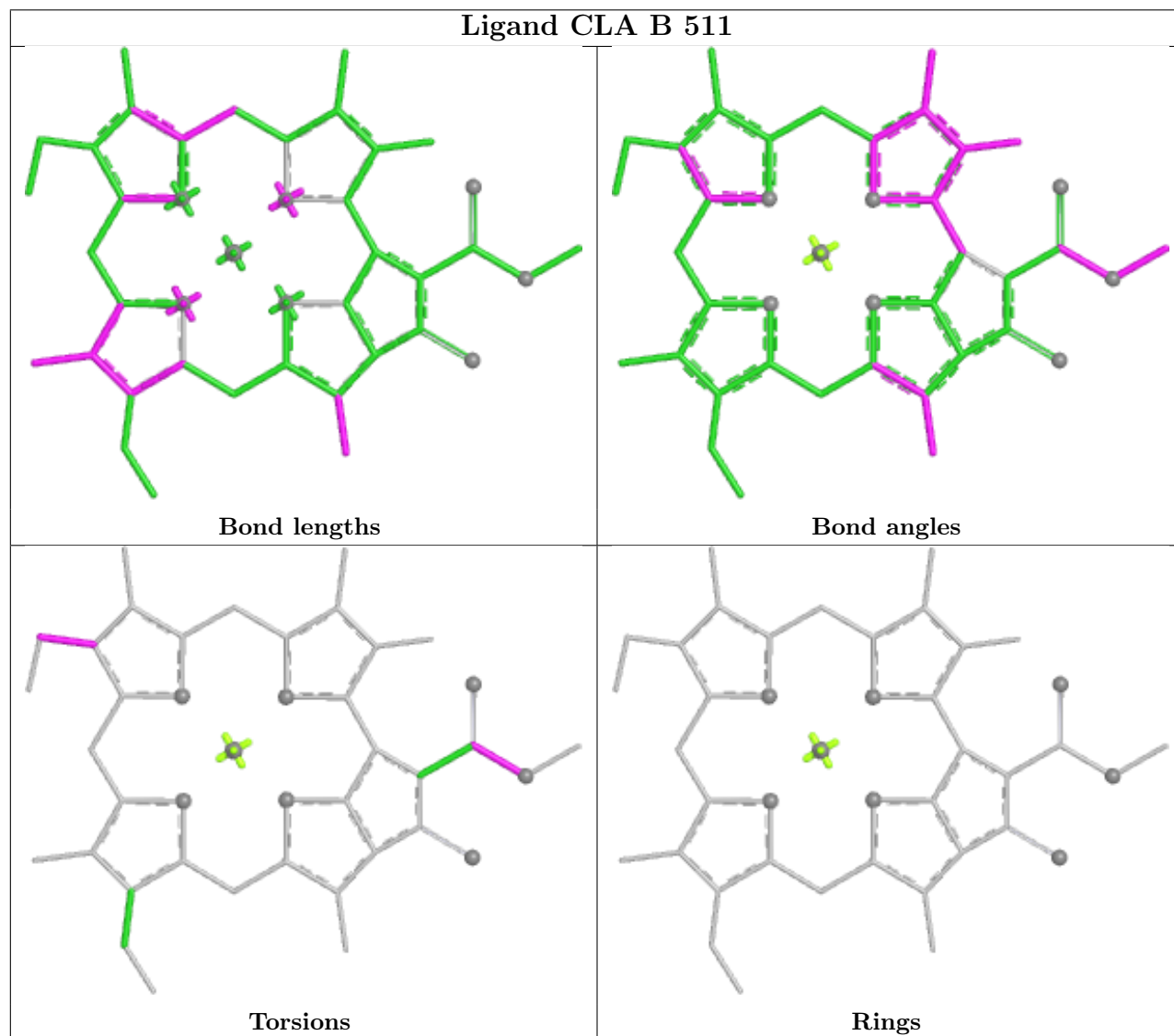
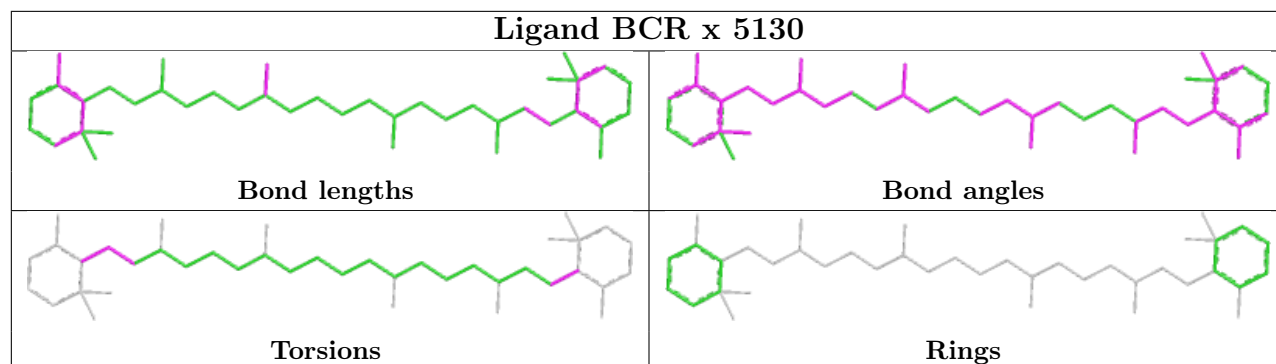


Ligand CLA b 5525

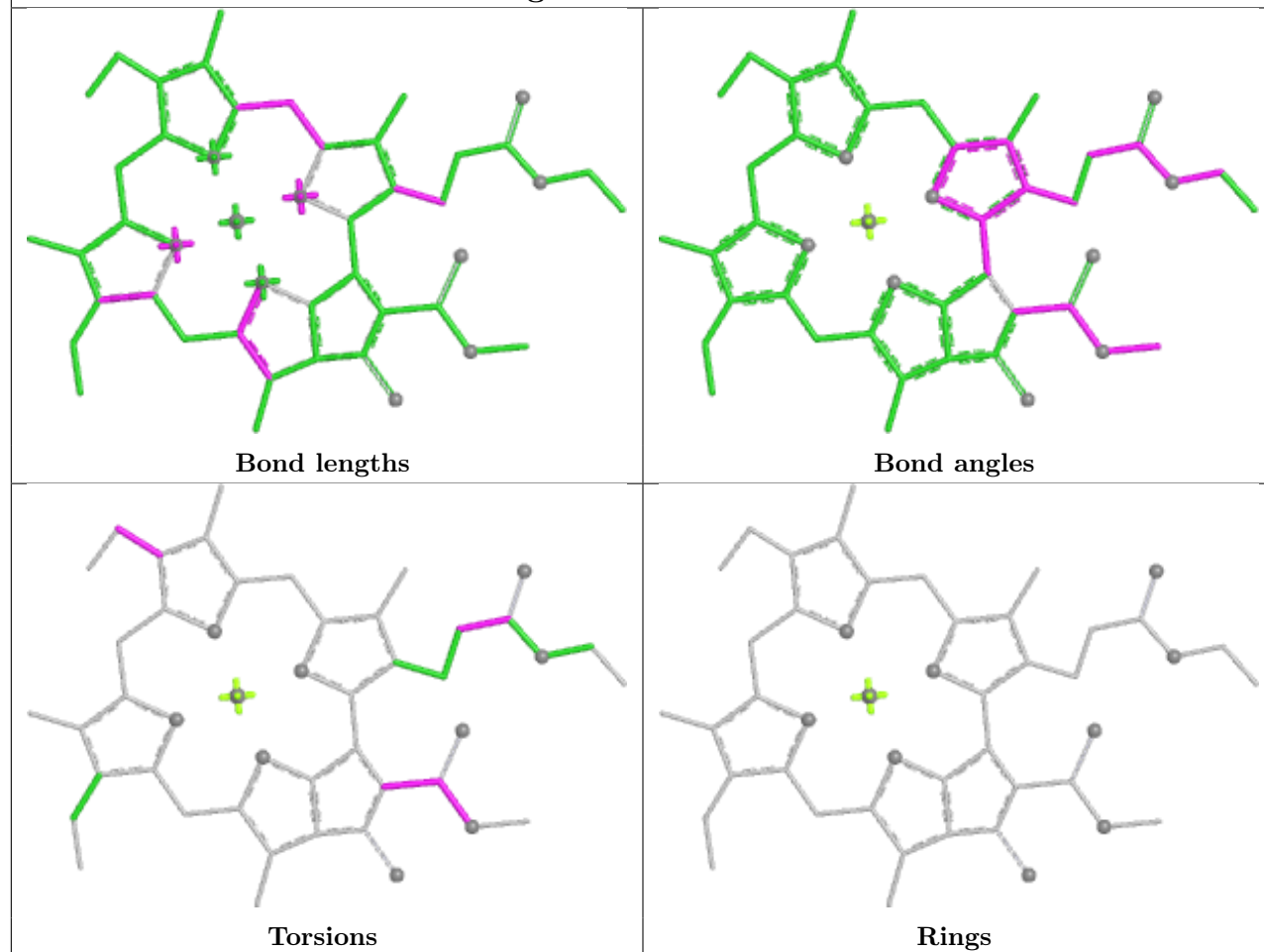


Ligand BCR d 5357

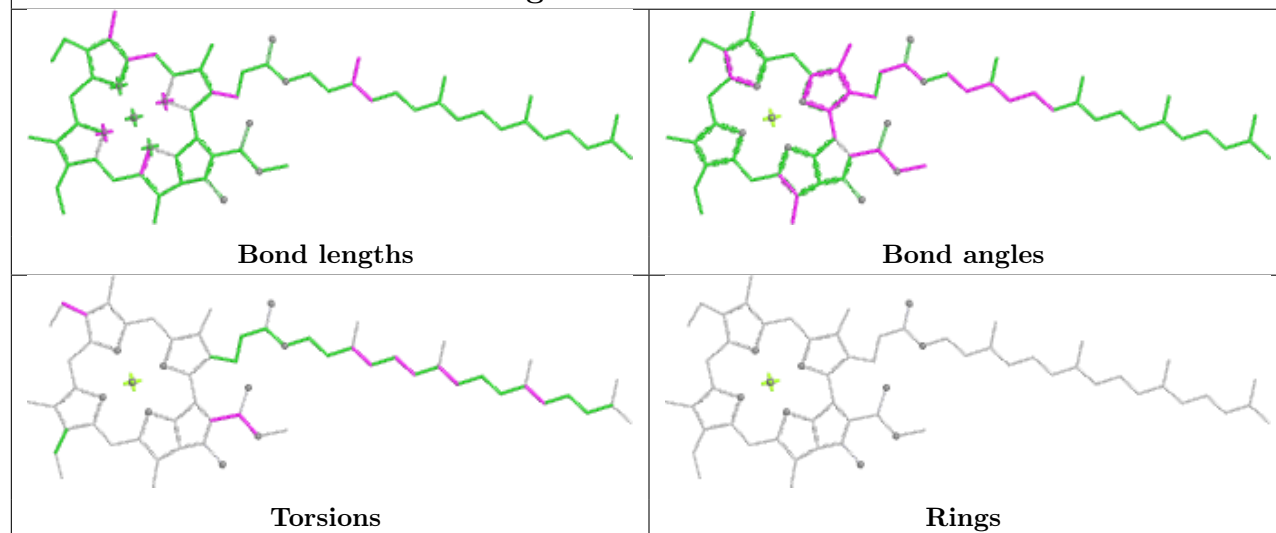


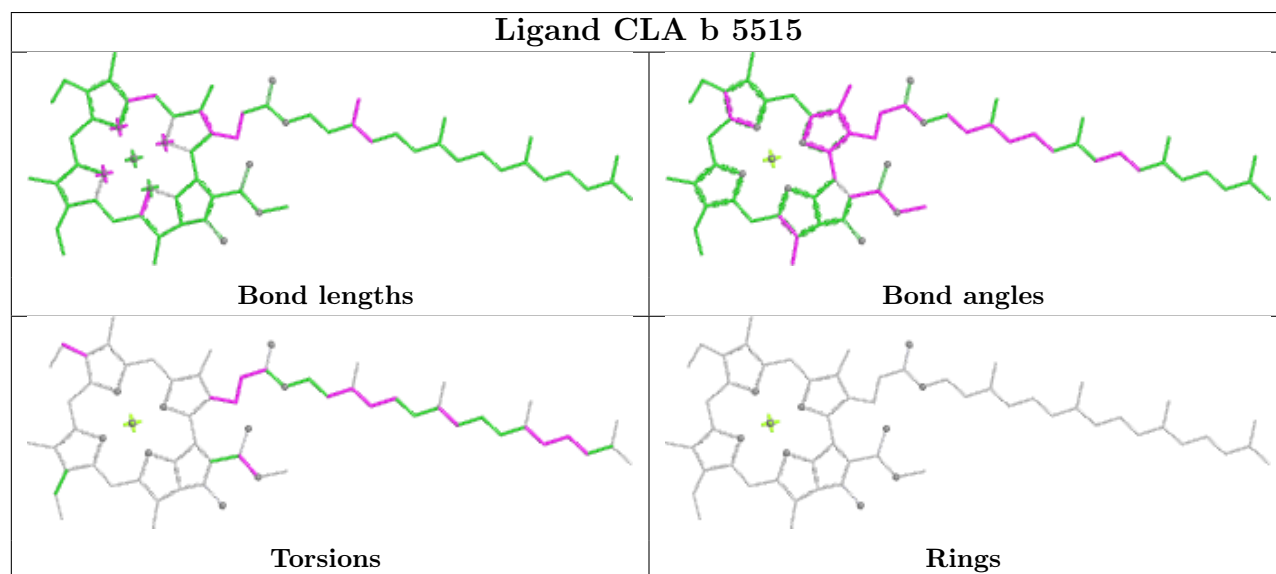
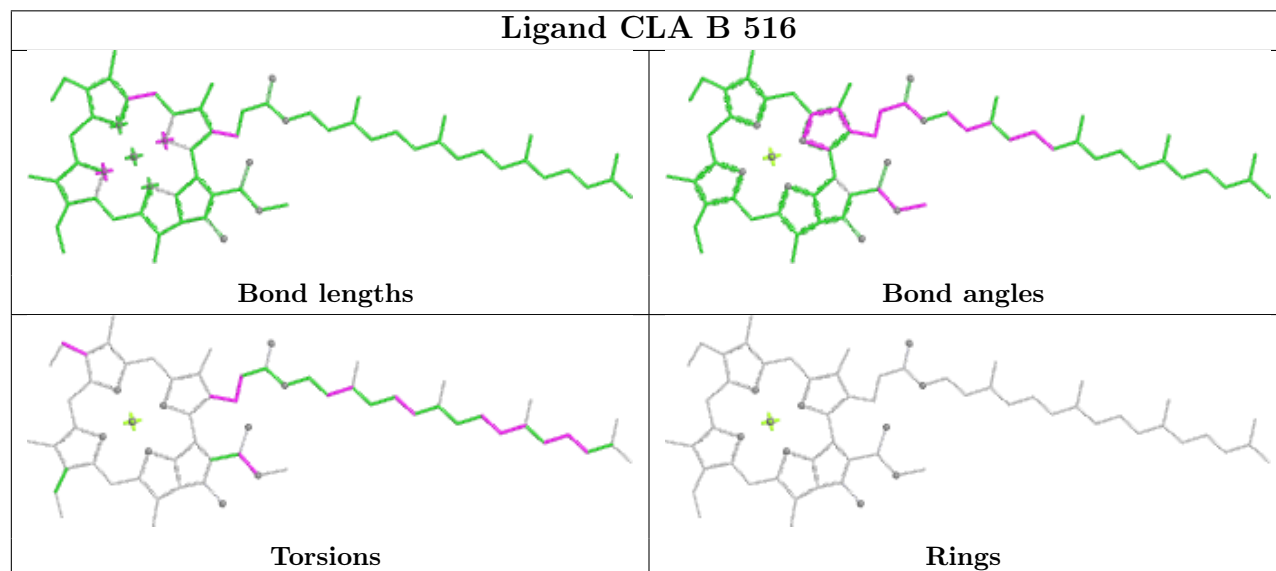
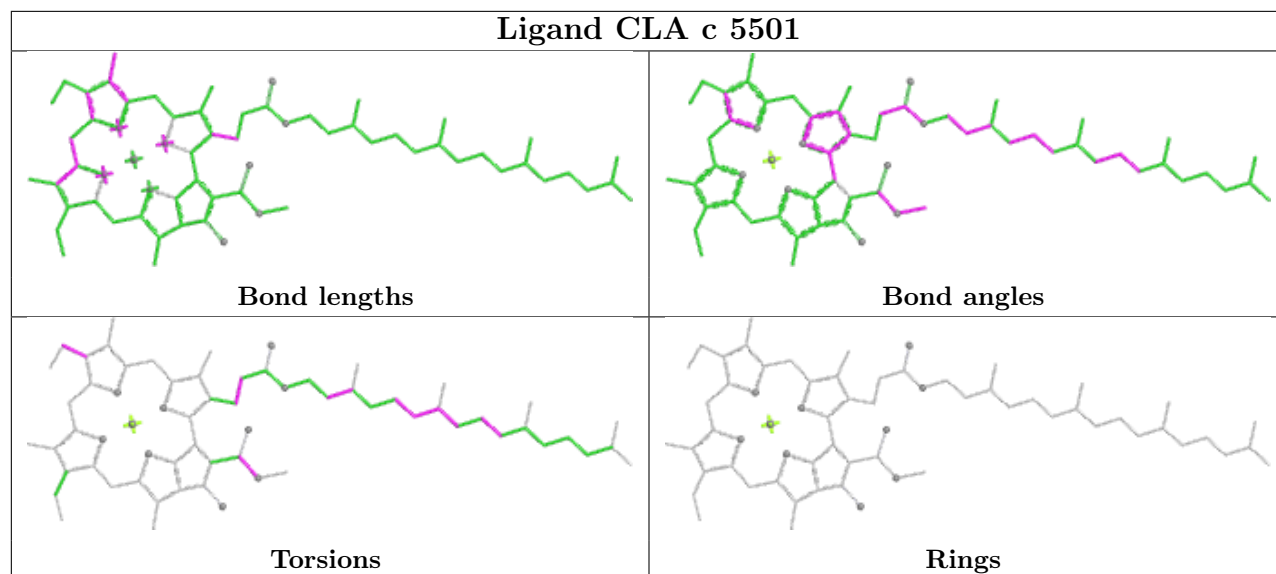


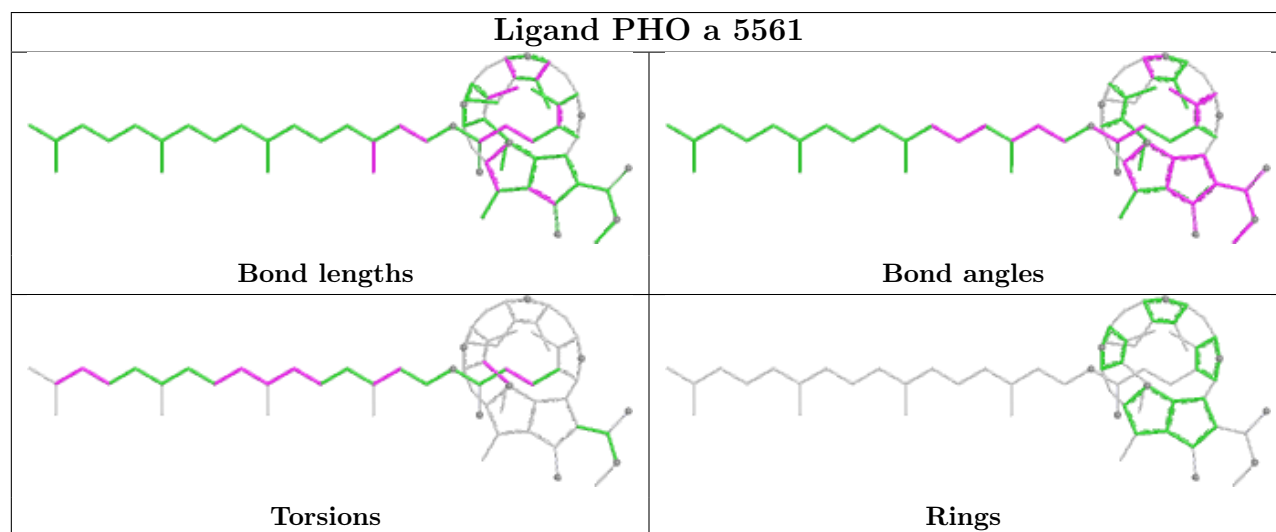
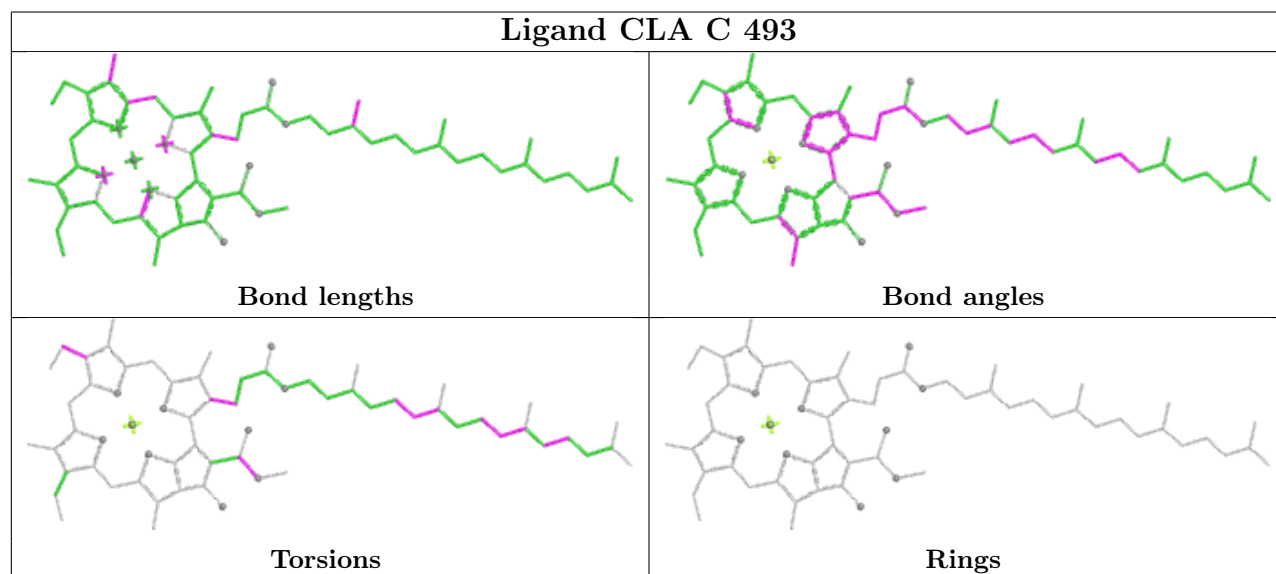
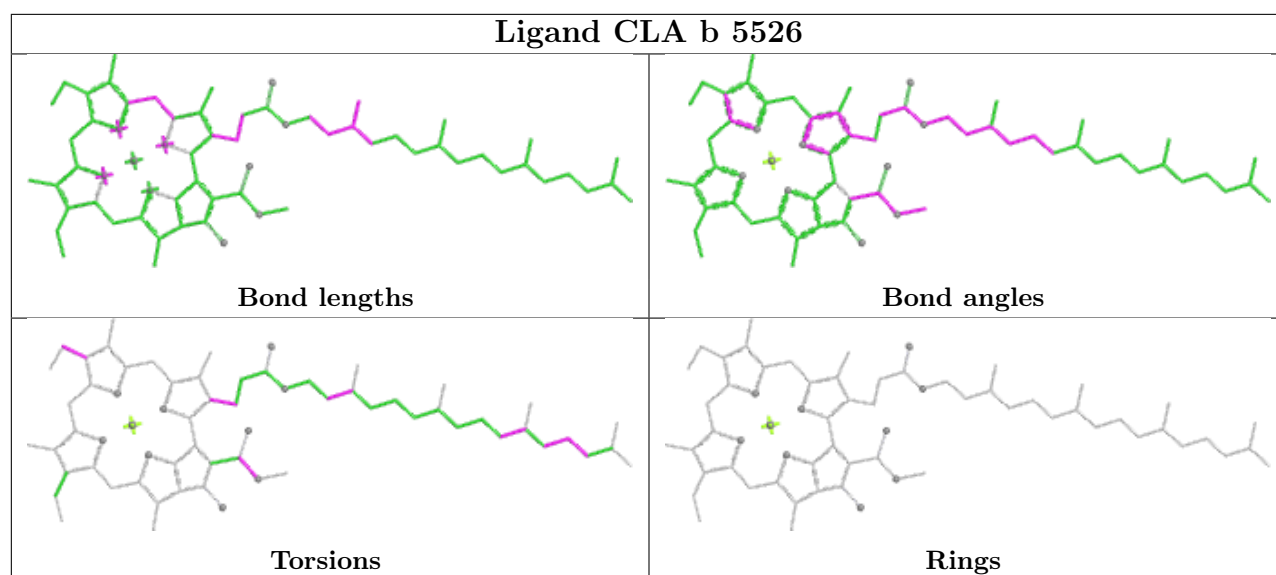
Ligand CLA C 499



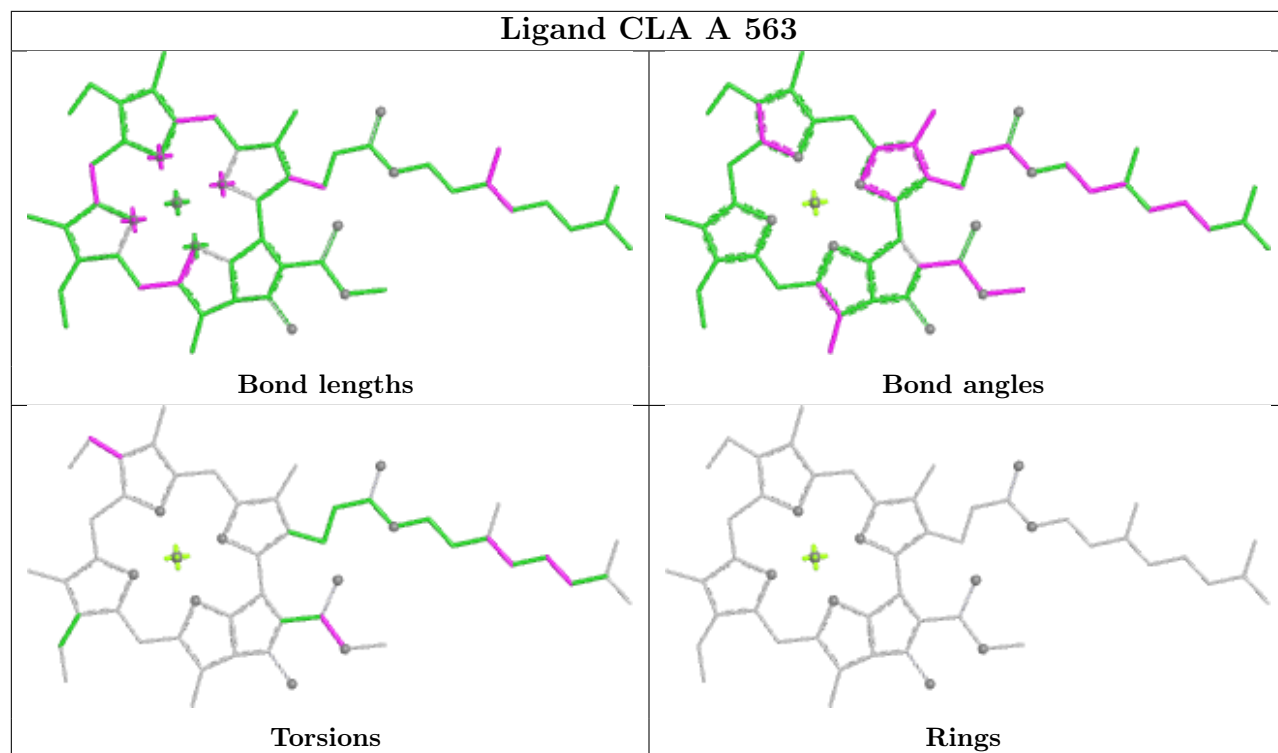
Ligand CLA b 5513



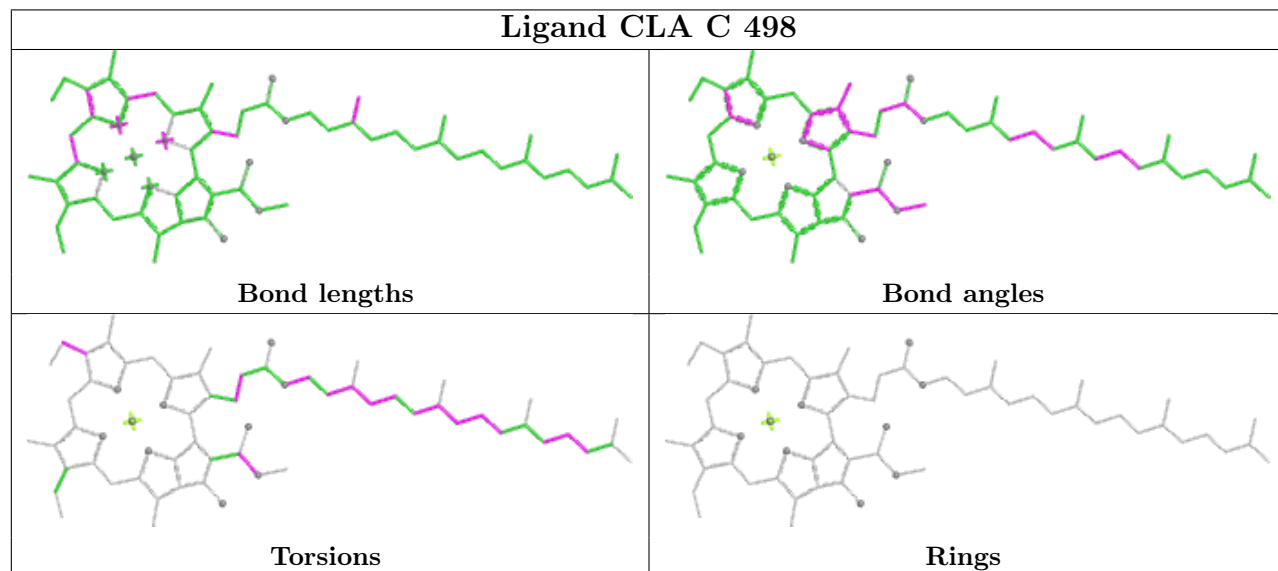




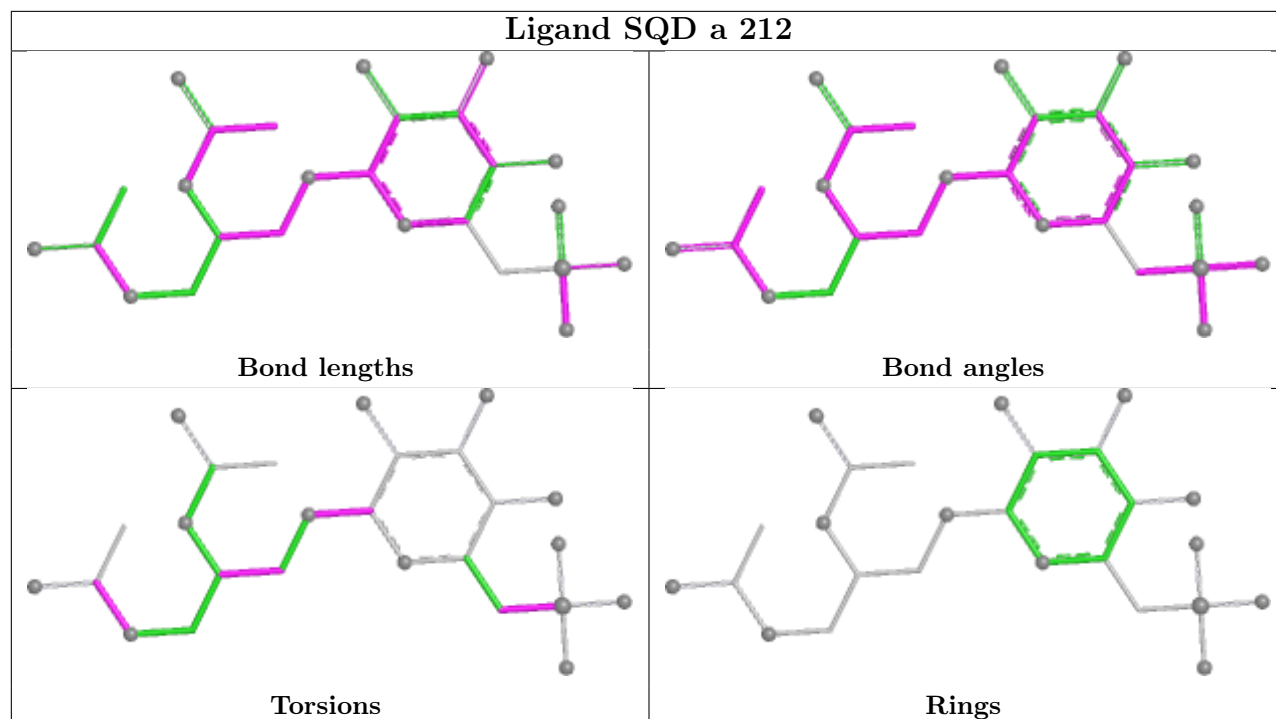
Ligand CLA A 563



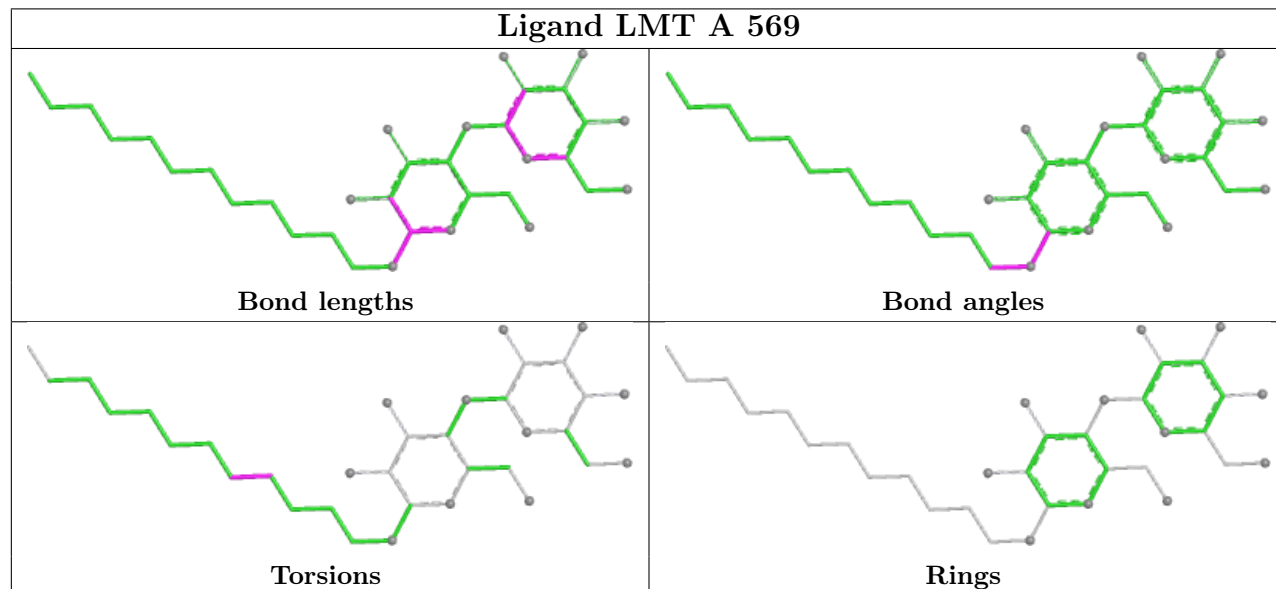
Ligand CLA C 498



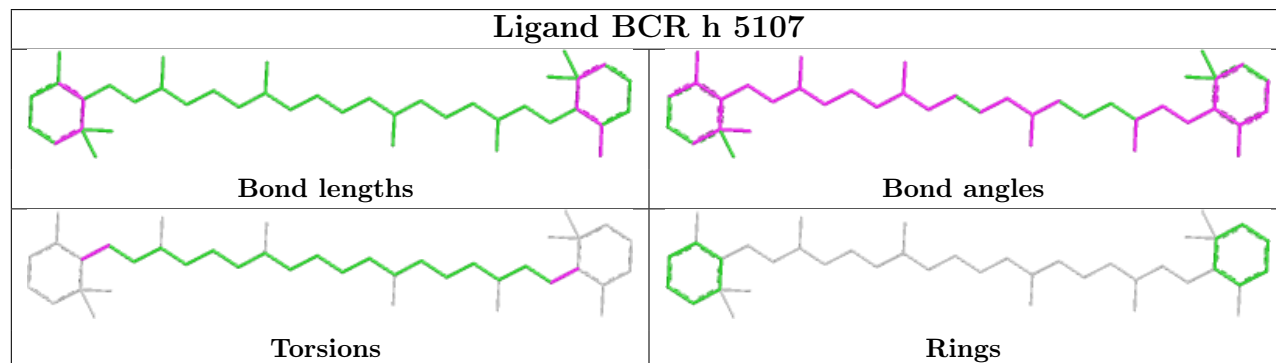
Ligand SQD a 212

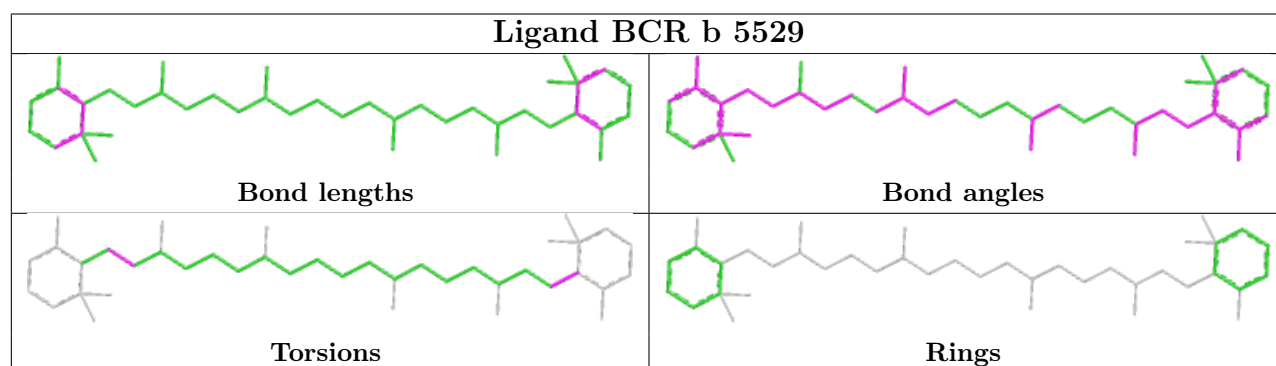
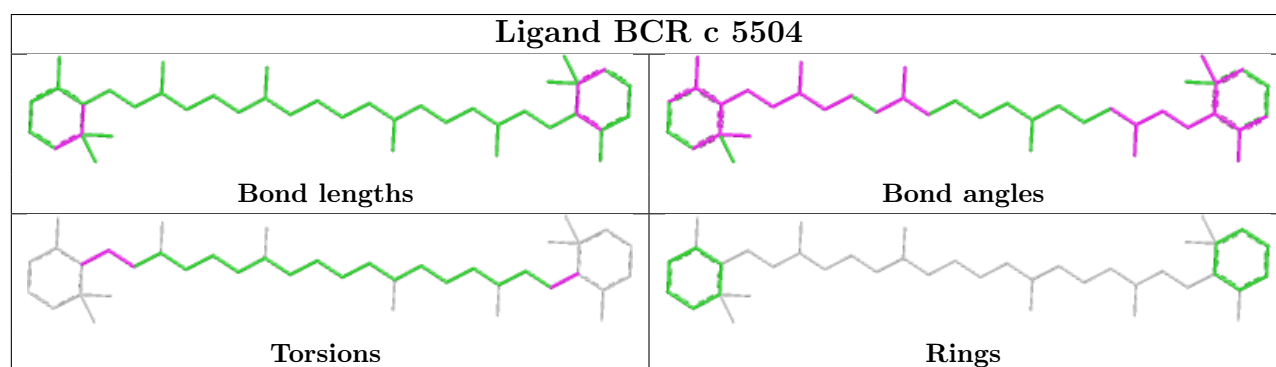
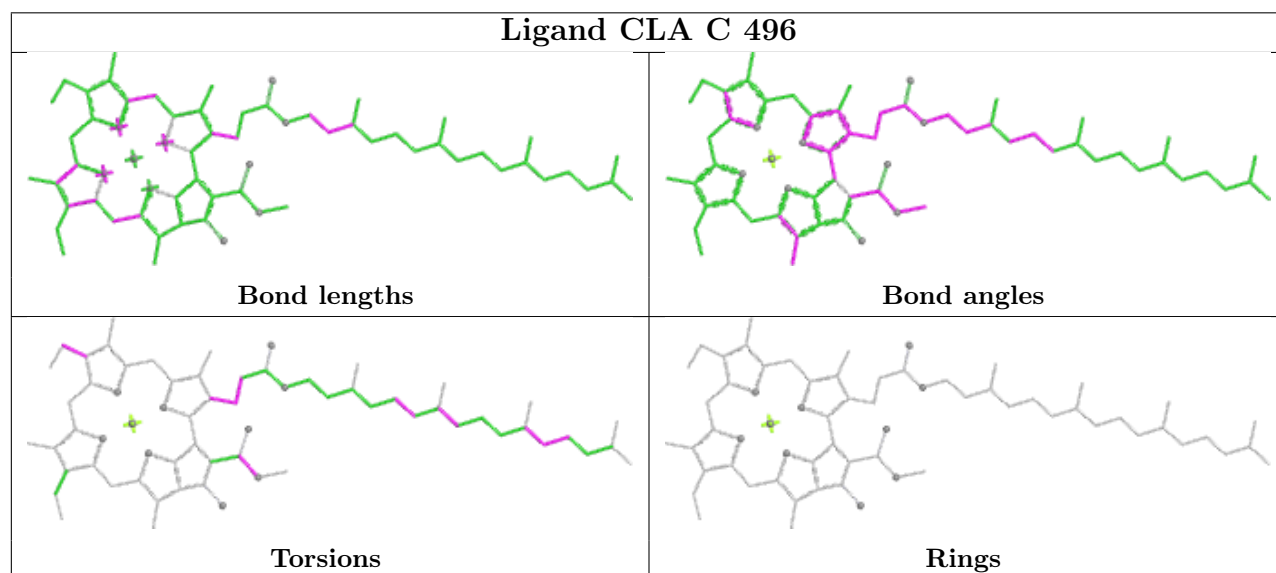
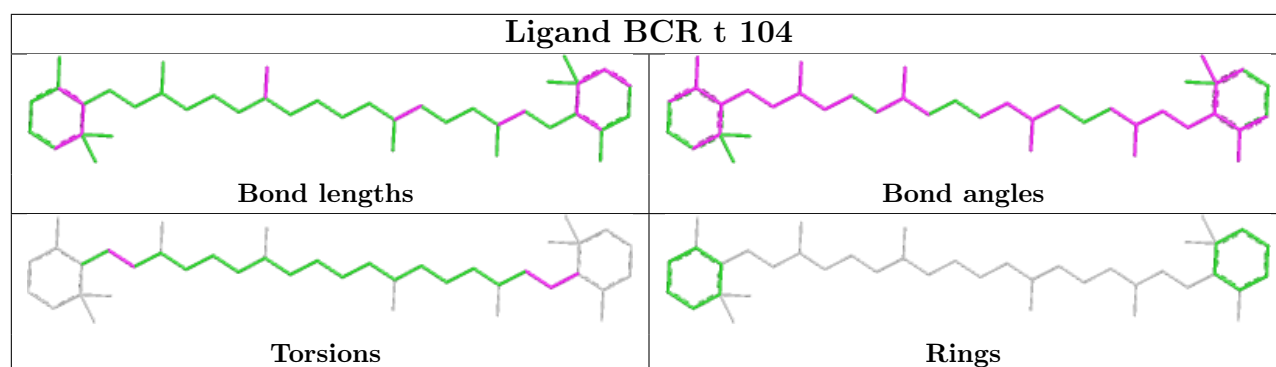


