



Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 07:30 AM JST

PDB ID : 7EDA / pdb_00007eda
EMDB ID : EMD-31062
Title : Structure of monomeric photosystem II
Authors : Yu, H.; Hamaguchi, T.; Nakajima, Y.; Kato, K.; kawakami, K.; Akita, F.;
Yonekura, K.; Shen, J.R.
Deposited on : 2021-03-15
Resolution : 2.78 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

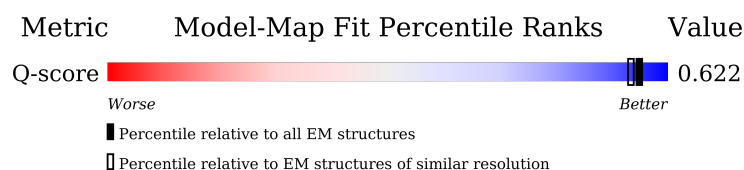
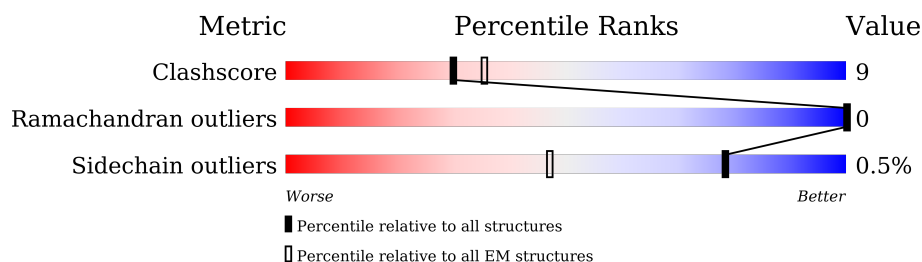
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.78 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10754 (2.28 - 3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	13% 69% 30%
2	B	504	81% 18%
3	C	451	6% 79% 21%
4	D	341	75% 25%

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Mol	Chain	Length	Quality of chain
5	E	84	
6	F	45	
7	H	62	
8	I	38	
9	J	40	
10	K	37	
11	L	37	
12	M	30	
13	O	244	
14	T	30	
15	U	104	
16	V	163	
17	Y	30	
18	X	40	
19	Z	62	
20	R	34	

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
35	HEC	V	201	X	-	-	-

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 22843 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	334	Total	C	N	O	S	0	0
			2598	1708	429	446	15		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	PRO	ARG	conflict	UNP P51765

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	504	Total	C	N	O	S	0	0
			3890	2560	652	665	13		

- Molecule 3 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	451	Total	C	N	O	S	0	0
			3453	2268	583	589	13		

- Molecule 4 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	341	Total	C	N	O	S	2	0
			2699	1796	443	448	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	80	Total	C	N	O	0	0
			622	412	100	110		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	34	Total	C	N	O	S	0	0
			274	187	45	41	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	62	Total	C	N	O	S	0	0
			484	326	78	78	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	32	Total	C	N	O	S	0	0
			255	176	37	41	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	36	Total	C	N	O	S	0	0
			251	171	37	42	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	K	37	Total	C	N	O	0	0
			280	194	42	44		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	33	LEU	PHE	conflict	UNP P19054
K	39	TRP	VAL	conflict	UNP P19054

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	L	30	Total	C	N	O	0	0
			244	166	36	42		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	30	Total	C	N	O	0	0
			223	150	33	40		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	8	LEU	PHE	conflict	UNP P12312

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	192	Total	C	N	O	S	0	0
			1415	907	237	267	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	29	Total	C	N	O	S	0	0
			230	161	32	36	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
15	U	84	Total	C	N	O	0	0
			629	409	110	110		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	135	Total	C	N	O	S	0	0
			1016	651	171	190	4		

- Molecule 17 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	27	Total	C	N	O	S	0	0
			190	125	32	31	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	X	38	Total	C	N	O	0	0
			269	179	44	46		

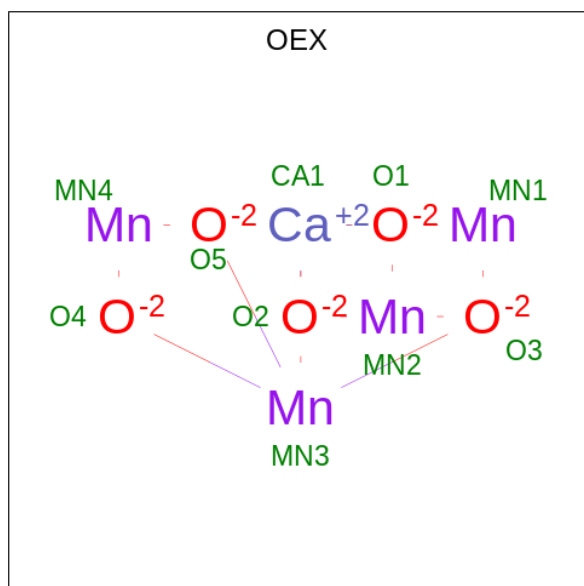
- Molecule 19 is a protein called Photosystem II reaction center protein Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	57	Total	C	N	O	S	0	0
			410	284	61	64	1		

- Molecule 20 is a protein called Photosystem II protein Y.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	34	Total	C	N	O	0	0
			186	115	36	35		

- Molecule 21 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: CaMn_4O_5).

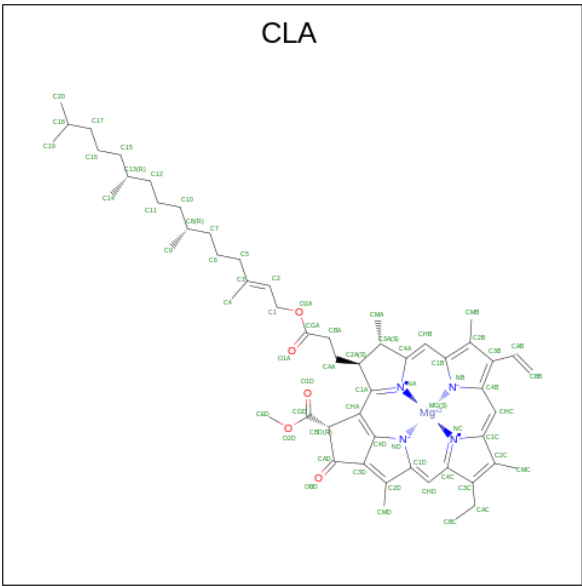


Mol	Chain	Residues	Atoms				AltConf
21	A	1	Total	Ca	Mn	O	0
			10	1	4	5	

- Molecule 22 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
22	A	1	Total	Fe	0
			1	1	

- Molecule 23 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	

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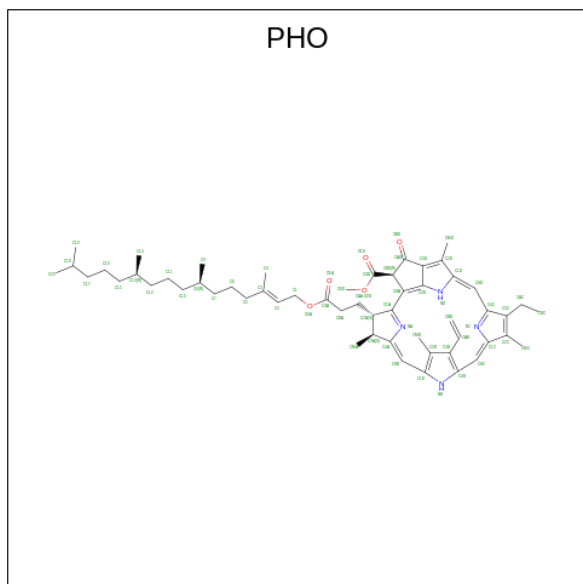
Mol	Chain	Residues	Atoms					AltConf
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
23	C	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
23	D	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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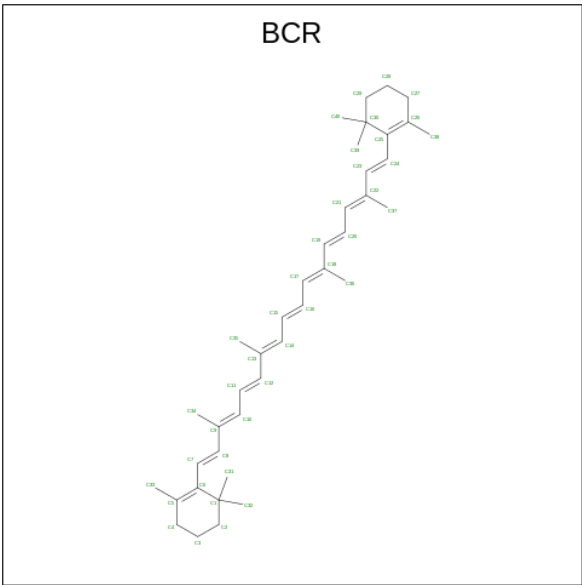
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
23	D	1	45	35	1	4	5	0