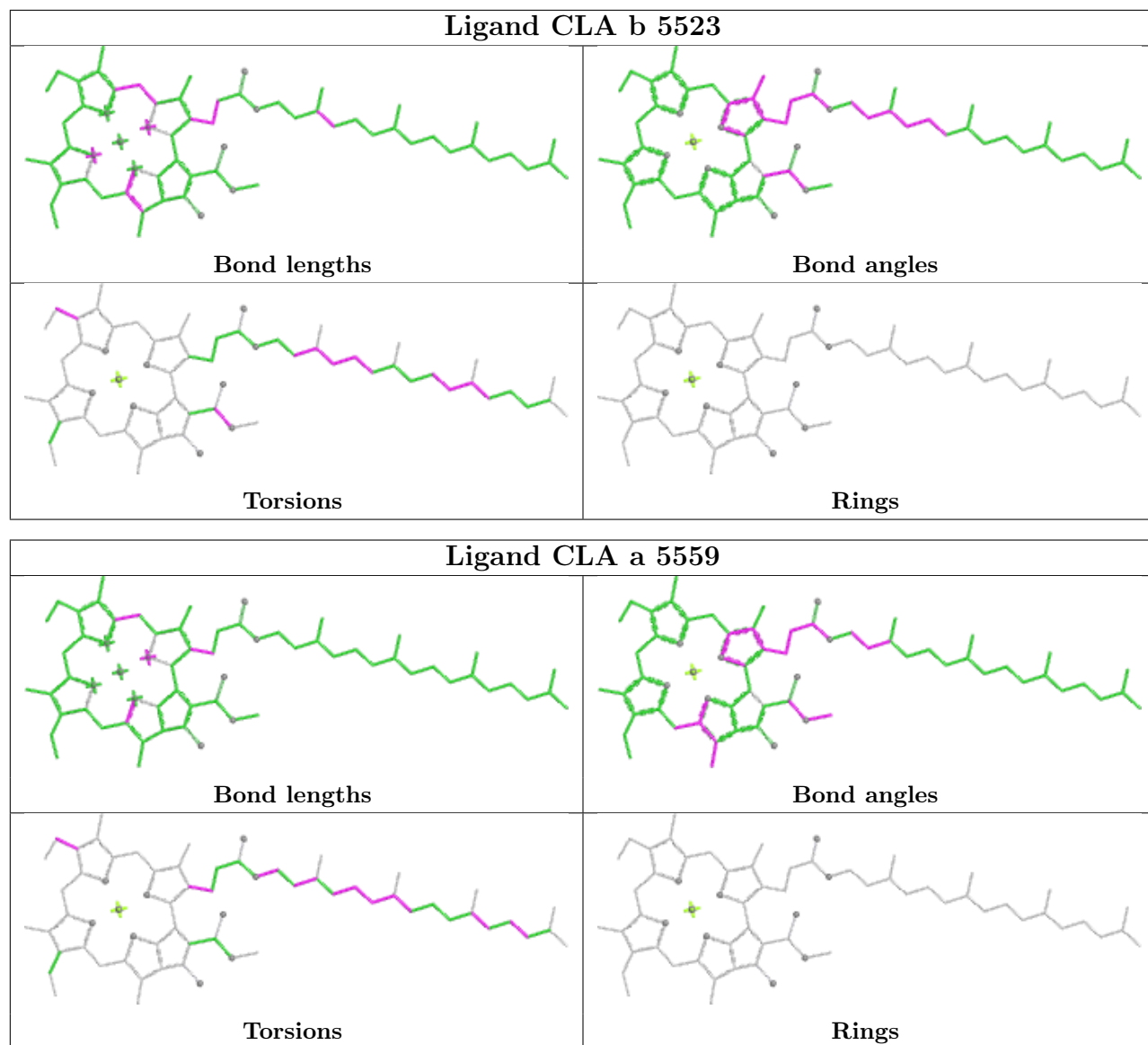
Ligand LMT A 569

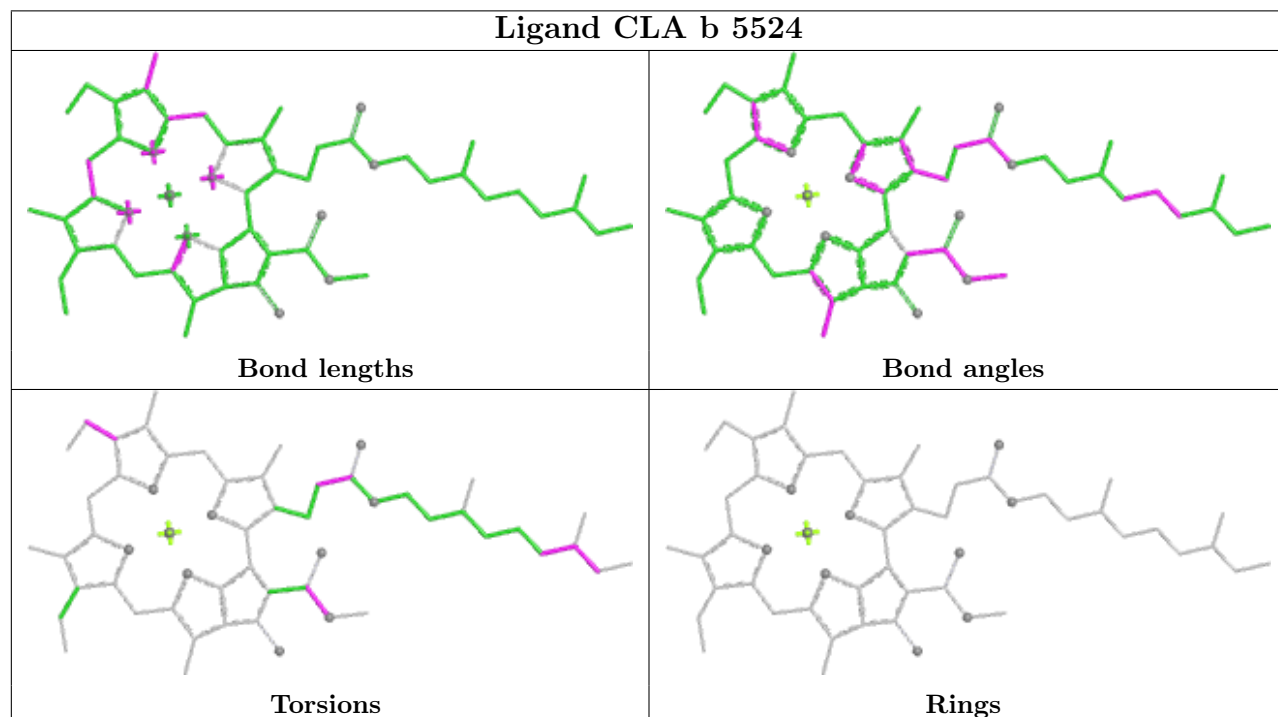
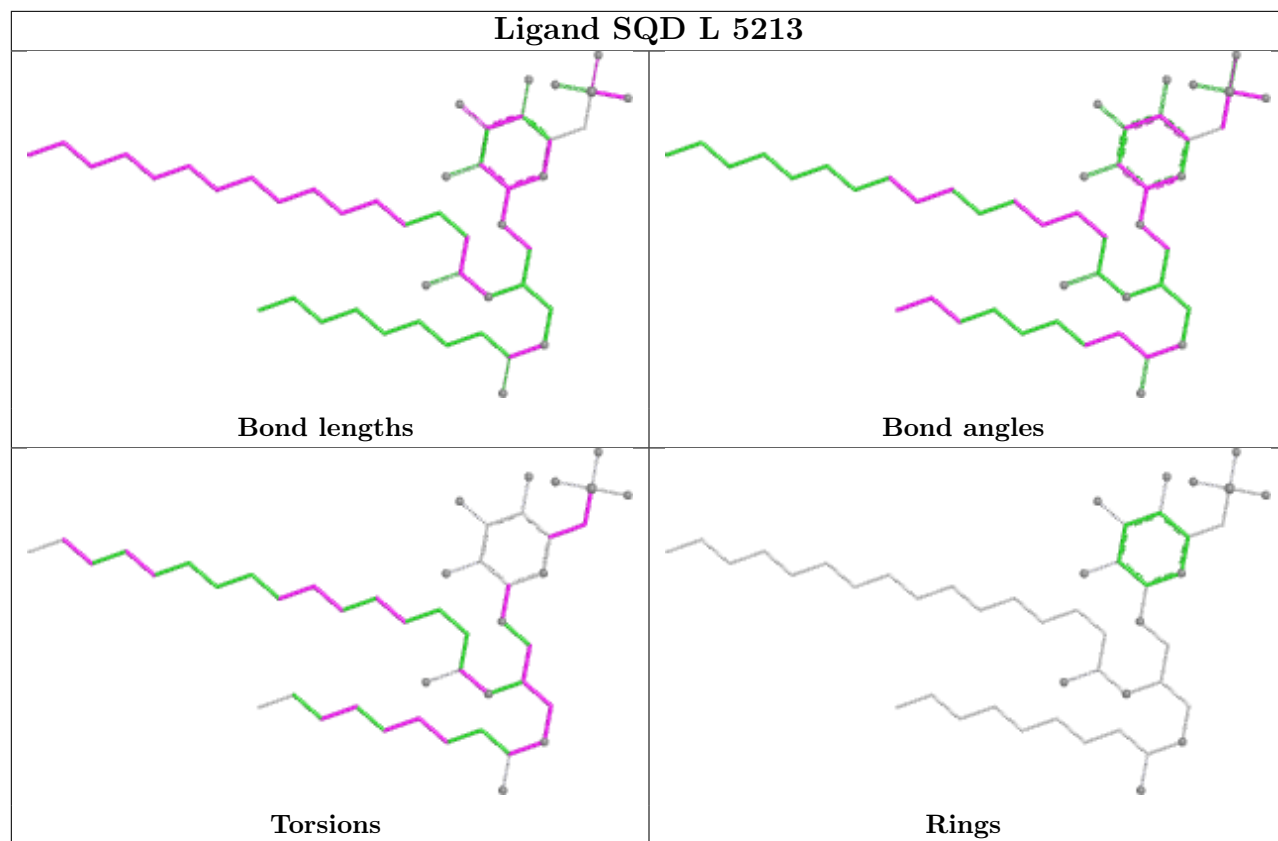


Ligand BCR h 5107

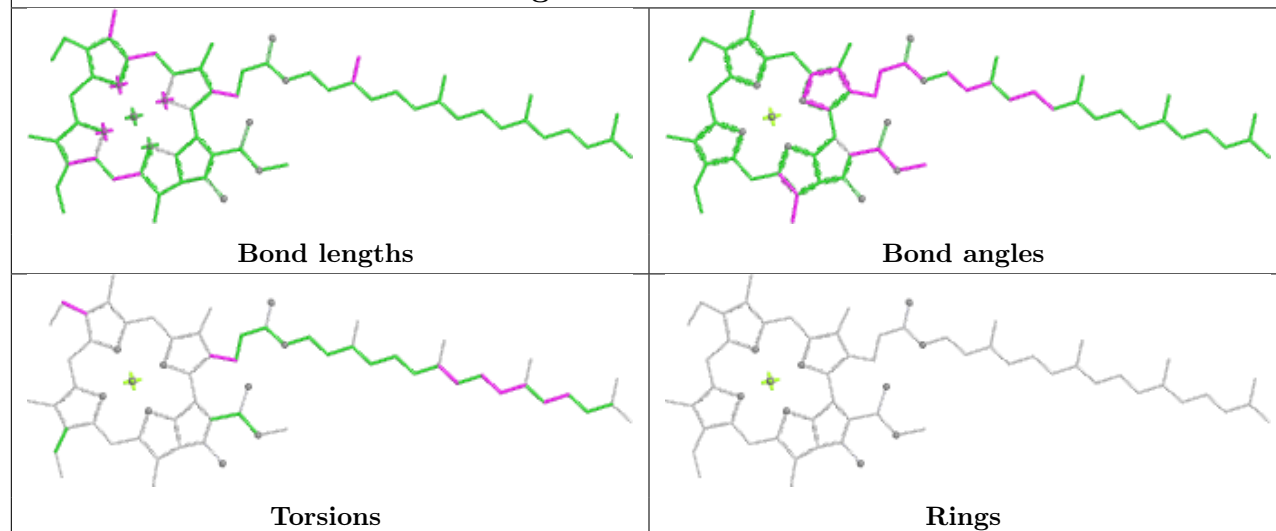




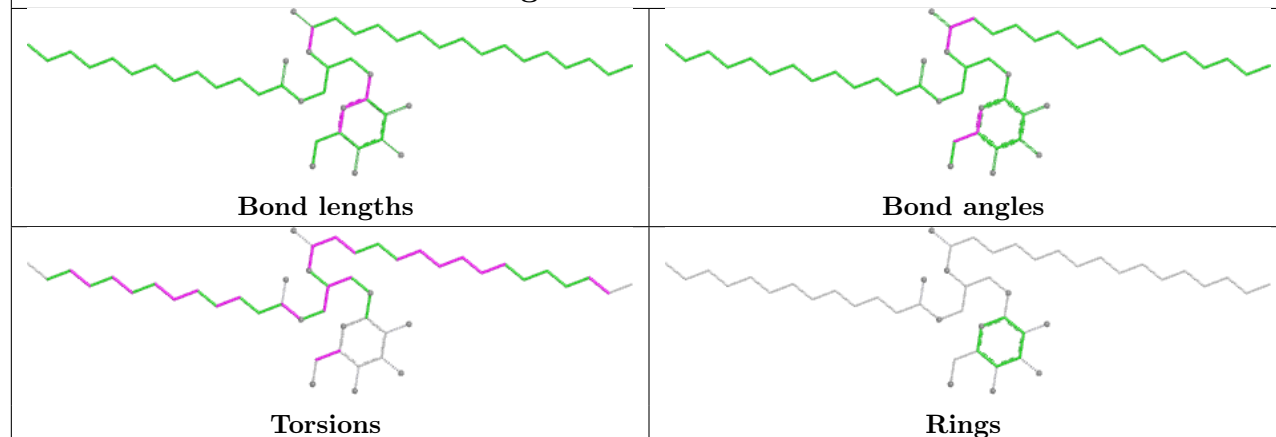




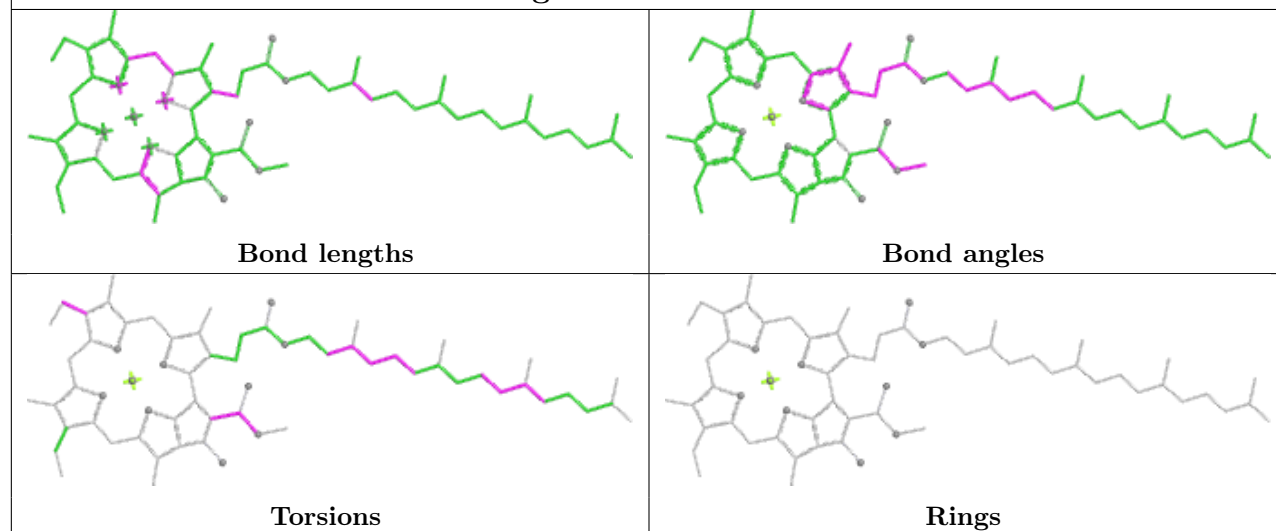
Ligand CLA A 560

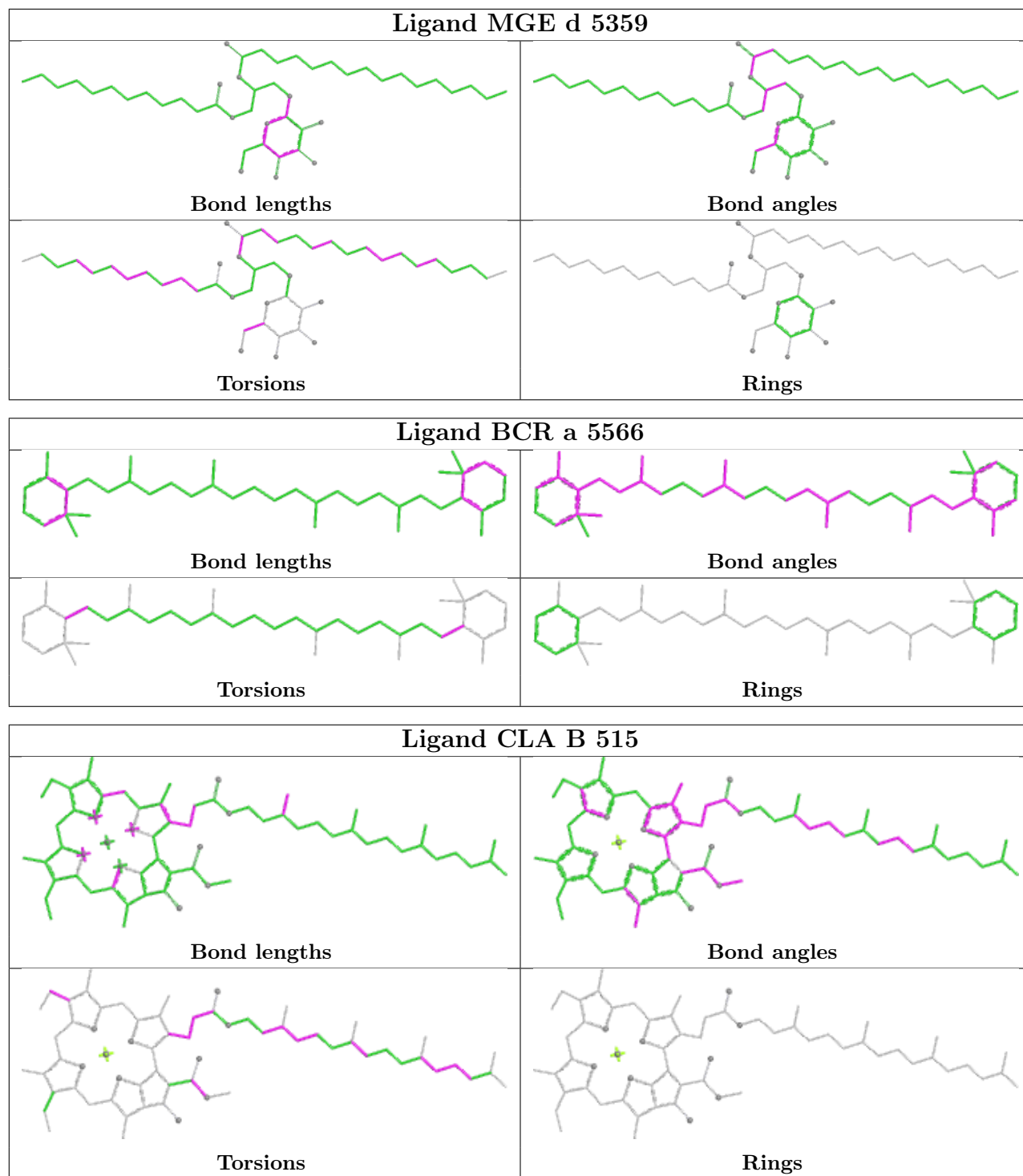


Ligand MGE d 5361

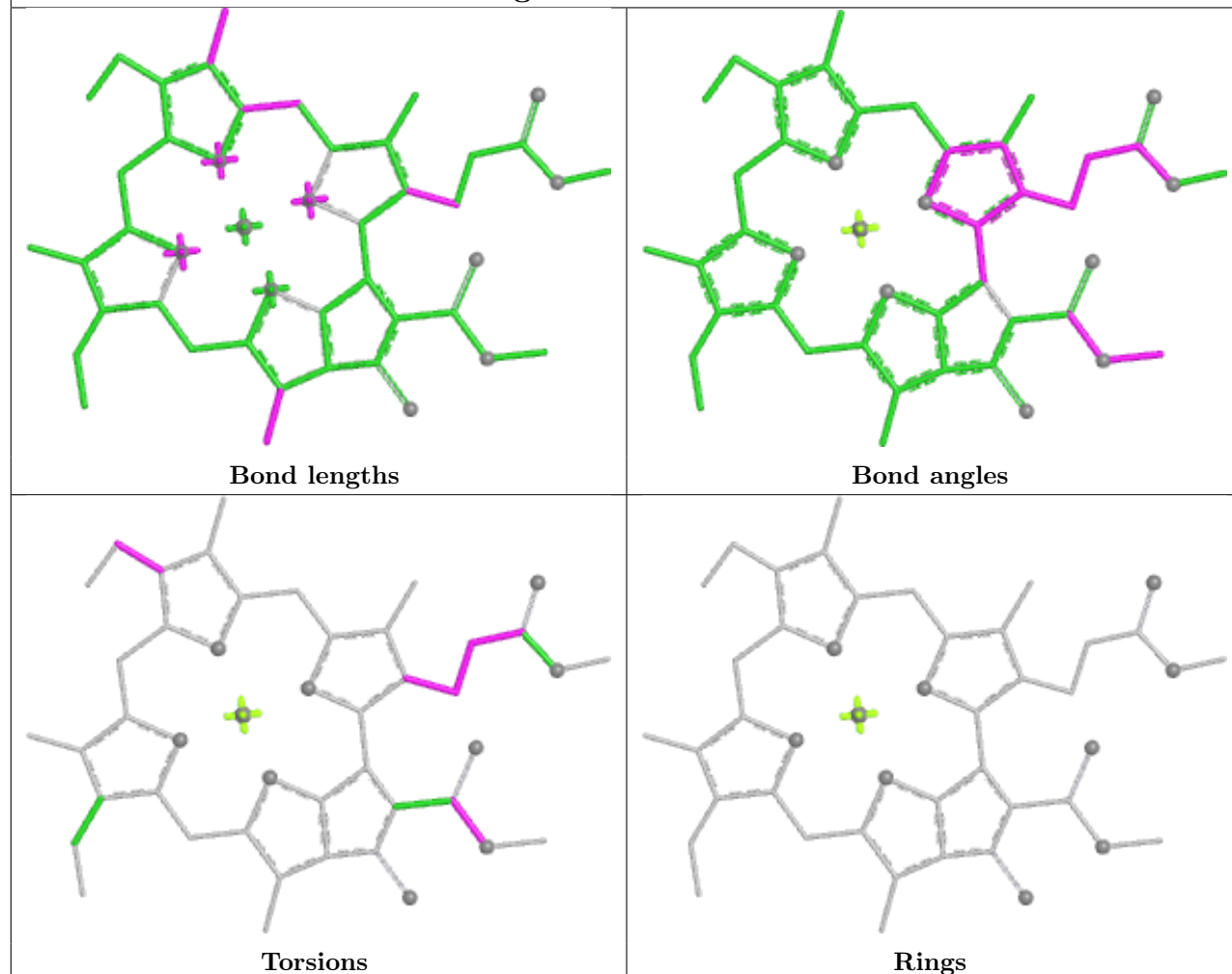


Ligand CLA B 523

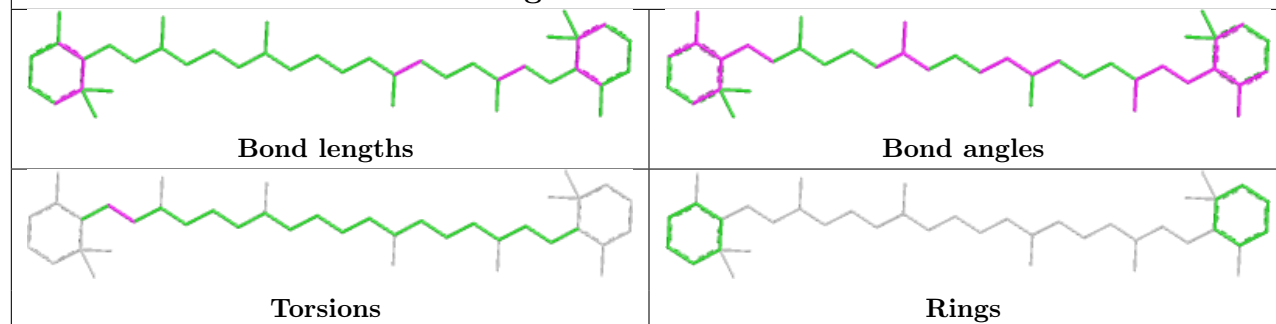


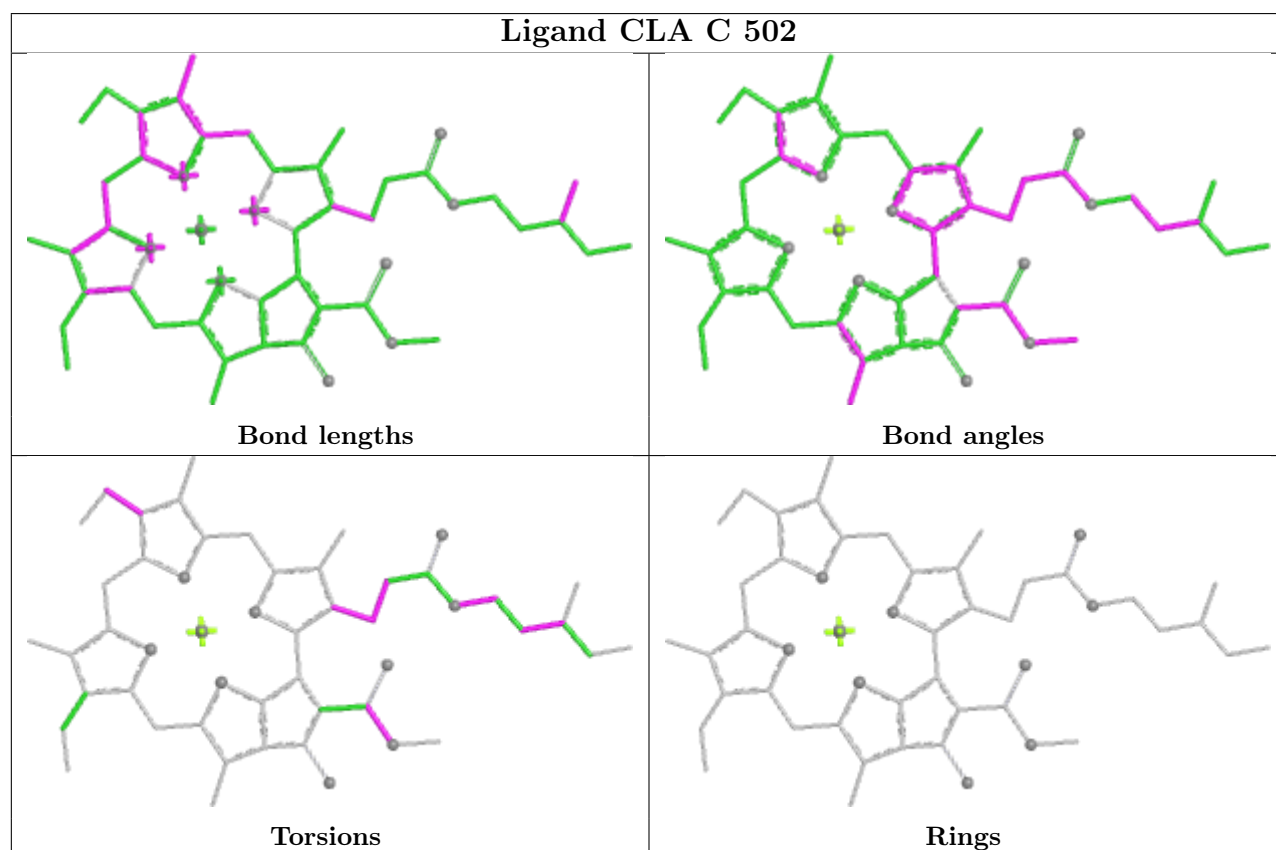
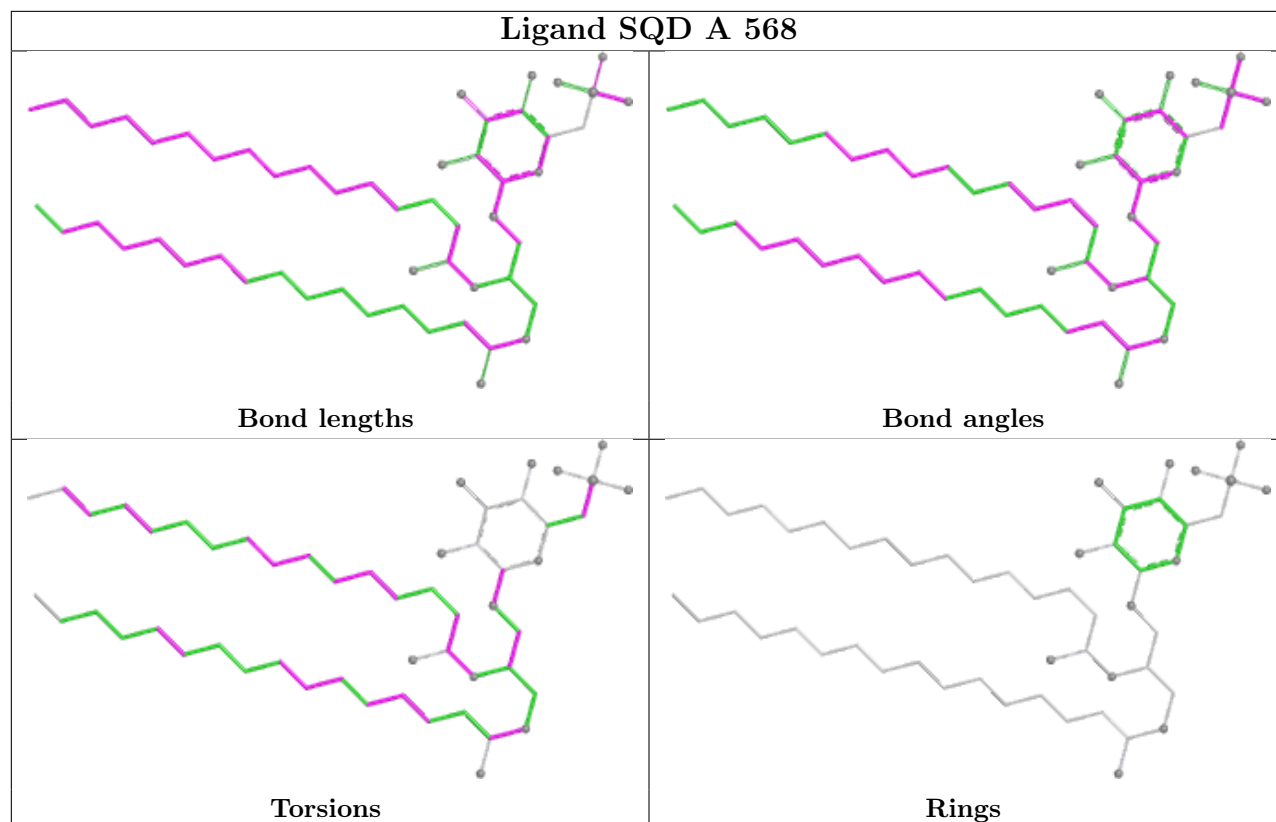


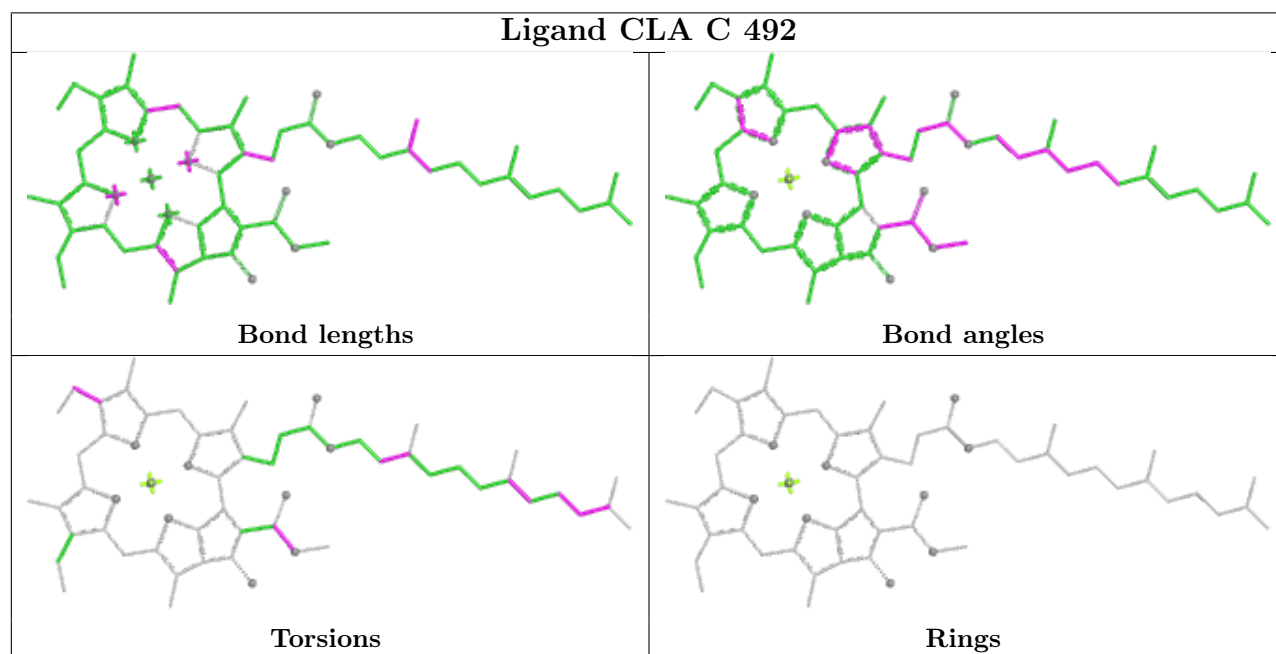
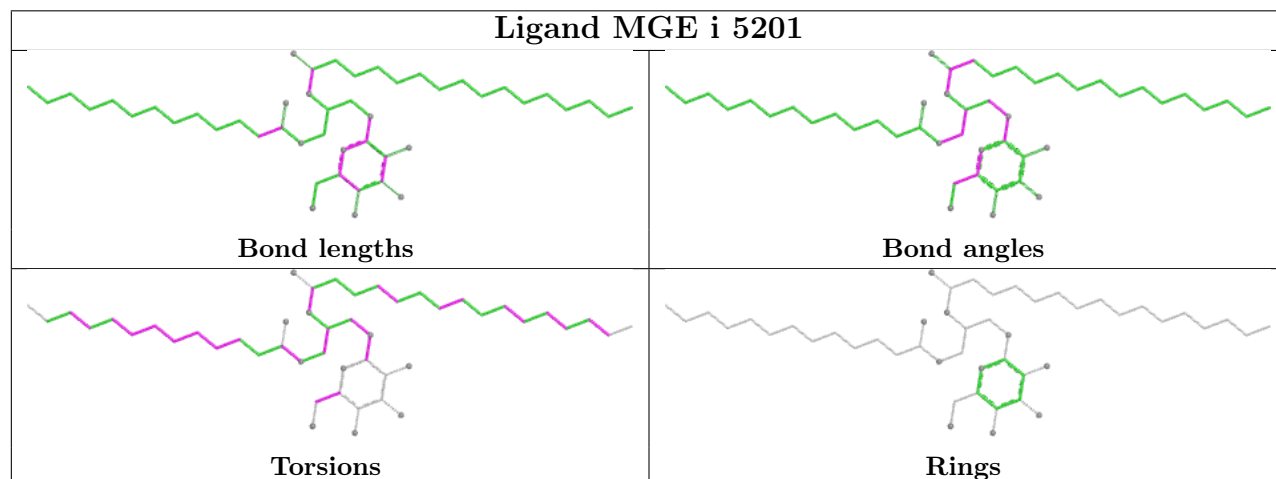
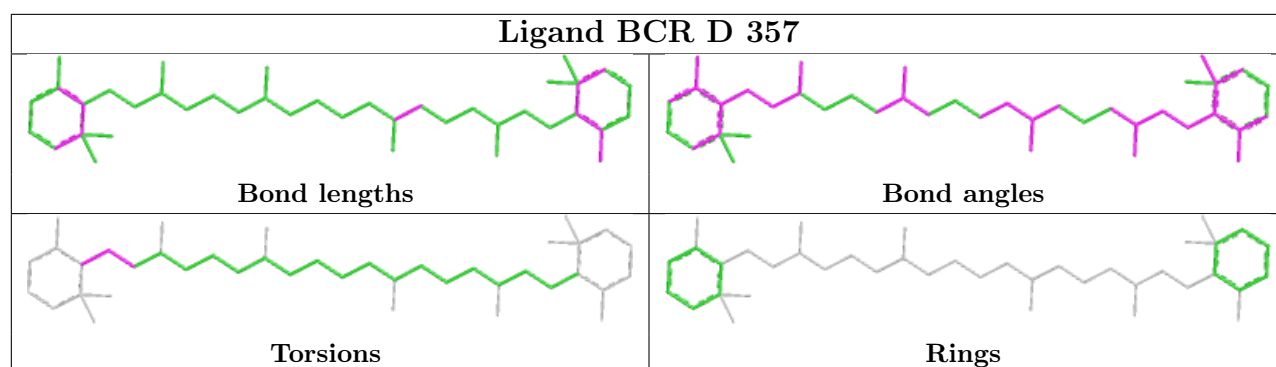
Ligand CLA C 494

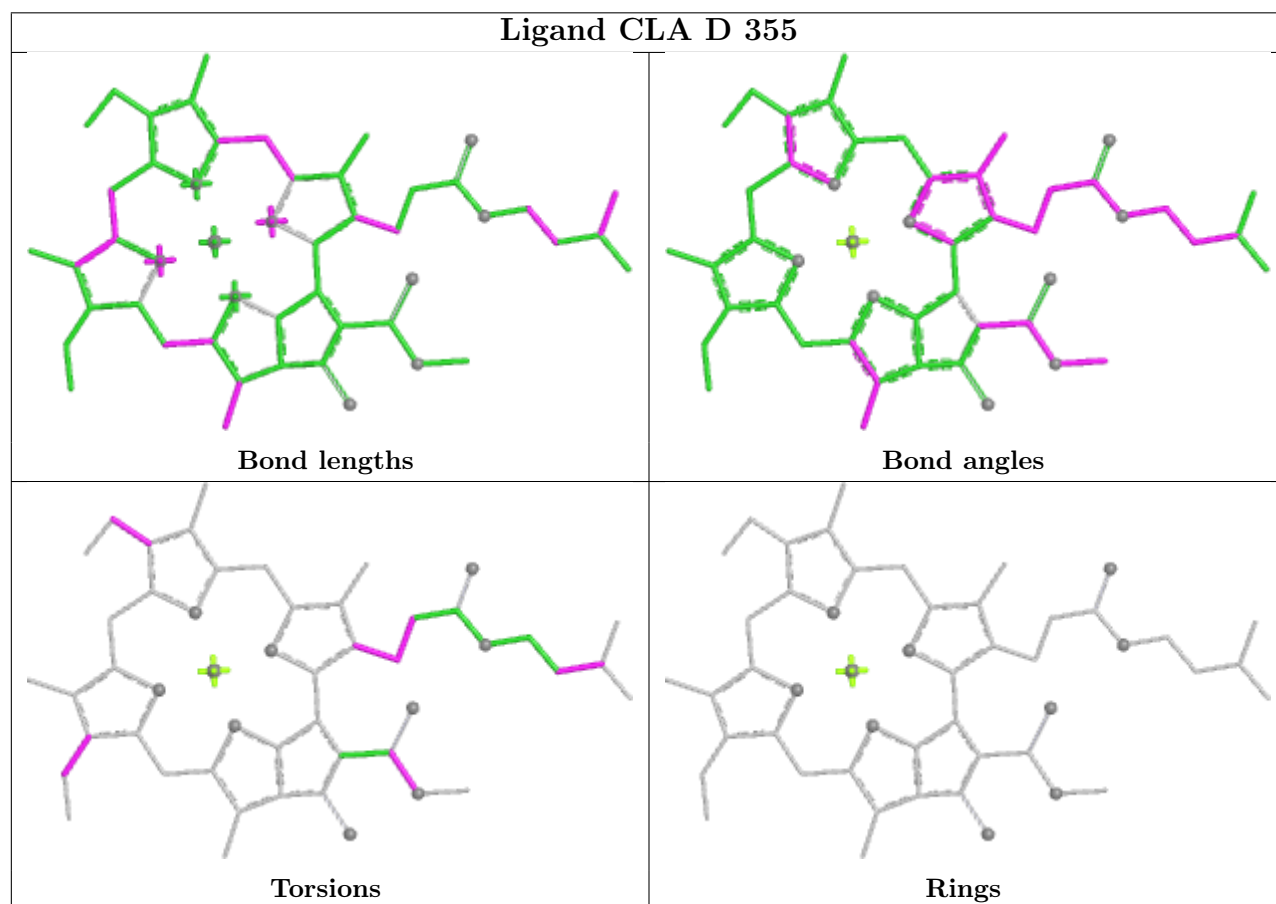
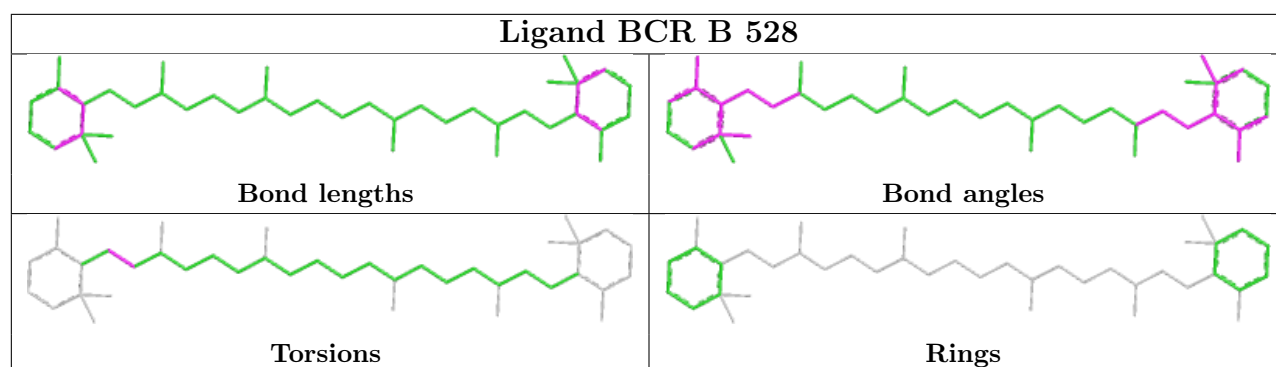


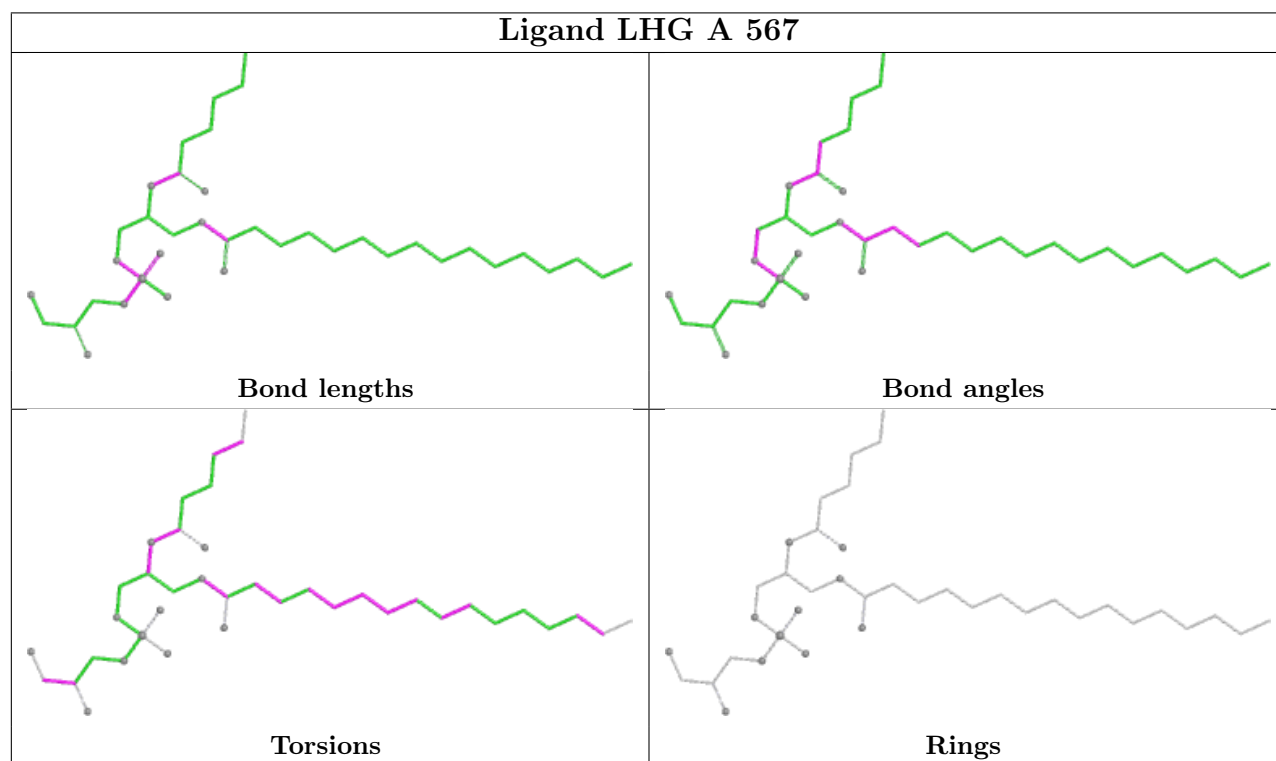
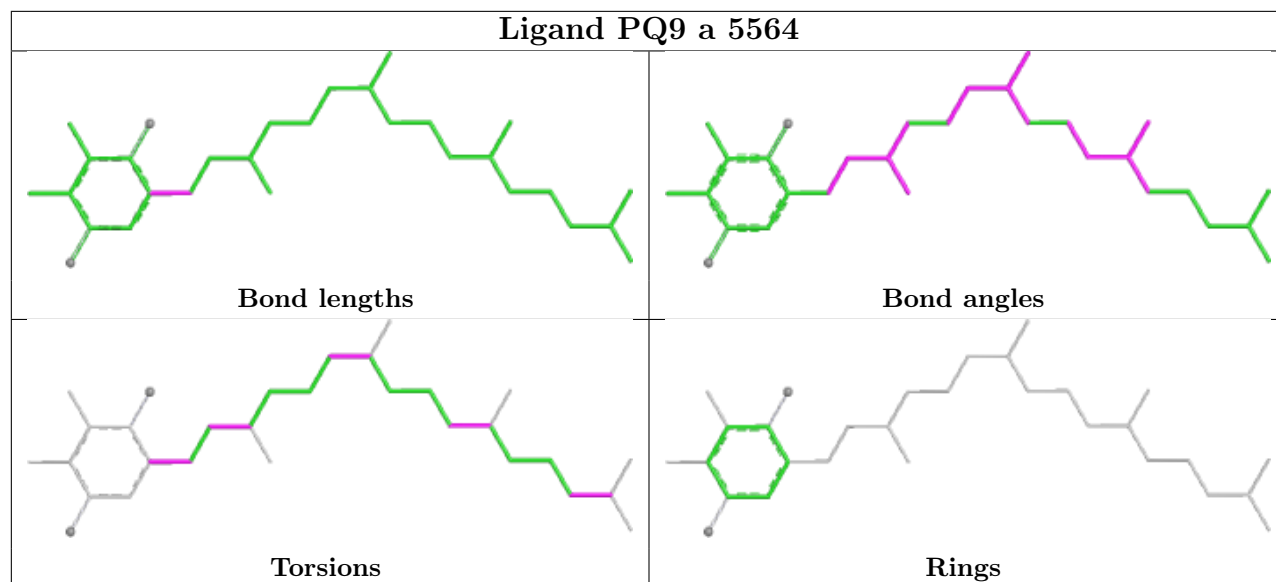
Ligand BCR b 5527

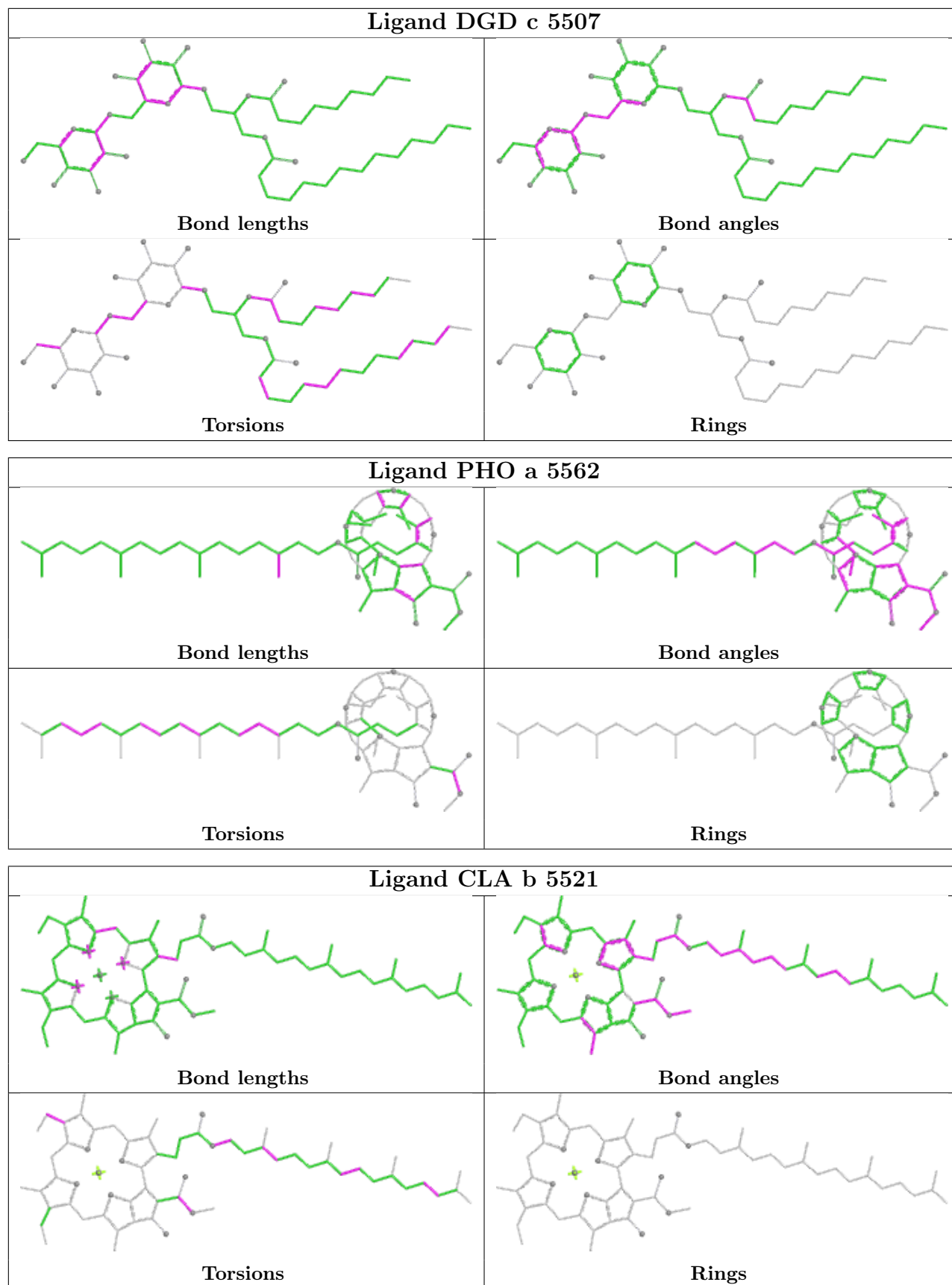




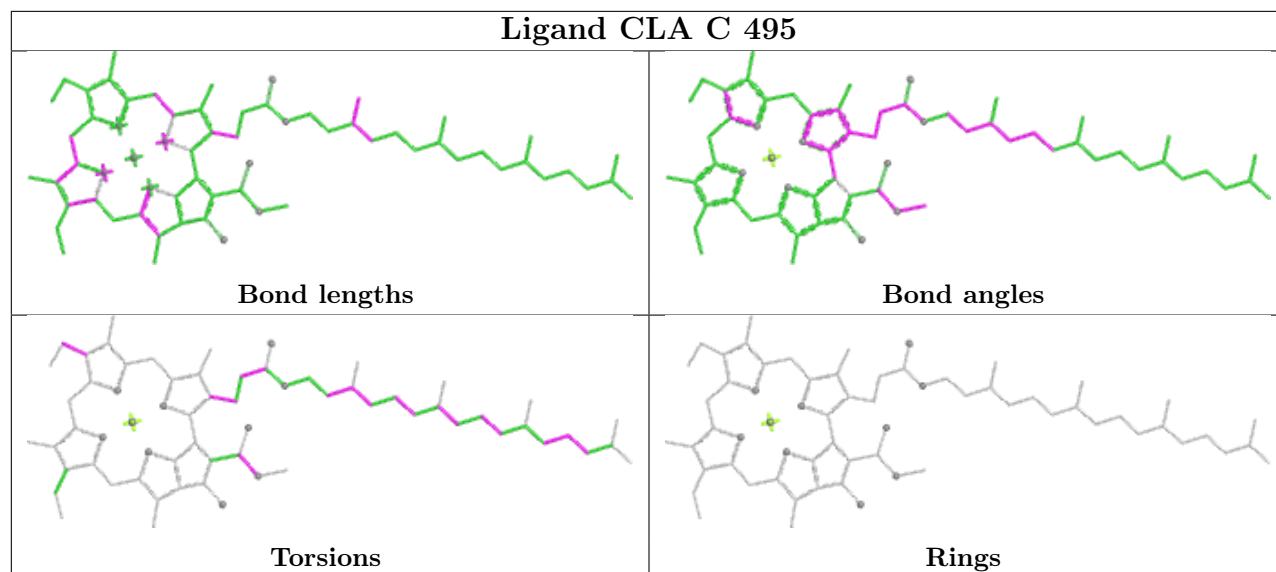




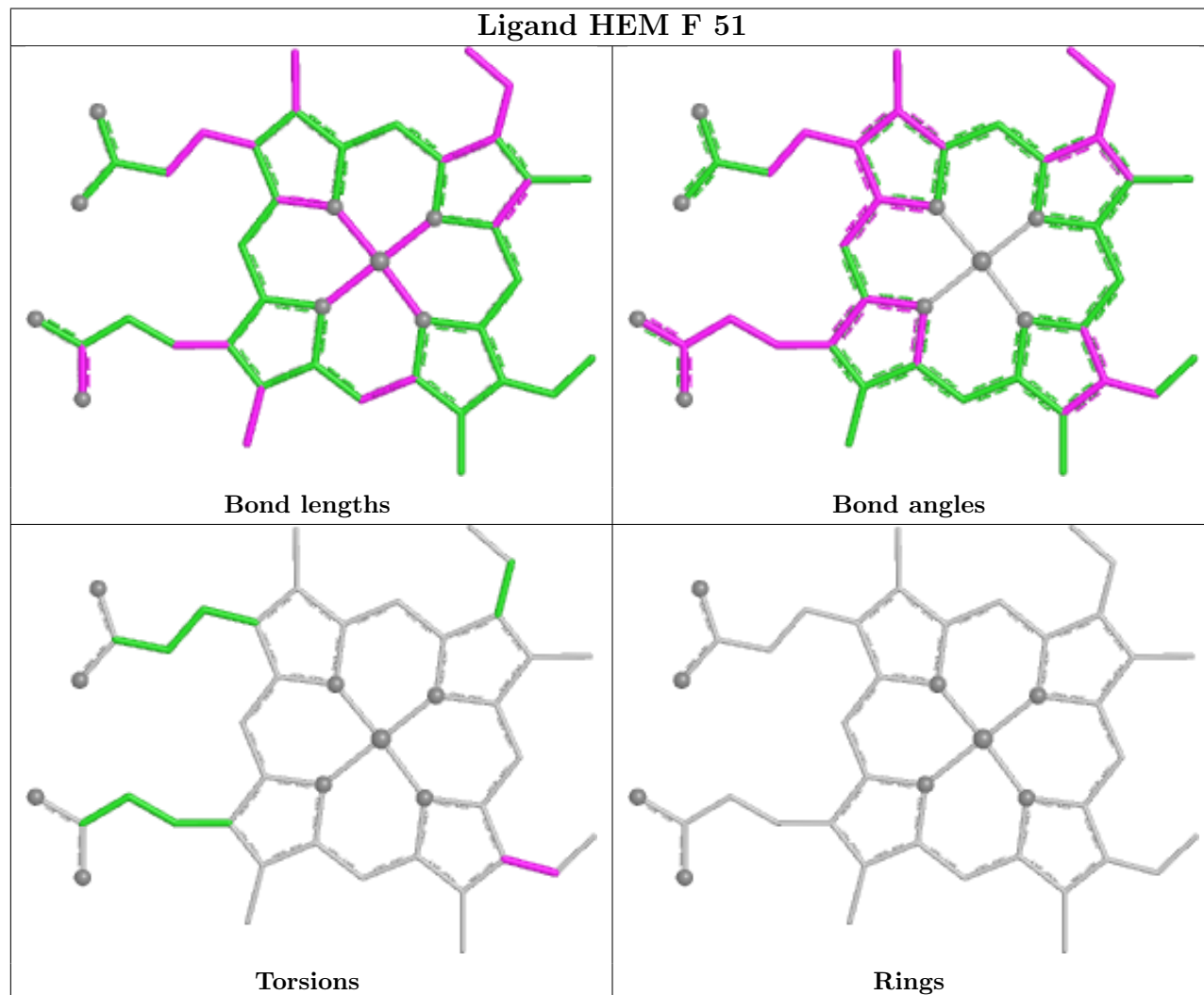


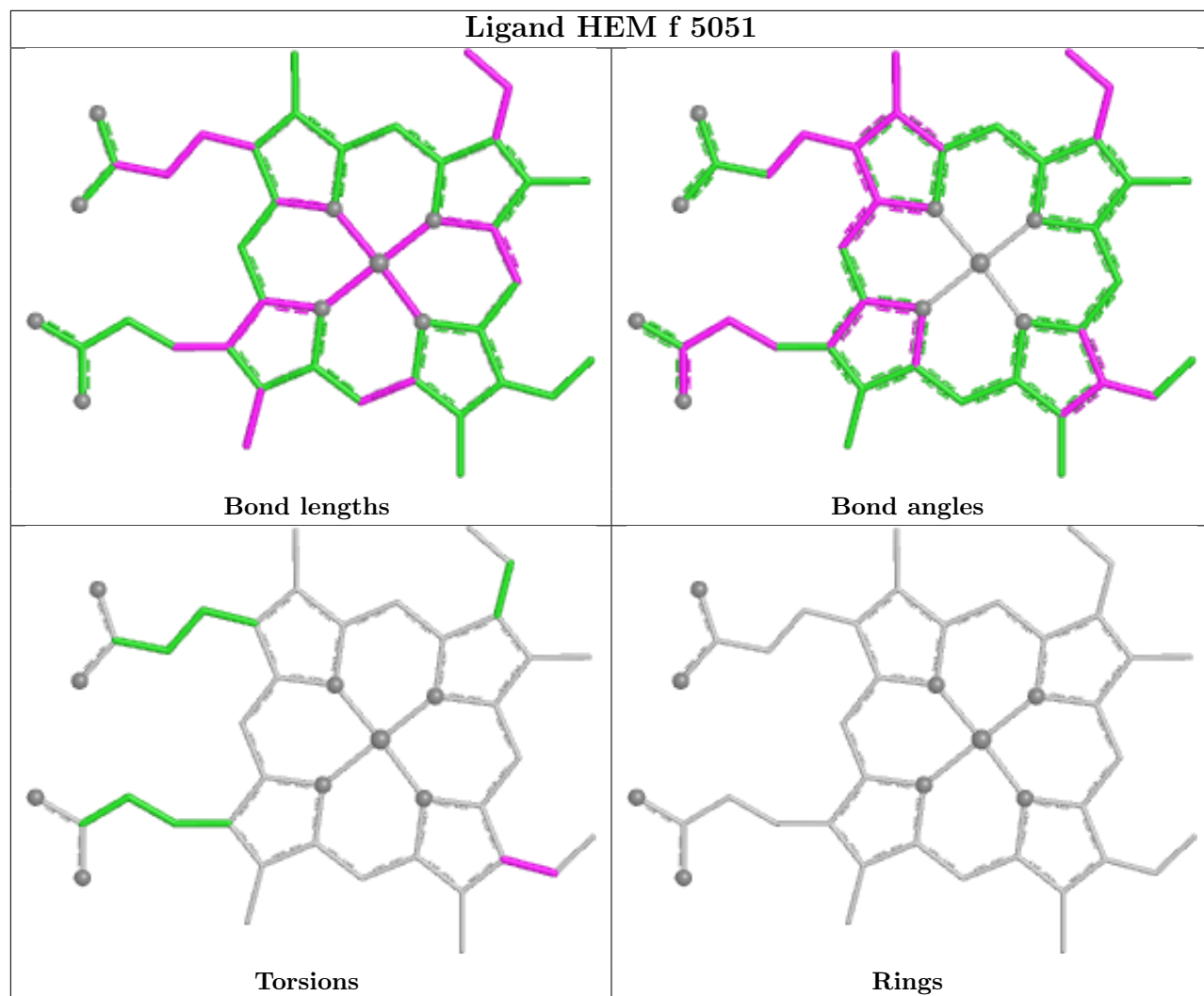


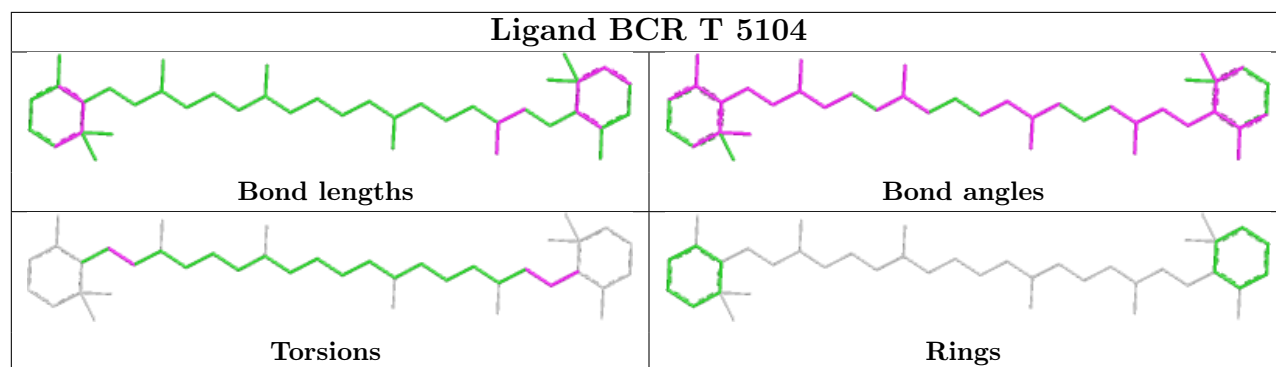
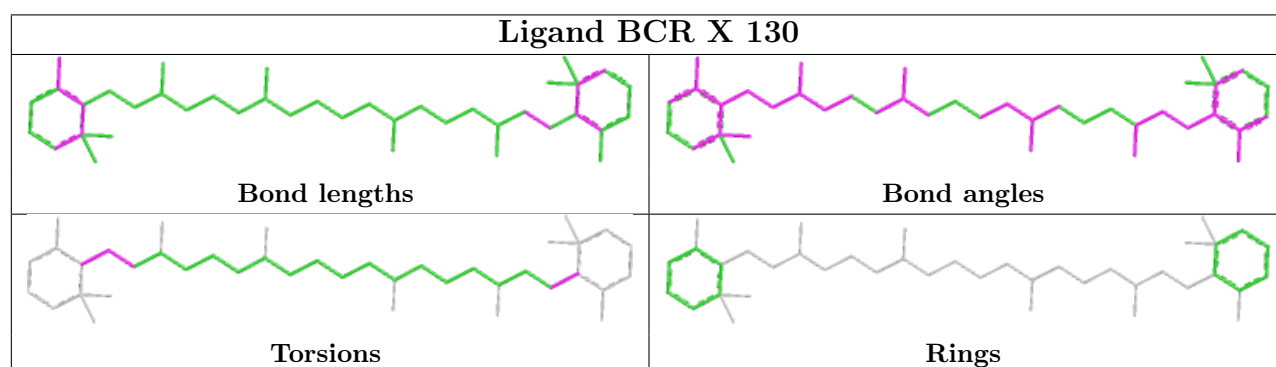
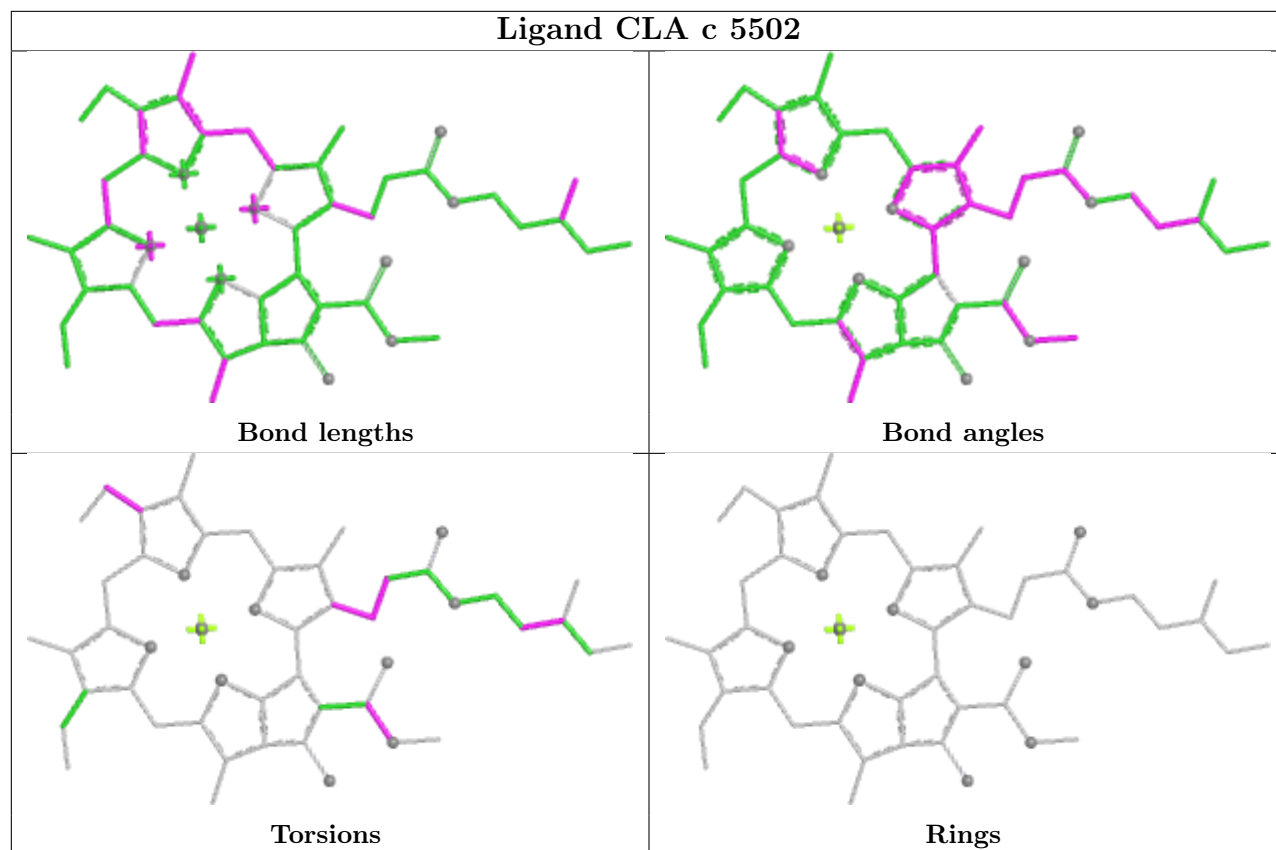
Ligand CLA C 495

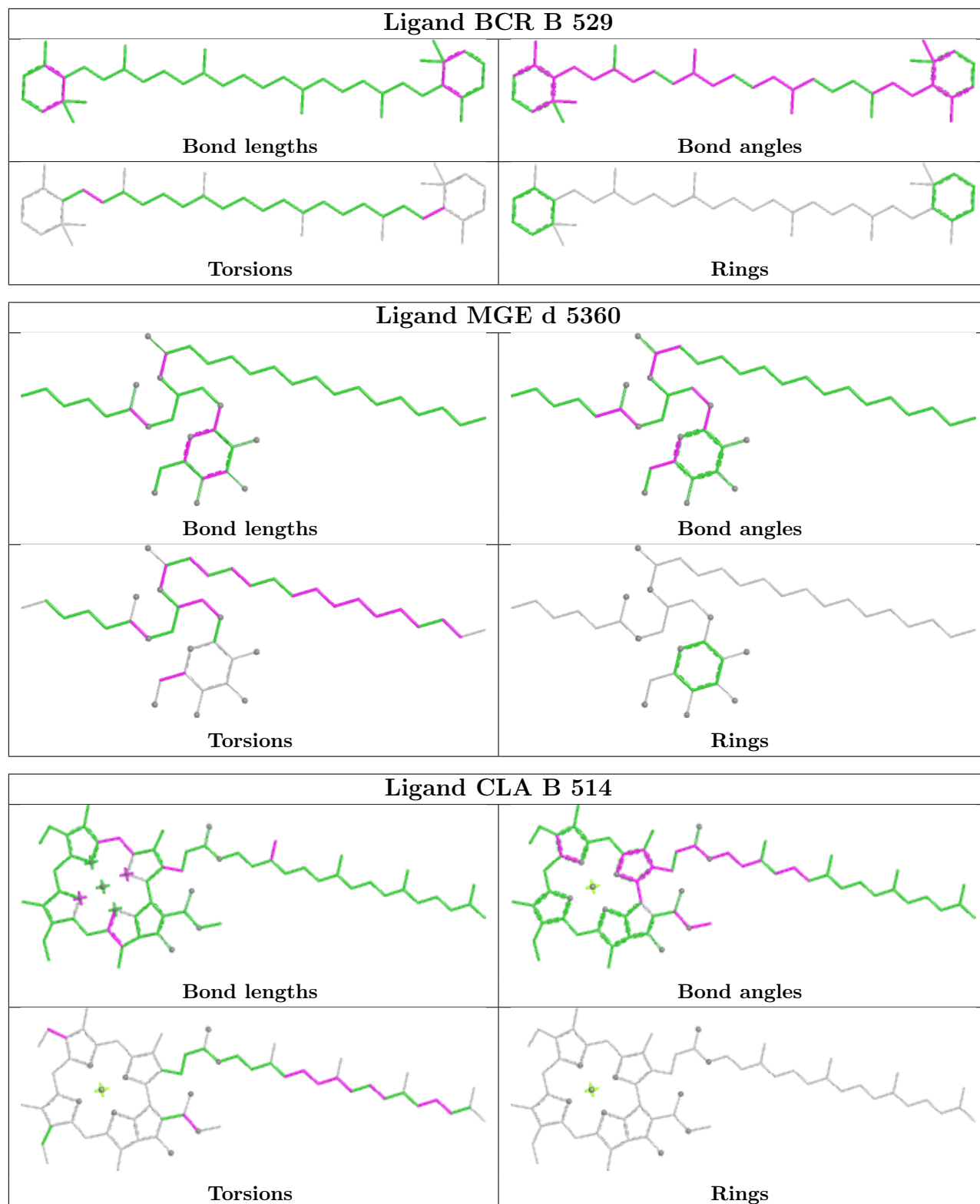


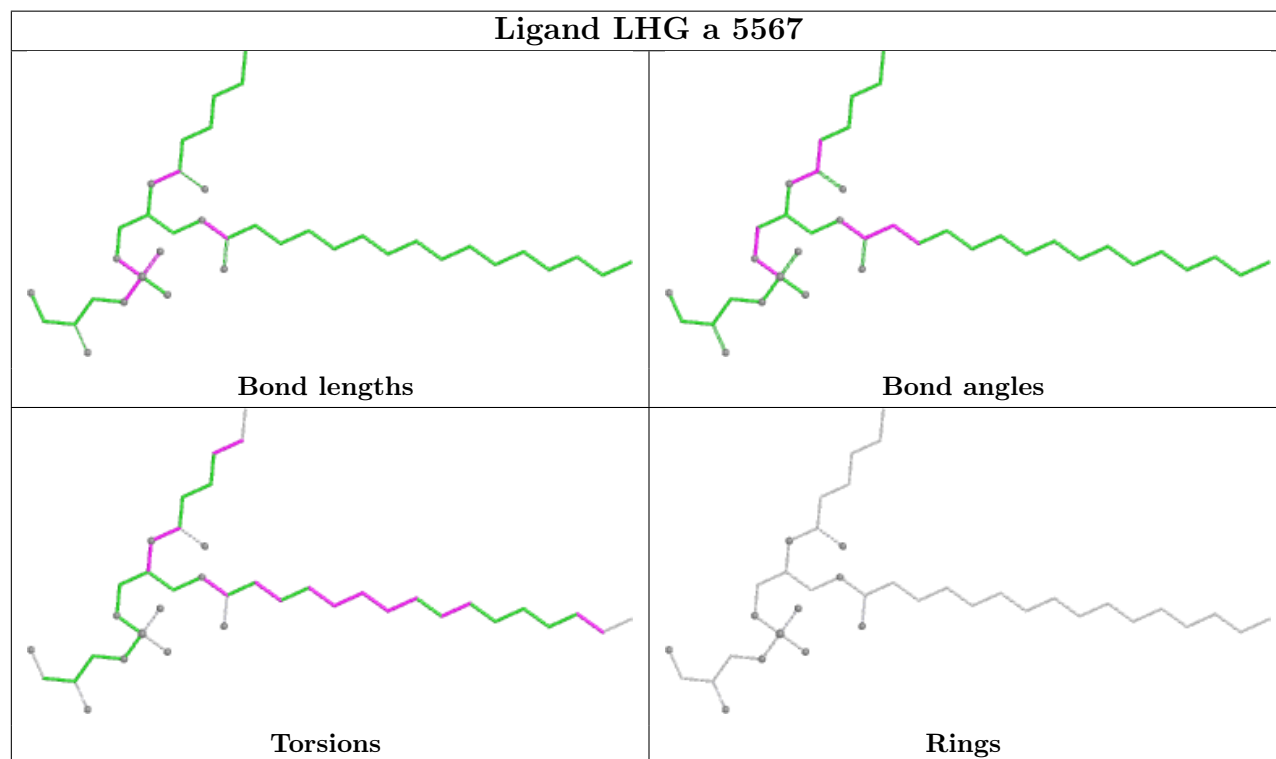
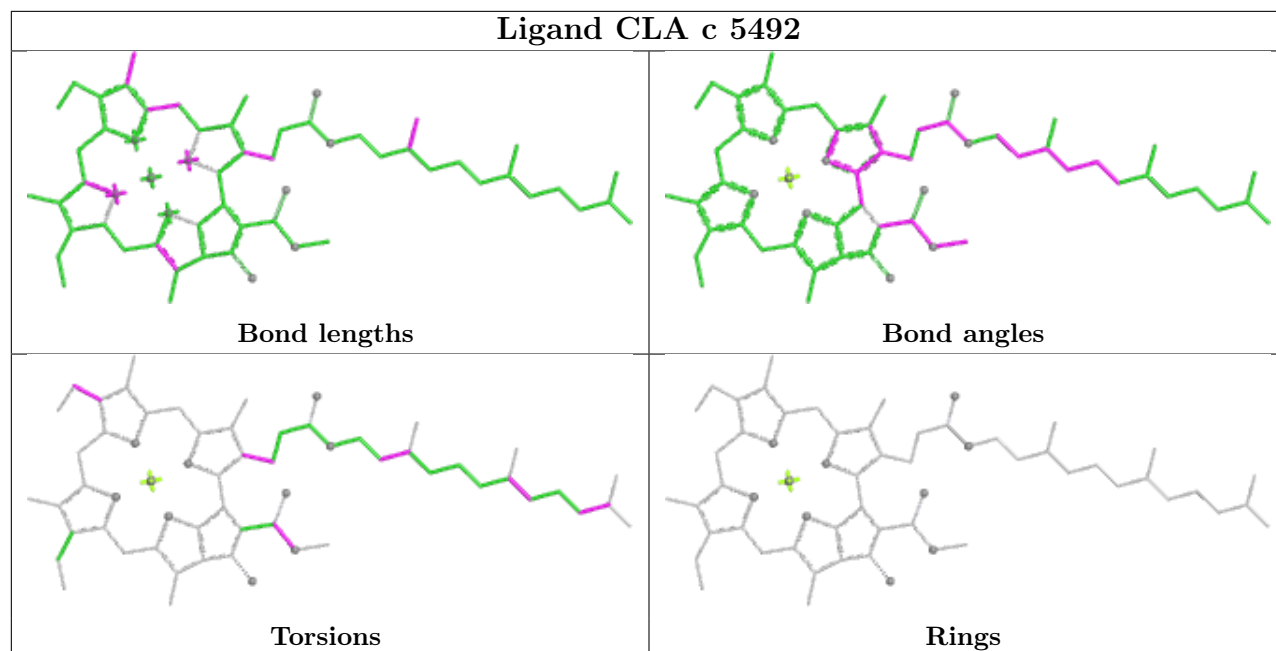
Ligand HEM F 51

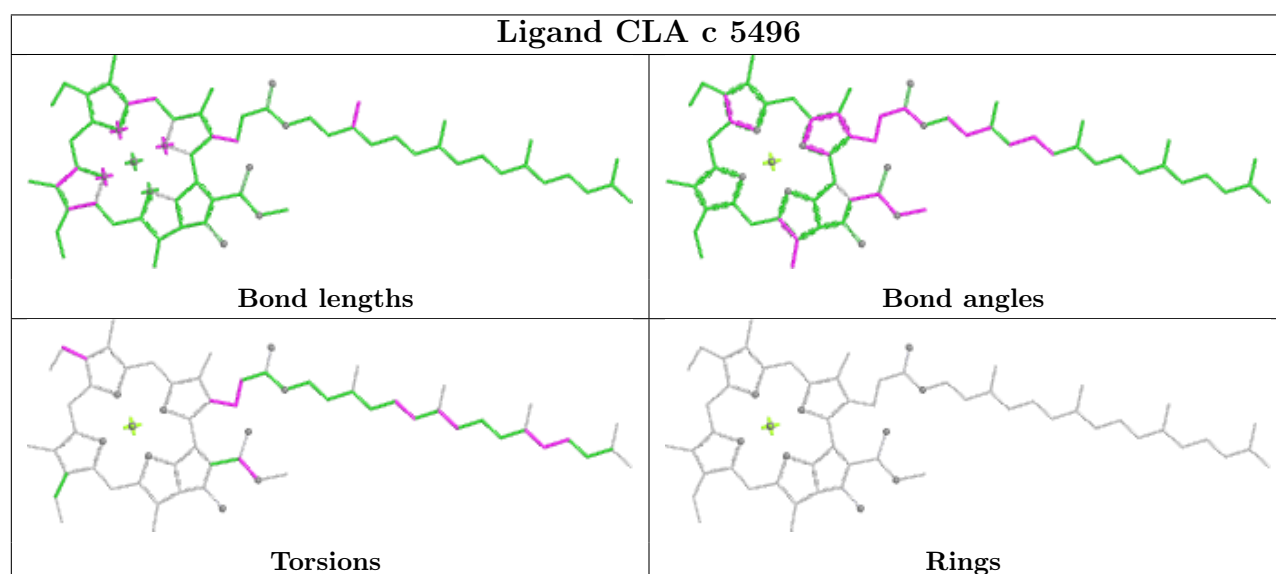
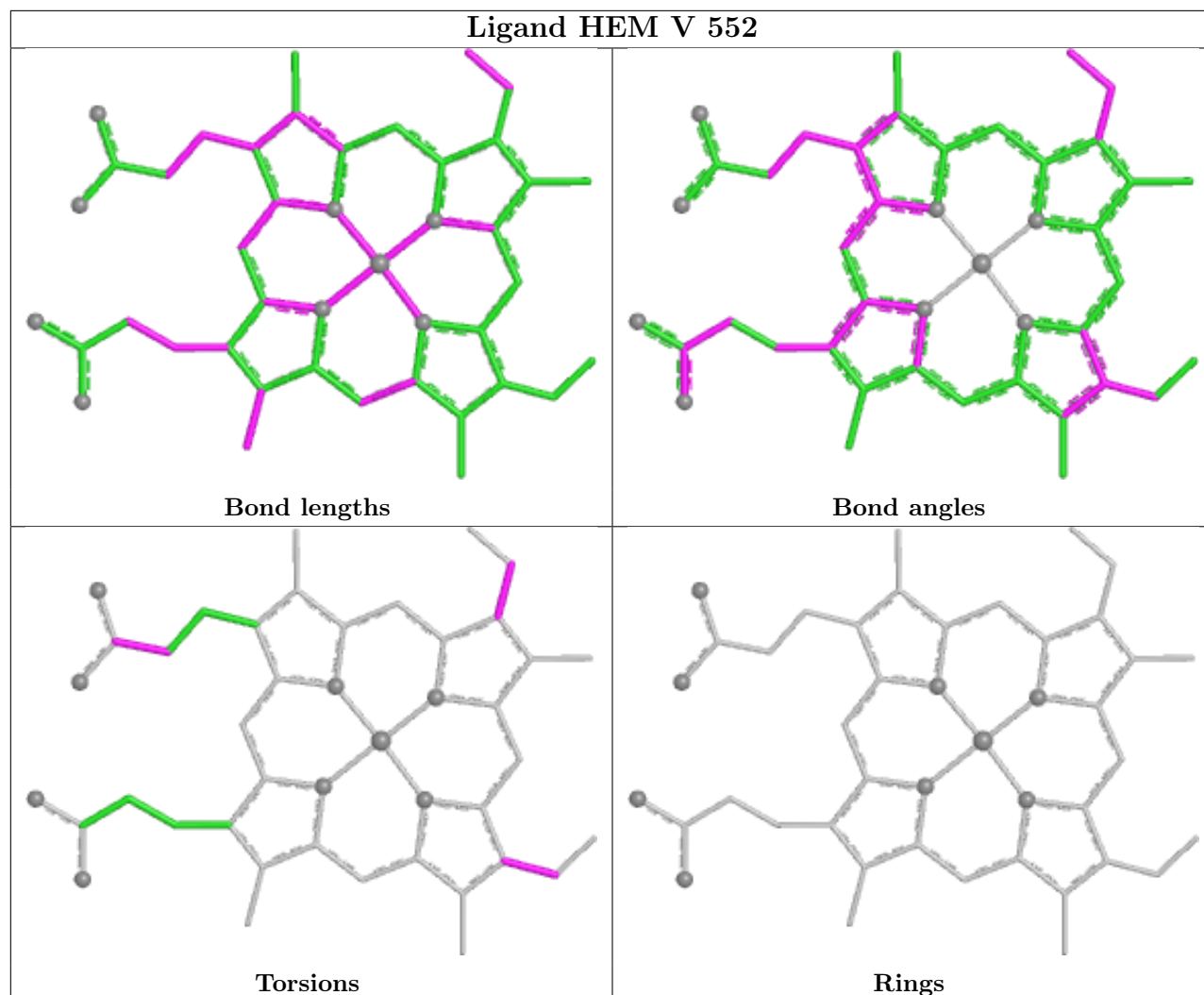


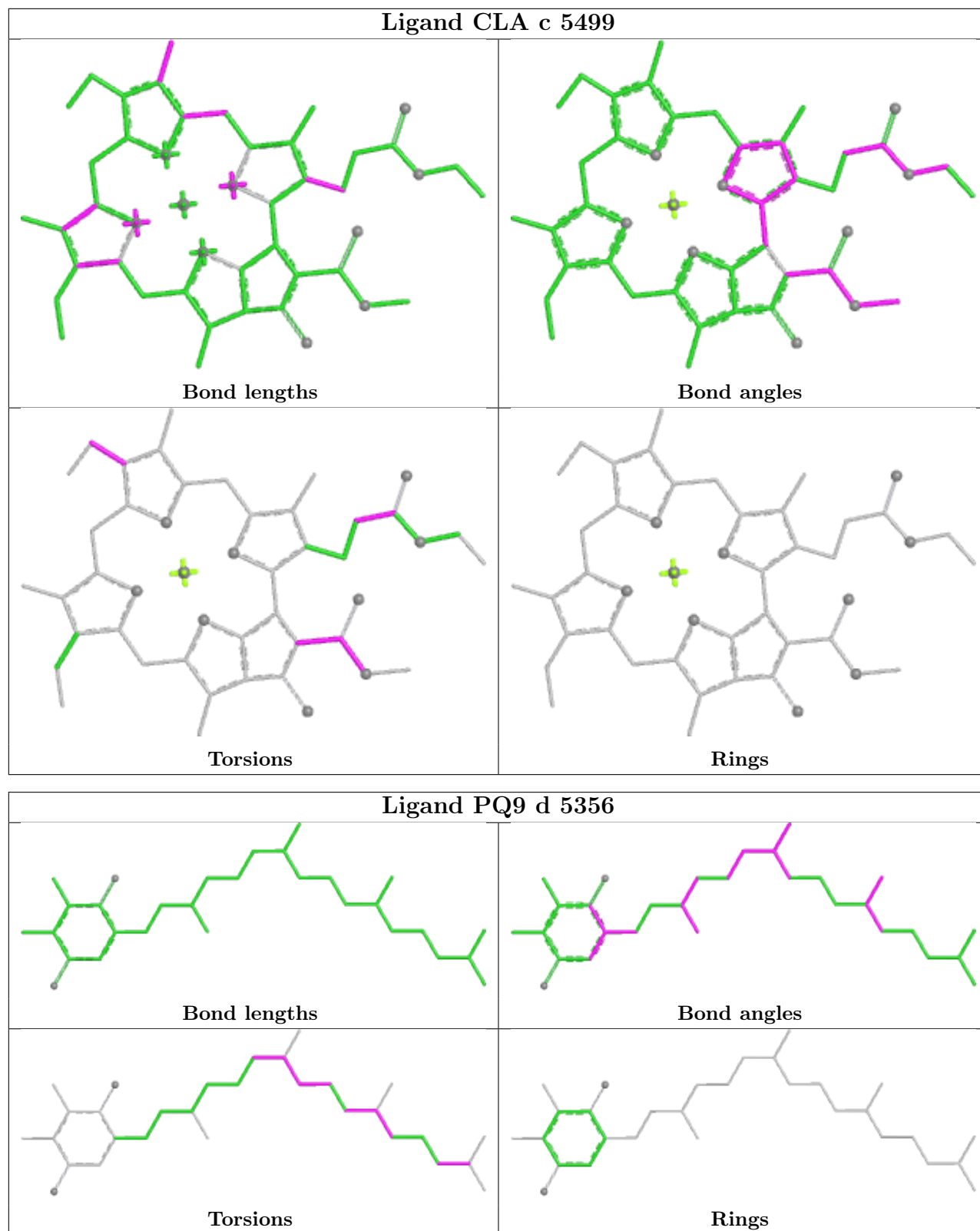


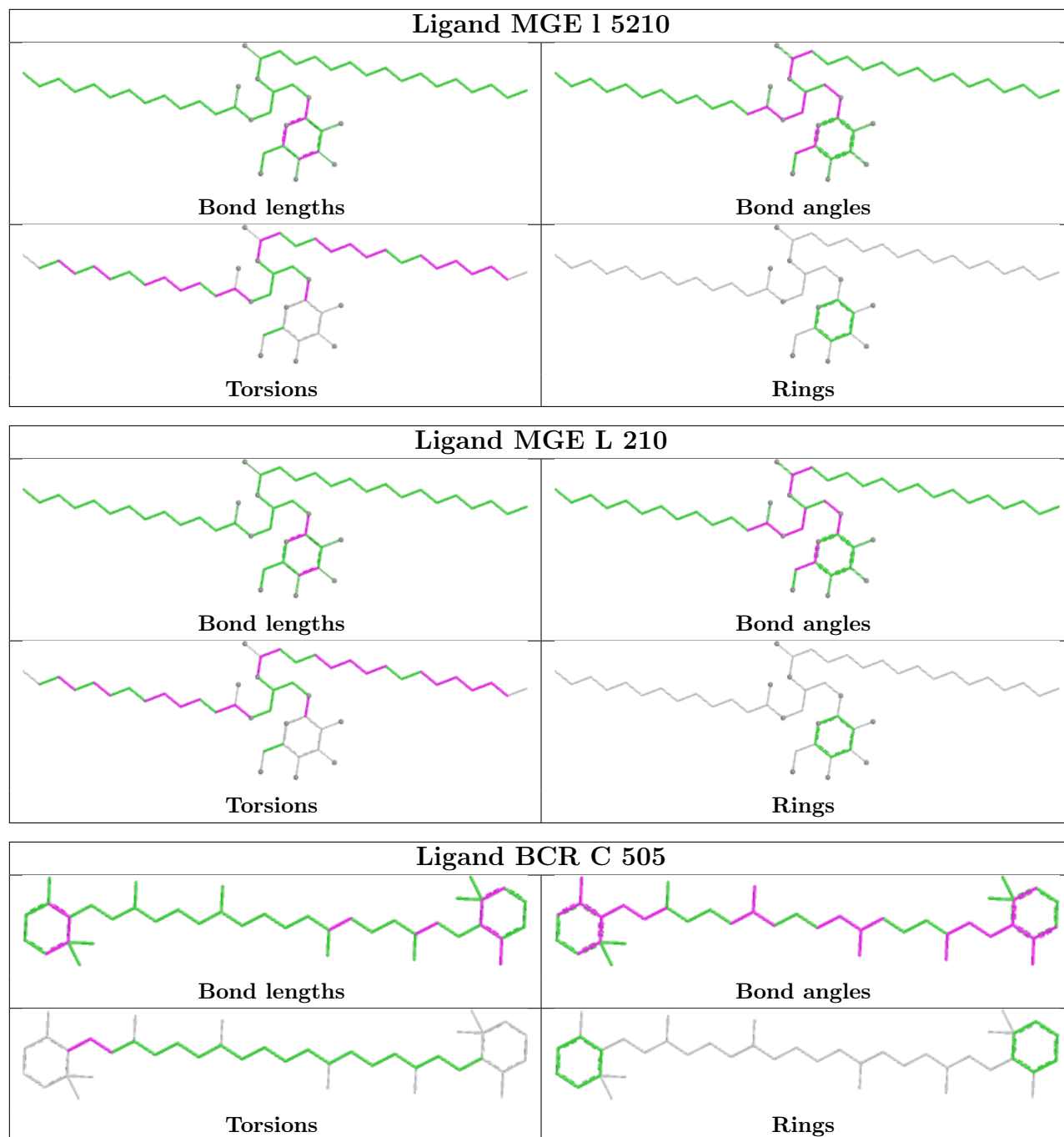


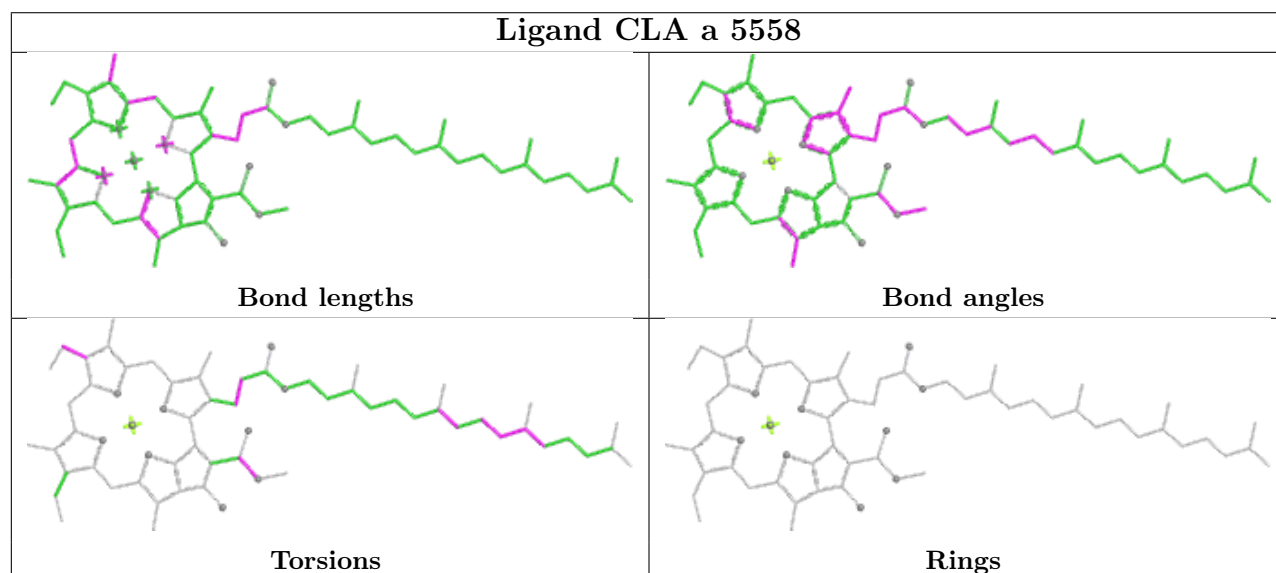
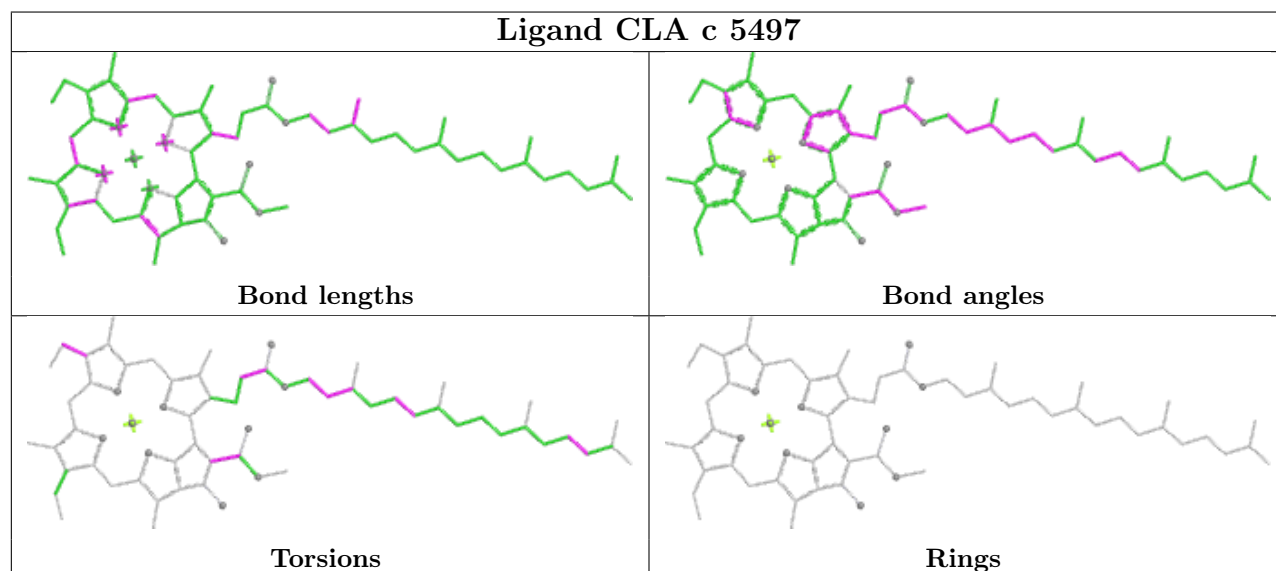
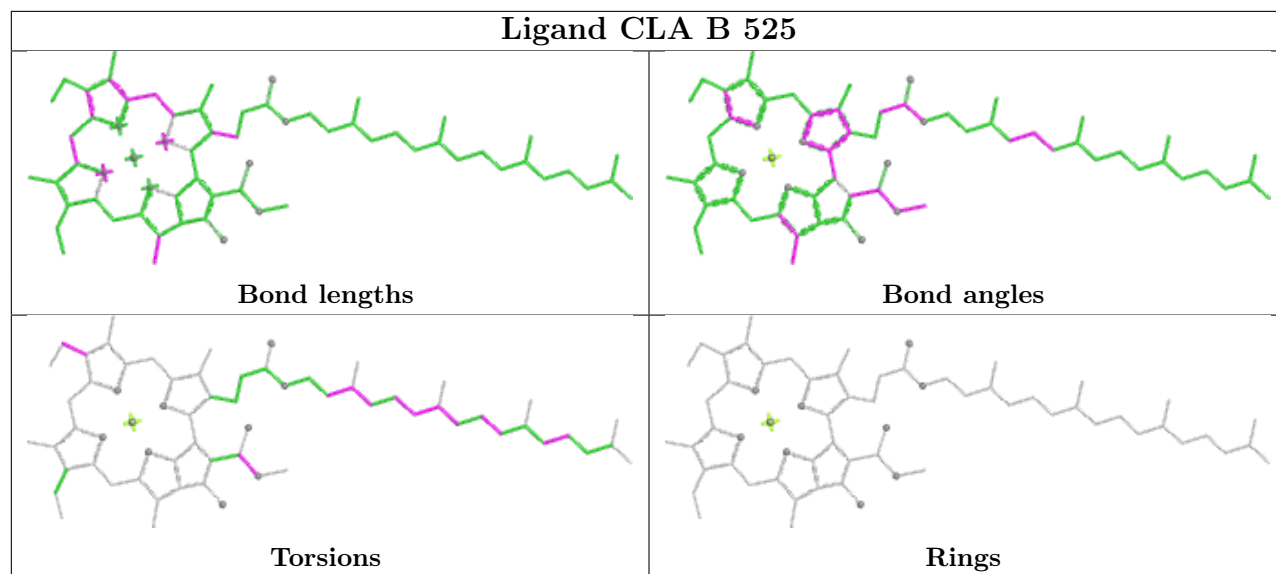