- Molecule 24 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



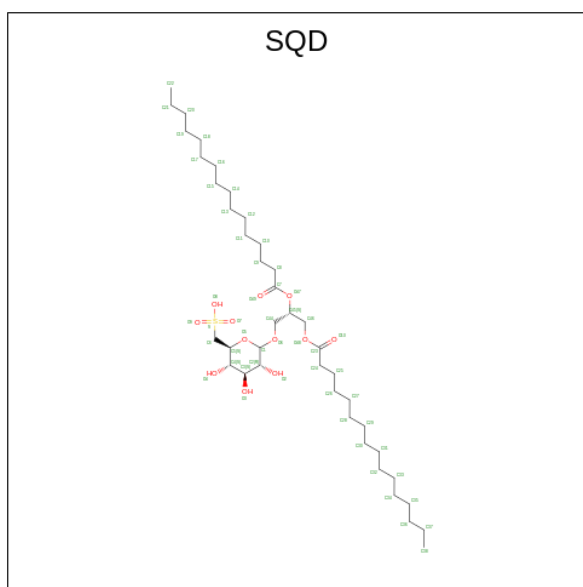
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
24	A	1	64	55	4	5	0
24	A	1	64	55	4	5	0

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



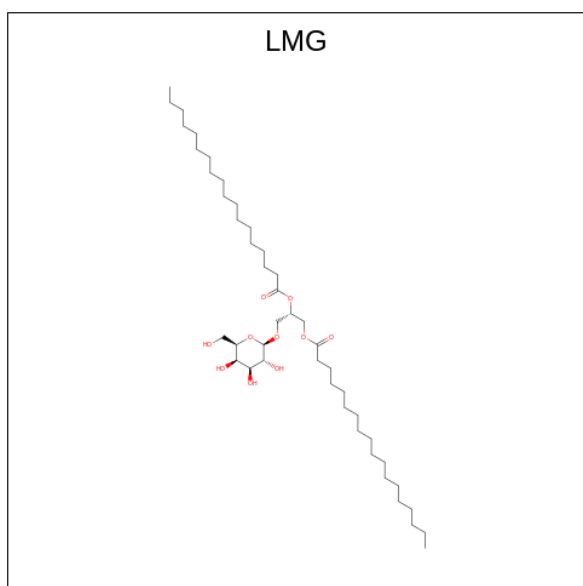
Mol	Chain	Residues	Atoms	AltConf
25	A	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	B	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	C	1	Total C 40 40	0
25	D	1	Total C 29 29	0
25	K	1	Total C 40 40	0
25	K	1	Total C 40 40	0

- Molecule 26 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	O	S	0
			54	41	12	1	
26	D	1	Total	C	O	S	0
			24	13	10	1	

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



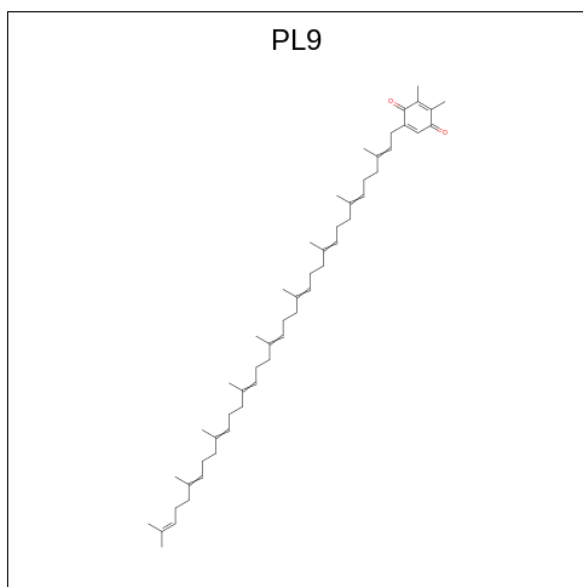
Mol	Chain	Residues	Atoms			AltConf
27	A	1	Total	C	O	0
			38	28	10	

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Mol	Chain	Residues	Atoms			AltConf
27	B	1	Total	C	O	0
			39	29	10	
27	D	1	Total	C	O	0
			24	14	10	

- Molecule 28 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (CCD ID: PL9) (formula: $C_{53}H_{80}O_2$).

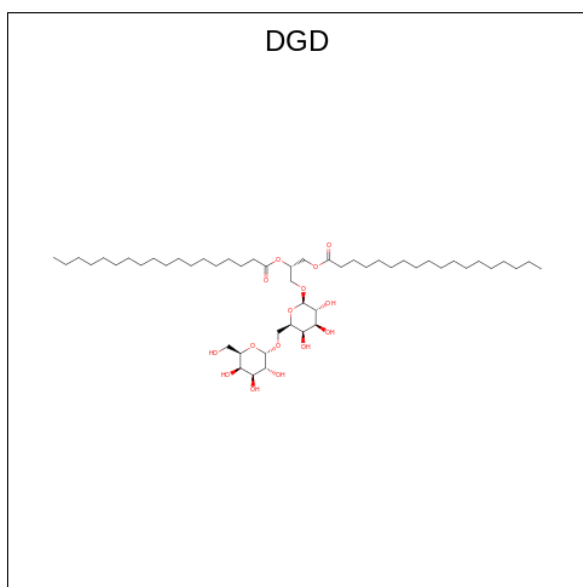


Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	C	O	0
			51	49	2	
28	D	1	Total	C	O	0
			43	41	2	

- Molecule 29 is UNKNOWN LIGAND (CCD ID: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

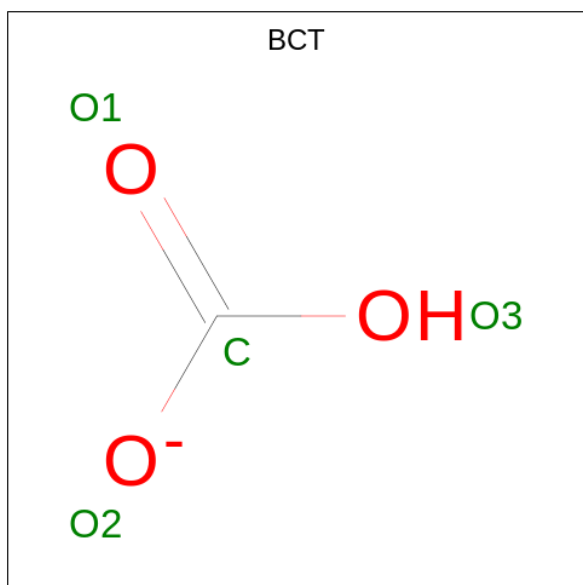
Mol	Chain	Residues	Atoms		AltConf
29	B	1	Total	C	0
			7	7	

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



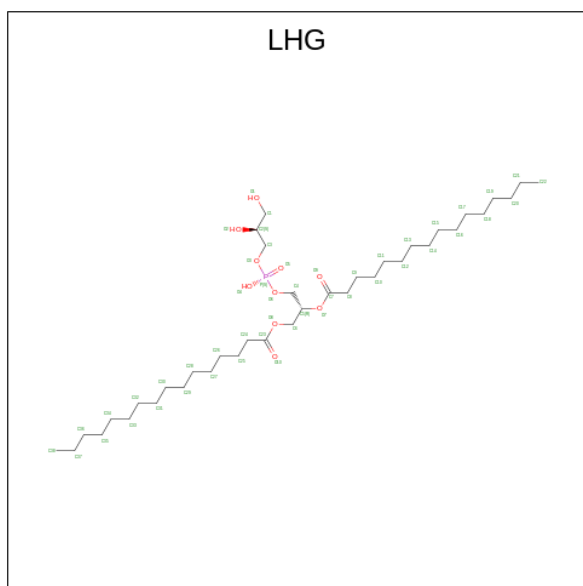
Mol	Chain	Residues	Atoms			AltConf
30	C	1	Total	C	O	0
			41	26	15	
30	C	1	Total	C	O	0
			49	34	15	
30	C	1	Total	C	O	0
			50	35	15	
30	H	1	Total	C	O	0
			50	35	15	