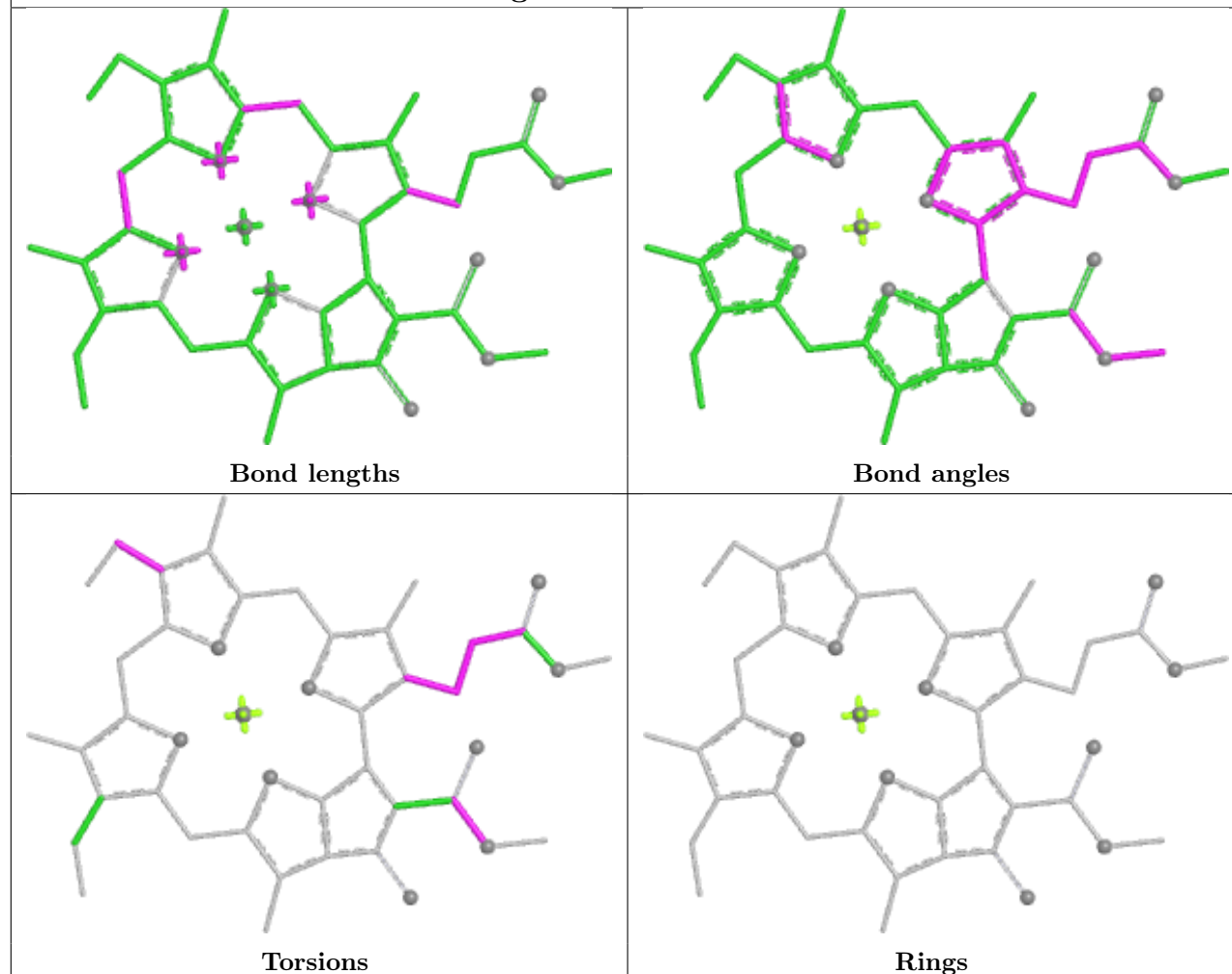




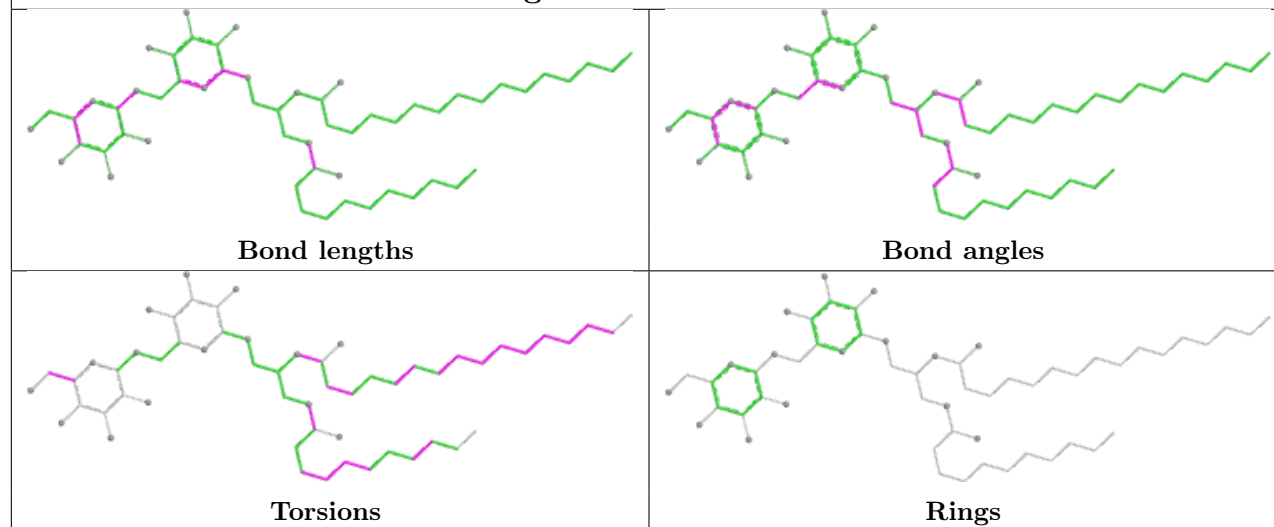


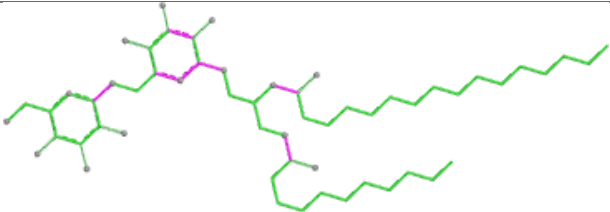
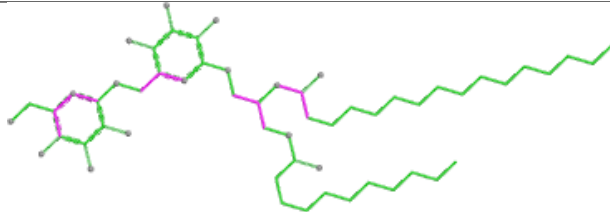
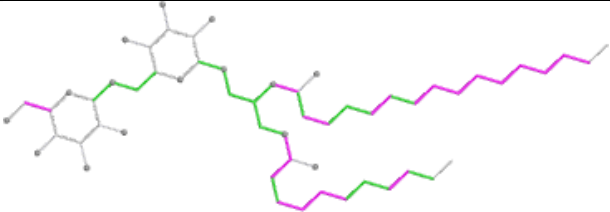
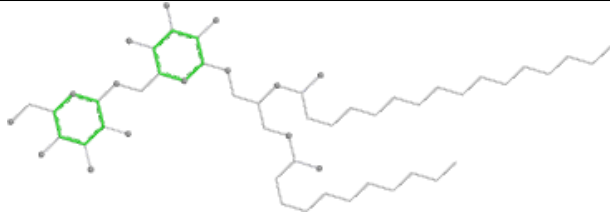


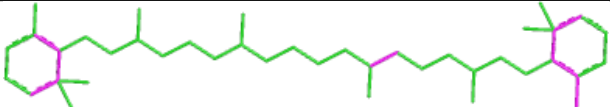
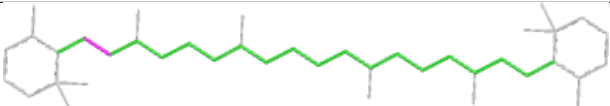
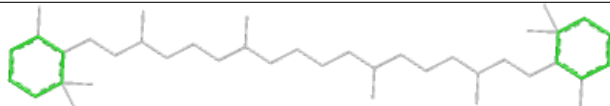
Ligand CLA c 5494

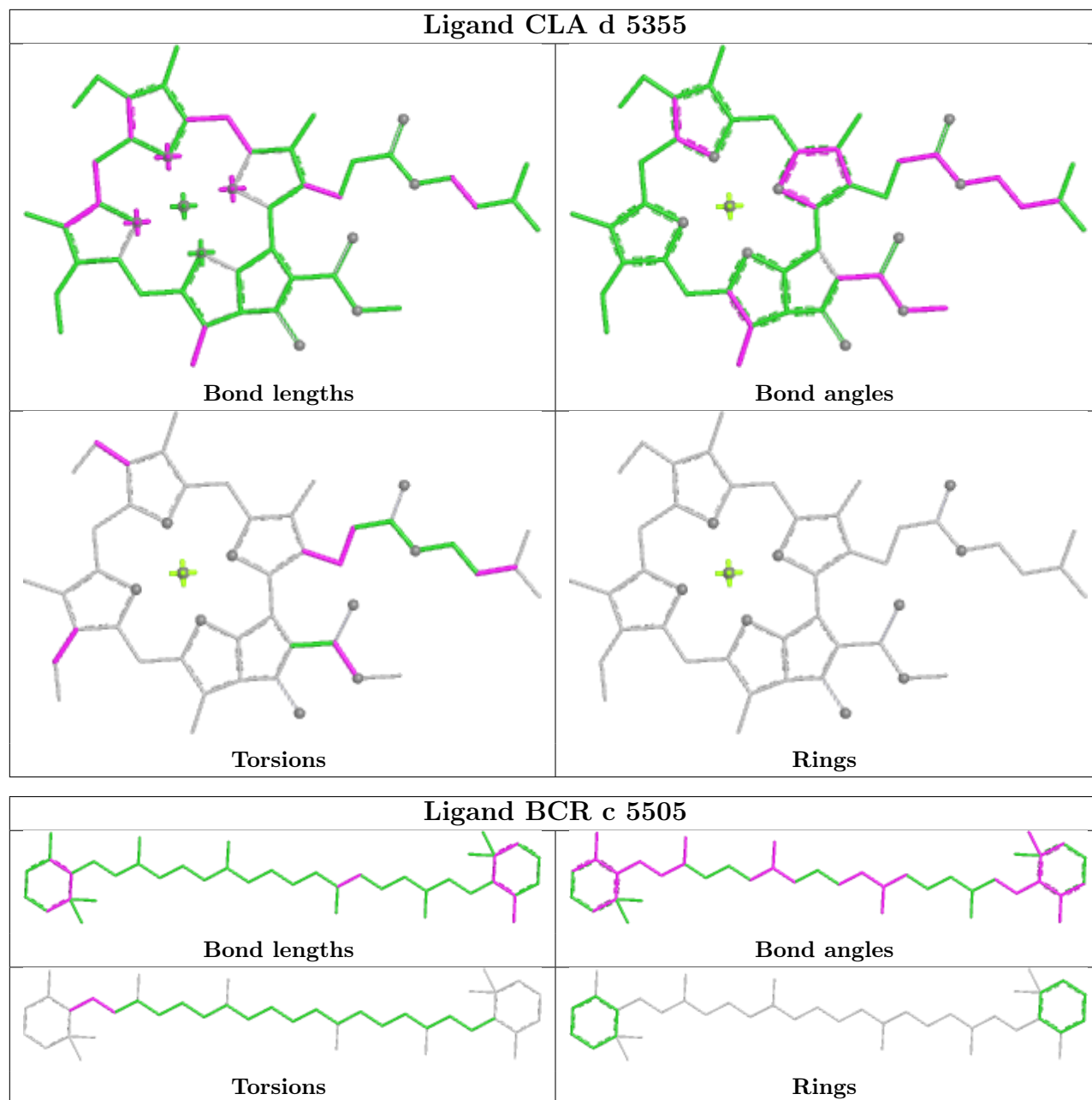


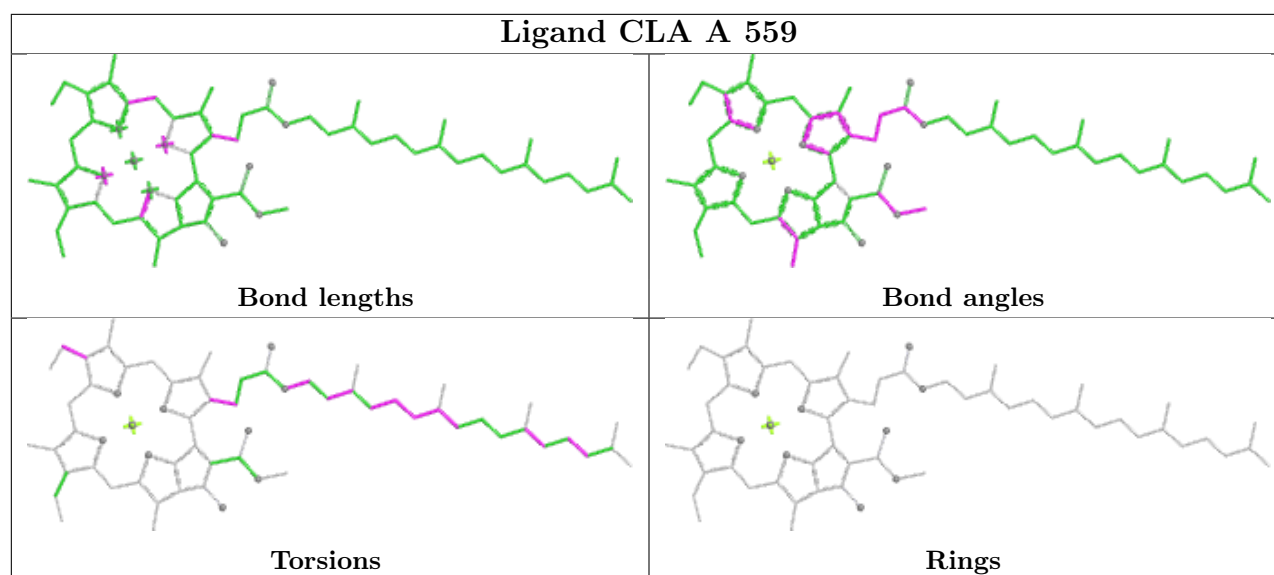
Ligand DGD c 5509



Ligand DGD C 509			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

Ligand BCR B 527			
			
Bond lengths	Bond angles		
			
Torsions	Rings		





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/344 (97%)	-0.62	0 100 100	40, 58, 78, 87	0
1	a	335/344 (97%)	-0.58	0 100 100	48, 65, 82, 98	0
2	B	488/510 (95%)	-0.63	0 100 100	40, 61, 78, 91	0
2	b	488/510 (95%)	-0.63	0 100 100	40, 62, 79, 91	0
3	C	447/473 (94%)	-0.57	2 (0%) 88 76	46, 68, 80, 88	0
3	c	447/473 (94%)	-0.43	1 (0%) 91 83	53, 75, 86, 98	0
4	D	340/352 (96%)	-0.75	0 100 100	35, 58, 76, 89	0
4	d	340/352 (96%)	-0.65	1 (0%) 90 79	42, 65, 83, 95	0
5	E	82/84 (97%)	-0.32	1 (1%) 76 55	55, 70, 86, 94	0
5	e	82/84 (97%)	-0.21	1 (1%) 76 55	65, 77, 90, 94	0
6	F	35/45 (77%)	-0.34	1 (2%) 53 31	55, 67, 82, 85	0
6	f	35/45 (77%)	-0.31	0 100 100	67, 75, 87, 89	0
7	H	64/66 (96%)	-0.40	0 100 100	57, 72, 81, 87	0
7	h	64/66 (96%)	-0.47	0 100 100	62, 71, 81, 93	0
8	I	35/38 (92%)	-0.47	0 100 100	57, 66, 80, 88	0
8	i	35/38 (92%)	-0.46	0 100 100	62, 72, 86, 88	0
9	J	34/40 (85%)	-0.28	0 100 100	55, 68, 72, 74	0
9	j	34/40 (85%)	-0.30	0 100 100	68, 74, 79, 86	0
10	K	37/37 (100%)	-0.62	0 100 100	60, 68, 80, 87	0
10	k	37/37 (100%)	-0.33	0 100 100	76, 80, 93, 97	0
11	L	37/37 (100%)	-0.39	0 100 100	43, 61, 95, 100	0
11	l	37/37 (100%)	-0.51	0 100 100	45, 56, 86, 91	0
12	M	36/36 (100%)	-0.43	0 100 100	52, 58, 89, 94	0
12	m	36/36 (100%)	-0.49	0 100 100	54, 60, 86, 91	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
13	O	242/247 (97%)	-0.47	1 (0%) 88 76	44, 65, 88, 101	0
13	o	242/247 (97%)	-0.43	0 100 100	43, 71, 88, 97	0
14	T	30/32 (93%)	-0.38	0 100 100	47, 61, 91, 97	0
14	t	30/32 (93%)	-0.43	0 100 100	48, 60, 89, 93	0
15	U	98/104 (94%)	-0.58	0 100 100	44, 60, 76, 83	0
15	u	98/104 (94%)	-0.56	0 100 100	52, 64, 74, 89	0
16	V	137/137 (100%)	-0.60	1 (0%) 84 66	47, 60, 75, 84	0
16	v	137/137 (100%)	-0.42	0 100 100	54, 74, 87, 99	0
17	X	0/129	-	-	-	-
17	x	0/129	-	-	-	-
18	Z	62/62 (100%)	-0.28	0 100 100	67, 76, 93, 96	0
18	z	62/62 (100%)	-0.04	0 100 100	73, 87, 94, 97	0
All	All	5078/5546 (91%)	-0.54	9 (0%) 91 83	35, 66, 85, 101	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	222	GLY	3.6
16	V	27	ALA	3.0
5	E	4	THR	2.5
5	e	5006	GLY	2.3
4	d	5013	GLY	2.3
13	O	61	SER	2.1
3	c	5159	THR	2.0
6	F	17	THR	2.0
3	C	78	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
29	UNL	C	486	8/-	0.49	0.12	55,56,59,60	0
29	UNL	c	5490	4/-	0.63	0.10	91,92,92,92	0
20	CLA	B	511	41/65	0.64	0.13	88,90,92,98	0
20	CLA	b	5511	41/65	0.65	0.13	88,92,95,96	0
29	UNL	c	5485	5/-	0.67	0.08	68,69,69,70	0
29	UNL	C	485	5/-	0.67	0.11	57,59,61,61	0
29	UNL	C	477	7/-	0.71	0.12	47,49,51,51	0
29	UNL	C	481	13/-	0.71	0.10	61,64,68,69	0
27	LMT	A	569	35/35	0.71	0.12	80,89,92,93	0
29	UNL	c	5479	11/-	0.72	0.12	76,77,77,77	0
29	UNL	c	5481	13/-	0.72	0.09	60,62,66,66	0
29	UNL	C	484	5/-	0.75	0.10	47,51,52,53	0
29	UNL	C	479	11/-	0.75	0.10	58,64,67,67	0
29	UNL	C	482	13/-	0.75	0.09	64,66,67,67	0
29	UNL	c	5486	8/-	0.75	0.08	63,64,65,66	0
29	UNL	C	487	7/-	0.75	0.07	49,52,52,53	0
29	UNL	c	5483	13/-	0.76	0.10	71,75,80,82	0
26	SQD	a	212	26/54	0.77	0.10	82,94,101,103	0
29	UNL	C	476	9/-	0.77	0.06	61,62,63,64	0
29	UNL	c	5478	11/-	0.77	0.09	76,79,81,81	0
26	SQD	A	5212	26/54	0.78	0.11	75,100,107,107	0
29	UNL	c	5484	5/-	0.78	0.09	69,69,70,72	0
27	LMT	a	5568	35/35	0.78	0.10	79,92,94,96	0
29	UNL	c	5480	7/-	0.78	0.13	65,66,66,67	0
29	UNL	c	5489	7/-	0.78	0.09	73,73,74,74	0
28	MGE	i	5201	48/48	0.78	0.10	67,83,88,90	0
27	LMT	m	216	35/35	0.79	0.10	62,87,89,91	0
29	UNL	C	488	5/-	0.79	0.09	41,45,47,47	0
29	UNL	C	478	11/-	0.79	0.08	58,65,66,66	0
29	UNL	c	5488	5/-	0.81	0.07	59,59,59,60	0
29	UNL	C	483	13/-	0.81	0.10	61,68,78,78	0
29	UNL	C	475	12/-	0.81	0.08	68,69,72,73	0
26	SQD	L	5213	47/54	0.82	0.10	52,85,106,108	0
29	UNL	C	480	7/-	0.82	0.12	35,36,38,38	0
24	BCR	c	5506	40/40	0.82	0.09	75,81,86,86	0
27	LMT	t	5217	35/35	0.82	0.13	76,95,104,105	0
29	UNL	c	5482	13/-	0.82	0.08	60,61,71,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
20	CLA	c	5501	65/65	0.82	0.10	82,91,94,95	0
24	BCR	C	505	40/40	0.83	0.11	75,81,91,92	0
27	LMT	T	217	35/35	0.83	0.12	83,93,96,97	0
24	BCR	c	5505	40/40	0.83	0.10	84,87,91,92	0
20	CLA	c	5502	51/65	0.83	0.10	93,96,97,98	0
26	SQD	d	5358	54/54	0.83	0.10	74,85,106,107	0
29	UNL	c	5477	7/-	0.83	0.14	67,68,70,70	0
28	MGE	d	5359	47/48	0.84	0.10	72,81,96,98	0
28	MGE	d	5360	41/48	0.84	0.09	68,72,78,80	0
22	PQ9	A	564	30/45	0.84	0.14	54,57,63,64	30
27	LMT	M	5216	35/35	0.84	0.09	58,83,90,90	0
20	CLA	c	5498	65/65	0.84	0.10	81,90,93,93	0
28	MGE	d	5361	48/48	0.85	0.09	61,68,78,83	0
24	BCR	H	107	40/40	0.85	0.10	77,83,88,89	0
28	MGE	l	5210	48/48	0.85	0.09	59,69,78,81	0
29	UNL	c	5475	12/-	0.85	0.07	74,78,84,84	0
29	UNL	c	5476	9/-	0.85	0.05	58,60,62,62	0
26	SQD	A	568	54/54	0.85	0.09	76,82,90,90	0
29	UNL	c	5487	7/-	0.85	0.06	57,57,58,58	0
28	MGE	D	358	47/48	0.85	0.10	65,72,79,81	0
20	CLA	c	5491	65/65	0.85	0.09	70,78,81,86	0
26	SQD	t	213	47/54	0.85	0.10	61,95,116,117	0
28	MGE	b	5530	48/48	0.86	0.09	59,64,71,73	0
22	PQ9	a	5564	30/45	0.86	0.10	51,55,62,62	30
20	CLA	B	526	65/65	0.86	0.10	71,82,97,98	0
20	CLA	b	5526	65/65	0.86	0.09	66,71,92,95	0
20	CLA	C	502	51/65	0.86	0.09	74,80,83,84	0
20	CLA	c	5503	50/65	0.86	0.10	88,91,92,93	0
20	CLA	c	5495	65/65	0.86	0.09	74,81,86,88	0
28	MGE	I	201	48/48	0.86	0.09	73,81,89,90	0
28	MGE	L	210	48/48	0.86	0.09	59,68,73,75	0
30	DGD	C	507	53/66	0.86	0.10	55,66,86,88	0
30	DGD	c	5507	53/66	0.86	0.09	66,74,90,91	0
30	DGD	c	5509	57/66	0.86	0.08	67,72,77,78	0
31	BCT	d	5353	4/4	0.86	0.06	75,75,76,77	0
20	CLA	B	516	65/65	0.87	0.10	61,76,92,97	0
20	CLA	c	5497	65/65	0.87	0.10	66,82,84,87	0
28	MGE	D	359	41/48	0.87	0.09	60,67,76,79	0
28	MGE	D	360	48/48	0.87	0.09	52,60,63,68	0
24	BCR	B	527	40/40	0.87	0.09	58,65,68,69	0
29	UNL	C	489	7/-	0.87	0.12	75,76,77,78	0
30	DGD	C	508	47/66	0.87	0.12	61,71,80,83	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
29	UNL	c	5474	15/-	0.87	0.06	39,50,56,56	0
30	DGD	c	5508	47/66	0.87	0.11	66,76,82,84	0
24	BCR	h	5107	40/40	0.87	0.09	74,79,82,83	0
20	CLA	b	5519	65/65	0.87	0.08	70,75,80,81	0
20	CLA	B	519	65/65	0.88	0.08	73,82,85,87	0
20	CLA	C	497	65/65	0.88	0.09	74,78,80,82	0
24	BCR	d	5357	40/40	0.88	0.09	61,72,86,88	0
30	DGD	C	509	57/66	0.88	0.09	52,60,69,70	0
29	UNL	C	474	15/-	0.88	0.05	26,37,40,40	0
20	CLA	b	5524	56/65	0.88	0.10	63,68,89,91	0
24	BCR	D	357	40/40	0.88	0.08	61,66,78,80	0
20	CLA	B	525	65/65	0.88	0.09	67,84,91,92	0
20	CLA	c	5493	65/65	0.89	0.09	67,81,86,86	0
20	CLA	B	524	56/65	0.89	0.09	67,72,77,80	0
24	BCR	B	528	40/40	0.89	0.09	54,68,74,75	0
20	CLA	C	495	65/65	0.89	0.08	58,68,74,76	0
28	MGE	B	530	48/48	0.89	0.09	55,64,70,72	0
24	BCR	C	506	40/40	0.89	0.08	68,72,79,80	0
24	BCR	x	5130	40/40	0.89	0.08	77,81,85,86	0
30	DGD	h	5208	54/66	0.89	0.08	57,68,73,75	0
20	CLA	b	5520	65/65	0.89	0.09	63,72,74,76	0
24	BCR	b	5529	40/40	0.90	0.08	69,72,74,74	0
24	BCR	c	5504	40/40	0.90	0.09	73,80,88,89	0
20	CLA	c	5496	65/65	0.90	0.08	79,83,95,97	0
20	CLA	b	5525	65/65	0.90	0.09	71,77,80,82	0
20	CLA	b	5518	65/65	0.90	0.08	60,64,69,75	0
20	CLA	C	498	65/65	0.90	0.09	64,74,98,101	0
24	BCR	t	104	40/40	0.90	0.07	65,72,84,85	0
24	BCR	B	529	40/40	0.90	0.07	62,69,80,80	0
25	LHG	A	567	39/49	0.90	0.08	57,73,79,81	0
25	LHG	a	5567	39/49	0.90	0.07	65,68,74,80	0
30	DGD	H	208	54/66	0.90	0.09	61,69,75,76	0
20	CLA	C	503	50/65	0.90	0.10	83,86,88,94	0
20	CLA	C	501	65/65	0.90	0.08	70,78,83,85	0
20	CLA	d	5355	50/65	0.90	0.08	74,77,80,81	0
21	PHO	a	5562	64/64	0.90	0.09	70,75,81,82	0
24	BCR	X	130	40/40	0.90	0.08	68,71,80,81	0
20	CLA	c	5500	65/65	0.91	0.09	64,69,82,83	0
20	CLA	a	5560	65/65	0.91	0.09	62,68,100,101	0
20	CLA	B	522	65/65	0.91	0.09	54,65,75,77	0
20	CLA	b	5512	65/65	0.91	0.09	68,72,75,76	0
20	CLA	b	5516	65/65	0.91	0.09	62,66,84,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
24	BCR	T	5104	40/40	0.91	0.09	67,71,78,79	0
20	CLA	C	500	65/65	0.91	0.09	59,63,73,74	0
24	BCR	b	5527	40/40	0.91	0.09	58,63,72,72	0
20	CLA	B	518	65/65	0.91	0.07	53,64,79,79	0
20	CLA	C	496	65/65	0.91	0.08	71,78,88,89	0
20	CLA	B	520	65/65	0.91	0.09	62,67,76,79	0
20	CLA	c	5499	47/65	0.91	0.09	60,69,76,78	0
20	CLA	b	5523	65/65	0.92	0.08	45,52,74,75	0
20	CLA	B	513	65/65	0.92	0.09	56,61,67,67	0
20	CLA	C	491	65/65	0.92	0.07	63,70,77,79	0
29	UNL	C	490	4/-	0.92	0.04	67,67,68,68	0
20	CLA	C	494	46/65	0.92	0.08	59,66,68,72	0
20	CLA	b	5517	65/65	0.92	0.07	54,58,66,71	0
20	CLA	c	5492	60/65	0.92	0.08	57,61,83,84	0
20	CLA	B	523	65/65	0.92	0.08	47,56,73,74	0
21	PHO	a	5561	64/64	0.92	0.08	51,55,66,68	0
20	CLA	c	5494	46/65	0.92	0.09	72,77,86,88	0
20	CLA	B	514	65/65	0.92	0.08	59,64,82,83	0
20	CLA	B	512	65/65	0.92	0.07	68,75,78,79	0
22	PQ9	d	5356	30/45	0.92	0.07	51,57,66,66	0
23	OEC	A	565	5/9	0.92	0.07	62,63,65,66	0
20	CLA	b	5521	65/65	0.92	0.07	48,57,63,64	0
20	CLA	B	515	65/65	0.93	0.08	55,66,71,72	0
21	PHO	A	561	64/64	0.93	0.07	32,52,55,59	0
21	PHO	A	562	64/64	0.93	0.07	47,53,63,66	0
20	CLA	A	560	65/65	0.93	0.07	49,57,86,88	0
20	CLA	D	355	50/65	0.93	0.07	63,65,68,70	0
24	BCR	a	5566	40/40	0.93	0.07	59,75,78,79	0
20	CLA	B	521	65/65	0.93	0.08	58,63,66,68	0
24	BCR	b	5528	40/40	0.93	0.07	61,64,72,73	0
20	CLA	b	5522	65/65	0.93	0.09	60,66,75,76	0
20	CLA	a	5563	55/65	0.93	0.09	59,65,102,103	0
20	CLA	B	517	65/65	0.93	0.07	37,44,56,57	0
24	BCR	A	566	40/40	0.93	0.07	50,57,64,66	0
20	CLA	C	499	47/65	0.93	0.09	57,60,66,69	0
20	CLA	b	5513	65/65	0.93	0.07	54,61,84,90	0
20	CLA	C	493	65/65	0.93	0.09	67,71,77,79	0
24	BCR	C	504	40/40	0.93	0.07	57,64,70,70	0
20	CLA	A	563	55/65	0.93	0.08	43,49,75,78	0
32	HEM	f	5051	43/43	0.93	0.11	80,84,97,101	0
20	CLA	D	354	65/65	0.94	0.07	35,43,63,66	0
20	CLA	b	5515	65/65	0.94	0.08	46,51,74,76	0

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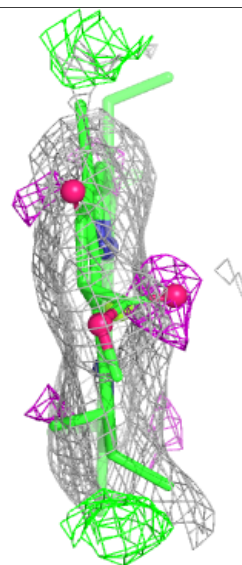
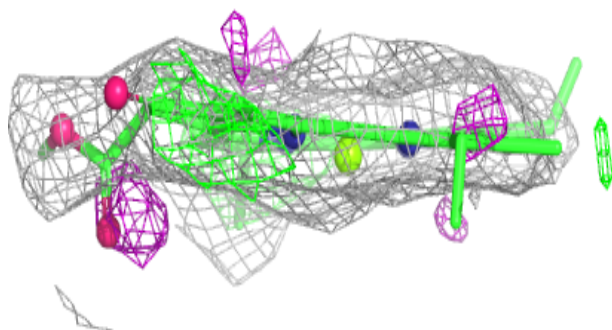
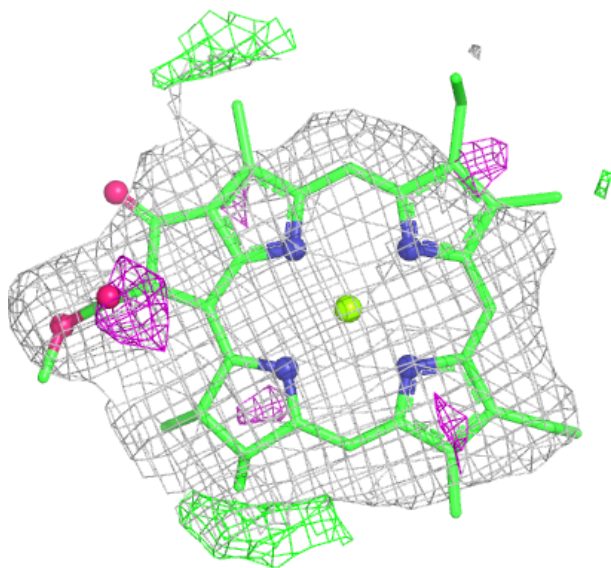
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
23	OEC	a	5565	5/9	0.94	0.05	63,64,71,87	0
22	PQ9	D	356	30/45	0.94	0.07	49,67,80,83	0
20	CLA	C	492	60/65	0.94	0.08	53,58,76,77	0
20	CLA	a	5559	65/65	0.95	0.07	42,49,60,60	0
20	CLA	d	5354	65/65	0.95	0.06	39,47,64,65	0
20	CLA	A	559	65/65	0.95	0.06	39,43,49,52	0
20	CLA	a	5558	65/65	0.95	0.07	41,50,55,61	0
32	HEM	F	51	43/43	0.95	0.10	78,84,92,95	0
20	CLA	b	5514	65/65	0.95	0.06	41,51,74,75	0
32	HEM	v	5552	43/43	0.95	0.08	65,67,70,70	0
33	CA	K	56	1/1	0.95	0.13	119,119,119,119	0
20	CLA	A	558	65/65	0.96	0.07	41,46,50,51	0
33	CA	k	5056	1/1	0.96	0.08	119,119,119,119	0
31	BCT	D	353	4/4	0.97	0.05	72,73,73,74	0
32	HEM	V	552	43/43	0.97	0.07	37,54,58,59	0
19	FE2	A	557	1/1	0.98	0.01	60,60,60,60	0
19	FE2	a	5557	1/1	1.00	0.03	75,75,75,75	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

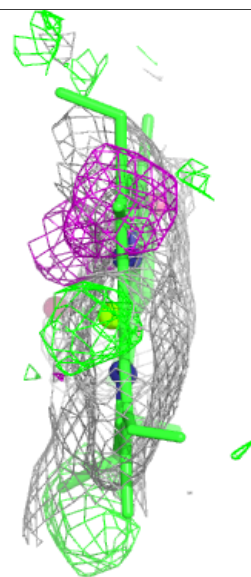
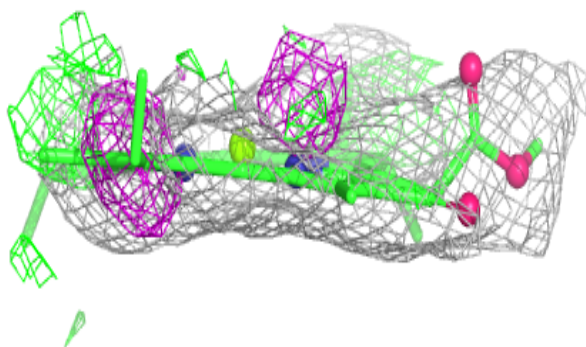
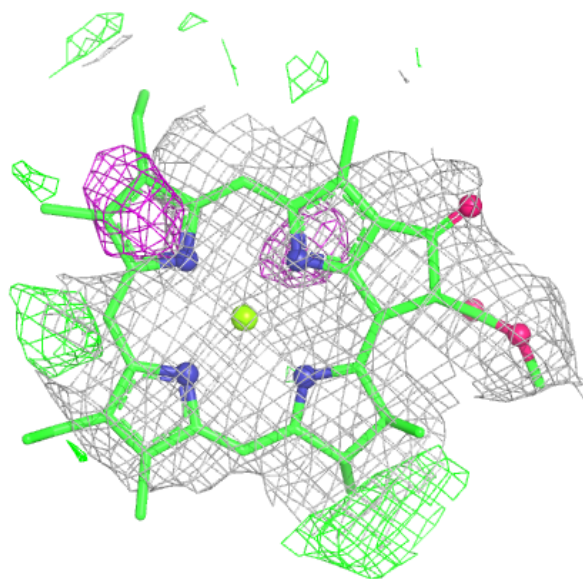
Electron density around CLA B 511:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



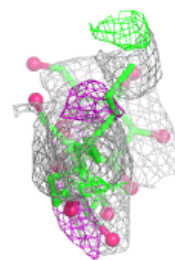
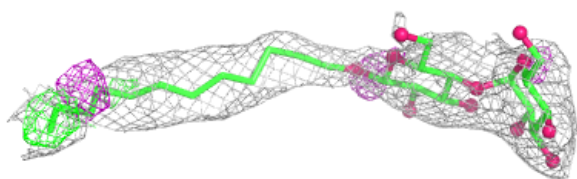
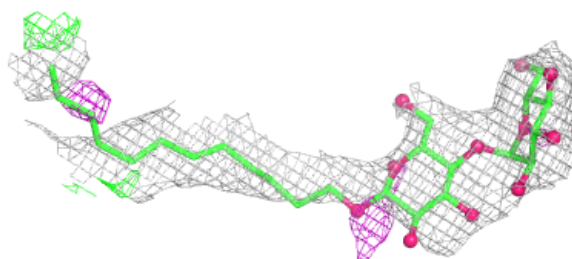
Electron density around CLA b 5511:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



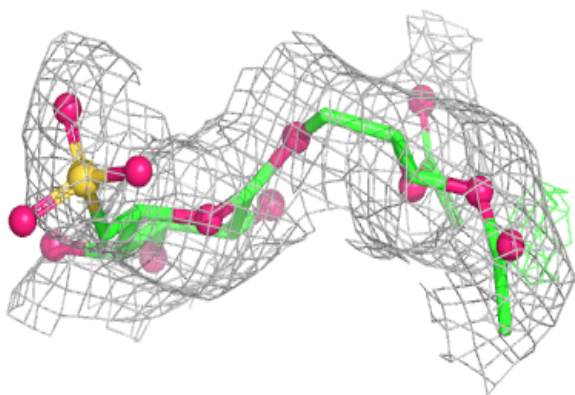
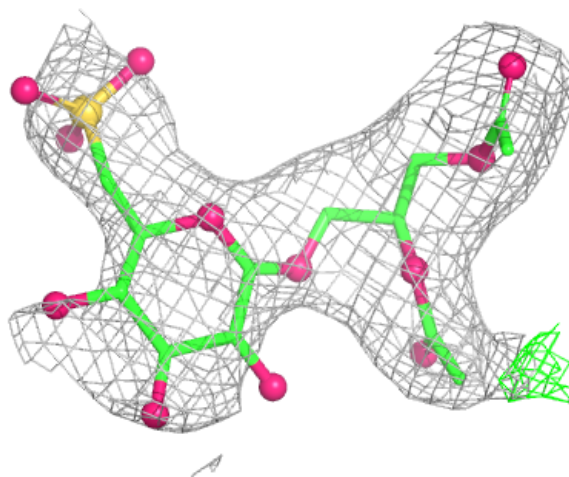
Electron density around LMT A 569:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



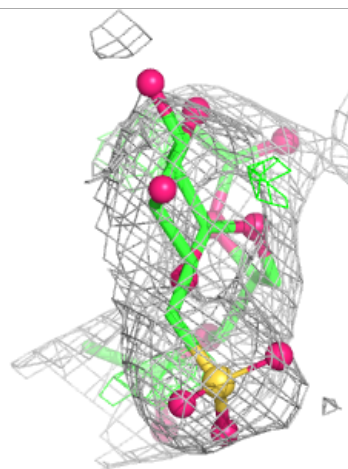
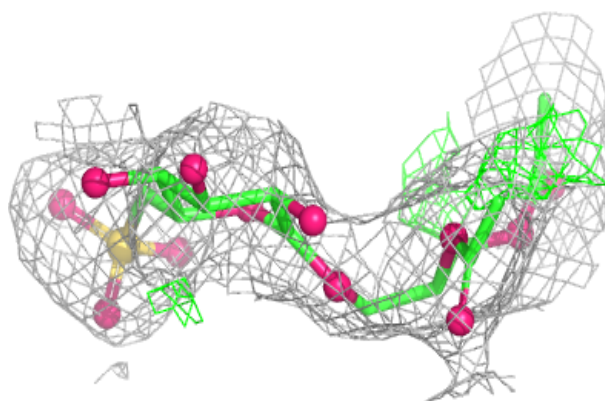
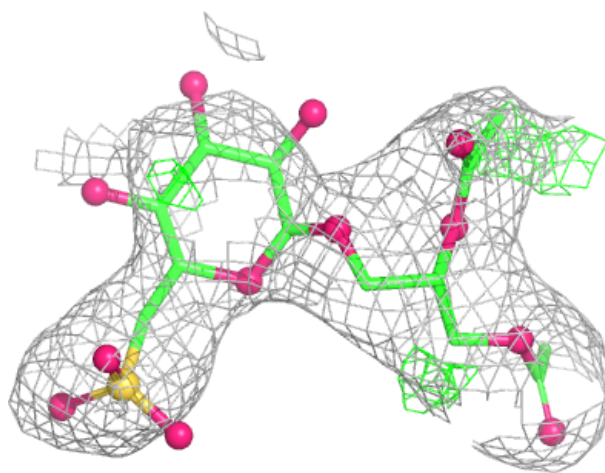
Electron density around SQD a 212:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



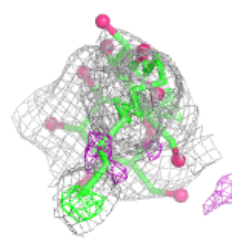
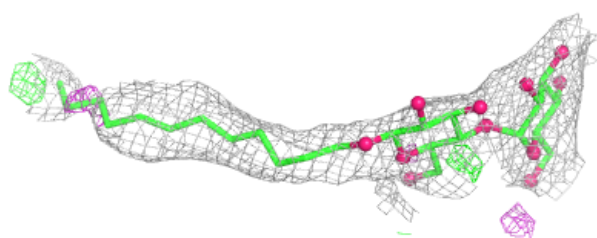
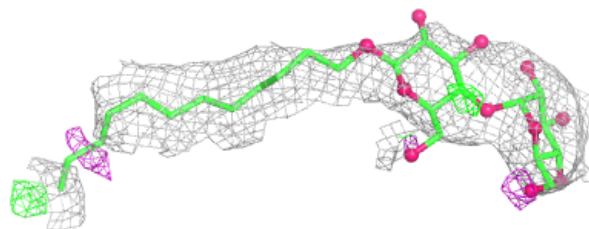
Electron density around SQD A 5212:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

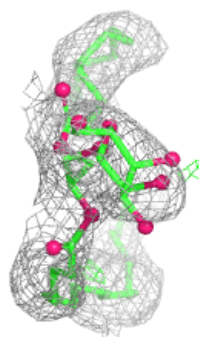
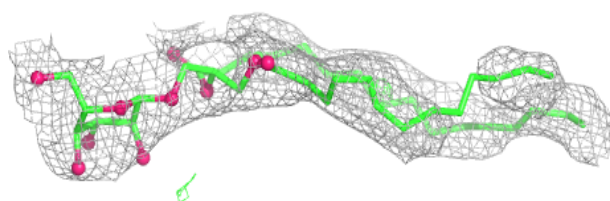
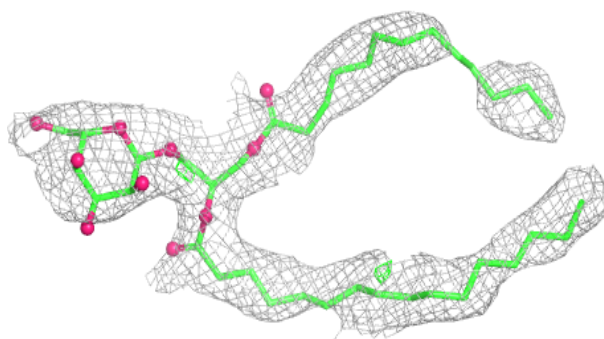


Electron density around LMT a 5568:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

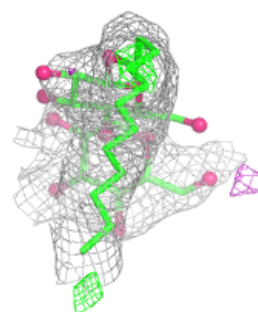
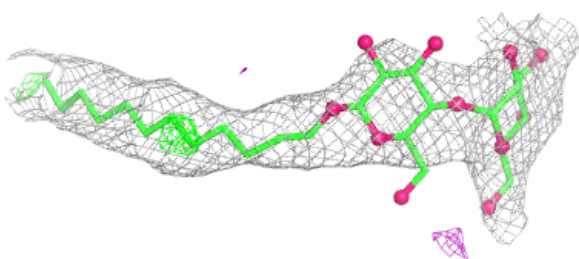
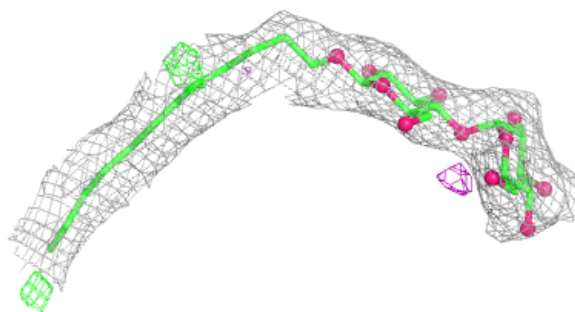
**Electron density around MGE i 5201:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

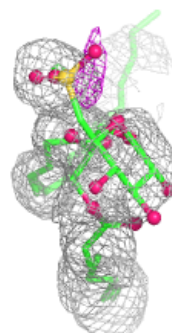
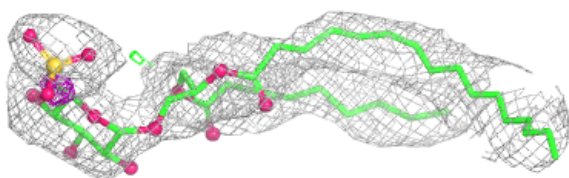
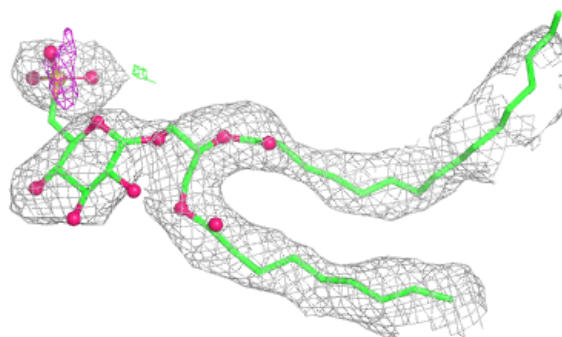


Electron density around LMT m 216:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

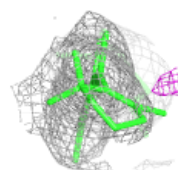
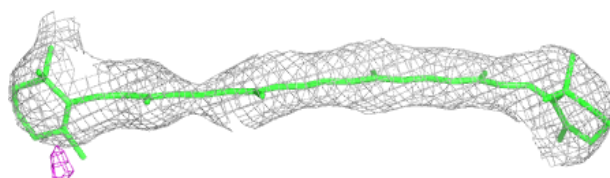
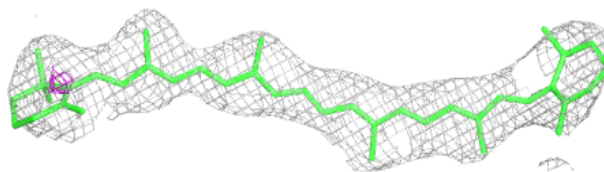
**Electron density around SQD L 5213:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

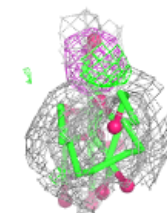
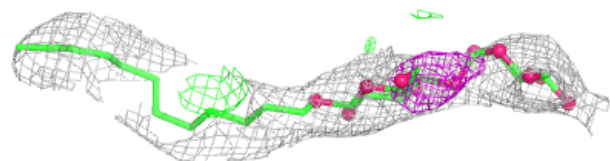
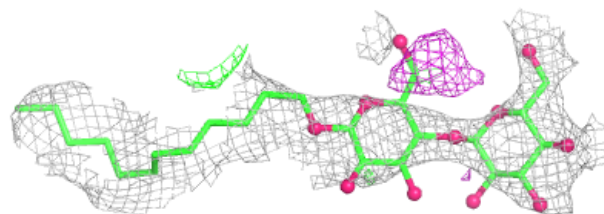


Electron density around BCR c 5506:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

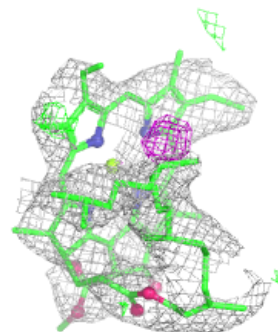
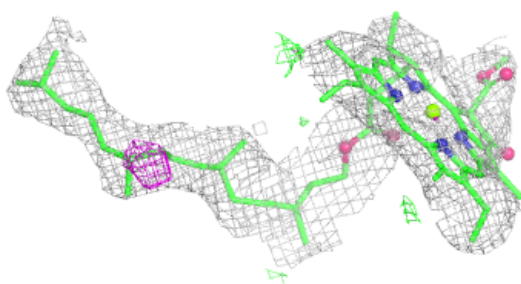
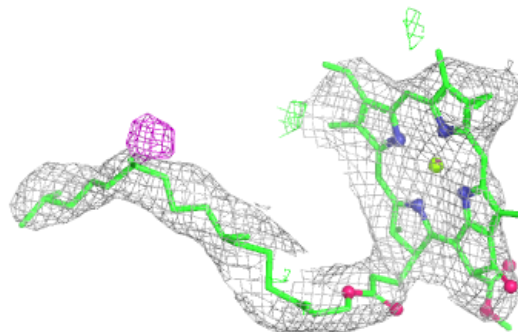
**Electron density around LMT t 5217:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

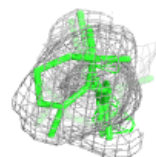
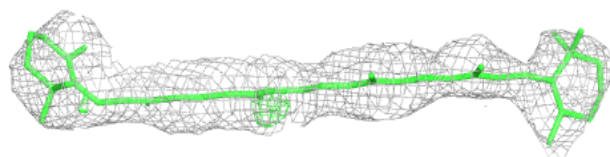
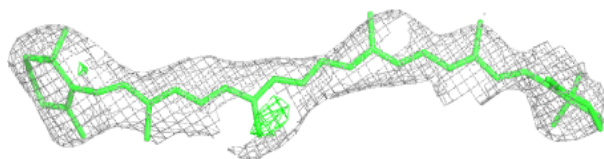


Electron density around CLA c 5501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

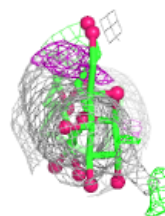
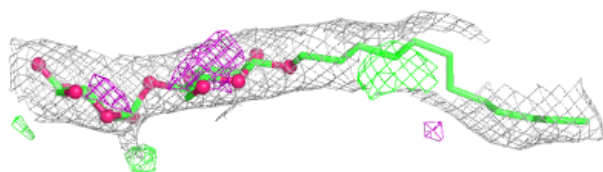
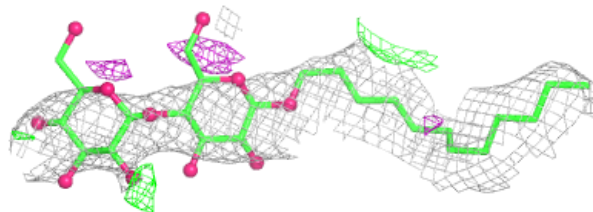
**Electron density around BCR C 505:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

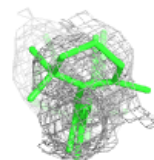
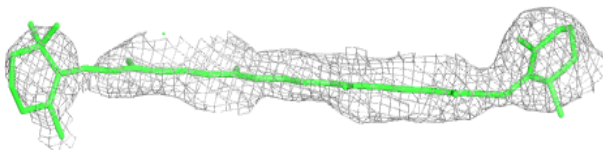
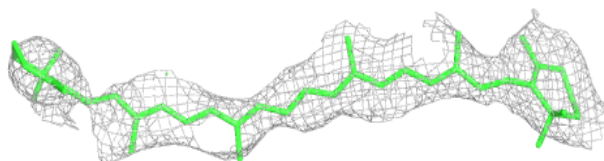


Electron density around LMT T 217:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

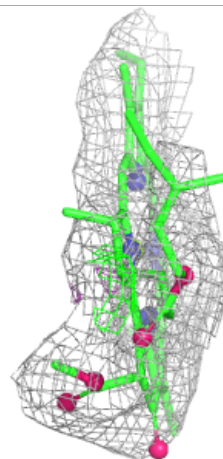
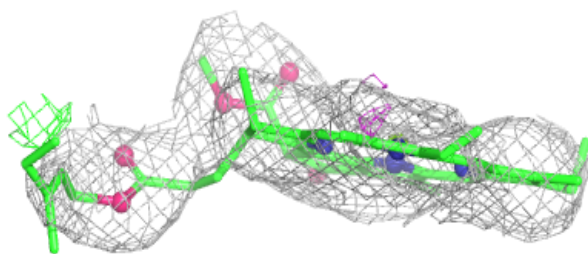
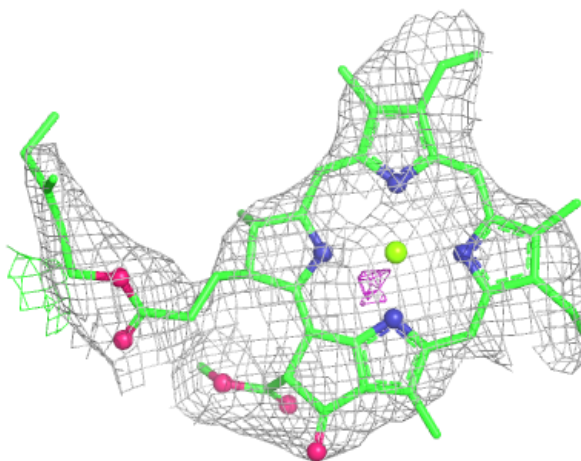
**Electron density around BCR c 5505:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



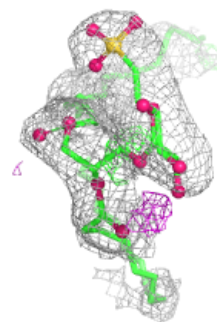
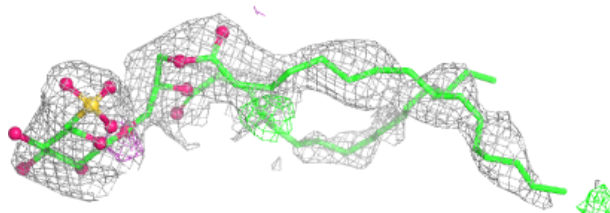
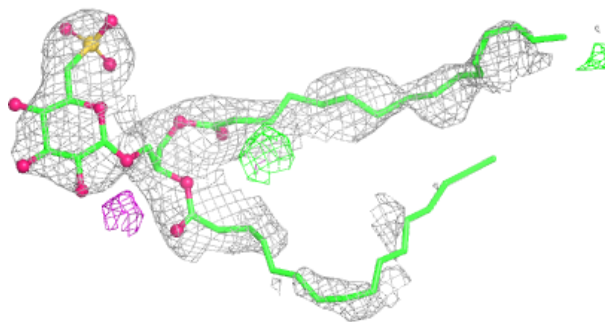
Electron density around CLA c 5502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

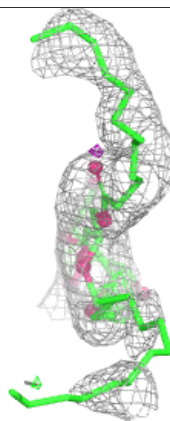
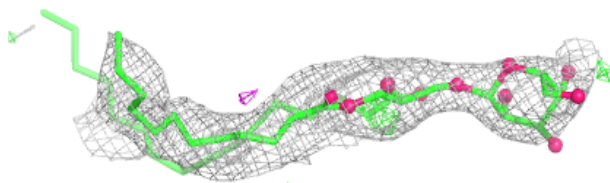
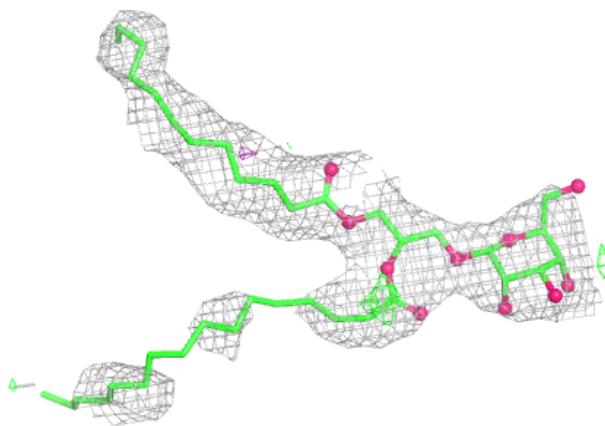


Electron density around SQD d 5358:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

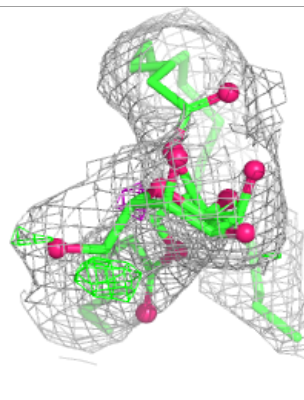
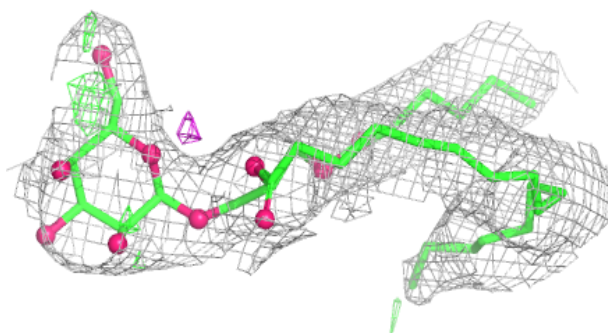
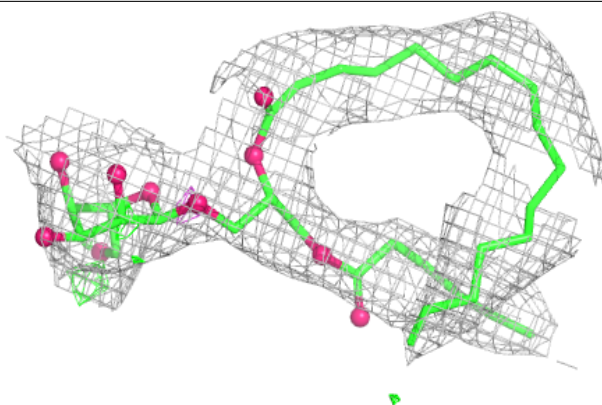
**Electron density around MGE d 5359:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

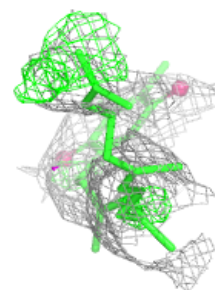
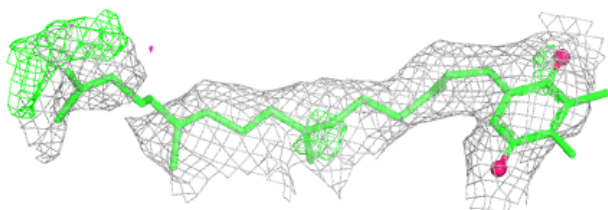
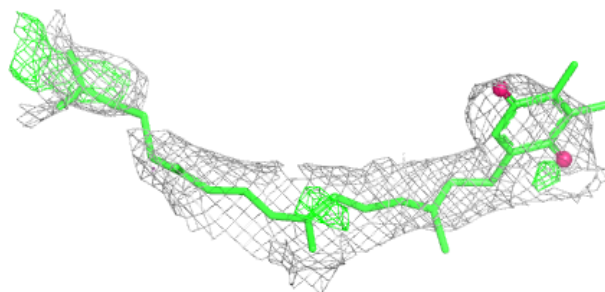


Electron density around MGE d 5360:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

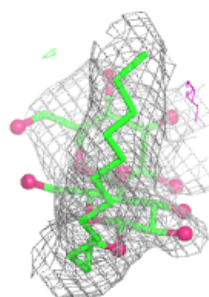
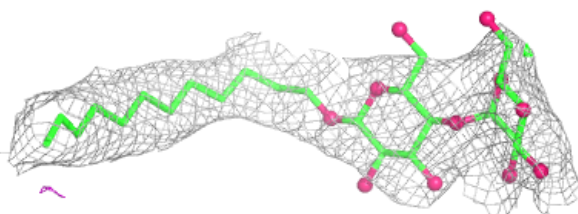
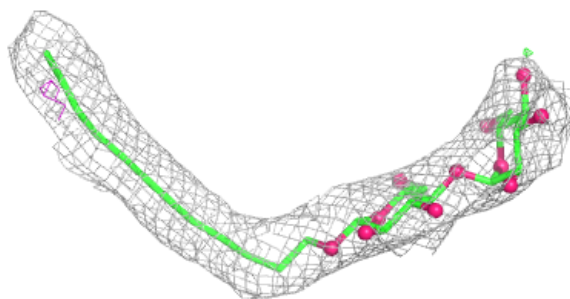
**Electron density around PQ9 A 564:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

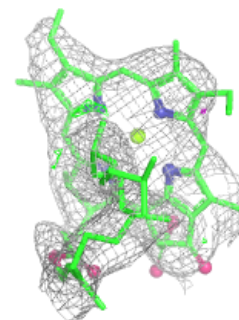
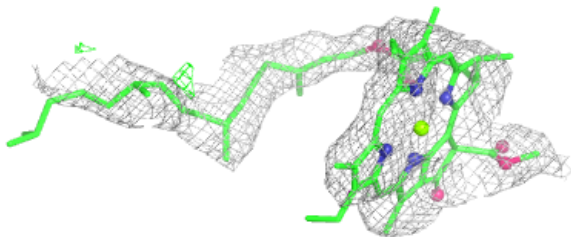
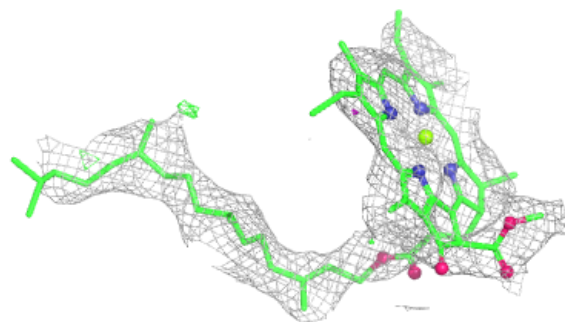


Electron density around LMT M 5216:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

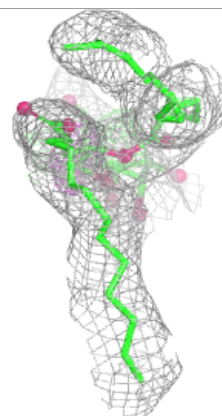
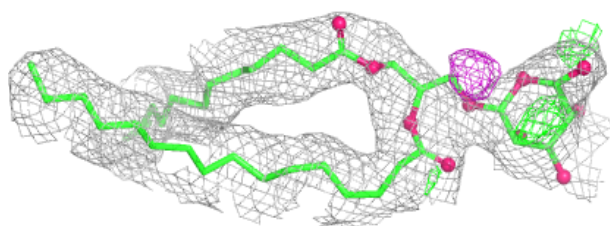
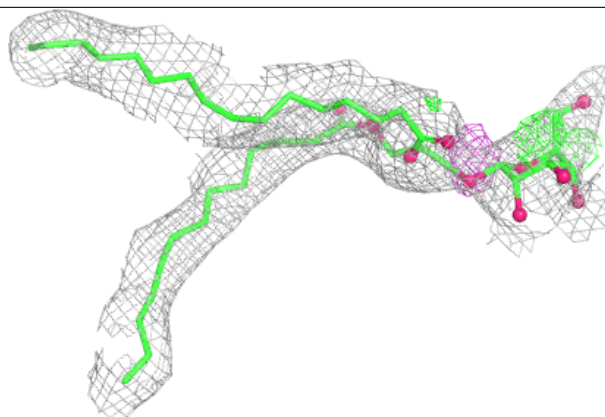
**Electron density around CLA c 5498:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

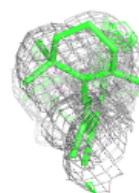
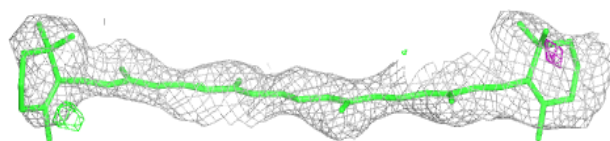
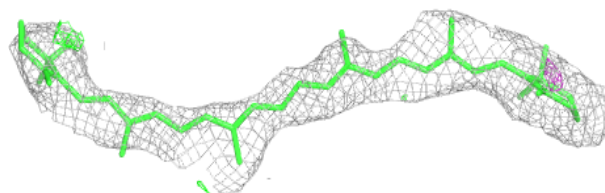


Electron density around MGE d 5361:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

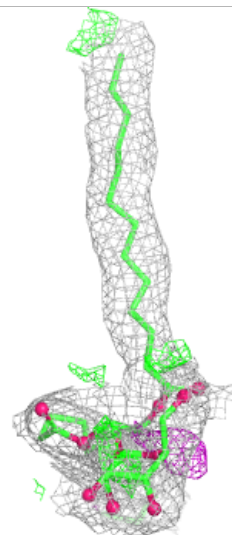
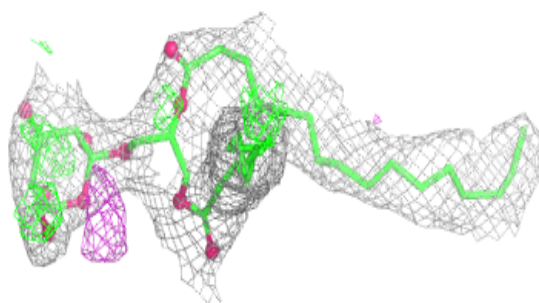
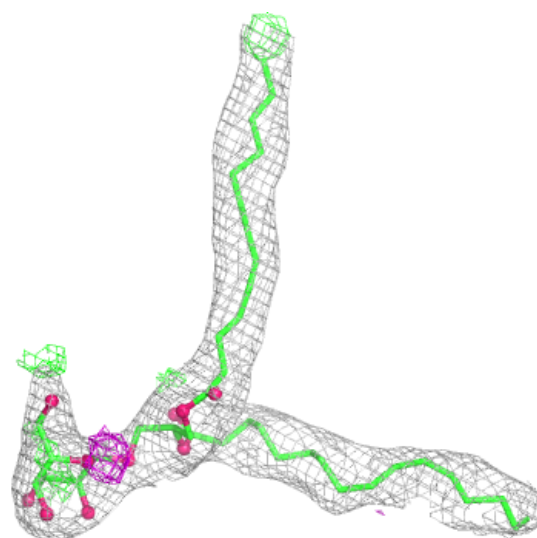
**Electron density around BCR H 107:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



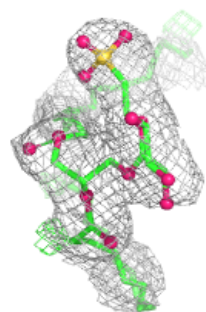
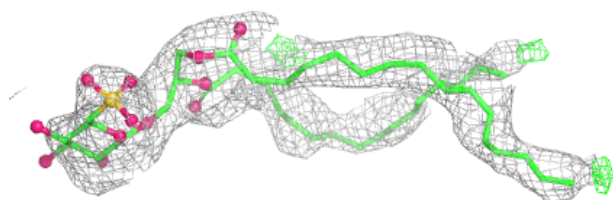
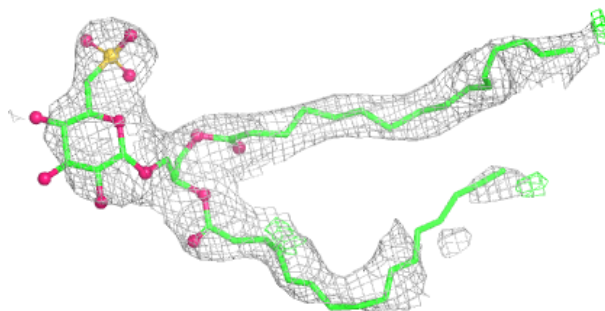
Electron density around MGE 1 5210:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

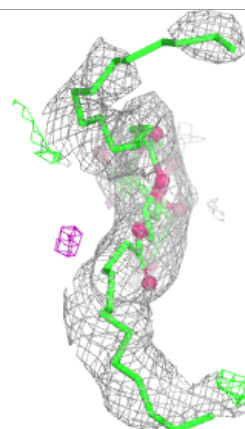
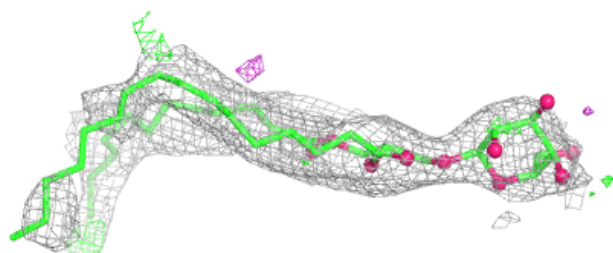
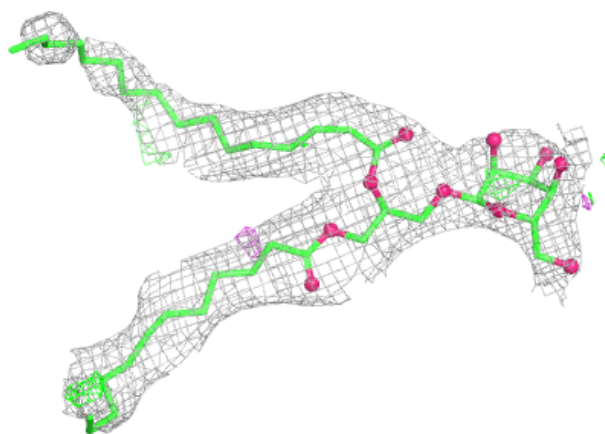


Electron density around SQD A 568:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

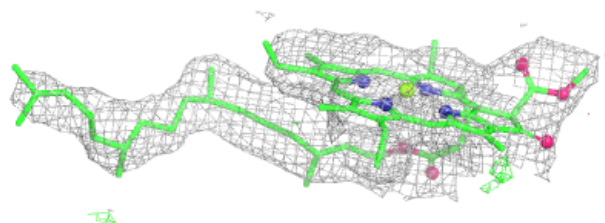
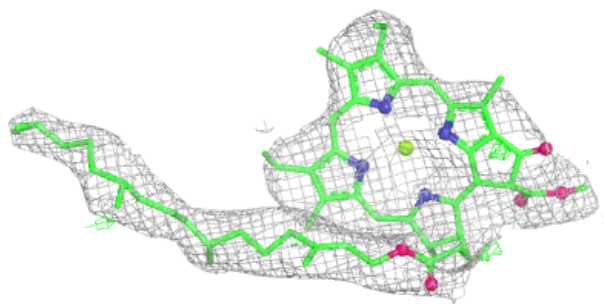
**Electron density around MGE D 358:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

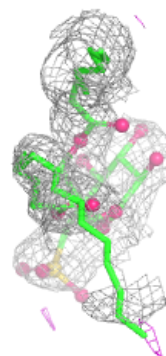
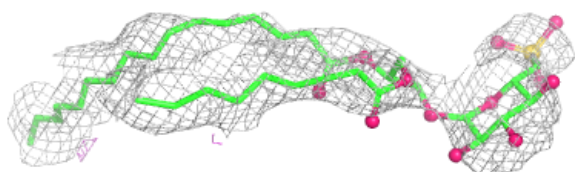
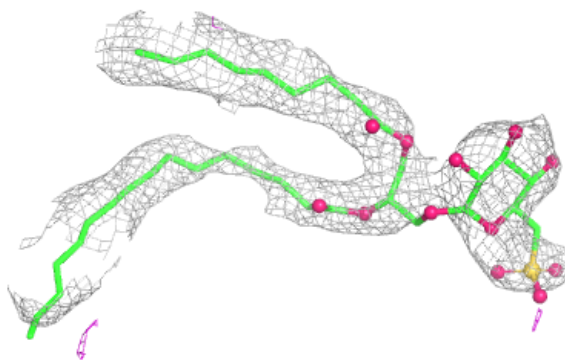


Electron density around CLA c 5491:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

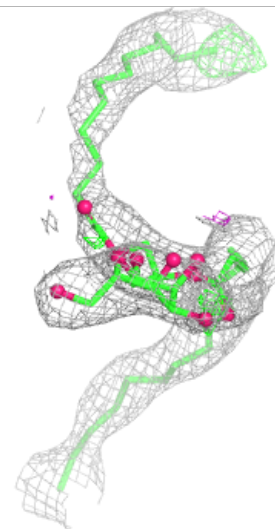
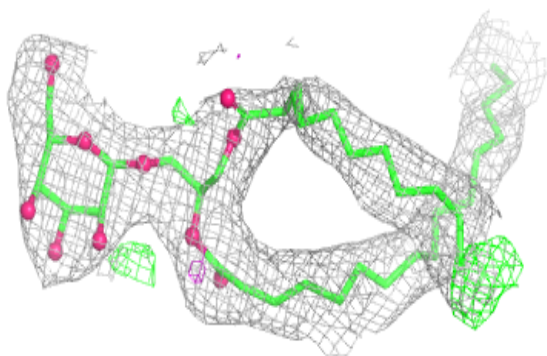
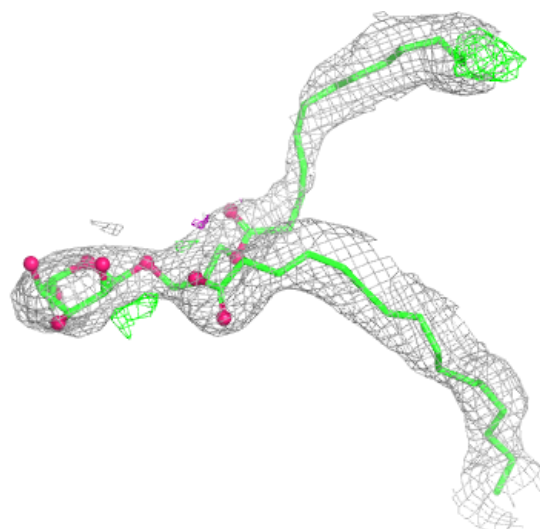
**Electron density around SQD t 213:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



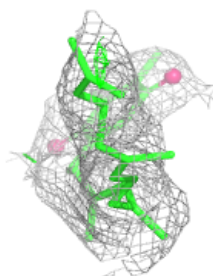
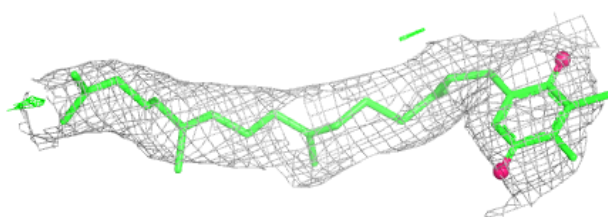
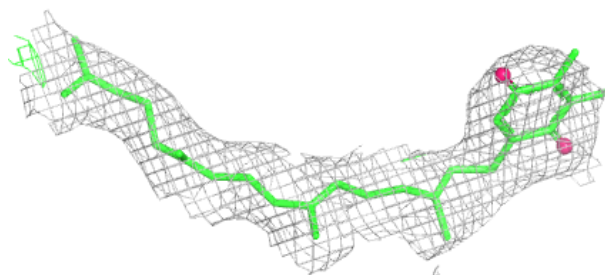
Electron density around MGE b 5530:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



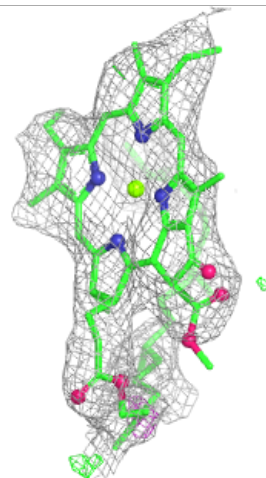
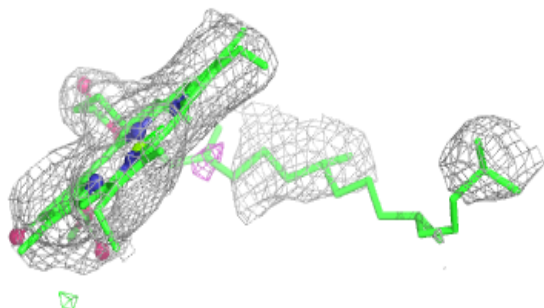
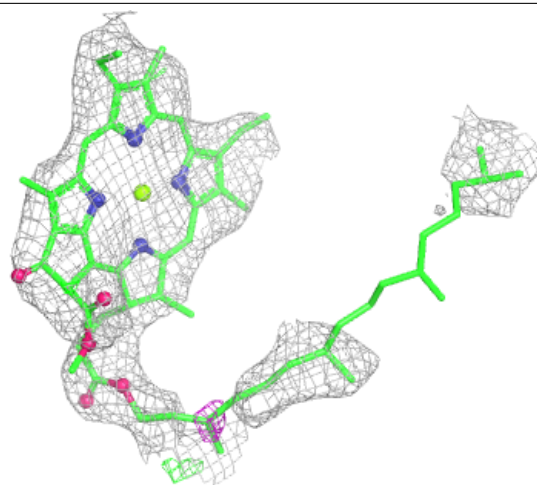
Electron density around PQ9 a 5564:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



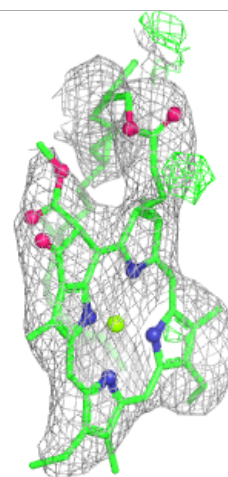
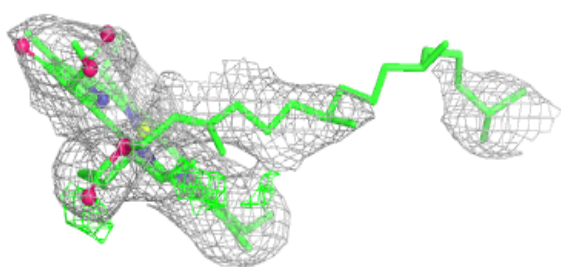
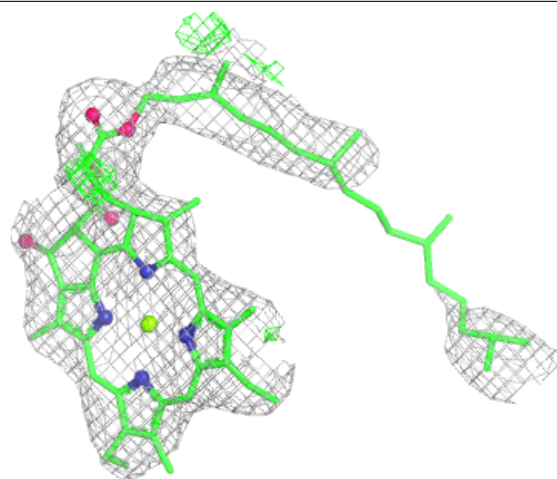
Electron density around CLA B 526:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



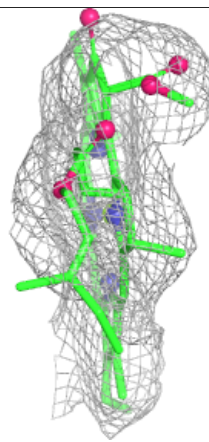
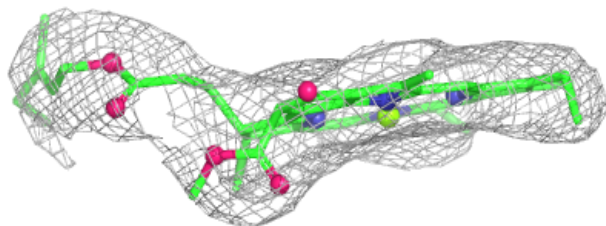
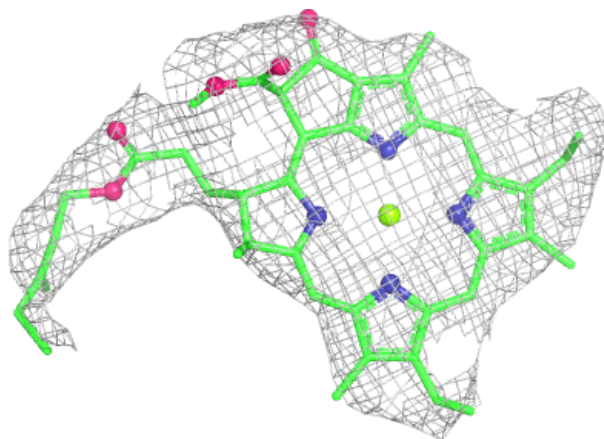
Electron density around CLA b 5526:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



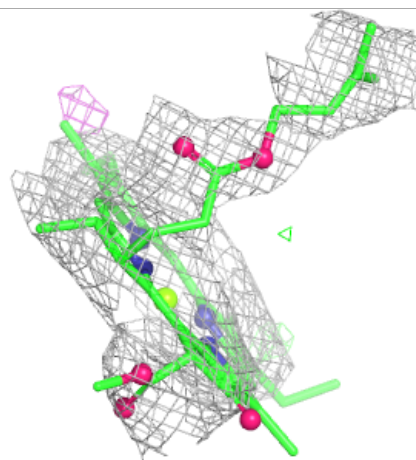
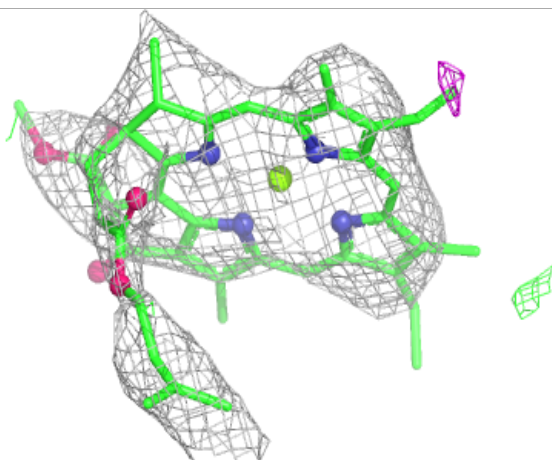
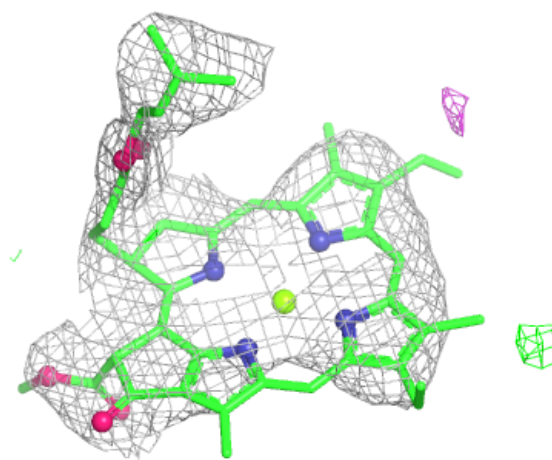
Electron density around CLA C 502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



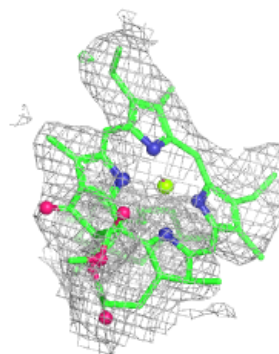
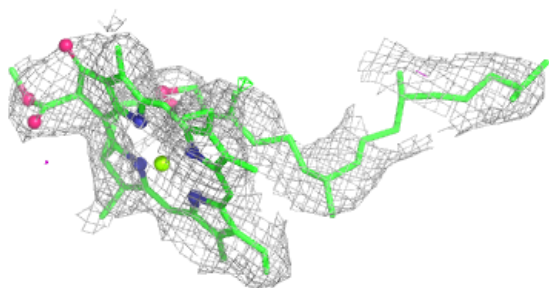
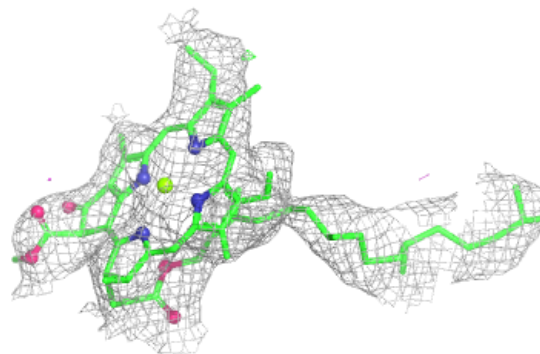
Electron density around CLA c 5503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

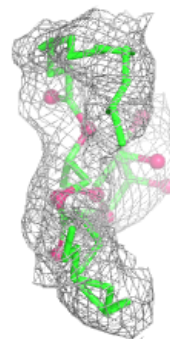
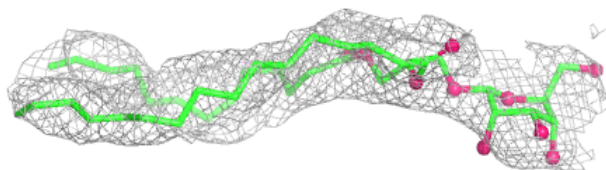
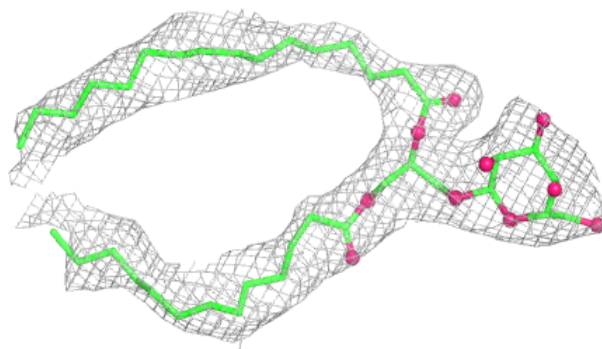


Electron density around CLA c 5495:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

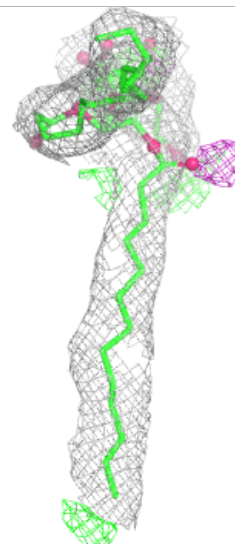
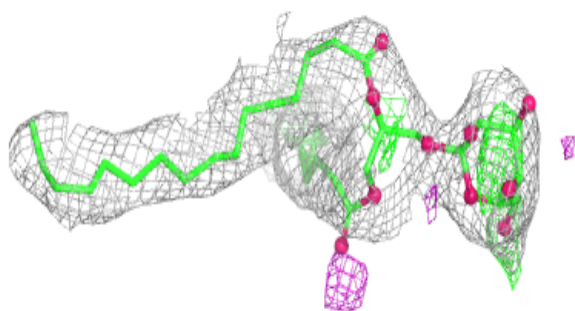
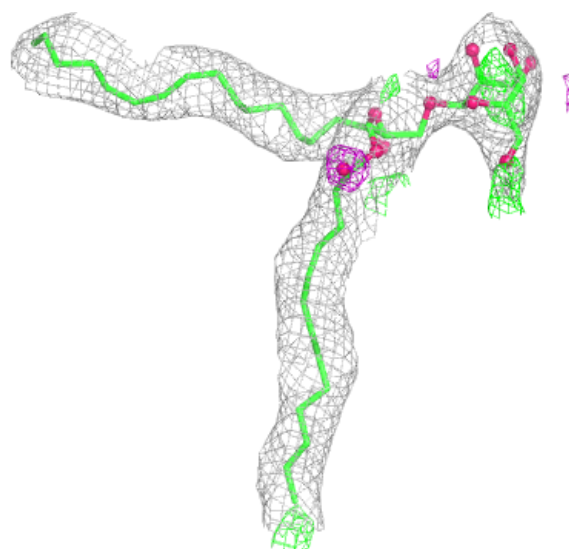
**Electron density around MGE I 201:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



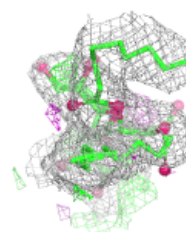
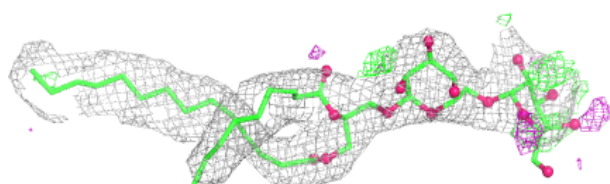
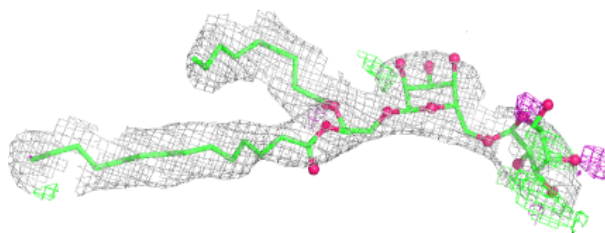
Electron density around MGE L 210:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

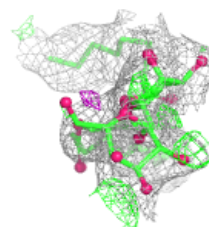
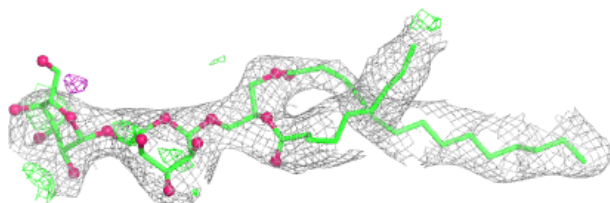
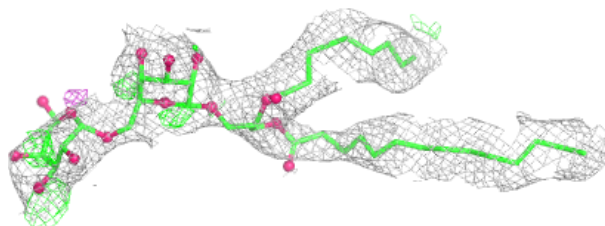


Electron density around DGD C 507:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

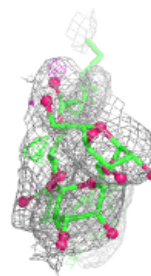
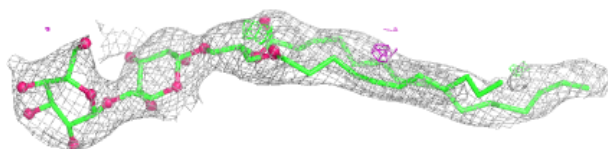
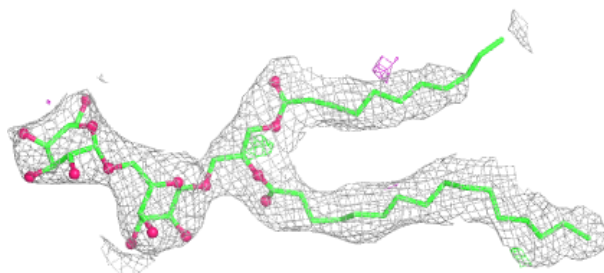
**Electron density around DGD c 5507:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

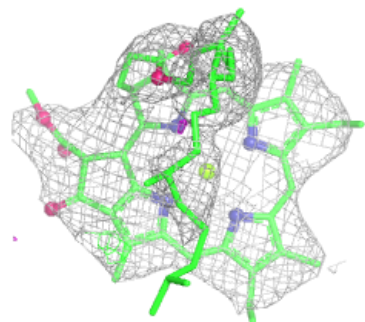
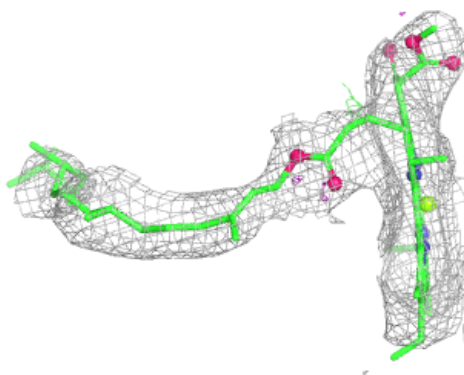
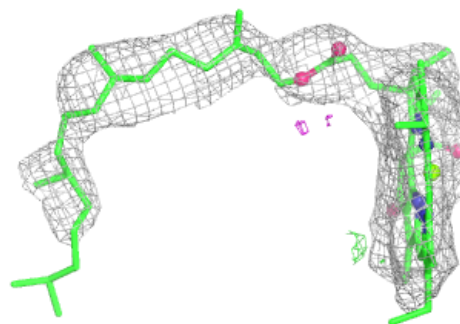


Electron density around DGD c 5509:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

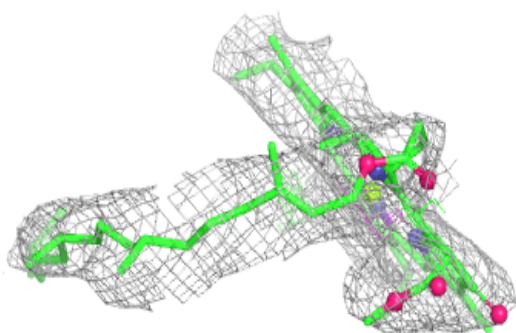
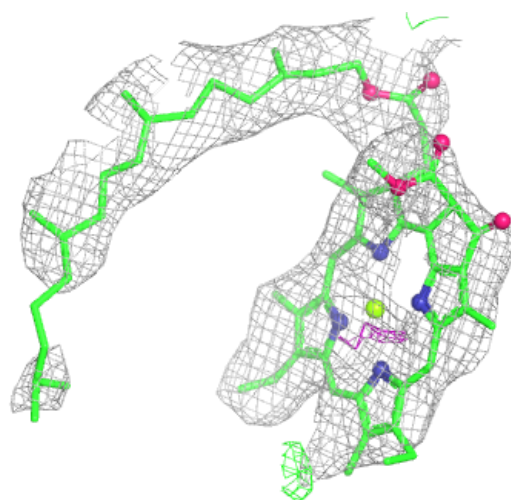
**Electron density around CLA B 516:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



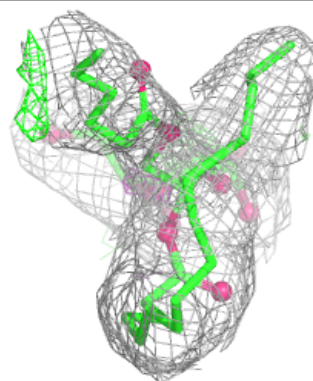
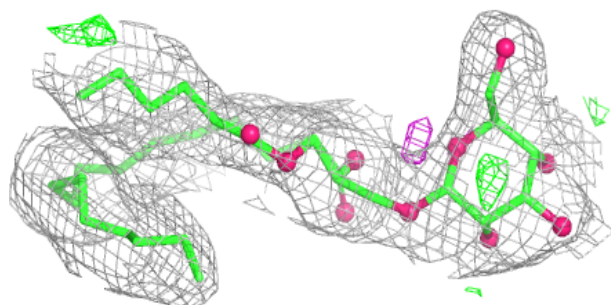
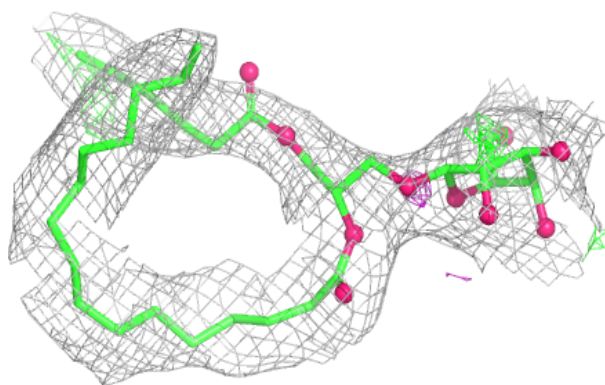
Electron density around CLA c 5497:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