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



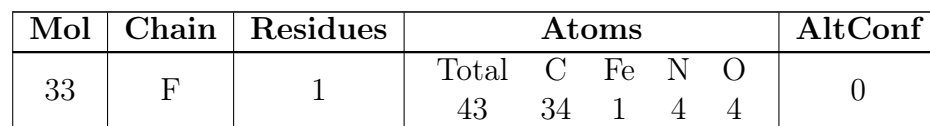
Mol	Chain	Residues	Atoms			AltConf
31	D	1	Total	C	O	
			4	1	3	0

- Molecule 32 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
32	D	1	Total	C	O	P	
			49	38	10	1	0
32	D	1	Total	C	O	P	
			32	21	10	1	0
32	D	1	Total	C	O	P	
			33	22	10	1	0
32	L	1	Total	C	O	P	
			40	29	10	1	0

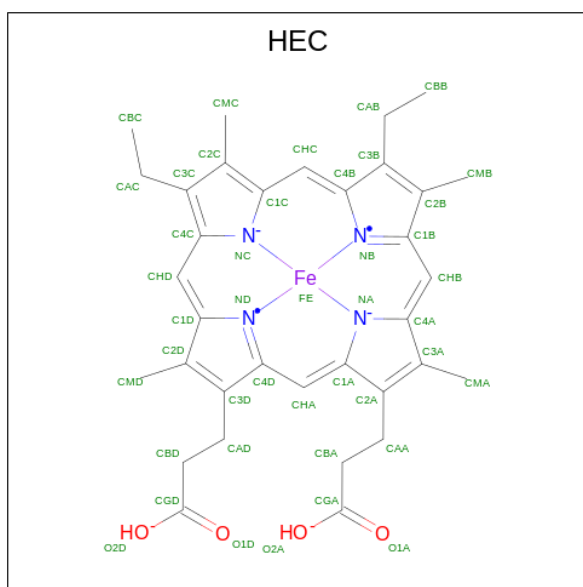
- Molecule 33 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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- The chemical structure shows a long, zig-zagging carbon chain with alternating double bonds. At the right end, there is a terminal diol group: a carbon atom bonded to two hydroxyl groups (OH) and two methyl groups (CH₃). The chain continues with several conjugated and non-conjugated double bonds, ending at a methyl group on the left. The structure is drawn in a skeletal format with grey lines for carbon-carbon bonds and red lines for the hydroxyl groups.

Mol	Chain	Residues	Atoms			AltConf
34	H	1	Total	C	O	0
			41	40	1	

- 



Mol	Chain	Residues	Atoms					AltConf
35	V	1	Total 43	C 34	Fe 1	N 4	O 4	0

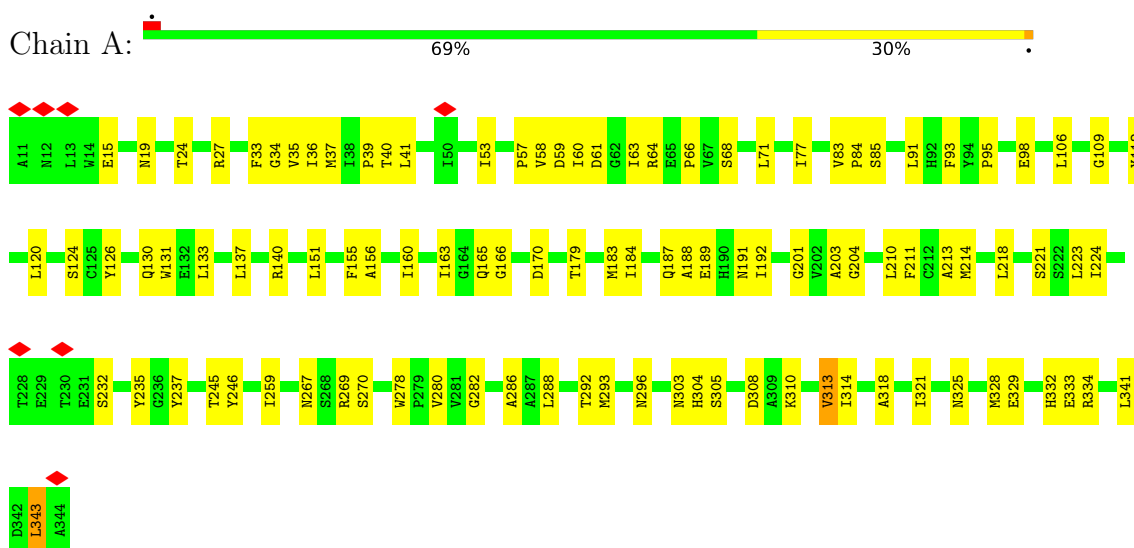
- Molecule 36 is water.

Mol	Chain	Residues	Atoms	AltConf
36	A	7	Total O 7 7	0
36	B	5	Total O 5 5	0
36	C	4	Total O 4 4	0

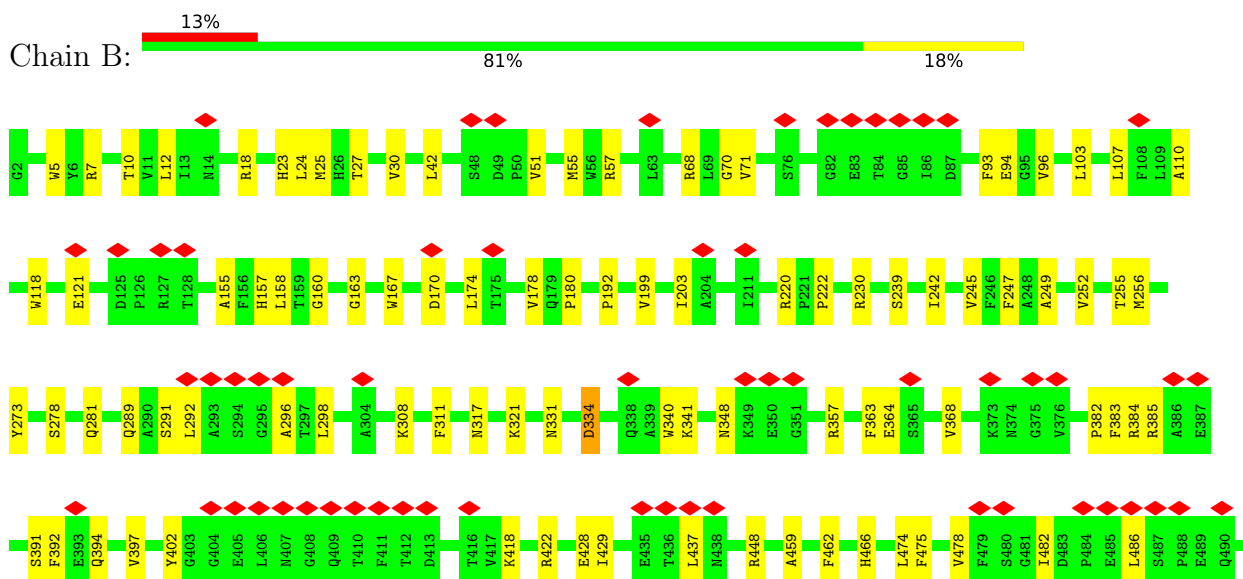
3 Residue-property plots

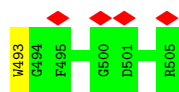
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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 II protein D1