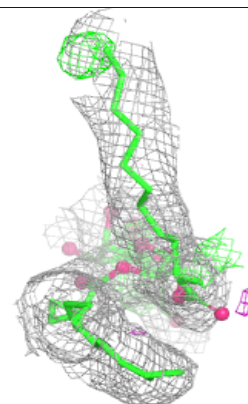
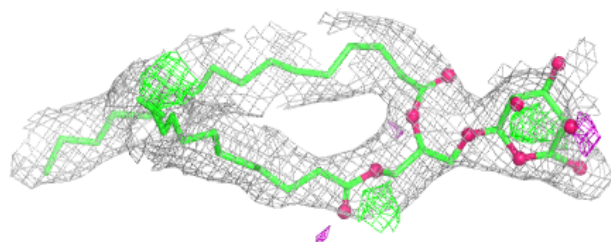
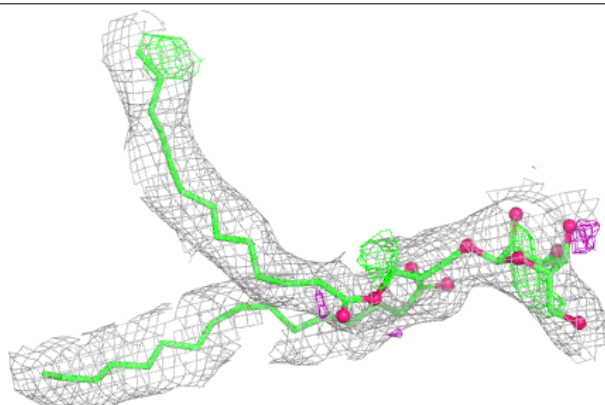


Electron density around MGE D 359:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

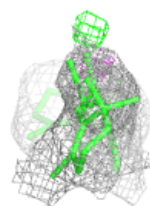
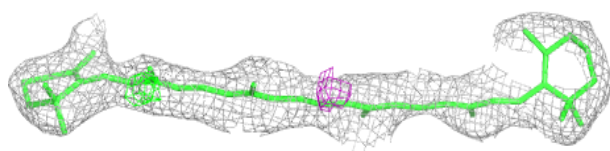
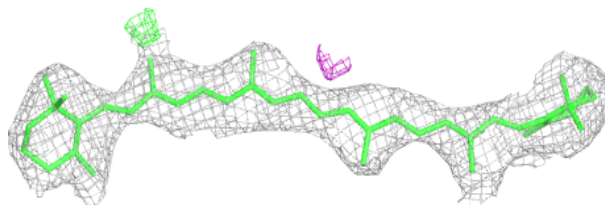
**Electron density around MGE D 360:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



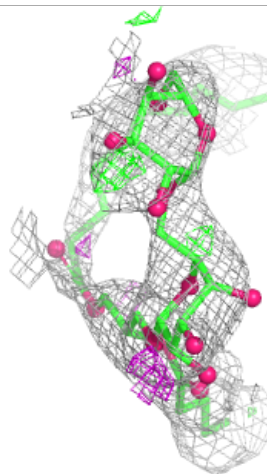
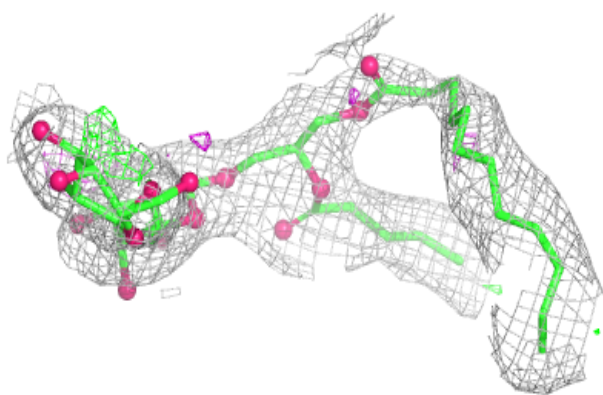
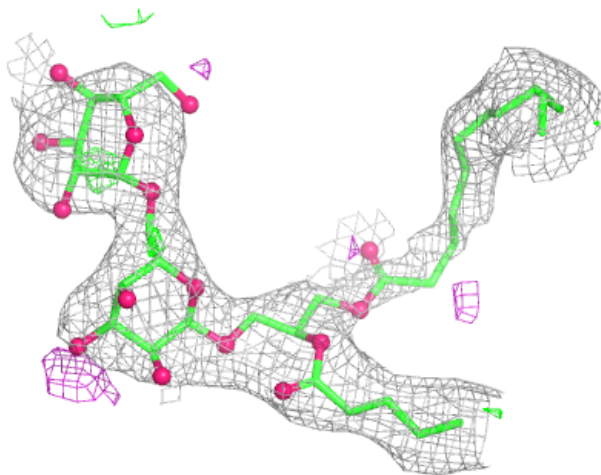
Electron density around BCR B 527:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



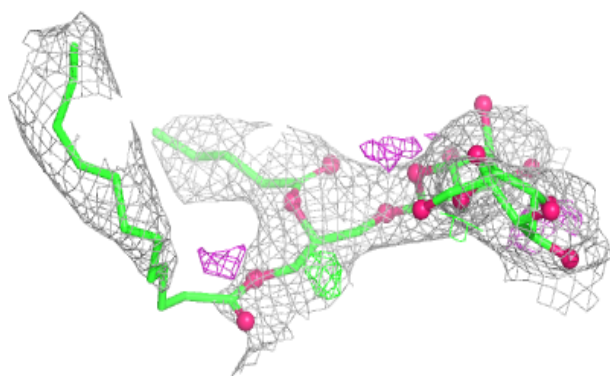
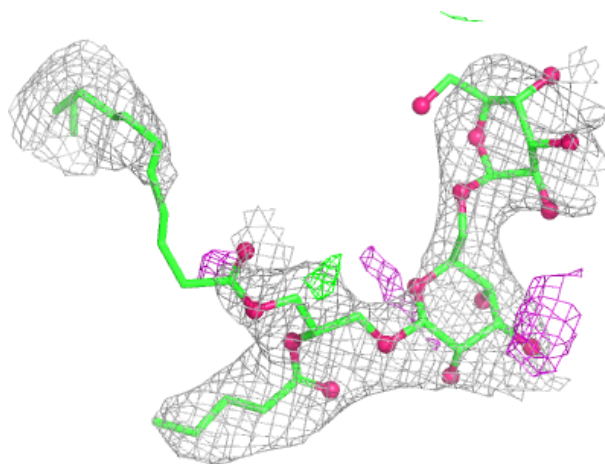
Electron density around DGD C 508:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



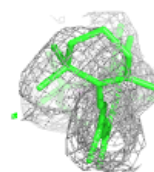
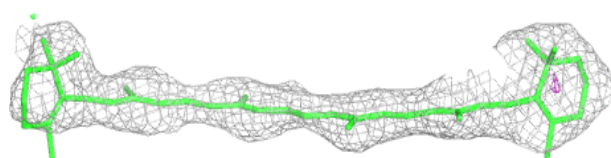
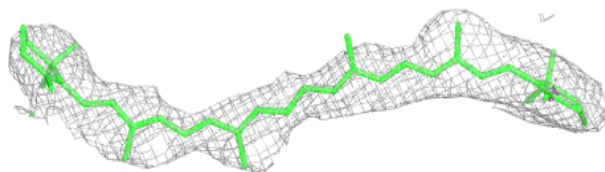
Electron density around DGD c 5508:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

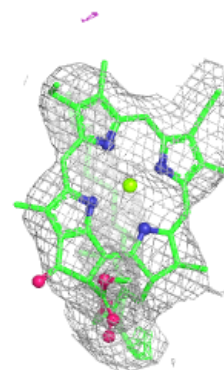
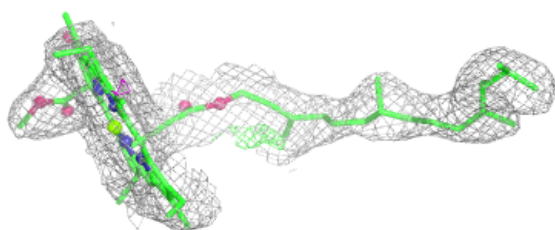
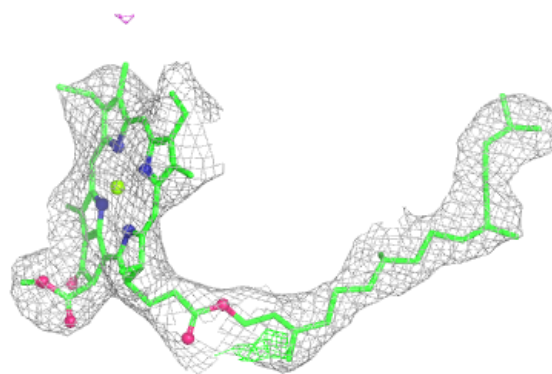


Electron density around BCR h 5107:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

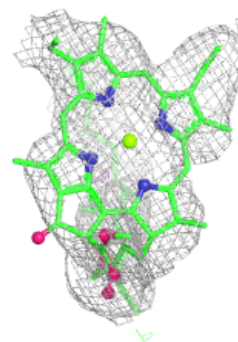
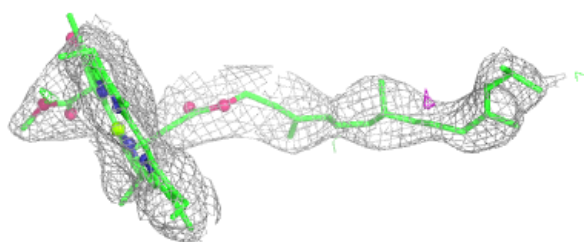
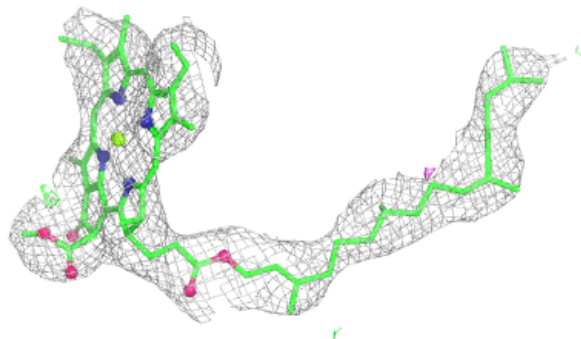
**Electron density around CLA b 5519:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



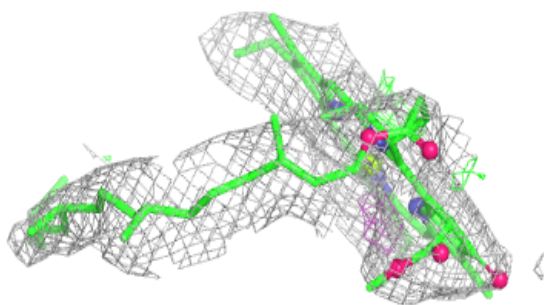
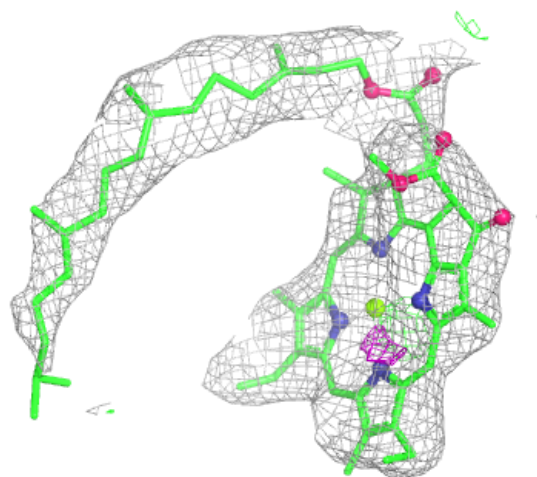
Electron density around CLA B 519:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



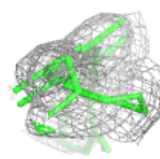
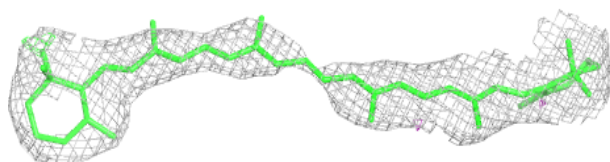
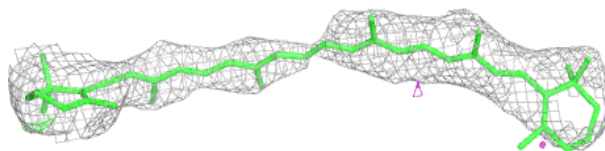
Electron density around CLA C 497:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

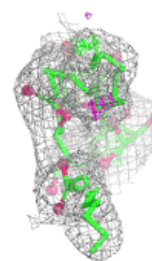
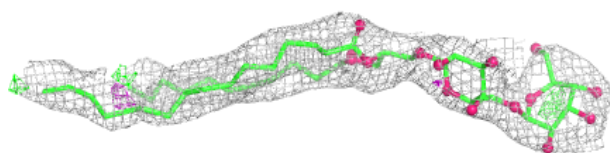


Electron density around BCR d 5357:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

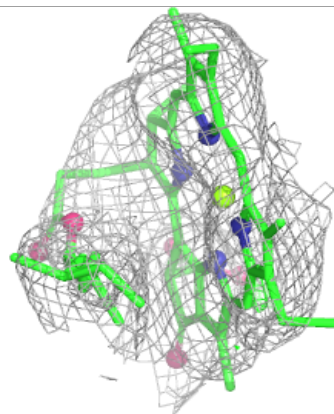
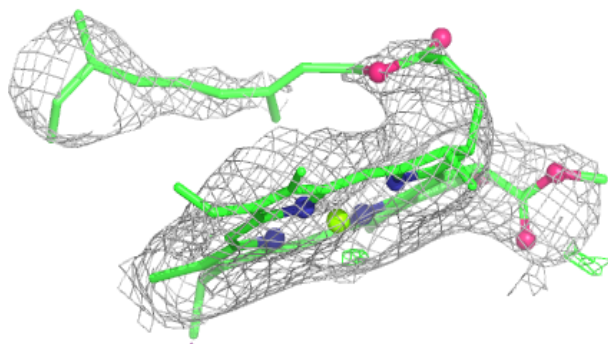
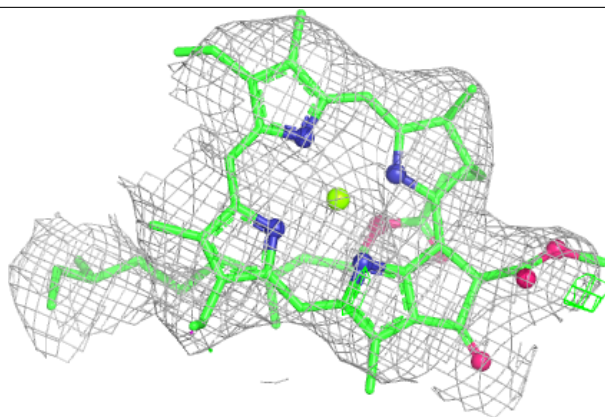
**Electron density around DGD C 509:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

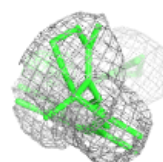
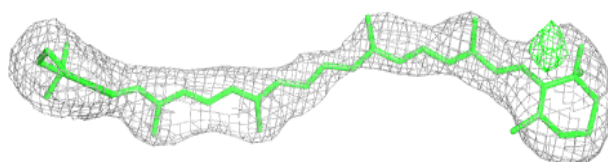


Electron density around CLA b 5524:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

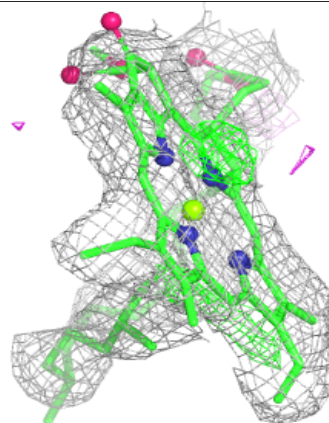
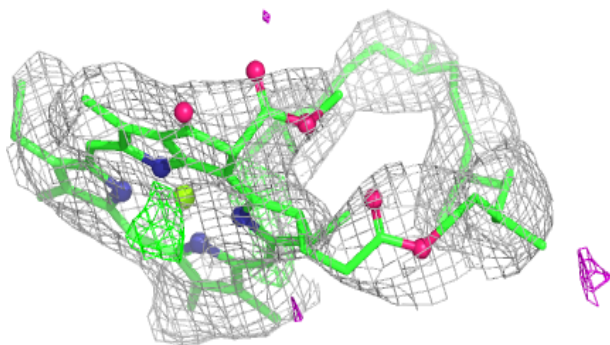
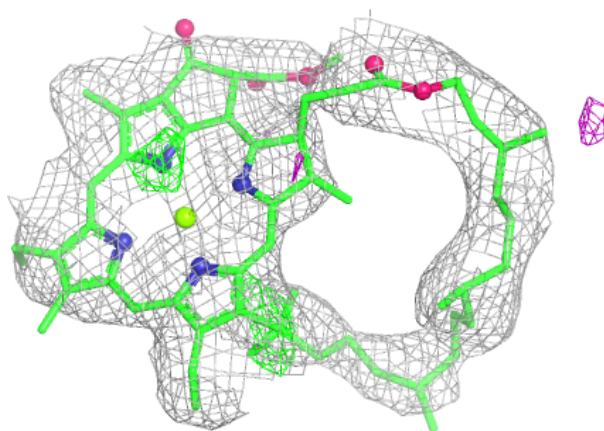
**Electron density around BCR D 357:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



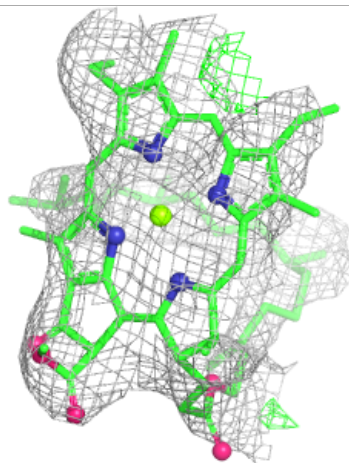
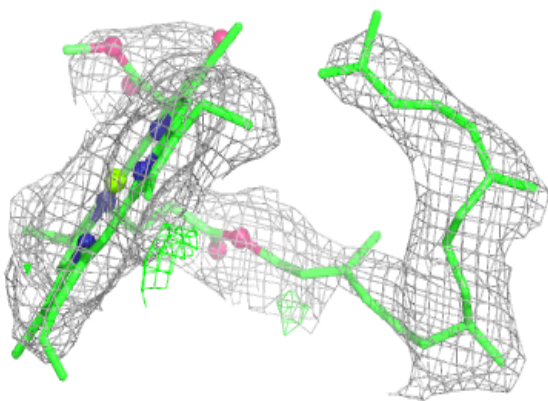
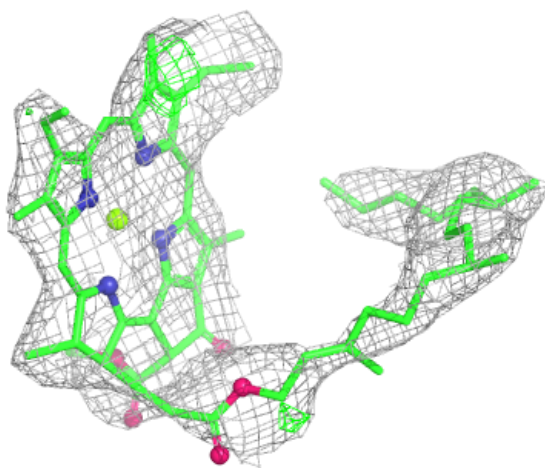
Electron density around CLA B 525:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



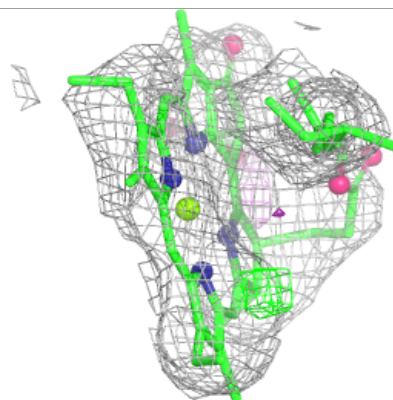
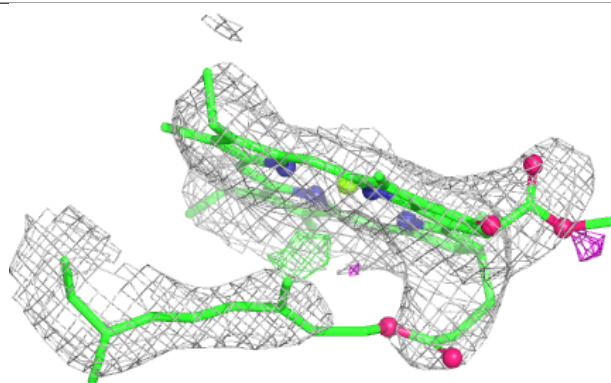
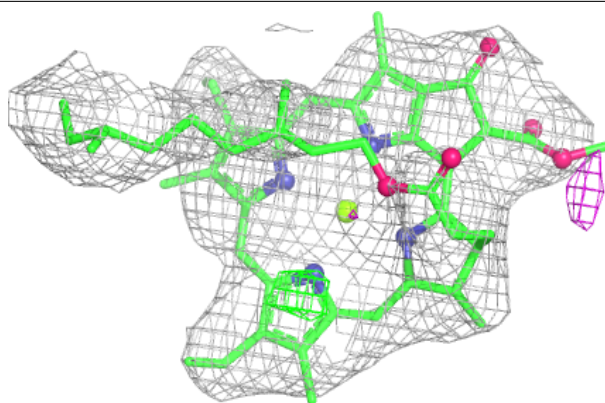
Electron density around CLA c 5493:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

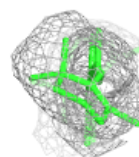
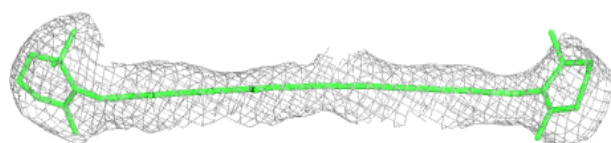
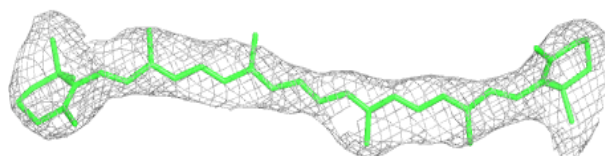


Electron density around CLA B 524:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

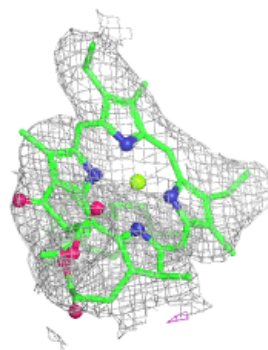
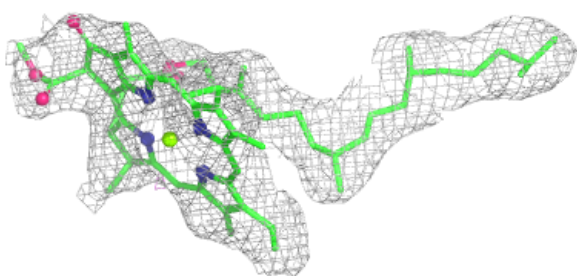
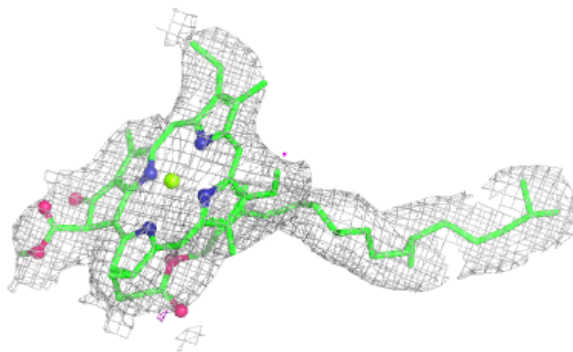
**Electron density around BCR B 528:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



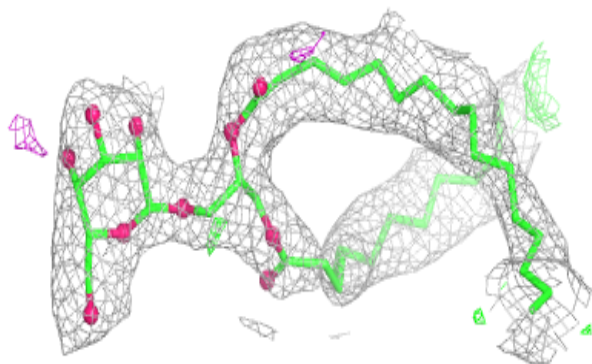
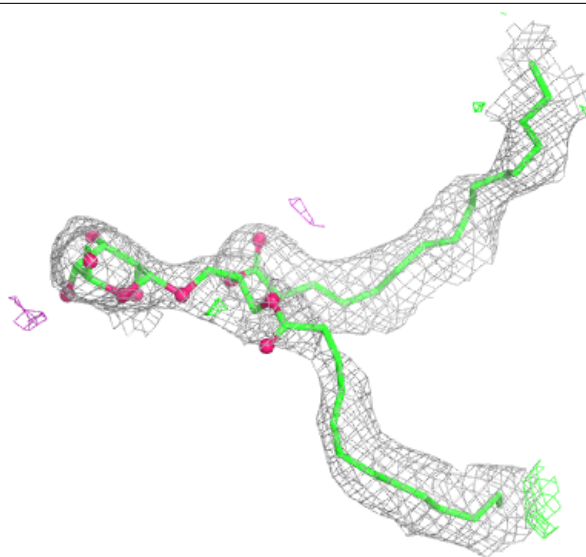
Electron density around CLA C 495:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



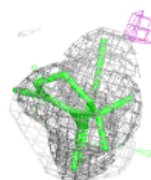
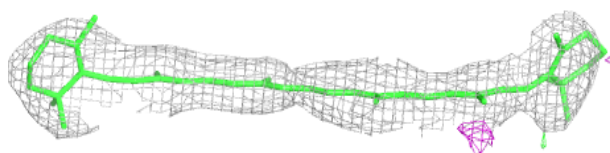
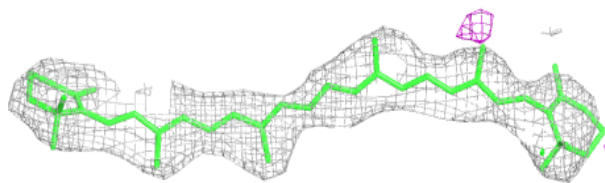
Electron density around MGE B 530:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

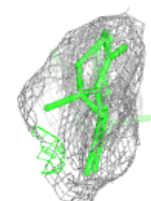
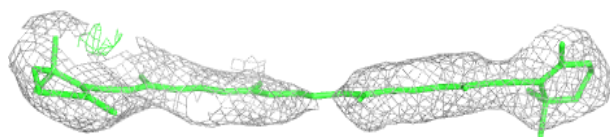
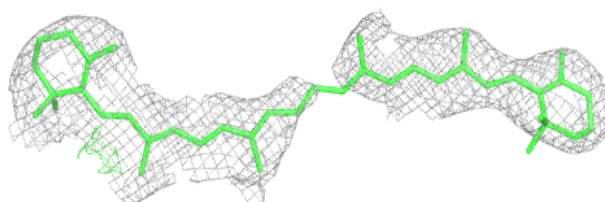


Electron density around BCR C 506:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

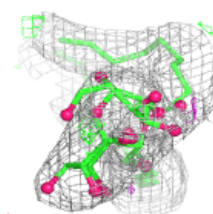
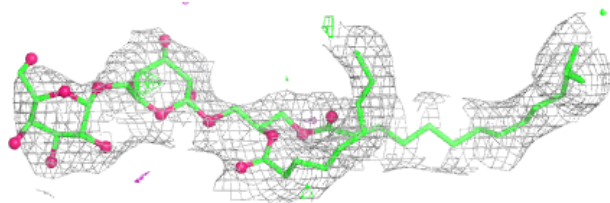
**Electron density around BCR x 5130:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

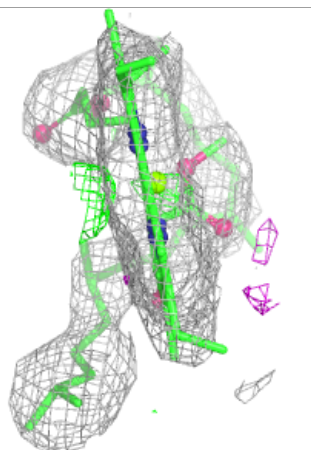
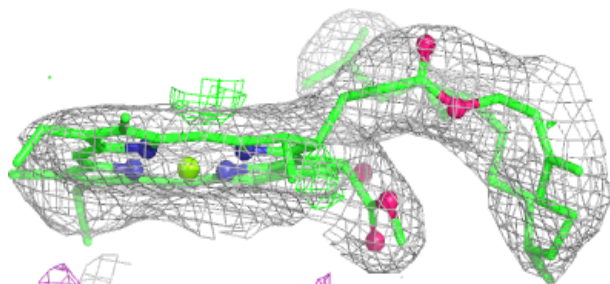
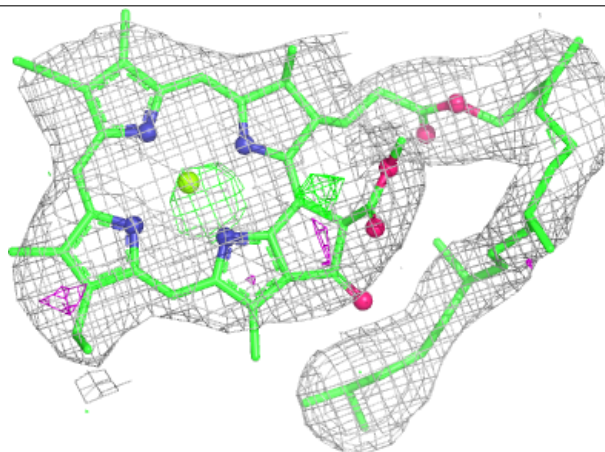


Electron density around DGD h 5208:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

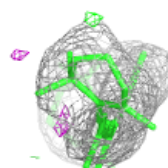
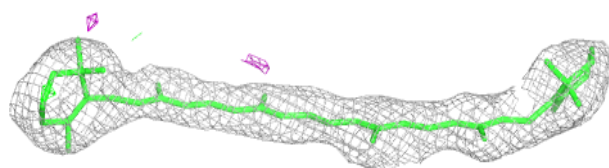
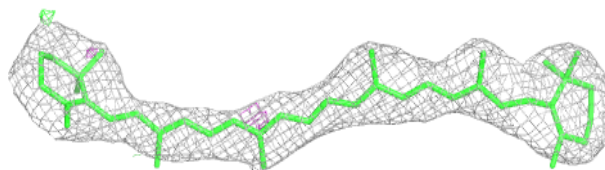
**Electron density around CLA b 5520:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

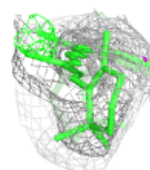
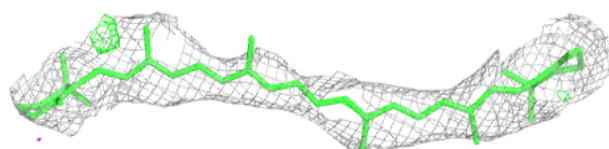


Electron density around BCR b 5529:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

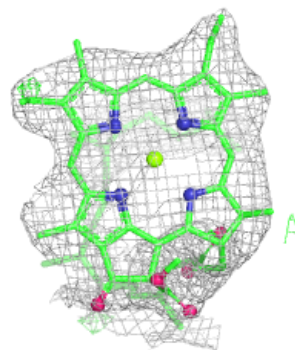
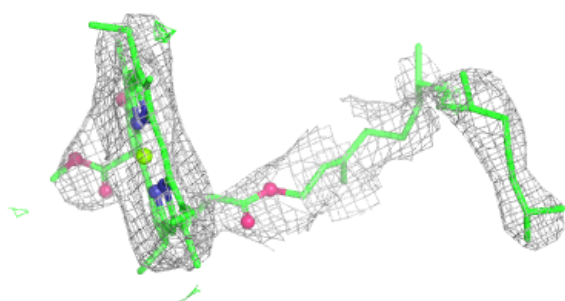
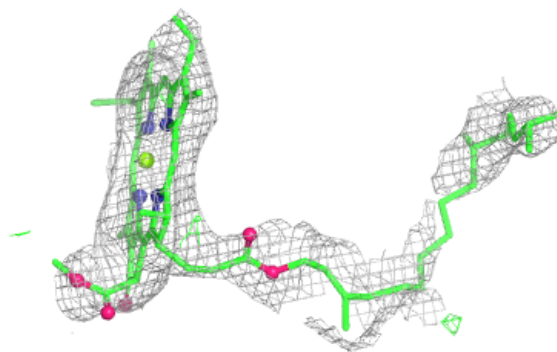
**Electron density around BCR c 5504:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



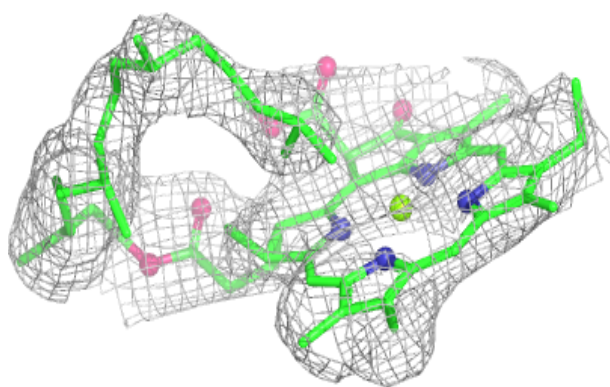
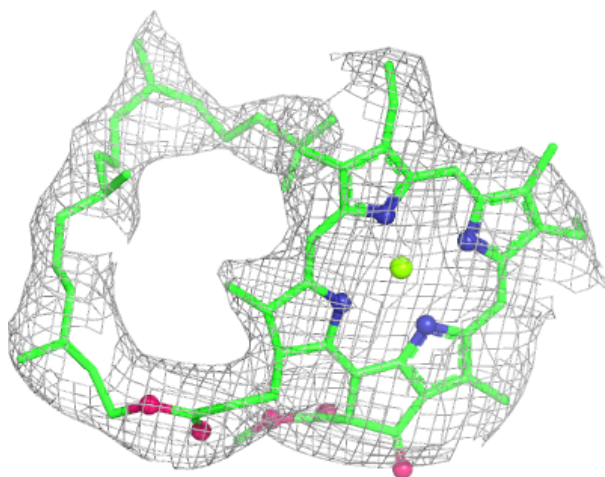
Electron density around CLA c 5496:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



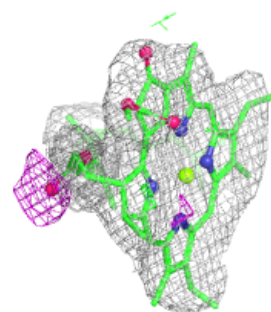
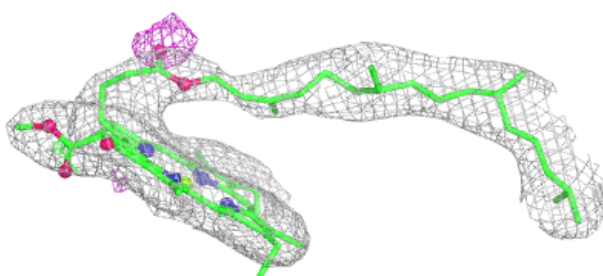
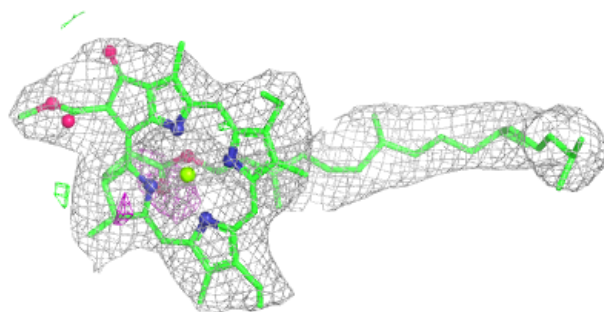
Electron density around CLA b 5525:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

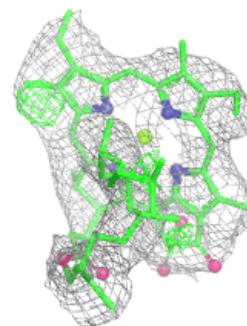
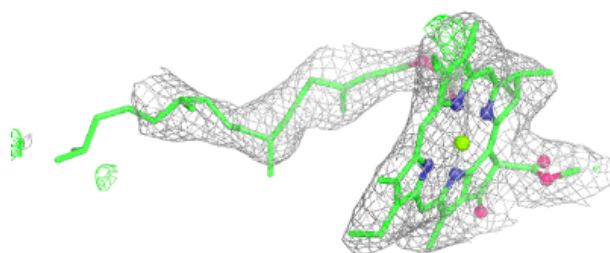
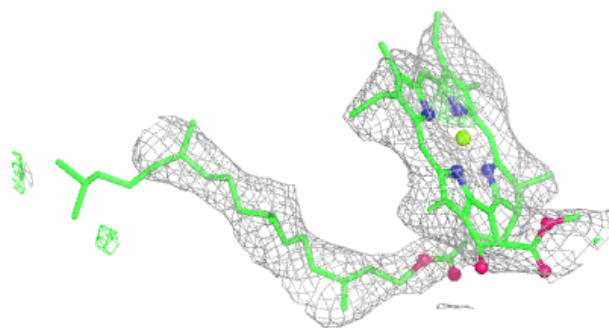


Electron density around CLA b 5518:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

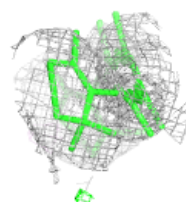
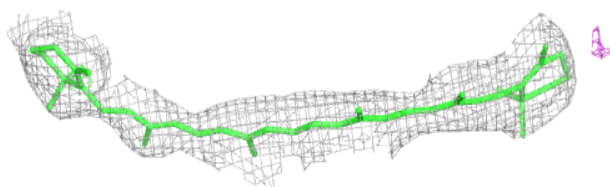
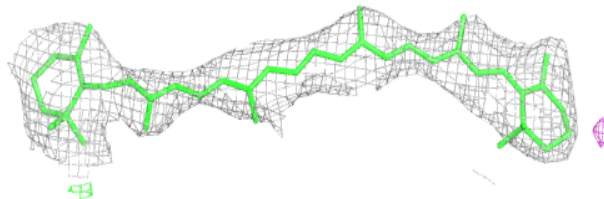
**Electron density around CLA C 498:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

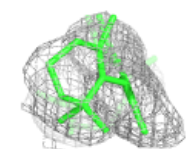
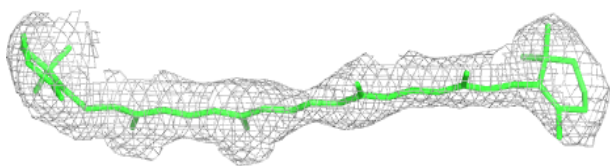
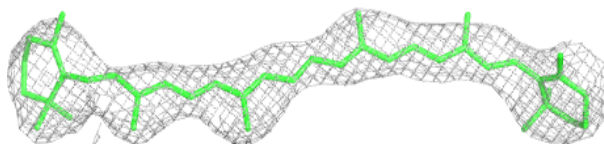


Electron density around BCR t 104:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

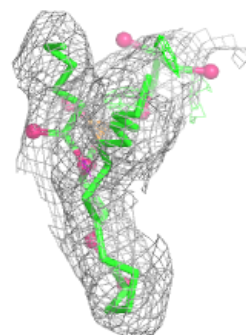
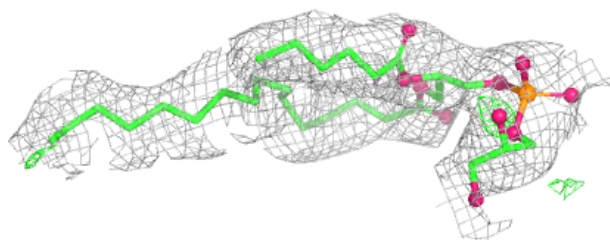
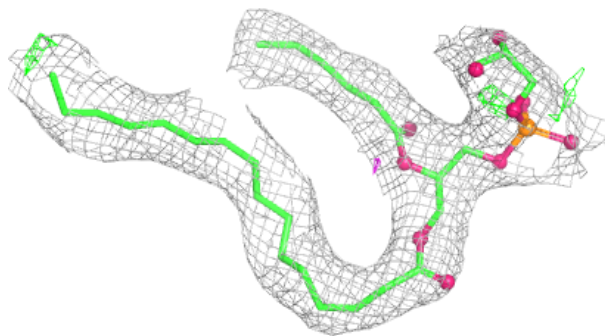
**Electron density around BCR B 529:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

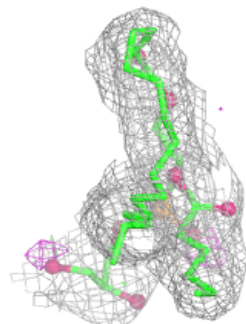
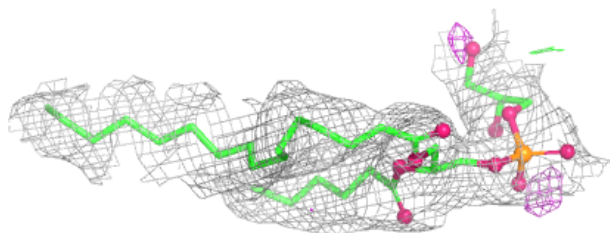
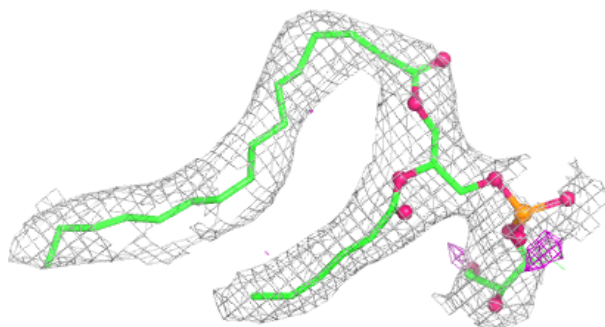


Electron density around LHG A 567:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

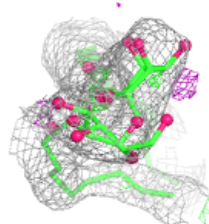
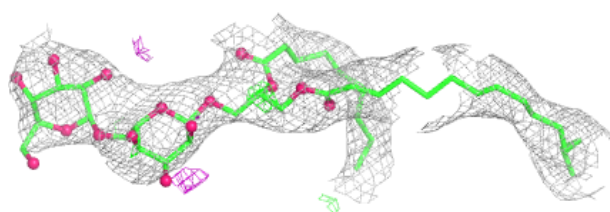
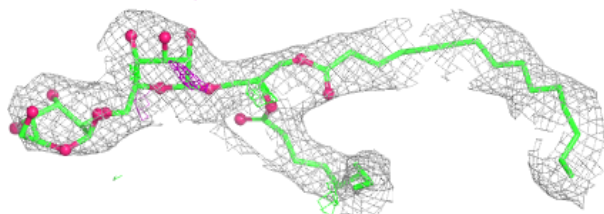
**Electron density around LHG a 5567:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

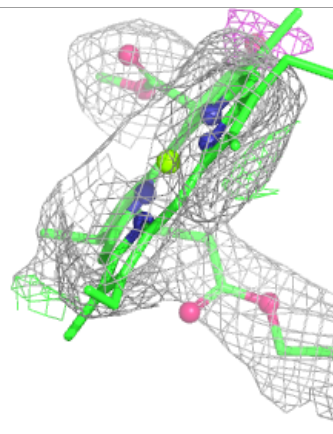
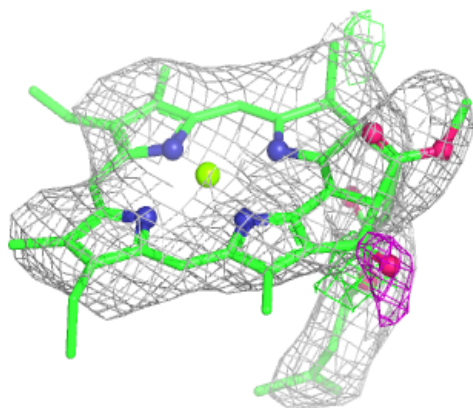
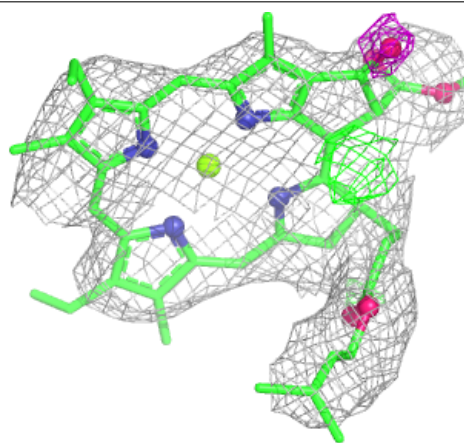


Electron density around DGD H 208:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

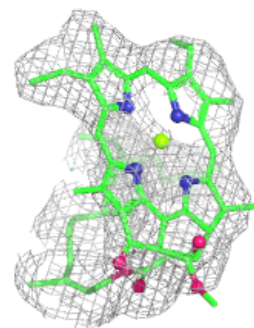
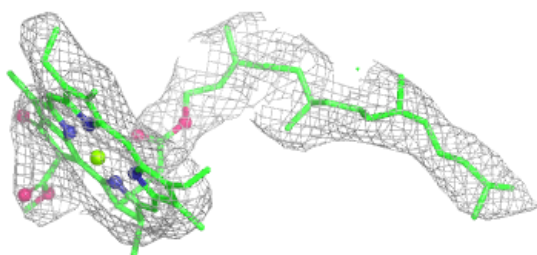
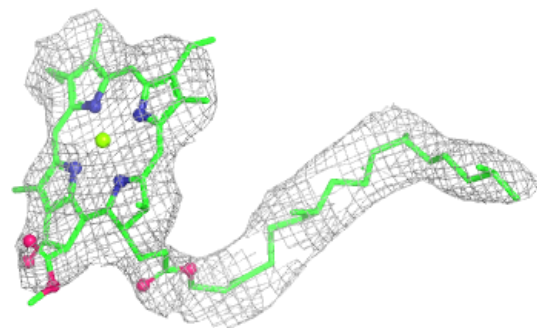
**Electron density around CLA C 503:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