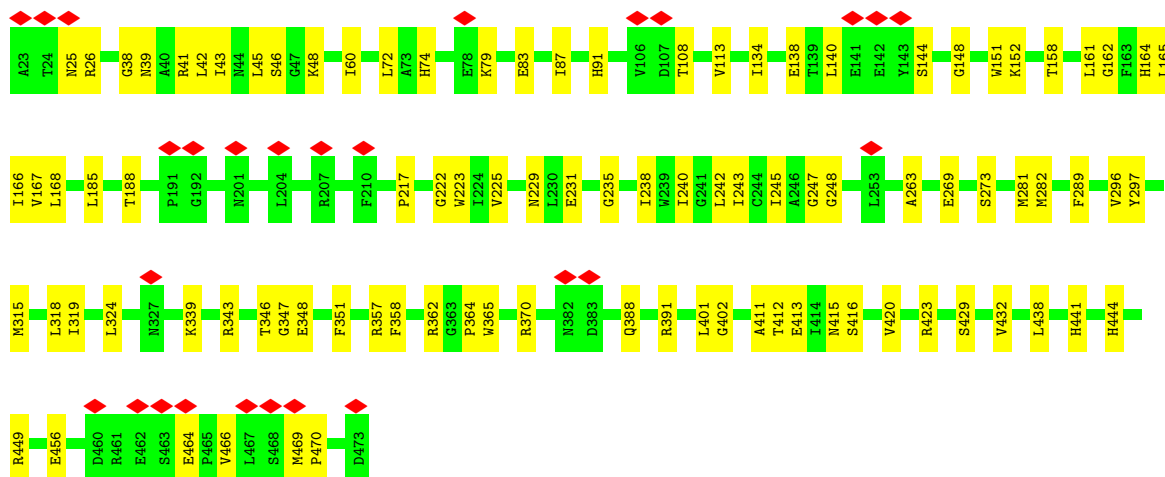
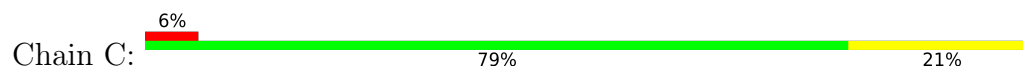


- Molecule 2: Photosystem II CP47 reaction center protein

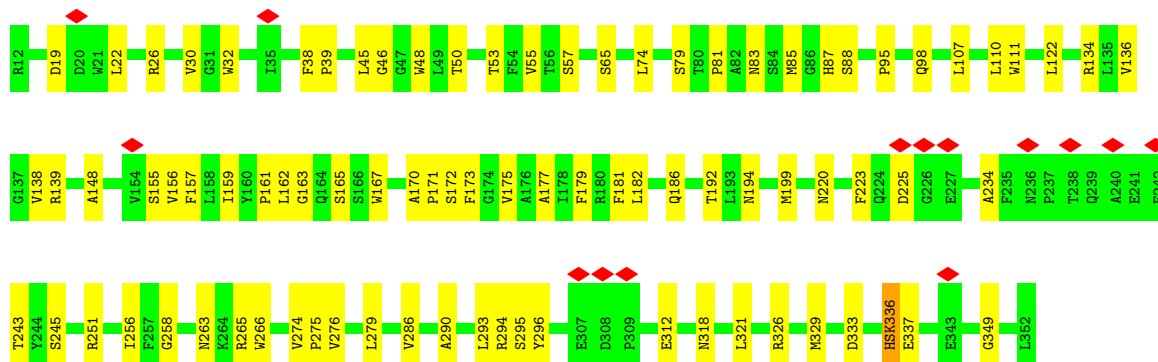
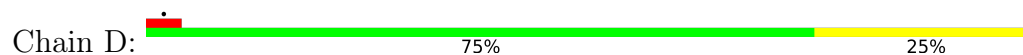




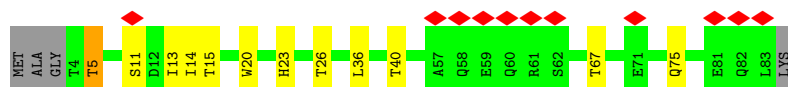
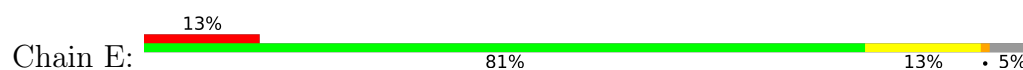
- Molecule 3: Photosystem II CP43 reaction center protein



- Molecule 4: Photosystem II D2 protein

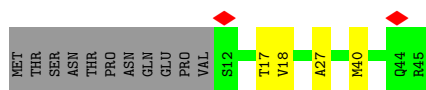


- Molecule 5: Cytochrome b559 subunit alpha

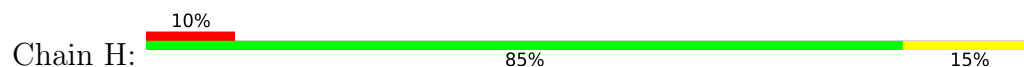


- Molecule 6: Cytochrome b559 subunit beta

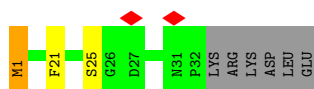
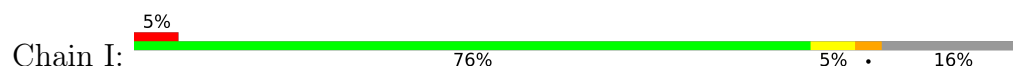




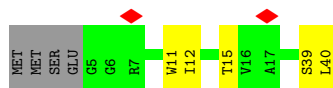
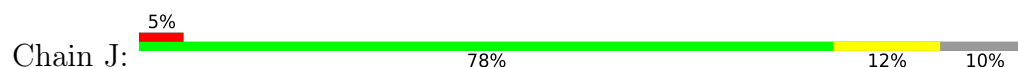
- Molecule 7: Photosystem II reaction center protein H



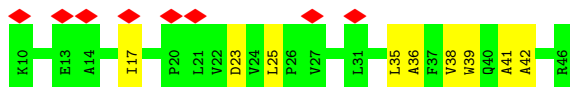
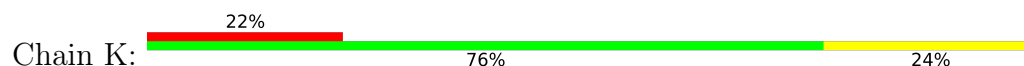
- Molecule 8: Photosystem II reaction center protein I



- Molecule 9: Photosystem II reaction center protein J



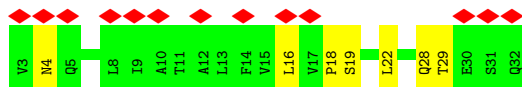
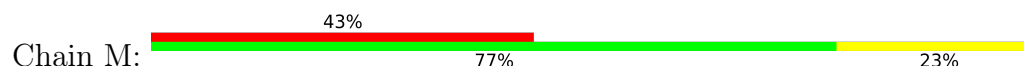
- Molecule 10: Photosystem II reaction center protein K



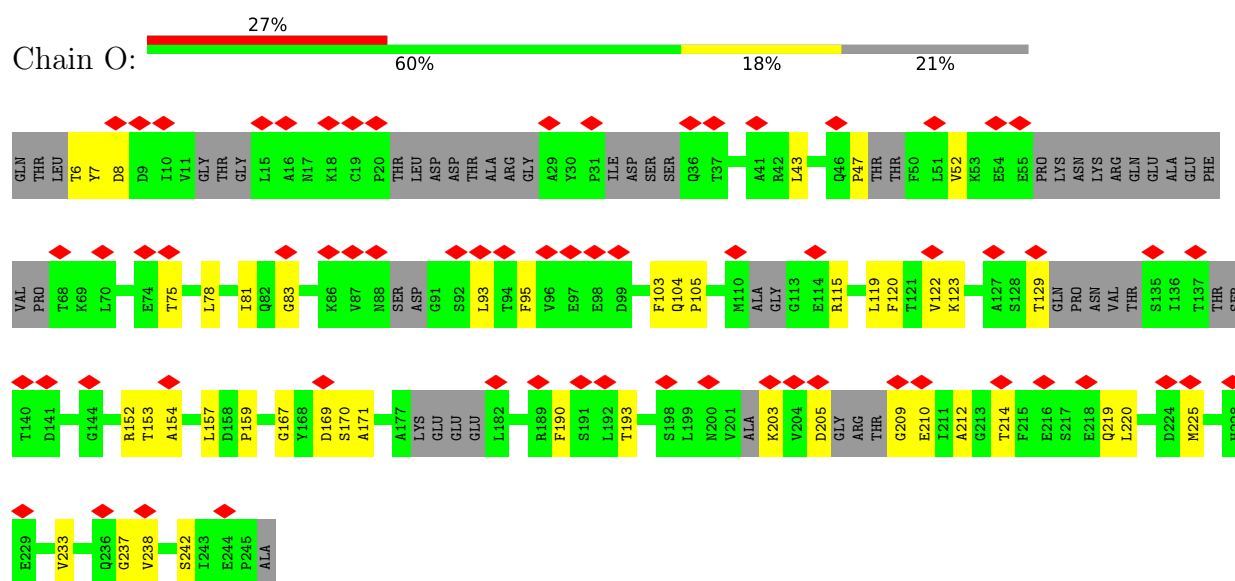
- Molecule 11: Photosystem II reaction center protein L



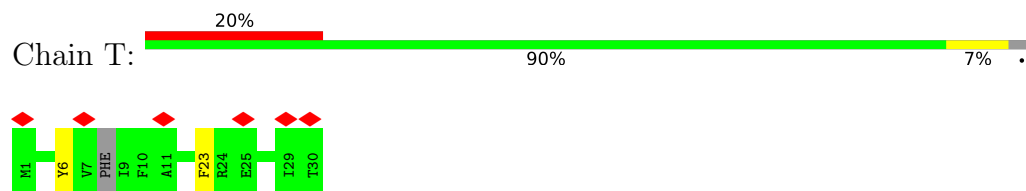
- Molecule 12: Photosystem II reaction center protein M



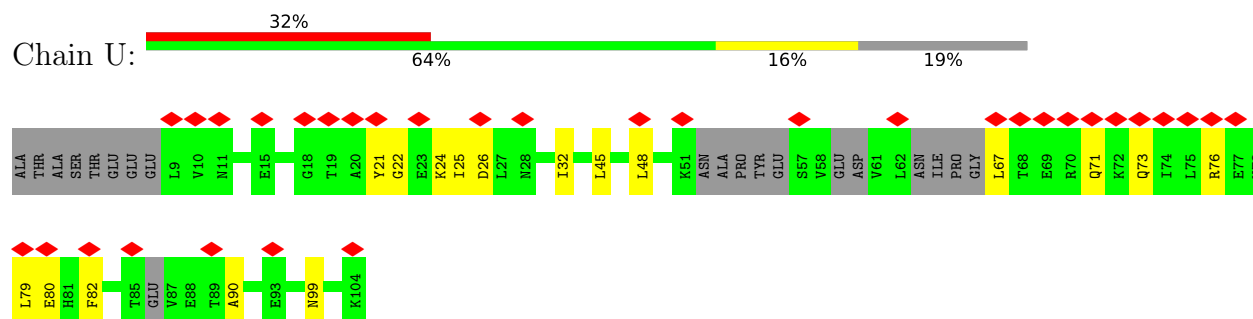
- Molecule 13: Photosystem II manganese-stabilizing polypeptide



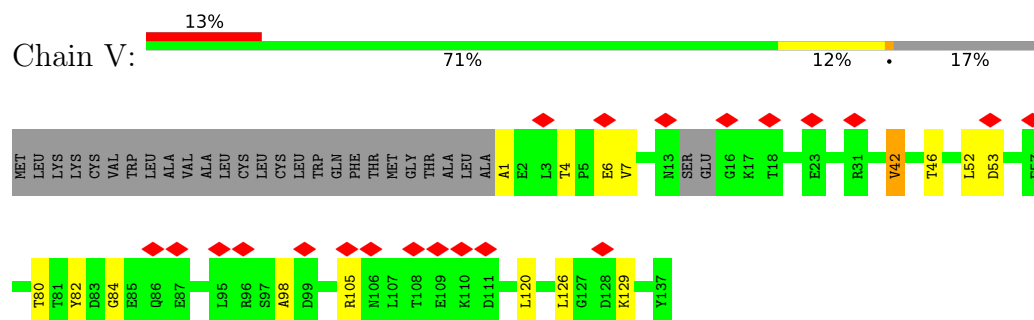
• Molecule 14: Photosystem II reaction center protein T



• Molecule 15: Photosystem II 12 kDa extrinsic protein

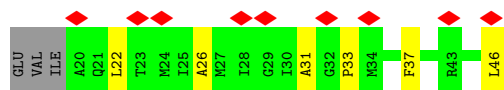


• Molecule 16: Cytochrome c-550



• Molecule 17: Photosystem II reaction center protein Ycf12





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	173875	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.180	Depositor
Minimum map value	-0.111	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0316	Depositor
Map size ($\text{\AA}$)	197.26031, 197.26031, 197.26031	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.82191795, 0.82191795, 0.82191795	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, RRX, DGD, HEC, CLA, FME, HEM, HSK, UNL, PHO, PL9, BCR, LMG, OEX, SQD, BCT, FE2

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	0.44	0/2683	0.60	0/3660
2	B	0.36	0/4028	0.53	0/5496
3	C	0.38	0/3566	0.53	0/4859
4	D	0.44	0/2777	0.59	0/3785
5	E	0.30	0/641	0.48	0/880
6	F	0.33	0/283	0.52	0/386
7	H	0.32	0/497	0.60	0/679
8	I	0.27	0/252	0.51	0/344
9	J	0.28	0/257	0.51	0/349
10	K	0.41	0/290	0.72	0/399
11	L	0.39	0/249	0.53	0/337
12	M	0.35	0/226	0.57	0/310
13	O	0.31	0/1430	0.59	2/1928 (0.1%)
14	T	0.25	0/231	0.45	0/313
15	U	0.27	0/633	0.55	0/853
16	V	0.30	0/1036	0.55	0/1410
17	Y	0.26	0/191	0.53	0/256
18	X	0.26	0/271	0.52	0/367
19	Z	0.25	0/417	0.53	0/570
20	R	0.23	0/186	0.46	0/257
All	All	0.37	0/20144	0.56	2/27438 (0.0%)

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
3	C	0	1
4	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	I	0	2
All	All	0	4

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	123	LYS	CA-C-N	5.13	131.33	121.54
13	O	123	LYS	C-N-CA	5.13	131.33	121.54

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	222	GLY	Peptide
4	D	294	ARG	Peptide
8	I	1	FME	Peptide,Mainchain

5.2 Too-close contacts [i](#)

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	2598	0	2498	91	0
2	B	3890	0	3702	71	0
3	C	3453	0	3367	72	0
4	D	2699	0	2600	68	0
5	E	622	0	595	9	0
6	F	274	0	279	4	0
7	H	484	0	500	9	0
8	I	255	0	264	1	0
9	J	251	0	257	4	0
10	K	280	0	272	7	0
11	L	244	0	252	7	0
12	M	223	0	228	6	0
13	O	1415	0	1337	28	0
14	T	230	0	223	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	U	629	0	628	12	0
16	V	1016	0	1012	12	0
17	Y	190	0	203	6	0
18	X	269	0	294	2	0
19	Z	410	0	427	4	0
20	R	186	0	124	1	0
21	A	10	0	0	2	0
22	A	1	0	0	0	0
23	A	207	0	175	7	0
23	B	920	0	888	32	0
23	C	774	0	780	37	0
23	D	105	0	88	4	0
24	A	128	0	148	8	0
25	A	40	0	56	4	0
25	B	80	0	112	6	0
25	C	80	0	112	4	0
25	D	29	0	36	0	0
25	K	80	0	112	8	0
26	A	54	0	78	4	0
26	D	24	0	18	1	0
27	A	38	0	46	1	0
27	B	39	0	48	2	0
27	D	24	0	18	0	0
28	A	51	0	71	5	0
28	D	43	0	58	4	0
29	B	7	0	0	0	0
30	C	140	0	154	7	0
30	H	50	0	58	3	0
31	D	4	0	0	1	0
32	D	114	0	144	4	0
32	L	40	0	50	5	0
33	F	43	0	30	4	0
34	H	41	0	56	4	0
35	V	43	0	30	0	0
36	A	7	0	0	0	0
36	B	5	0	0	0	0
36	C	4	0	0	0	0
All	All	22843	0	22428	413	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 9.