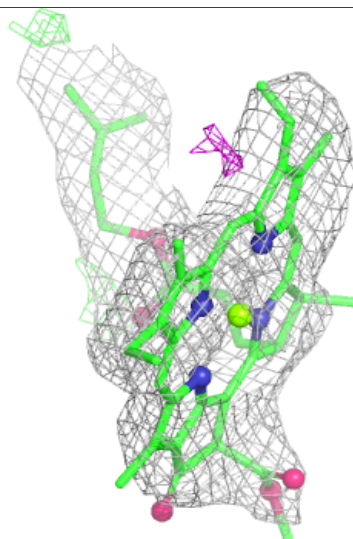
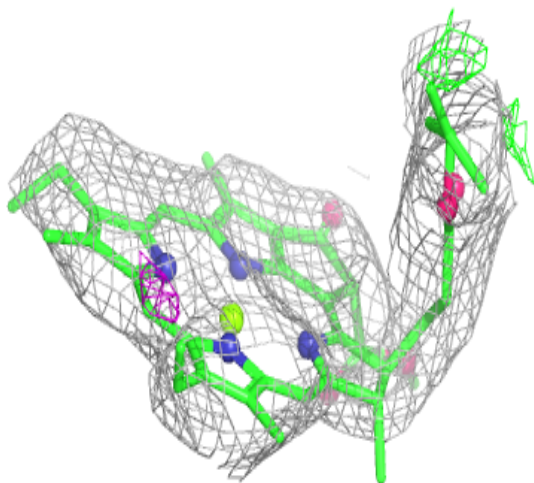
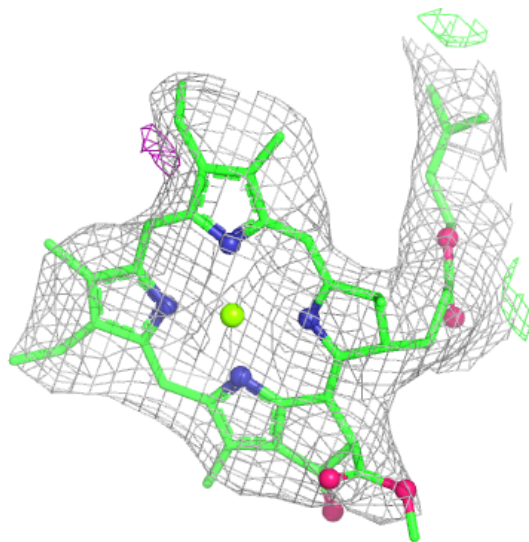
Electron density around CLA C 501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



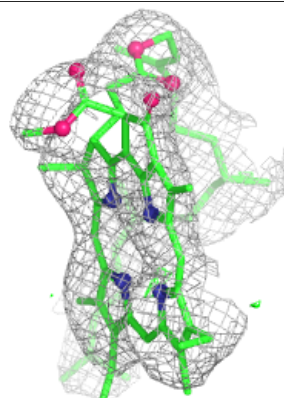
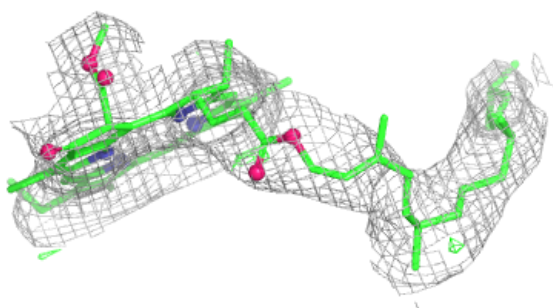
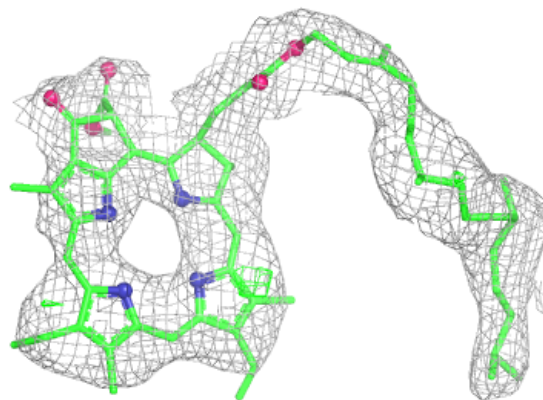
Electron density around CLA d 5355:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

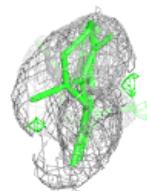
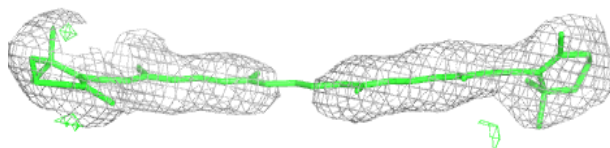
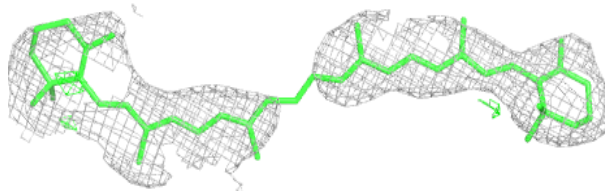


Electron density around PHO a 5562:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

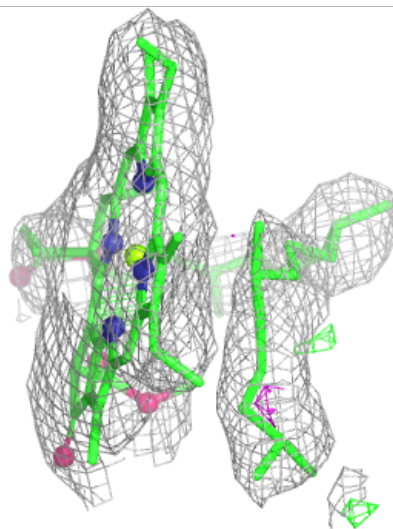
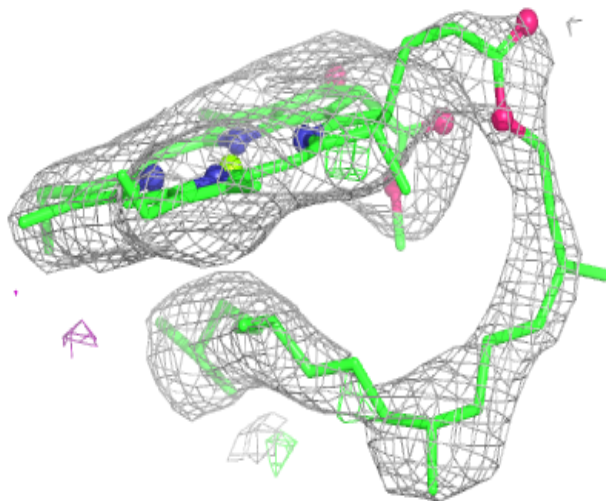
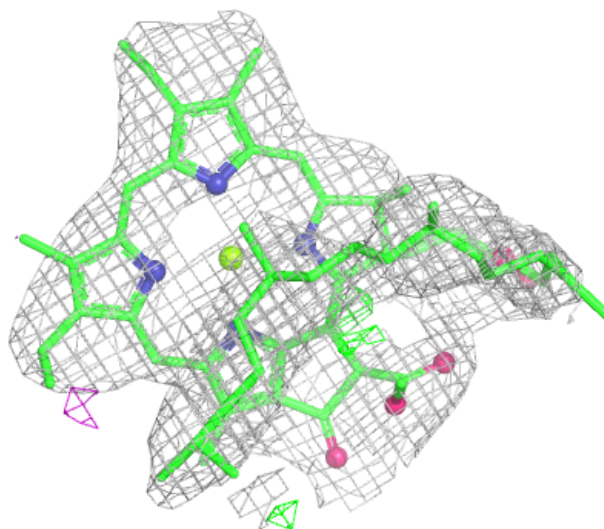
**Electron density around BCR X 130:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



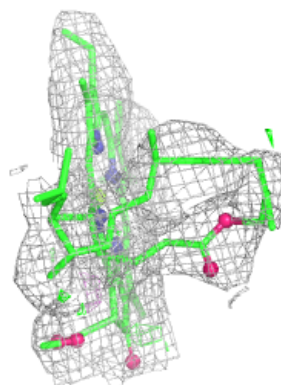
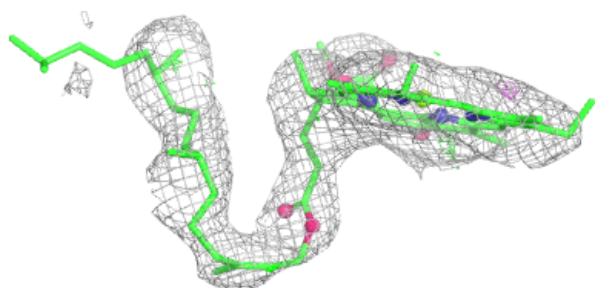
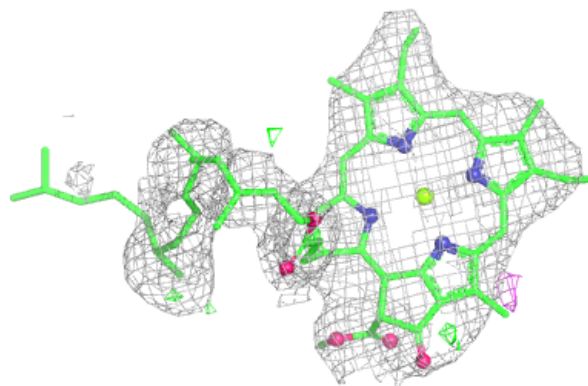
Electron density around CLA c 5500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

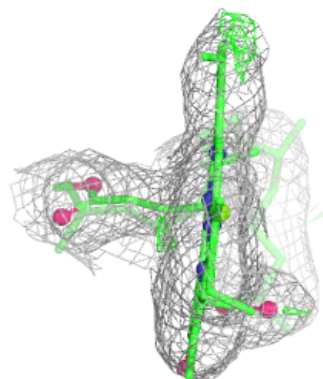
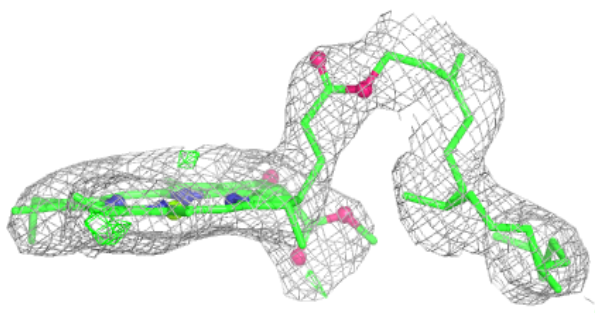
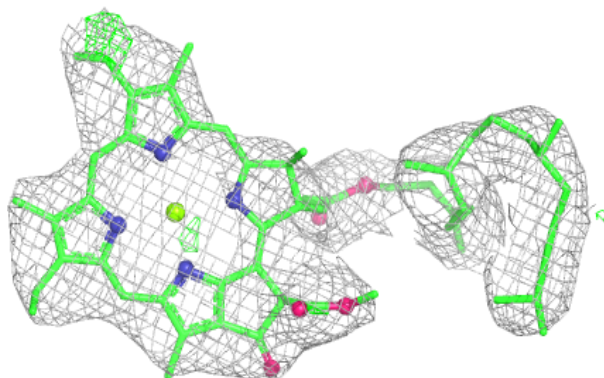


Electron density around CLA a 5560:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

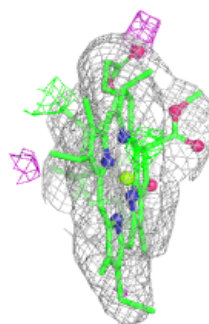
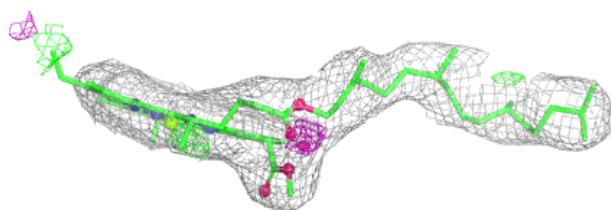
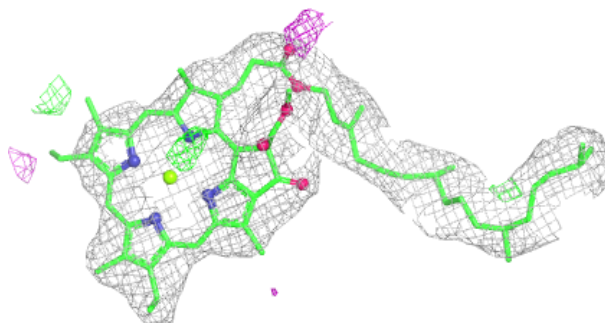
**Electron density around CLA B 522:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

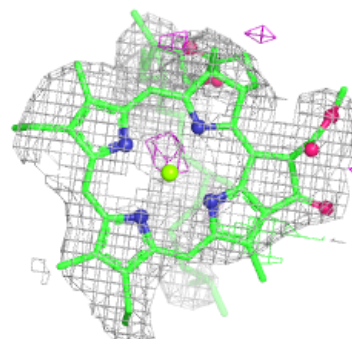
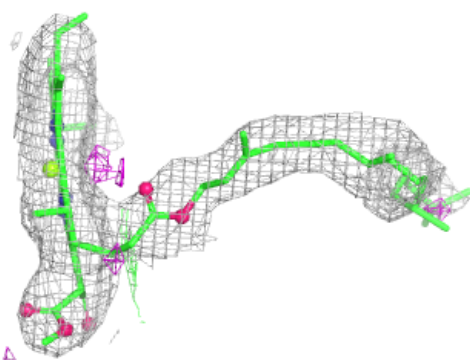
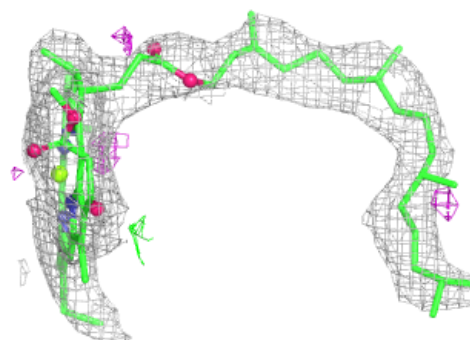


Electron density around CLA b 5512:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

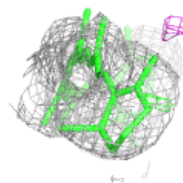
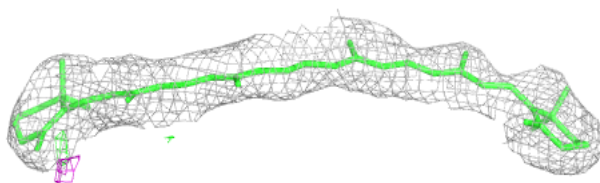
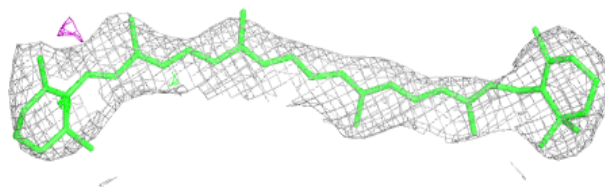
**Electron density around CLA b 5516:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



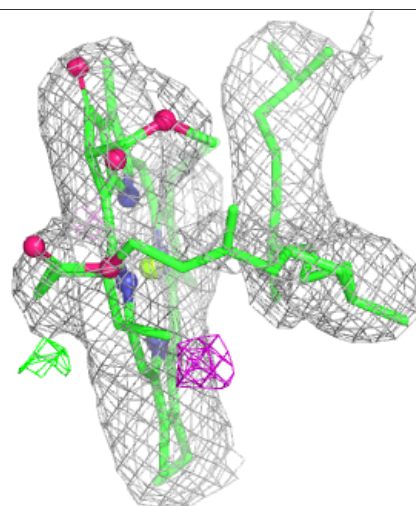
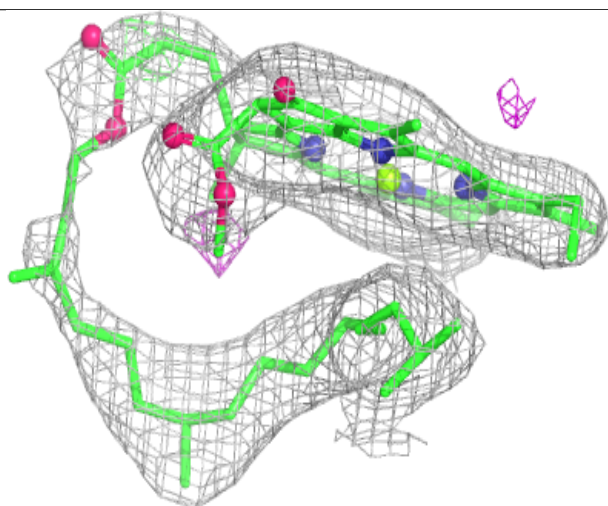
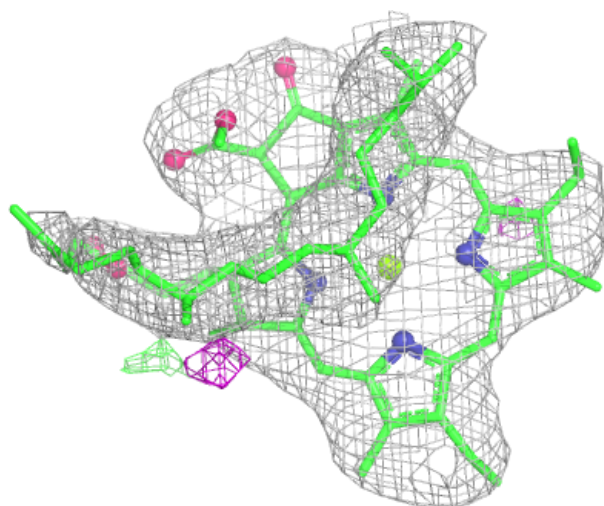
Electron density around BCR T 5104:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



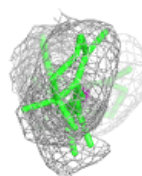
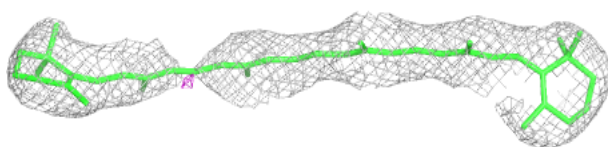
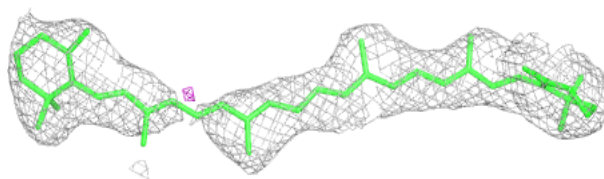
Electron density around CLA C 500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

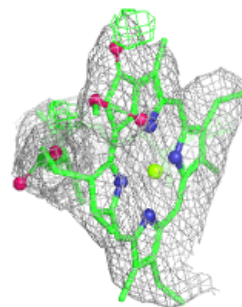
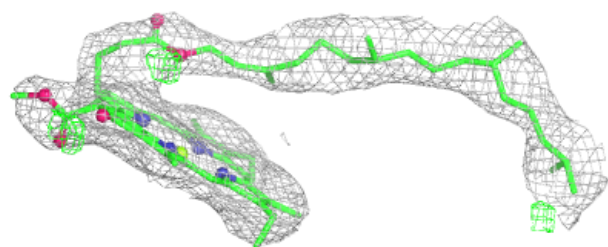
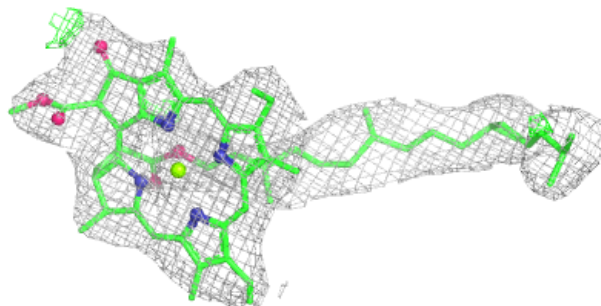


Electron density around BCR b 5527:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

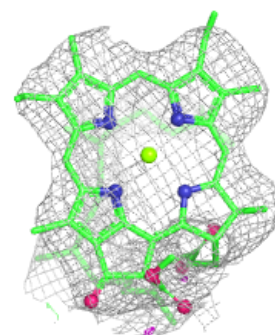
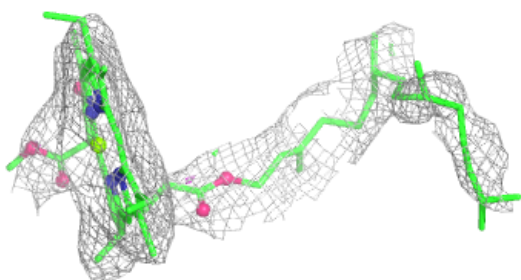
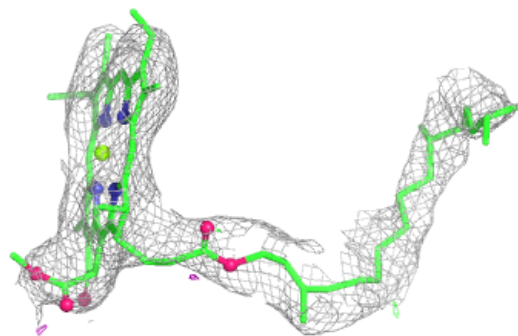
**Electron density around CLA B 518:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



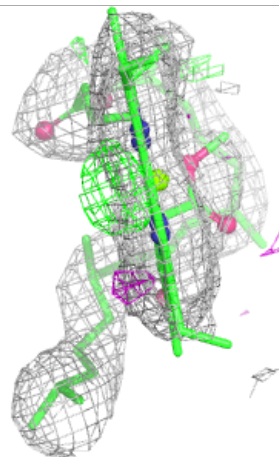
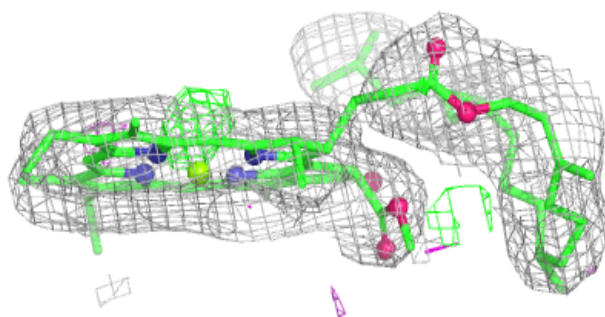
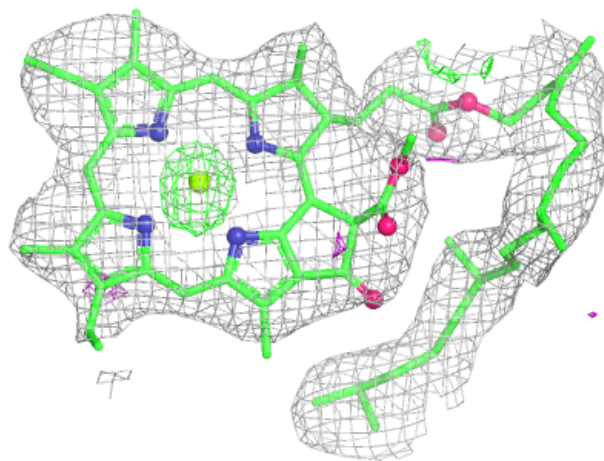
Electron density around CLA C 496:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



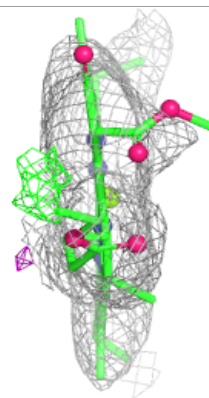
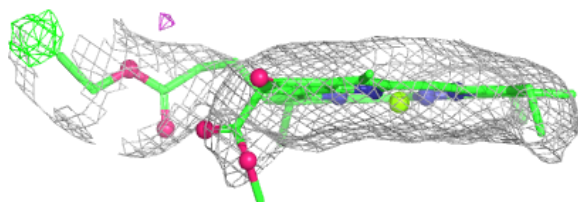
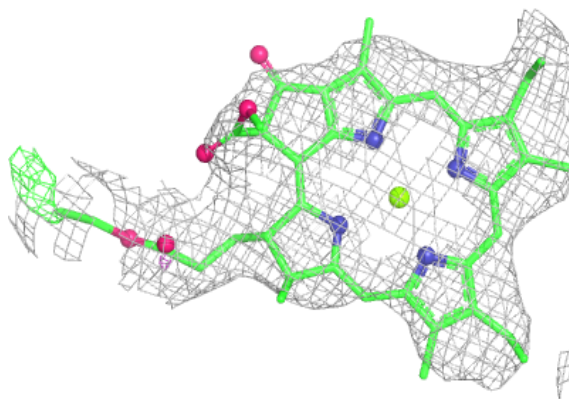
Electron density around CLA B 520:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

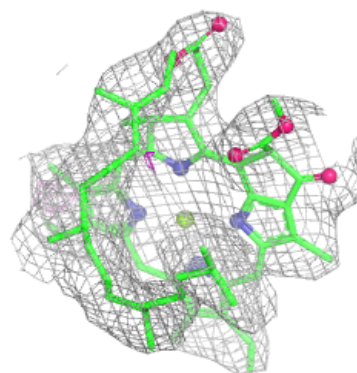
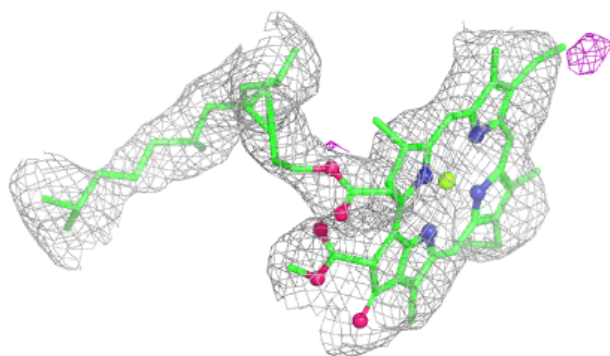
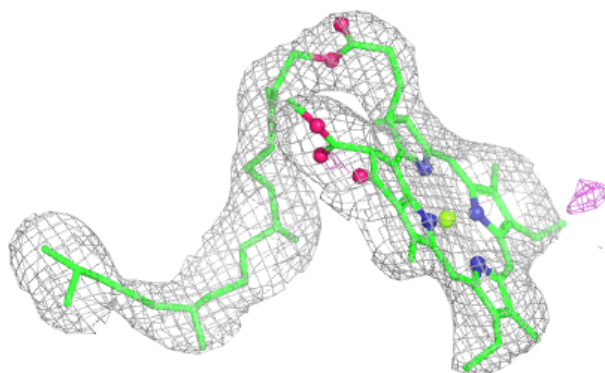


Electron density around CLA c 5499:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

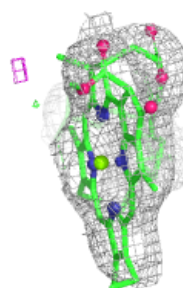
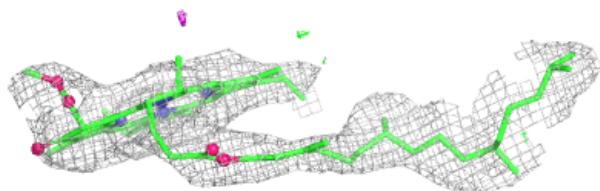
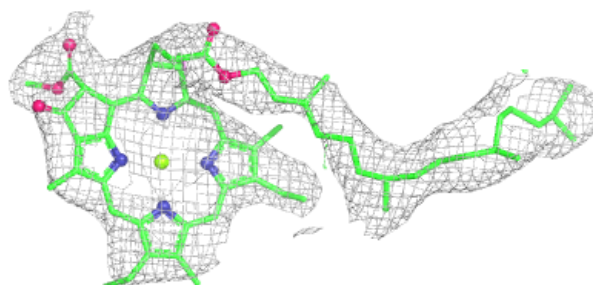
**Electron density around CLA b 5523:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

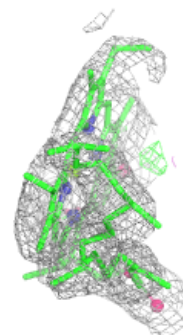
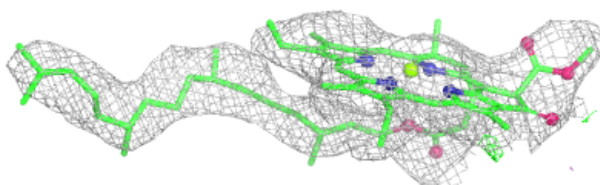
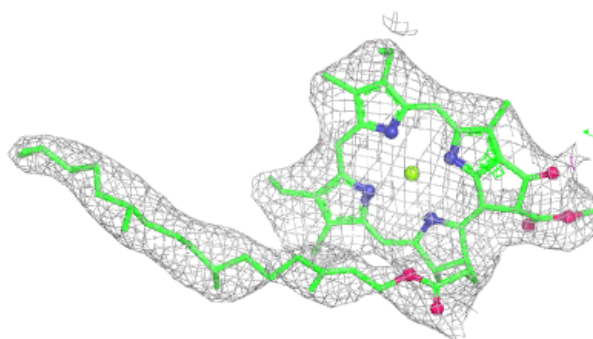


Electron density around CLA B 513:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

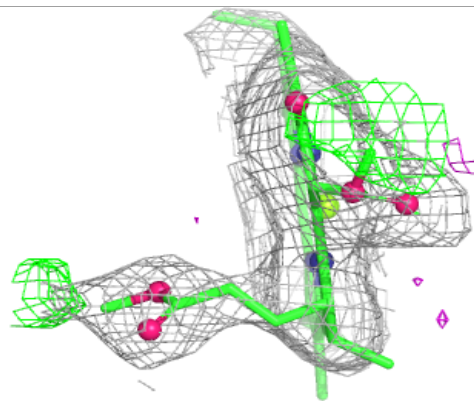
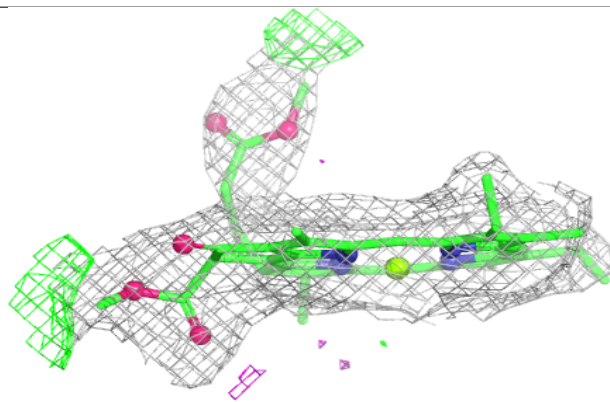
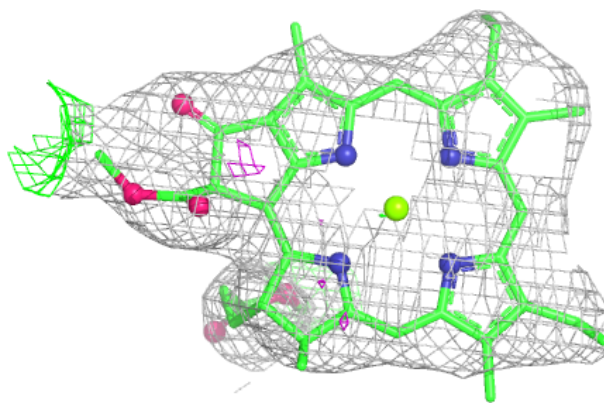
**Electron density around CLA C 491:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

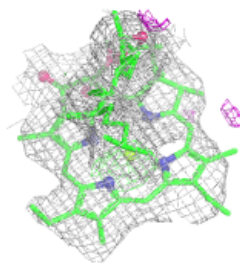
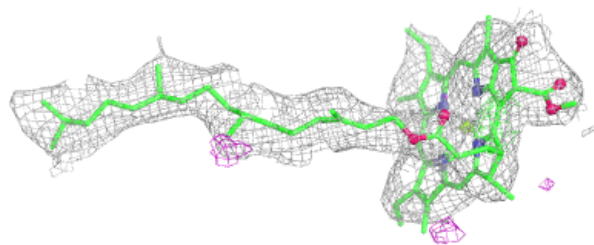
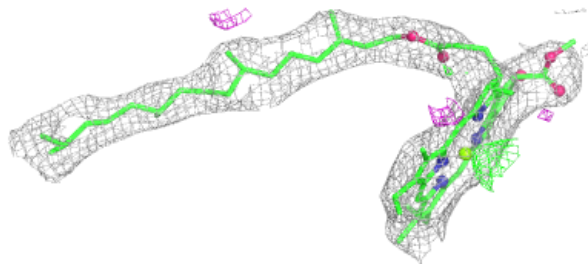


Electron density around CLA C 494:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

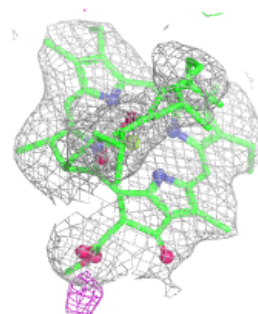
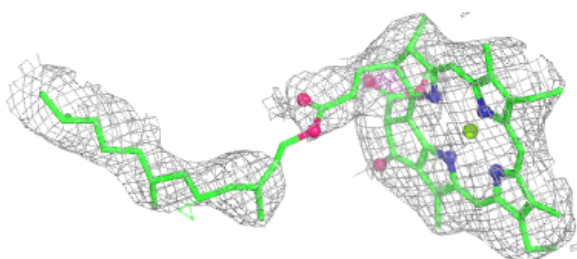
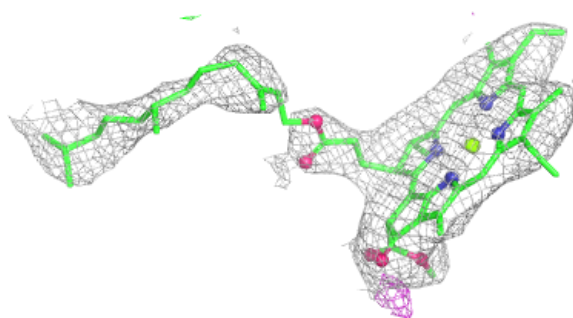
**Electron density around CLA b 5517:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

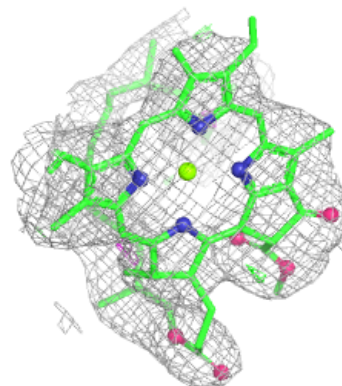
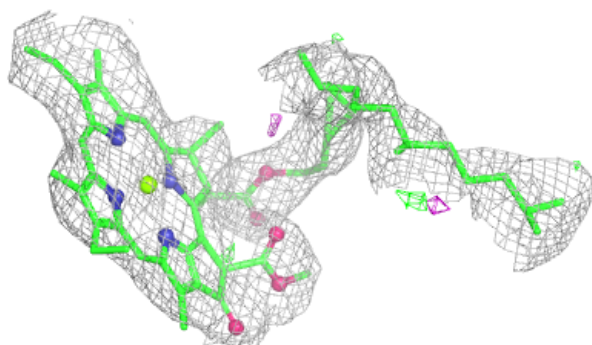
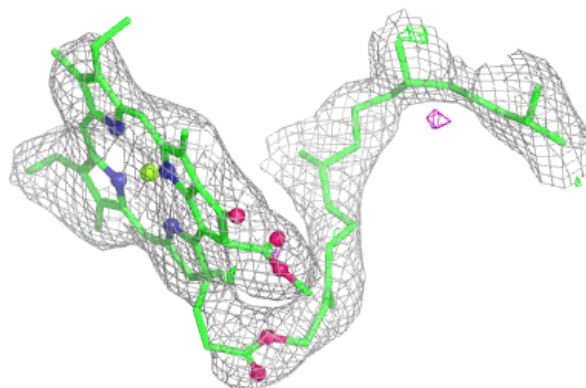


Electron density around CLA c 5492:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

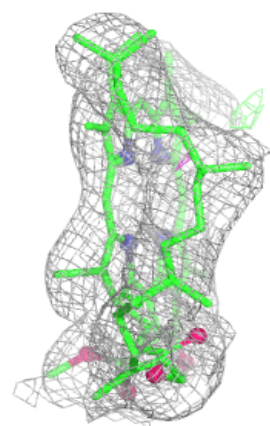
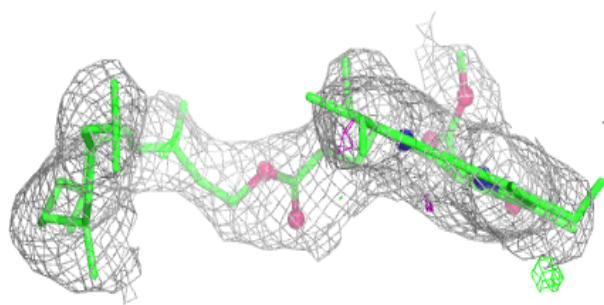
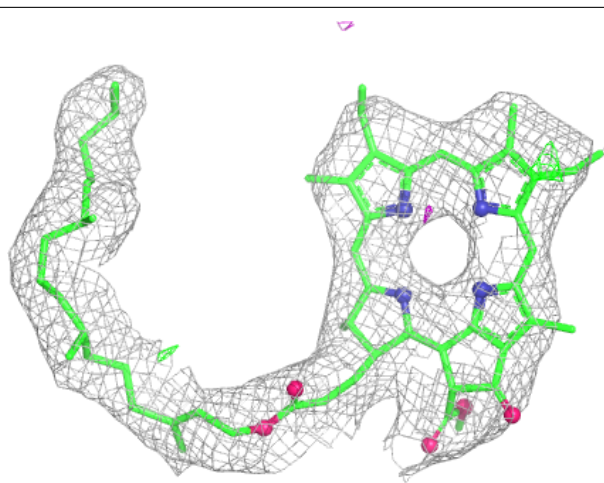
**Electron density around CLA B 523:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



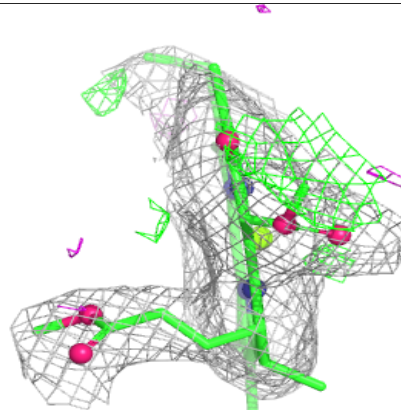
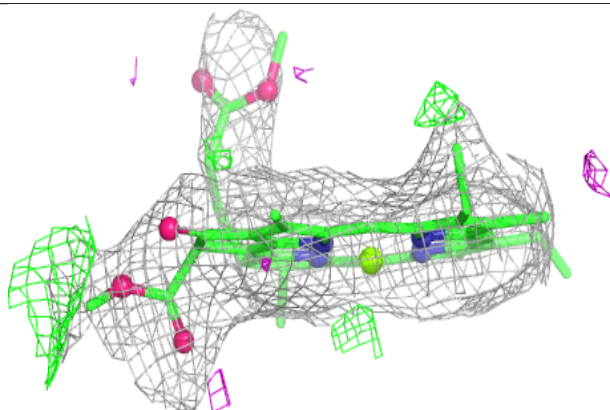
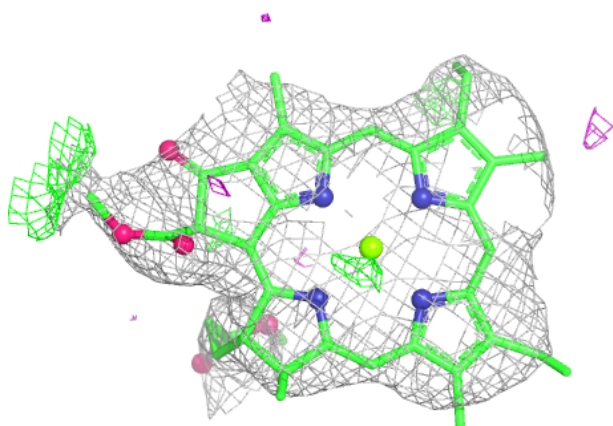
Electron density around PHO a 5561:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

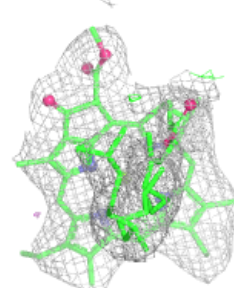
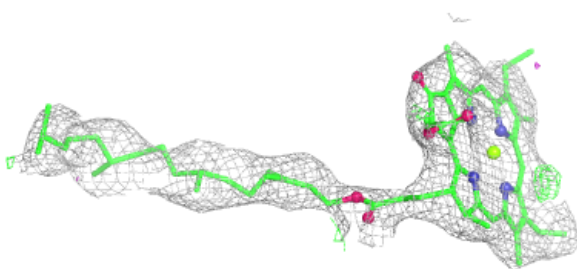
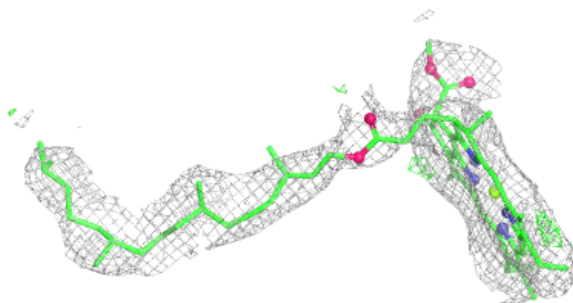


Electron density around CLA c 5494:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

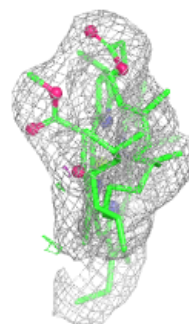
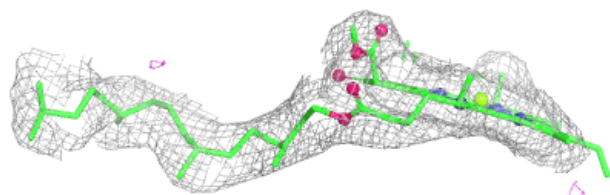
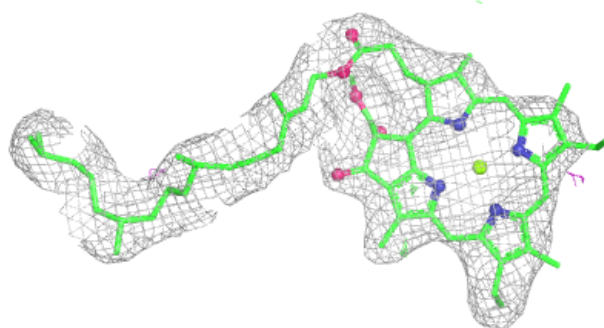
**Electron density around CLA B 514:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

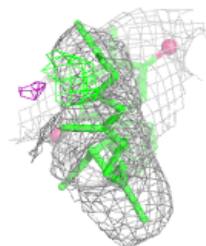
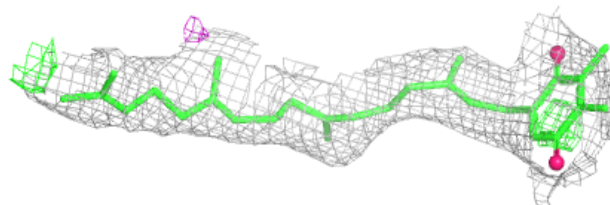
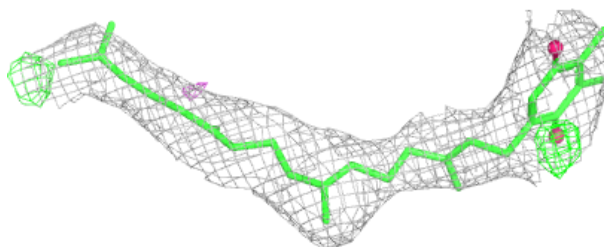


Electron density around CLA B 512:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

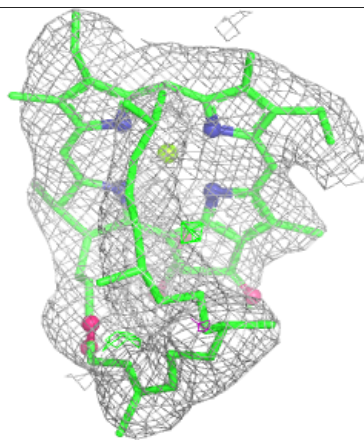
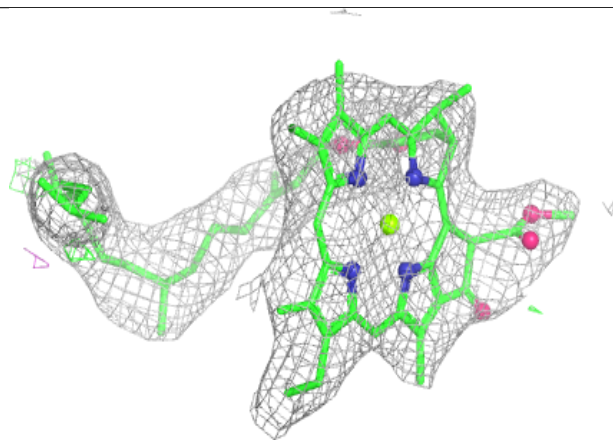
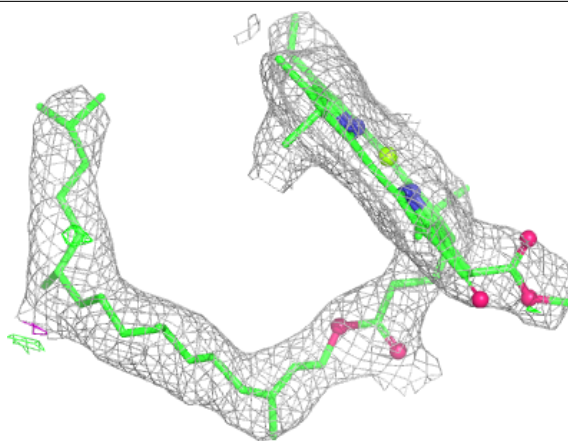
**Electron density around PQ9 d 5356:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



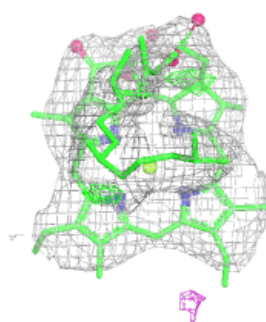
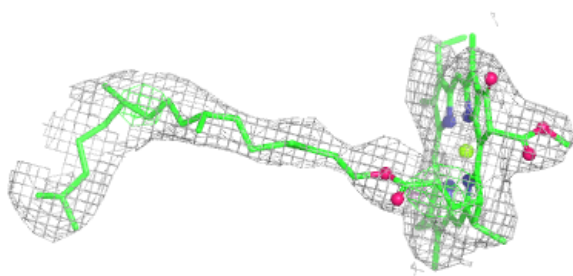
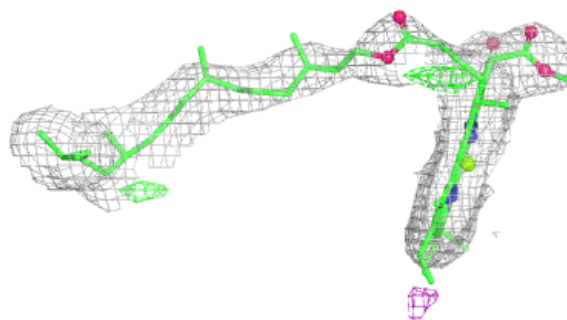
Electron density around CLA b 5521:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



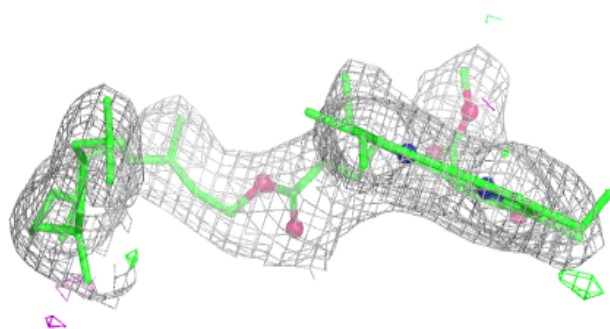
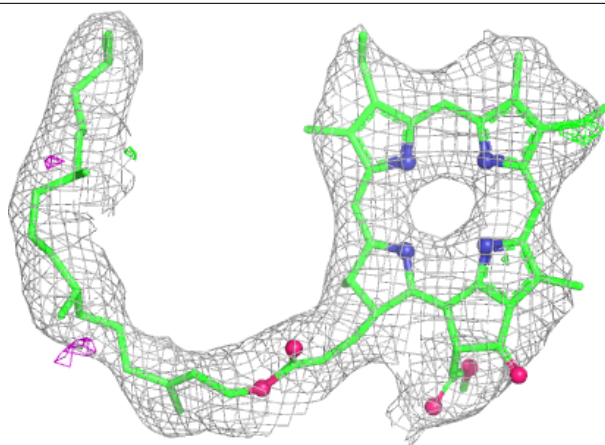
Electron density around CLA B 515:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