All (413) 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)
1:A:343:LEU:O	3:C:401:LEU:HD11	1.65	0.96
1:A:334:ARG:HG3	13:O:157:LEU:HB2	1.51	0.92
1:A:334:ARG:HB2	13:O:157:LEU:HD12	1.53	0.88
23:B:610:CLA:H2	23:B:611:CLA:HBB2	1.66	0.76
2:B:30:VAL:HG12	23:B:606:CLA:HHD	1.71	0.72
4:D:192:THR:HG23	23:D:402:CLA:HBC2	1.72	0.72
1:A:329:GLU:O	1:A:332:HIS:CE1	2.46	0.69
23:B:604:CLA:HAC2	23:B:607:CLA:HBB2	1.77	0.67
1:A:61:ASP:OD2	1:A:333:GLU:HG2	1.95	0.67
1:A:246:TYR:HE1	31:D:401:BCT:O2	1.79	0.66
1:A:189:GLU:OE2	21:A:401:OEX:MN1	1.54	0.65
23:B:613:CLA:H171	23:B:614:CLA:HBB2	1.77	0.65
16:V:126:LEU:HB3	16:V:129:LYS:HB2	1.78	0.65
1:A:34:GLY:HA2	1:A:37:MET:HB3	1.78	0.65
1:A:201:GLY:HA3	1:A:286:ALA:HB2	1.78	0.65
27:A:413:LMG:H322	3:C:217:PRO:HD3	1.78	0.65
13:O:93:LEU:H	13:O:129:THR:HG22	1.61	0.65
2:B:23:HIS:ND1	23:B:616:CLA:OBD	2.24	0.64
3:C:167:VAL:HG13	23:C:512:CLA:H61	1.79	0.64
3:C:438:LEU:HD11	23:C:505:CLA:HBB1	1.78	0.64
3:C:25:ASN:HB3	3:C:41:ARG:HB3	1.81	0.63
4:D:87:HIS:O	7:H:50:ASN:ND2	2.30	0.62
4:D:318:ASN:HA	4:D:321:LEU:HD12	1.81	0.62
1:A:95:PRO:HD2	1:A:98:GLU:HB2	1.83	0.61
1:A:85:SER:HA	1:A:109:GLY:HA3	1.81	0.61
23:B:604:CLA:H2	23:B:606:CLA:H91	1.83	0.61
2:B:255:THR:HG21	23:B:603:CLA:HED1	1.83	0.60
3:C:429:SER:HA	30:C:517:DGD:HBW1	1.83	0.60
1:A:189:GLU:OE2	21:A:401:OEX:O1	2.19	0.60
23:C:501:CLA:H193	23:C:507:CLA:HBB1	1.84	0.60
1:A:188:ALA:HB2	1:A:328:MET:HB2	1.84	0.60
17:Y:31:ALA:HB1	19:Z:21:ILE:HD11	1.84	0.60
1:A:35:VAL:HG13	25:A:411:BCR:HC21	1.84	0.59
16:V:4:THR:HG22	16:V:7:VAL:HG23	1.85	0.59
1:A:305:SER:HA	9:J:39:SER:HB3	1.83	0.59
2:B:392:PHE:HB2	2:B:418:LYS:HE3	1.84	0.59
2:B:25:MET:HG2	25:B:618:BCR:H23C	1.84	0.59
1:A:267:ASN:HB3	1:A:270:SER:HB3	1.84	0.59
3:C:39:ASN:ND2	23:C:510:CLA:O1A	2.33	0.59
1:A:310:LYS:HD2	16:V:1:ALA:HB3	1.85	0.58
1:A:57:PRO:O	13:O:115:ARG:NH1	2.34	0.58
1:A:329:GLU:O	1:A:332:HIS:ND1	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:155:SER:HA	4:D:159:ILE:HB	1.85	0.58
2:B:384:ARG:NH2	4:D:349:GLY:O	2.37	0.58
2:B:158:LEU:HB3	2:B:199:VAL:HG22	1.86	0.58
3:C:464:GLU:OE2	4:D:245:SER:OG	2.21	0.57
1:A:237:TYR:HB2	4:D:265:ARG:HG3	1.86	0.57
1:A:93:PHE:HZ	23:A:410:CLA:HAA1	1.69	0.57
23:A:407:CLA:HBB1	23:D:402:CLA:H2	1.86	0.57
3:C:415:ASN:ND2	30:C:518:DGD:O4D	2.38	0.57
3:C:339:LYS:NZ	15:U:99:ASN:O	2.37	0.56
1:A:39:PRO:HG3	25:A:411:BCR:HC8	1.87	0.56
1:A:77:ILE:HD11	14:T:6:TYR:HB3	1.87	0.56
11:L:14:ARG:NH2	14:T:23:PHE:O	2.38	0.56
13:O:119:LEU:O	13:O:219:GLN:NE2	2.37	0.56
3:C:229:ASN:HD22	3:C:231:GLU:HB2	1.71	0.56
1:A:140:ARG:NH1	3:C:456:GLU:O	2.35	0.56
1:A:288:LEU:HD13	3:C:432:VAL:HG22	1.87	0.56
2:B:5:TRP:HE1	32:L:101:LHG:HC62	1.70	0.56
2:B:23:HIS:HB3	23:B:616:CLA:HED2	1.87	0.56
1:A:191:ASN:HB2	3:C:411:ALA:HB1	1.87	0.56
1:A:213:ALA:HB2	4:D:275:PRO:HG2	1.88	0.56
1:A:334:ARG:HH22	4:D:312:GLU:CD	2.13	0.56
2:B:311:PHE:O	2:B:317:ASN:ND2	2.39	0.56
3:C:26:ARG:NH2	17:Y:46:LEU:O	2.39	0.56
3:C:343:ARG:NH1	3:C:347:GLY:O	2.39	0.56
13:O:214:THR:HA	13:O:238:VAL:HA	1.88	0.56
3:C:72:LEU:HD11	3:C:108:THR:HB	1.87	0.55
4:D:225:ASP:HB2	4:D:234:ALA:HB1	1.88	0.55
2:B:348:ASN:HA	2:B:397:VAL:HA	1.88	0.55
13:O:170:SER:OG	13:O:171:ALA:N	2.38	0.55
19:Z:10:ALA:HA	19:Z:13:VAL:HG22	1.89	0.55
4:D:179:PHE:HA	4:D:182:LEU:HD12	1.86	0.55
3:C:282:MET:HE2	23:C:501:CLA:H122	1.87	0.55
4:D:329:MET:HG2	4:D:333:ASP:HB2	1.87	0.55
13:O:152:ARG:HB2	13:O:225:MET:HE3	1.89	0.55
23:C:502:CLA:HBA2	23:C:503:CLA:H171	1.89	0.55
1:A:64:ARG:NH1	13:O:105:PRO:O	2.40	0.55
3:C:297:TYR:O	3:C:423:ARG:NH2	2.33	0.55
1:A:156:ALA:HA	1:A:160:ILE:HB	1.90	0.54
23:C:501:CLA:C4D	23:C:503:CLA:H2	2.37	0.54
23:C:502:CLA:H61	23:C:512:CLA:H11	1.89	0.54
24:A:409:PHO:HBC3	4:D:279:LEU:HD22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:168:LEU:HD21	23:C:509:CLA:H61	1.89	0.54
3:C:466:VAL:HA	3:C:469:MET:HB2	1.90	0.54
4:D:186:GLN:HB2	23:D:402:CLA:HBC1	1.89	0.54
2:B:18:ARG:HG3	2:B:118:TRP:HB3	1.90	0.54
2:B:157:HIS:HA	2:B:163:GLY:HA3	1.90	0.54
3:C:365:TRP:HB3	3:C:391:ARG:HD2	1.90	0.54
28:A:414:PL9:H461	4:D:39:PRO:HD3	1.89	0.53
23:B:612:CLA:H112	23:B:614:CLA:H52	1.90	0.53
23:C:508:CLA:H61	23:C:510:CLA:HED3	1.90	0.53
2:B:357:ARG:NH2	4:D:337:GLU:O	2.39	0.53
13:O:43:LEU:HB3	13:O:81:ILE:HB	1.89	0.53
2:B:230:ARG:NH2	2:B:474:LEU:O	2.42	0.53
1:A:192:ILE:HG13	1:A:293:MET:HE1	1.91	0.53
5:E:13:ILE:HG21	33:F:101:HEM:HAD2	1.89	0.53
3:C:346:THR:OG1	3:C:348:GLU:OE2	2.27	0.53
1:A:223:LEU:HD23	1:A:246:TYR:HB3	1.90	0.52
3:C:166:ILE:HG13	3:C:248:GLY:HA3	1.90	0.52
1:A:15:GLU:O	1:A:19:ASN:ND2	2.42	0.52
2:B:482:ILE:HD12	2:B:486:LEU:HD13	1.91	0.52
23:B:605:CLA:H42	23:B:606:CLA:H52	1.92	0.52
1:A:40:THR:HG23	23:A:410:CLA:HBB1	1.92	0.52
3:C:113:VAL:HG22	25:C:514:BCR:H313	1.90	0.52
3:C:362:ARG:NH2	13:O:8:ASP:OD1	2.36	0.52
2:B:278:SER:HB2	2:B:281:GLN:HB3	1.92	0.52
1:A:318:ALA:HA	1:A:321:ILE:HD12	1.92	0.52
13:O:47:PRO:HA	13:O:237:GLY:HA3	1.92	0.52
1:A:204:GLY:HA3	1:A:282:GLY:HA3	1.92	0.51
3:C:225:VAL:HG13	3:C:289:PHE:HA	1.91	0.51
3:C:45:LEU:HD22	3:C:138:GLU:HG2	1.91	0.51
3:C:60:ILE:HG23	23:C:510:CLA:HMC2	1.92	0.51
3:C:273:SER:O	3:C:441:HIS:ND1	2.36	0.51
23:C:504:CLA:HAA1	30:C:517:DGD:HD61	1.92	0.51
1:A:325:ASN:HA	1:A:328:MET:HE2	1.92	0.51
17:Y:33:PRO:O	17:Y:37:PHE:N	2.43	0.51
23:C:506:CLA:H43	25:C:515:BCR:H323	1.93	0.51
4:D:87:HIS:NE2	4:D:161:PRO:O	2.44	0.51
13:O:210:GLU:HA	13:O:242:SER:HA	1.92	0.51
1:A:58:VAL:HB	1:A:83:VAL:HB	1.92	0.51
1:A:188:ALA:HB1	1:A:329:GLU:HB3	1.93	0.51
3:C:165:LEU:HG	23:C:507:CLA:HED1	1.92	0.51
3:C:402:GLY:HA3	3:C:420:VAL:HG22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:95:PRO:O	4:D:98:GLN:NE2	2.43	0.51
16:V:69:ILE:HG13	16:V:120:LEU:HD12	1.93	0.51
16:V:98:ALA:O	16:V:105:ARG:NE	2.40	0.51
4:D:81:PRO:HD3	4:D:111:TRP:HB3	1.92	0.50
13:O:83:GLY:HA3	13:O:95:PHE:HE1	1.77	0.50
13:O:193:THR:HG21	13:O:220:LEU:HD12	1.92	0.50
27:B:622:LMG:HC92	12:M:4:ASN:HD21	1.76	0.50
3:C:185:LEU:HD13	23:C:501:CLA:HED2	1.92	0.50
2:B:493:TRP:HB3	5:E:5:THR:HG22	1.93	0.50
4:D:30:VAL:HA	4:D:38:PHE:HE2	1.76	0.50
26:D:407:SQD:H61	6:F:17:THR:HG22	1.94	0.50
3:C:188:THR:HG22	3:C:364:PRO:HG3	1.94	0.50
8:I:21:PHE:O	8:I:25:SER:N	2.45	0.50
4:D:263:ASN:HB3	4:D:266:TRP:HB3	1.93	0.50
23:C:506:CLA:HBB2	23:C:507:CLA:H52	1.94	0.50
1:A:210:LEU:HD23	1:A:214:MET:HG2	1.94	0.49
2:B:42:LEU:HD21	2:B:93:PHE:HB2	1.93	0.49
4:D:55:VAL:HG21	4:D:110:LEU:HD12	1.93	0.49
4:D:172:SER:HB2	4:D:177:ALA:HB1	1.93	0.49
3:C:315:MET:HE2	3:C:319:ILE:HD11	1.93	0.49
23:C:511:CLA:H71	25:K:102:BCR:H272	1.93	0.49
7:H:40:VAL:HG22	18:X:14:LEU:HD11	1.94	0.49
1:A:24:THR:O	4:D:251:ARG:NH2	2.45	0.49
3:C:74:HIS:NE2	10:K:23:ASP:OD1	2.43	0.49
13:O:78:LEU:HD13	13:O:122:VAL:HG22	1.94	0.49
1:A:27:ARG:NH2	4:D:258:GLY:O	2.37	0.49
1:A:334:ARG:NH2	4:D:312:GLU:OE2	2.31	0.49
3:C:235:GLY:HA2	3:C:238:ILE:HD12	1.93	0.49
23:C:503:CLA:HBB1	23:C:503:CLA:HHC	1.94	0.49
1:A:124:SER:HA	1:A:151:LEU:HD21	1.93	0.49
1:A:140:ARG:HB2	4:D:220:ASN:HA	1.94	0.49
2:B:174:LEU:HA	2:B:308:LYS:HD3	1.93	0.49
32:L:101:LHG:H291	12:M:22:LEU:HD11	1.93	0.49
1:A:187:GLN:HG3	1:A:328:MET:HE1	1.94	0.49
4:D:74:LEU:HD23	4:D:175:VAL:HG11	1.95	0.49
32:D:409:LHG:H251	11:L:18:TYR:HB3	1.95	0.49
3:C:38:GLY:HA3	23:C:511:CLA:HMD2	1.93	0.49
3:C:48:LYS:HG3	3:C:138:GLU:HG3	1.94	0.49
19:Z:26:ALA:HB1	19:Z:36:SER:HB3	1.95	0.49
1:A:232:SER:OG	32:L:101:LHG:O5	2.28	0.49
1:A:282:GLY:HA2	26:A:412:SQD:H223	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:PRO:HA	1:A:112:TYR:CG	2.48	0.48
1:A:221:SER:HA	4:D:139:ARG:HB2	1.94	0.48
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.94	0.48
23:B:611:CLA:HAB	34:H:101:RRX:H4	1.95	0.48
23:C:501:CLA:C3D	23:C:503:CLA:H2	2.43	0.48
1:A:211:PHE:HA	1:A:214:MET:HB2	1.95	0.48
32:D:408:LHG:H222	12:M:18:PRO:HD3	1.95	0.48
4:D:87:HIS:ND1	30:H:102:DGD:O2D	2.43	0.48
3:C:158:THR:HA	3:C:161:LEU:HB3	1.96	0.48
13:O:103:PHE:HD2	13:O:119:LEU:HD11	1.79	0.48
2:B:170:ASP:OD1	2:B:170:ASP:N	2.46	0.48
4:D:26:ARG:HD2	4:D:30:VAL:HG23	1.96	0.48
1:A:53:ILE:HG12	1:A:71:LEU:HD12	1.95	0.48
4:D:163:GLY:HA3	4:D:290:ALA:HB1	1.96	0.48
4:D:122:LEU:HD21	23:D:402:CLA:H8	1.96	0.47
4:D:274:VAL:HG22	28:D:405:PL9:H222	1.96	0.47
15:U:45:LEU:HD21	15:U:71:GLN:HB3	1.96	0.47
16:V:59:LEU:HD22	16:V:66:ARG:HB2	1.97	0.47
2:B:155:ALA:HB2	2:B:203:ILE:HG12	1.97	0.47
24:A:409:PHO:NC	24:A:409:PHO:ND	2.62	0.47
2:B:27:THR:HG22	2:B:107:LEU:HD13	1.96	0.47
15:U:24:LYS:NZ	15:U:80:GLU:O	2.46	0.47
11:L:12:LEU:H	12:M:29:THR:HG21	1.80	0.47
23:A:405:CLA:H102	24:A:408:PHO:HAA1	1.95	0.47
4:D:53:THR:HG22	6:F:40:MET:HE1	1.96	0.47
7:H:50:ASN:OD1	7:H:52:THR:OG1	2.29	0.47
1:A:106:LEU:HD11	25:A:411:BCR:H402	1.97	0.47