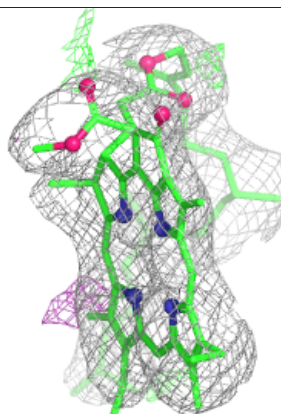
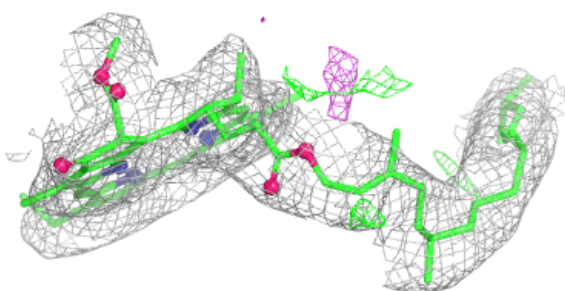
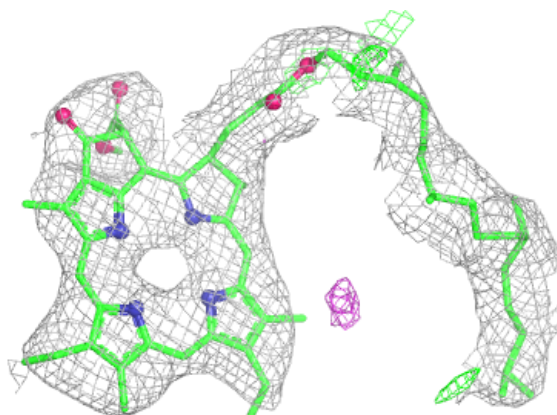
Electron density around PHO A 561:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

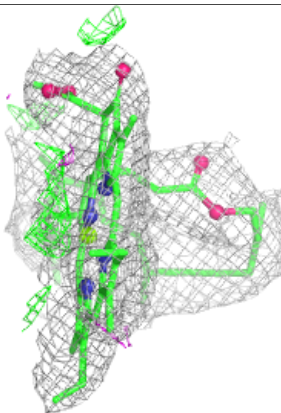
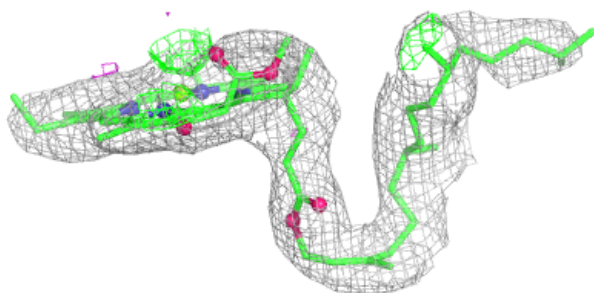
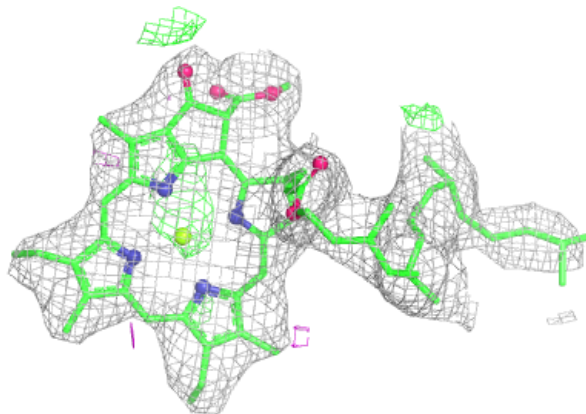


Electron density around PHO A 562:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

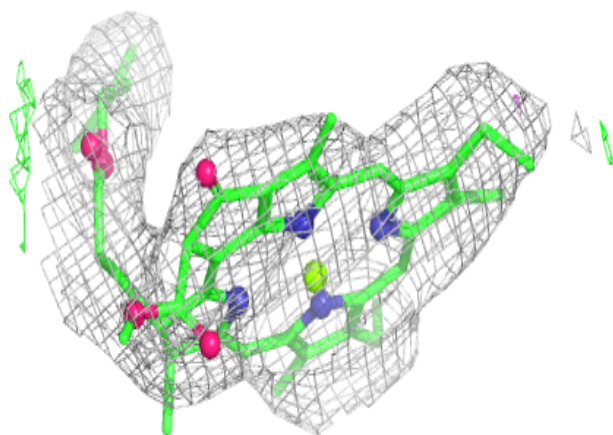
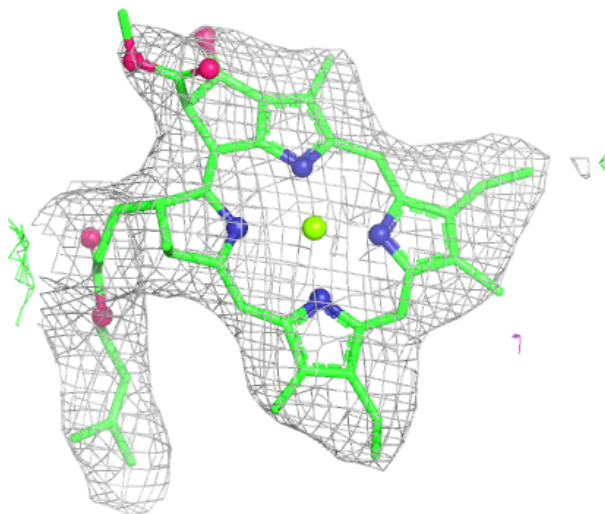
**Electron density around CLA A 560:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



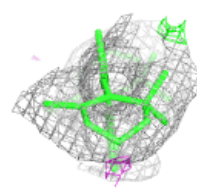
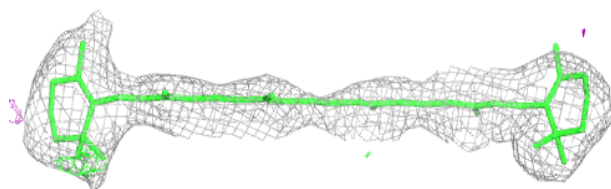
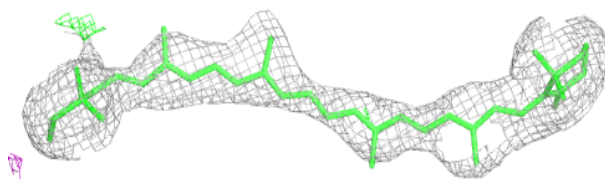
Electron density around CLA D 355:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



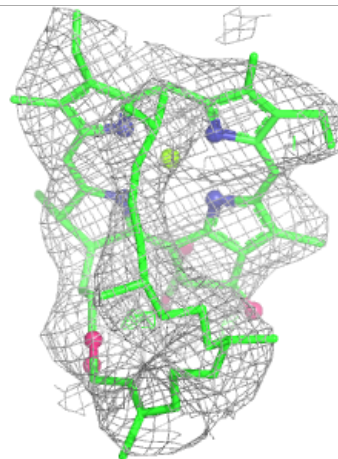
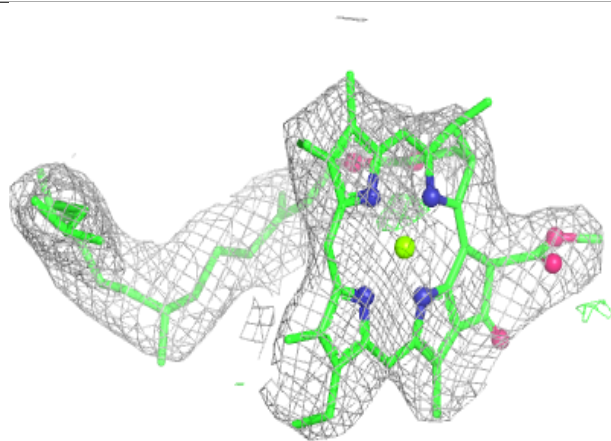
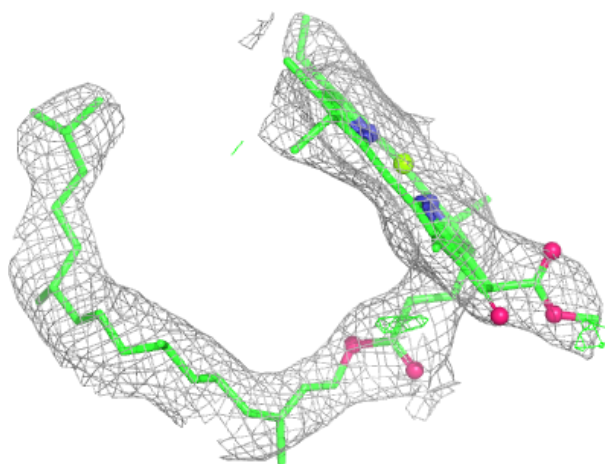
Electron density around BCR a 5566:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



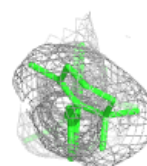
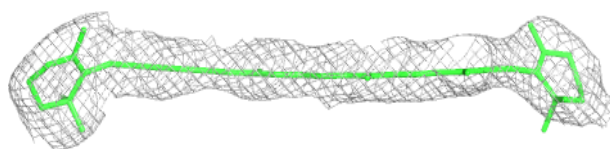
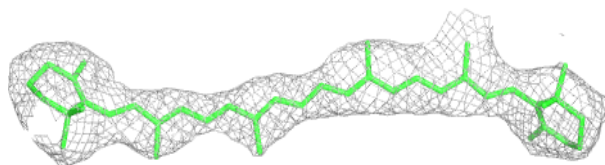
Electron density around CLA B 521:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

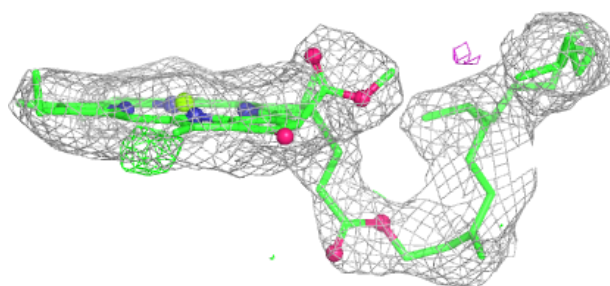
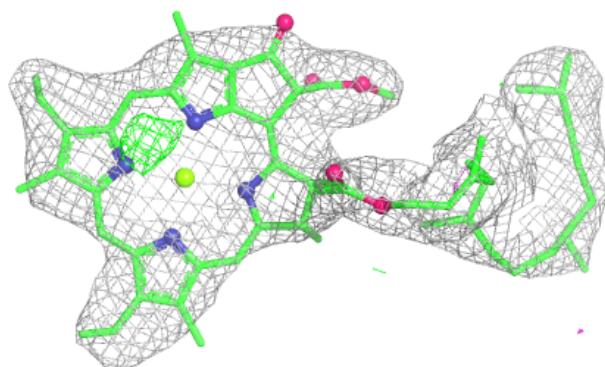


Electron density around BCR b 5528:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

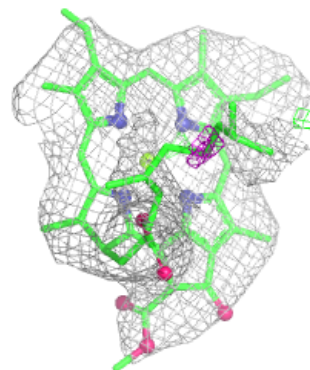
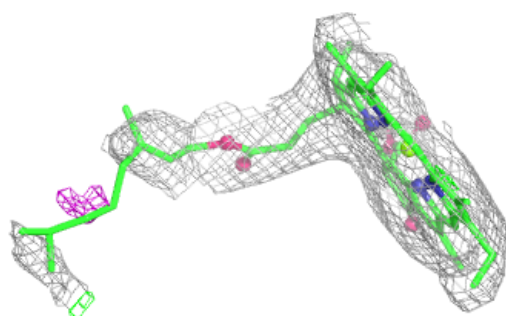
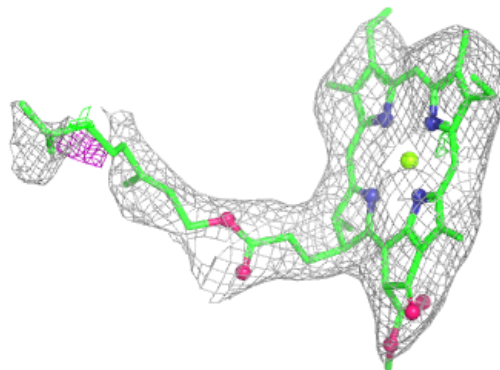
**Electron density around CLA b 5522:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

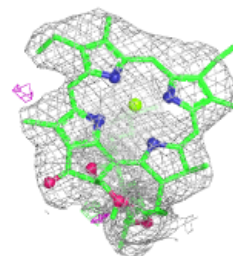
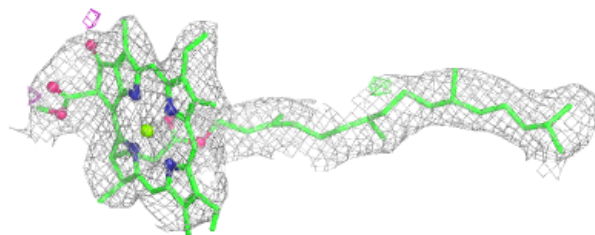
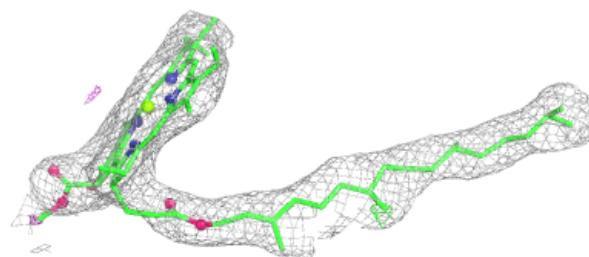


Electron density around CLA a 5563:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

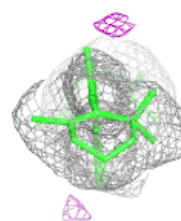
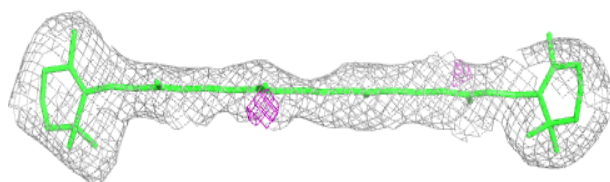
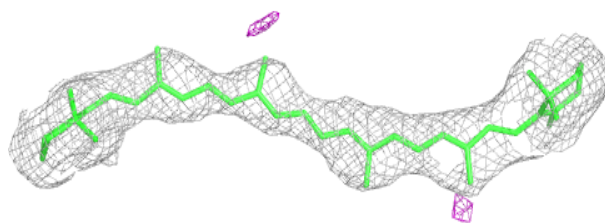
**Electron density around CLA B 517:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

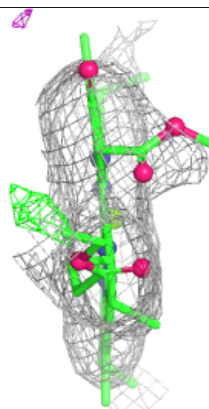
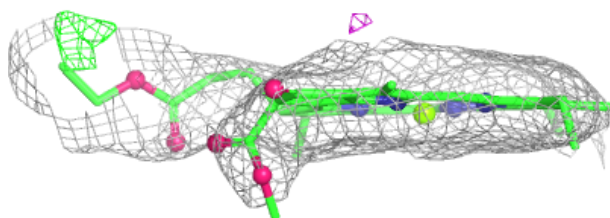
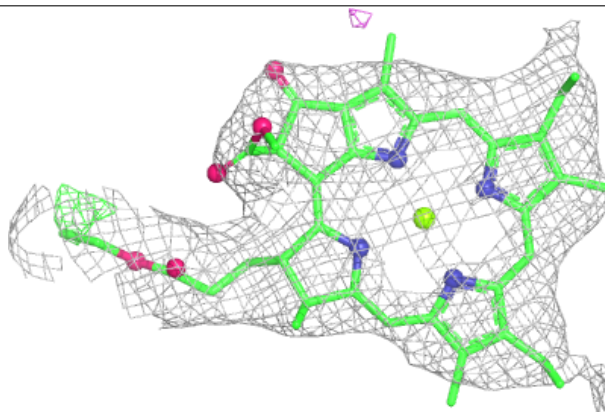


Electron density around BCR A 566:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

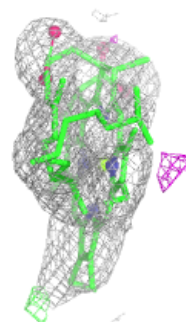
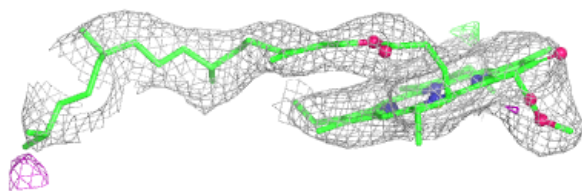
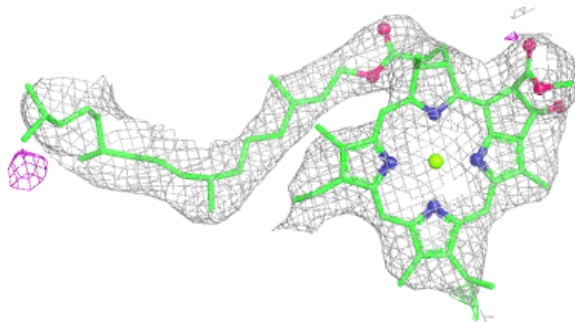
**Electron density around CLA C 499:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



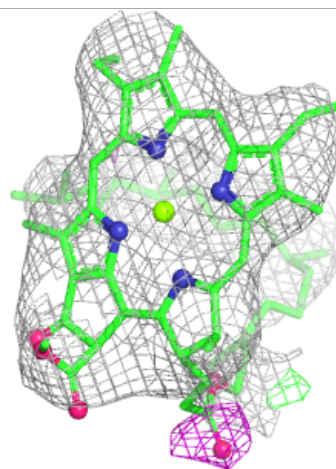
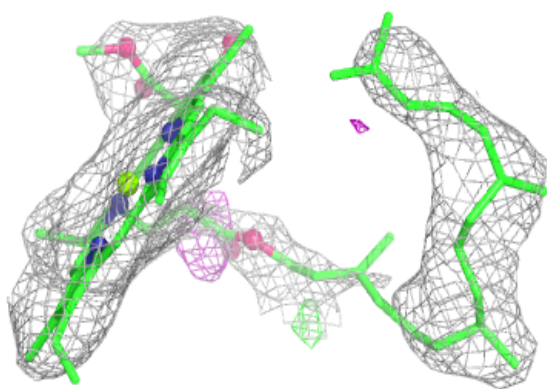
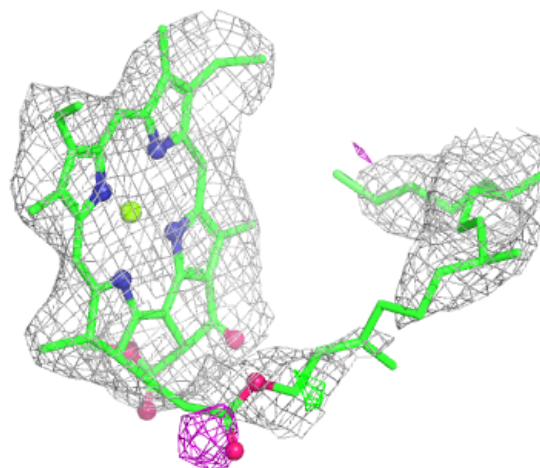
Electron density around CLA b 5513:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



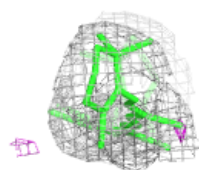
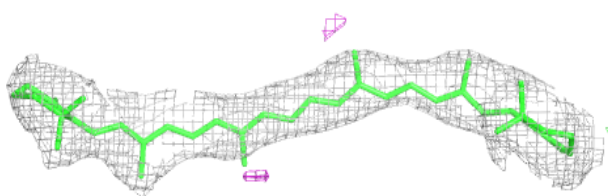
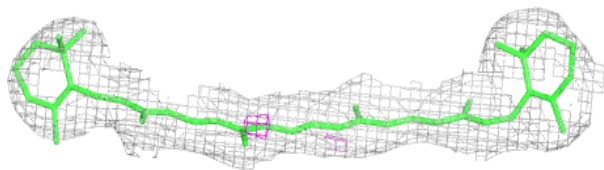
Electron density around CLA C 493:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

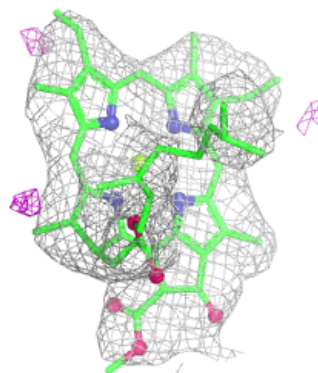
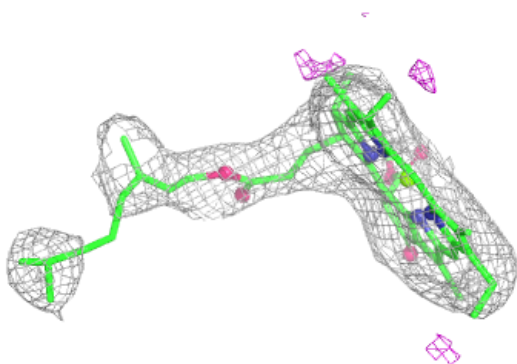
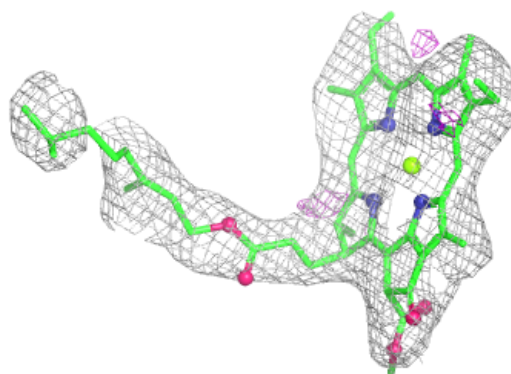


Electron density around BCR C 504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

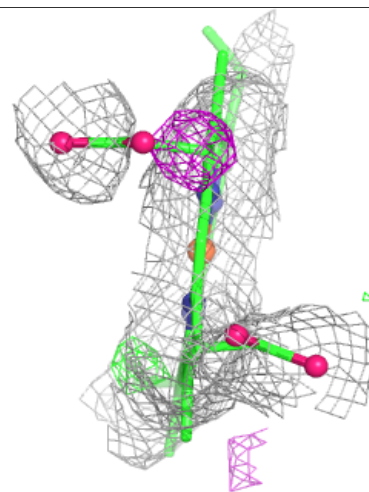
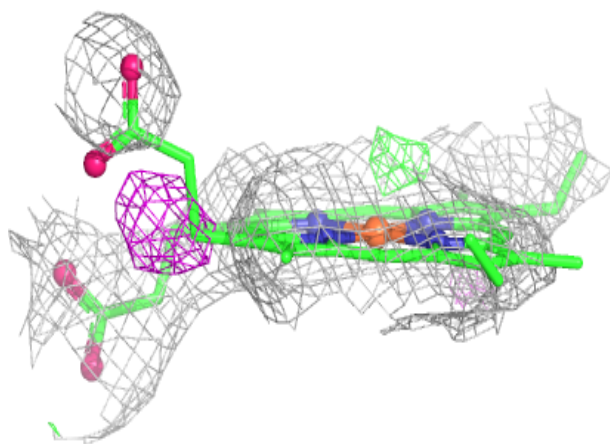
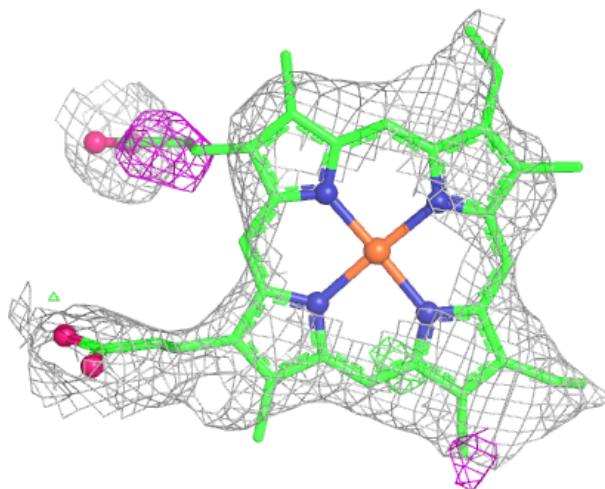
**Electron density around CLA A 563:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



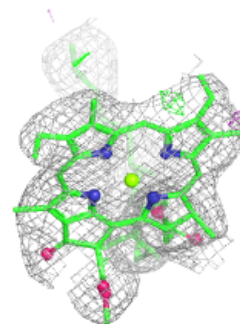
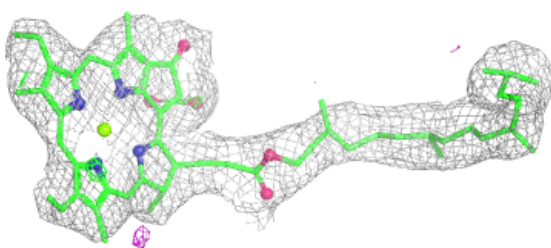
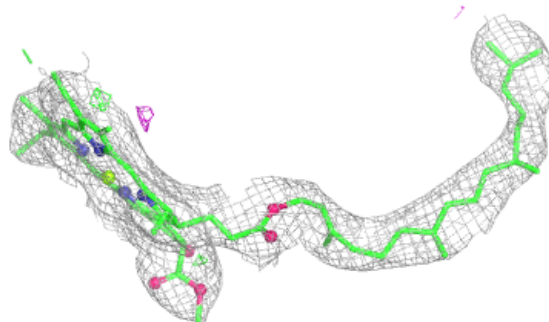
Electron density around HEM f 5051:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

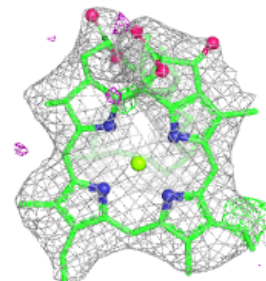
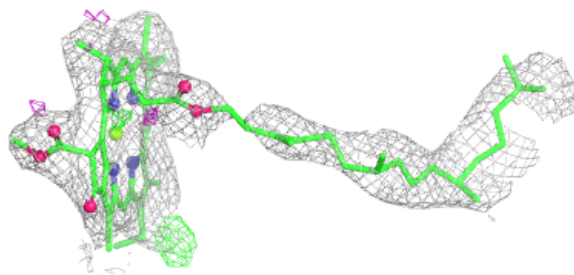
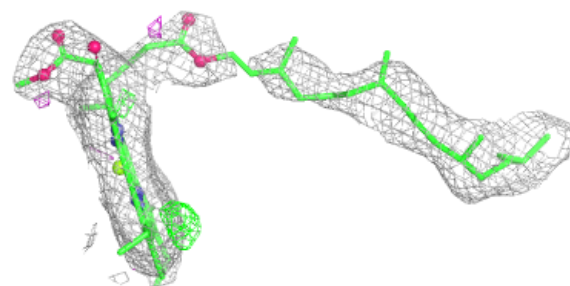


Electron density around CLA D 354:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

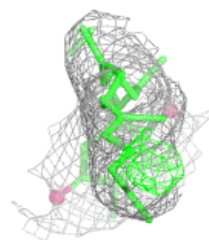
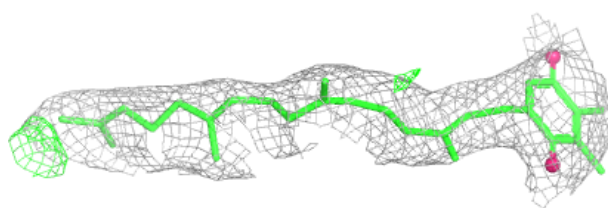
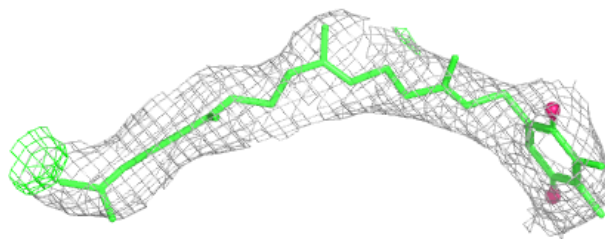
**Electron density around CLA b 5515:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

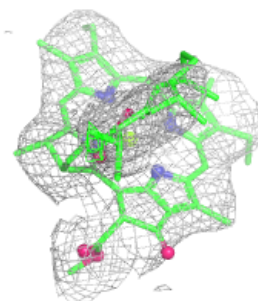
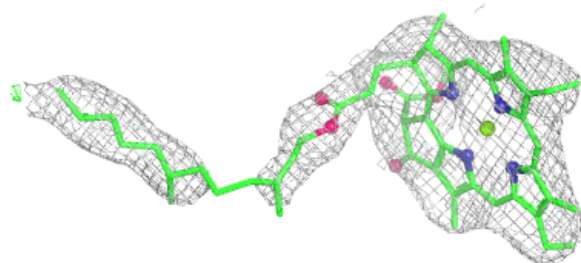
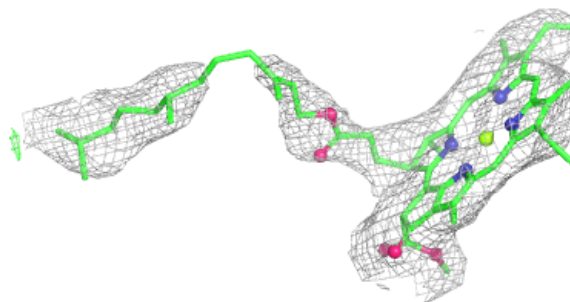


Electron density around PQ9 D 356:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

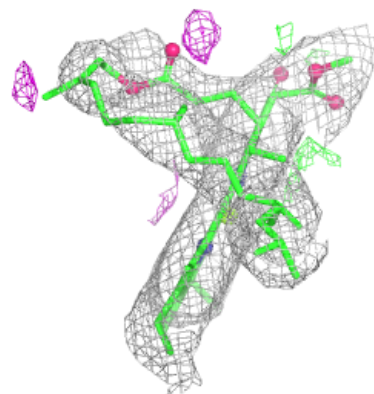
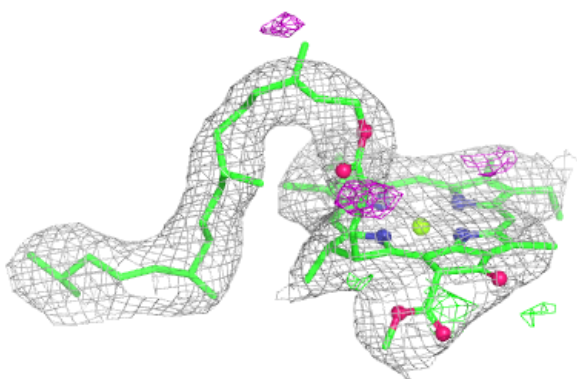
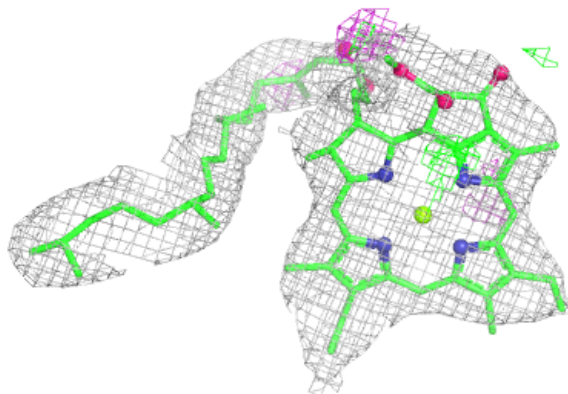
**Electron density around CLA C 492:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

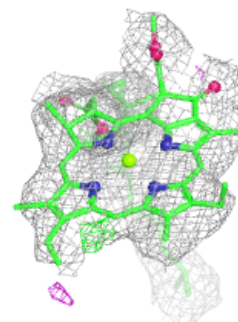
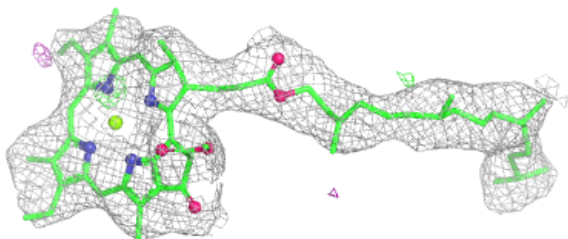
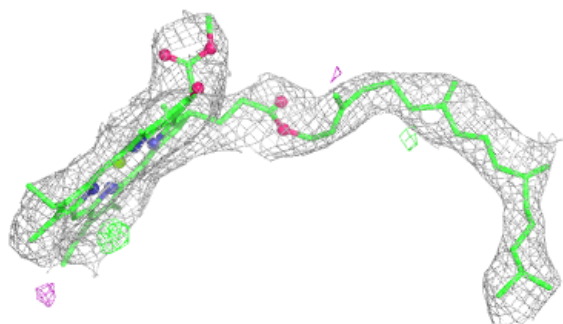


Electron density around CLA a 5559:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

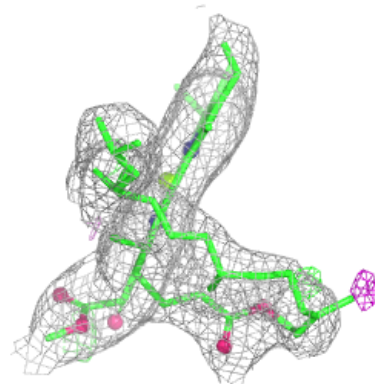
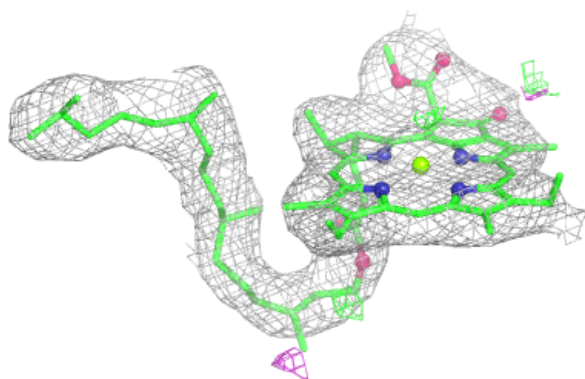
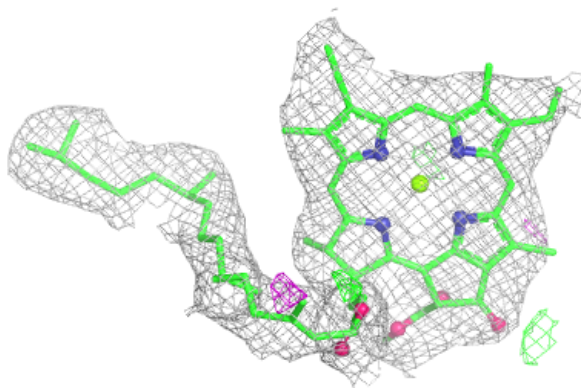
**Electron density around CLA d 5354:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

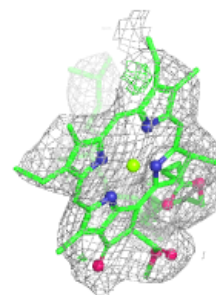
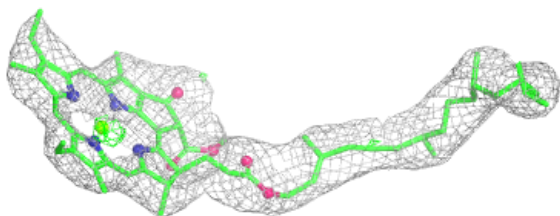
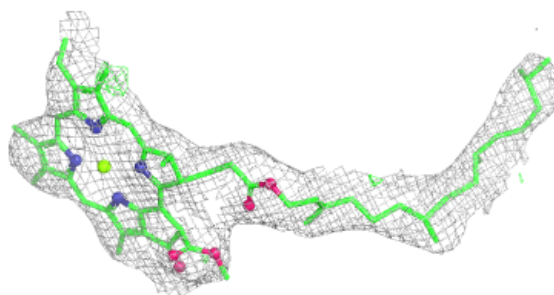


Electron density around CLA A 559:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

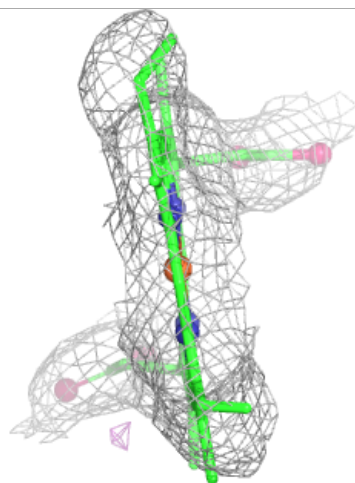
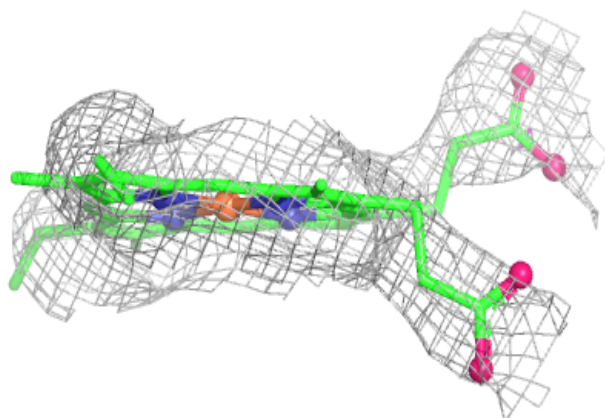
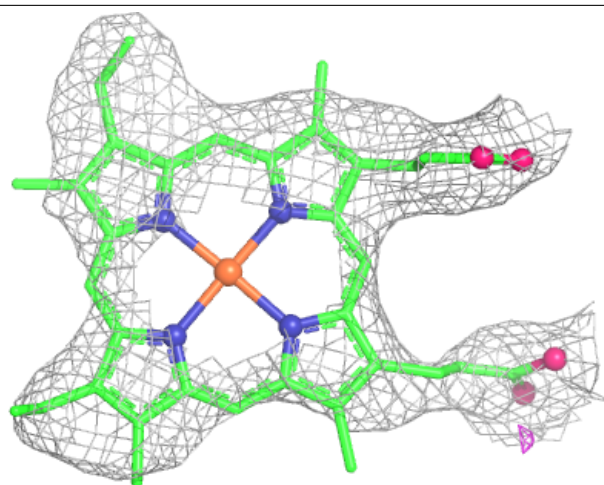
**Electron density around CLA a 5558:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



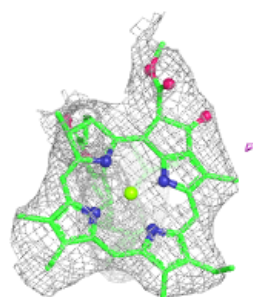
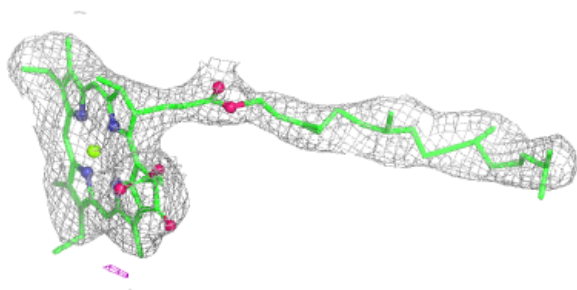
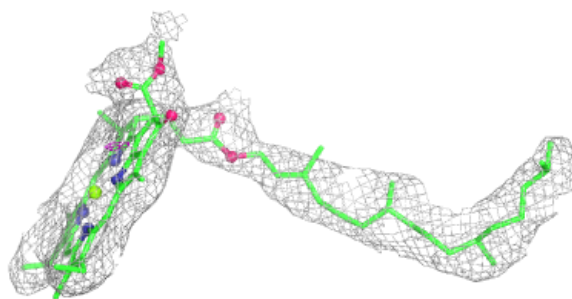
Electron density around HEM F 51:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



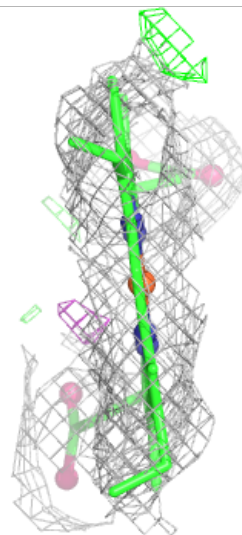
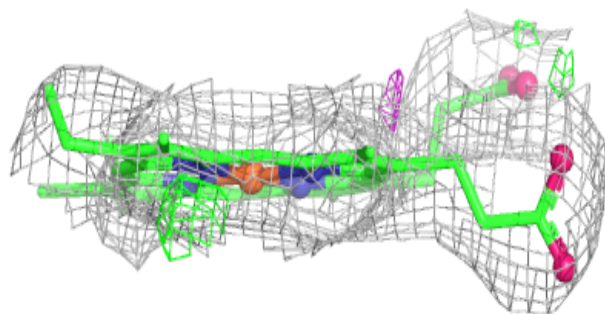
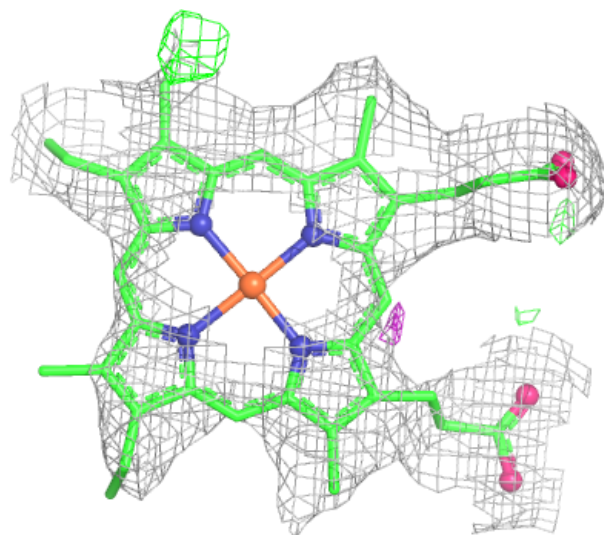
Electron density around CLA b 5514:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



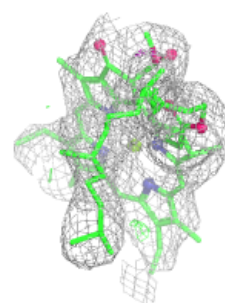
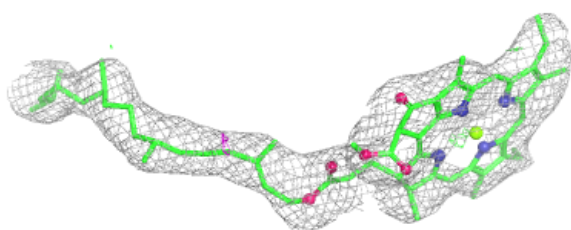
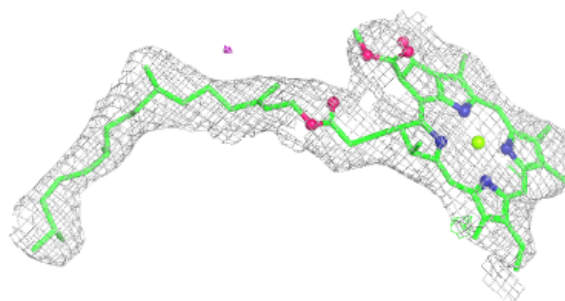
Electron density around HEM v 5552:

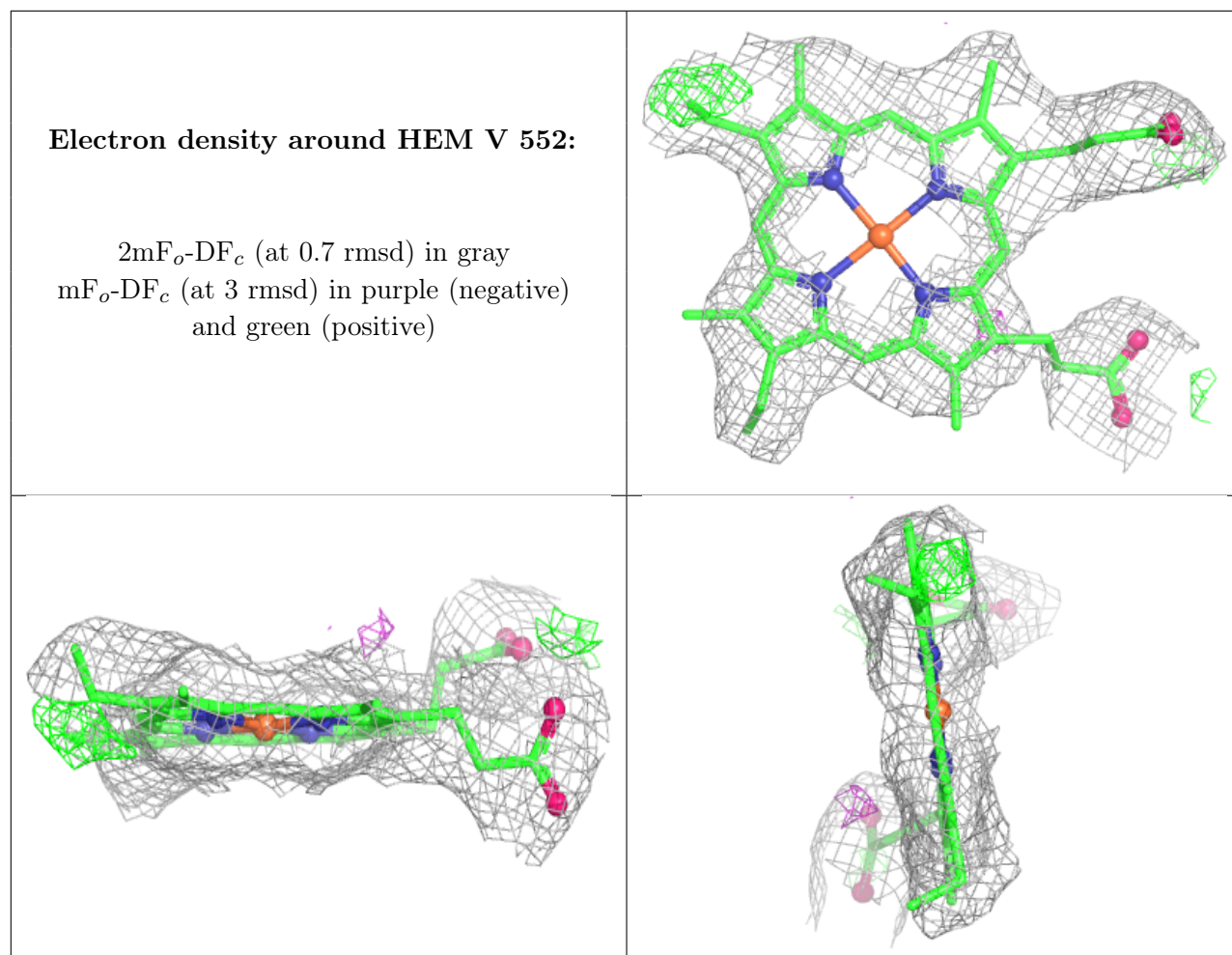
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around CLA A 558:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.