2:B:331:ASN:HB3	2:B:437:LEU:HD21	1.96	0.47
23:B:617:CLA:HHC	23:B:617:CLA:HBB1	1.97	0.47
23:C:502:CLA:H2	23:C:503:CLA:ND	2.30	0.47
34:H:101:RRX:H9	18:X:7:LEU:HD21	1.97	0.47
1:A:280:VAL:HG11	32:D:410:LHG:H282	1.97	0.47
24:A:409:PHO:H72	24:A:409:PHO:H112	1.58	0.47
16:V:53:ASP:OD1	16:V:53:ASP:N	2.43	0.47
1:A:303:ASN:ND2	3:C:413:GLU:O	2.39	0.46
4:D:79:SER:HA	4:D:172:SER:HB3	1.97	0.46
23:B:606:CLA:H92	23:B:606:CLA:H41	1.97	0.46
4:D:19:ASP:OD1	4:D:32:TRP:NE1	2.42	0.46
2:B:24:LEU:HD21	23:B:617:CLA:C3B	2.45	0.46
2:B:30:VAL:HG11	23:B:613:CLA:H111	1.98	0.46
23:C:511:CLA:HBA1	25:K:102:BCR:H271	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:336[B]:HSK:CD2	4:D:337:GLU:HG2	2.45	0.46
13:O:154:ALA:HB2	15:U:90:ALA:HB1	1.98	0.46
1:A:235:TYR:OH	11:L:11:GLU:OE2	2.30	0.46
3:C:242:LEU:HD23	3:C:245:ILE:HD12	1.98	0.46
3:C:296:VAL:HG12	23:C:501:CLA:HED3	1.98	0.46
11:L:10:VAL:O	12:M:28:GLN:NE2	2.37	0.46
16:V:58:THR:O	16:V:82:TYR:OH	2.33	0.46
2:B:391:SER:HB3	2:B:394:GLN:HG3	1.98	0.46
2:B:422:ARG:NH2	13:O:169:ASP:OD2	2.49	0.46
15:U:25:ILE:HD12	15:U:82:PHE:HE1	1.81	0.46
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.98	0.46
23:C:503:CLA:H18	23:C:510:CLA:HBB2	1.98	0.46
30:C:518:DGD:HE4	9:J:40:LEU:HD11	1.97	0.46
4:D:161:PRO:HB3	4:D:170:ALA:HB2	1.98	0.46
2:B:7:ARG:NH2	32:D:408:LHG:O5	2.40	0.45
4:D:83:ASN:HD22	4:D:336[A]:HSK:CD2	2.29	0.45
23:B:616:CLA:H13	23:B:616:CLA:H101	1.76	0.45
13:O:6:THR:OG1	13:O:7:TYR:N	2.42	0.45
1:A:133:LEU:HD23	4:D:256:ILE:HG12	1.99	0.45
2:B:239:SER:O	2:B:466:HIS:ND1	2.42	0.45
2:B:247:PHE:HB2	23:B:609:CLA:HBC1	1.97	0.45
2:B:475:PHE:HB3	2:B:478:VAL:HG12	1.98	0.45
23:C:507:CLA:H62	23:C:507:CLA:H41	1.69	0.45
25:K:101:BCR:H15C	25:K:101:BCR:H351	1.82	0.45
15:U:73:GLN:OE1	15:U:76:ARG:NH2	2.45	0.45
1:A:64:ARG:O	13:O:152:ARG:NH1	2.36	0.45
1:A:203:ALA:O	1:A:278:TRP:NE1	2.44	0.45
3:C:144:SER:O	3:C:148:GLY:N	2.44	0.45
4:D:46:GLY:O	4:D:50:THR:OG1	2.30	0.45
2:B:192:PRO:HD2	7:H:60:VAL:HG13	1.99	0.45
2:B:474:LEU:O	4:D:134:ARG:NH1	2.40	0.45
3:C:217:PRO:HB2	30:C:516:DGD:HA21	1.99	0.45
10:K:39:TRP:HD1	17:Y:46:LEU:HD22	1.82	0.45
2:B:273:TYR:HE1	4:D:165:SER:HA	1.82	0.45
2:B:474:LEU:HD11	23:B:609:CLA:HAA2	1.98	0.45
3:C:315:MET:HE1	3:C:388:GLN:HB3	1.99	0.45
3:C:416:SER:HB2	16:V:42:VAL:HG23	1.99	0.45
4:D:85:MET:HE3	4:D:107:LEU:HB3	1.99	0.45
2:B:30:VAL:HG13	23:B:614:CLA:HMC2	1.98	0.45
4:D:83:ASN:HD22	4:D:336[B]:HSK:CD2	2.29	0.45
11:L:31:PHE:HA	11:L:34:TYR:HD2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:PHE:HE1	23:C:505:CLA:H8	1.82	0.44
1:A:341:LEU:HB3	1:A:343:LEU:CD2	2.47	0.44
2:B:242:ILE:HG23	2:B:462:PHE:HD2	1.82	0.44
3:C:470:PRO:O	4:D:251:ARG:NH1	2.50	0.44
4:D:57:SER:OG	4:D:65:SER:OG	2.32	0.44
4:D:157:PHE:CE2	4:D:171:PRO:HG2	2.52	0.44
15:U:48:LEU:HD13	15:U:67:LEU:HD11	1.99	0.44
1:A:329:GLU:HG2	3:C:412:THR:HG21	1.99	0.44
3:C:79:LYS:NZ	3:C:83:GLU:O	2.42	0.44
3:C:269:GLU:OE2	3:C:444:HIS:ND1	2.44	0.44
1:A:36:ILE:O	1:A:40:THR:OG1	2.28	0.44
1:A:218:LEU:HD12	28:A:414:PL9:C3	2.47	0.44
3:C:217:PRO:HA	3:C:223:TRP:H	1.83	0.44
1:A:292:THR:HG21	30:C:517:DGD:HBF1	1.99	0.44
3:C:158:THR:O	3:C:162:GLY:N	2.44	0.44
13:O:203:LYS:N	13:O:212:ALA:O	2.51	0.44
23:B:606:CLA:HBC2	23:B:613:CLA:H112	2.00	0.44
2:B:51:VAL:HG13	2:B:308:LYS:HB2	2.00	0.44
3:C:42:LEU:HD21	23:C:511:CLA:H2A	2.00	0.44
5:E:26:THR:HB	33:F:101:HEM:HBB2	2.00	0.44
23:C:511:CLA:H13	25:K:102:BCR:H19C	1.99	0.44
1:A:165:GLN:NE2	1:A:296:ASN:OD1	2.41	0.43
2:B:249:ALA:HB3	2:B:459:ALA:HB2	1.99	0.43
2:B:394:GLN:NE2	15:U:22:GLY:O	2.45	0.43
2:B:110:ALA:HB2	25:B:620:BCR:H17C	1.99	0.43
23:B:602:CLA:H171	34:H:101:RRX:H33	2.00	0.43
25:B:620:BCR:H24C	25:B:620:BCR:H371	1.73	0.43
30:H:102:DGD:O5D	30:H:102:DGD:O4D	2.29	0.43
1:A:245:THR:OG1	4:D:265:ARG:NE	2.41	0.43
2:B:220:ARG:NE	7:H:20:LYS:O	2.50	0.43
2:B:249:ALA:HA	2:B:252:VAL:HG22	1.99	0.43
5:E:23:HIS:HE1	33:F:101:HEM:NA	2.16	0.43
2:B:222:PRO:HG3	7:H:26:GLY:HA3	2.00	0.43
10:K:36:ALA:HB2	25:K:102:BCR:H391	1.99	0.43
1:A:179:THR:O	1:A:183:MET:HG3	2.18	0.43
2:B:291:SER:HB3	2:B:296:ALA:HB3	1.99	0.43
12:M:16:LEU:HA	12:M:19:SER:HB2	2.00	0.43
2:B:12:LEU:HB2	23:B:613:CLA:HMC2	2.00	0.43
2:B:103:LEU:HD22	23:B:607:CLA:H51	2.01	0.43
4:D:194:ASN:HA	4:D:295:SER:HB3	2.00	0.43
2:B:68:ARG:HA	2:B:167:TRP:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:87:ILE:O	3:C:91:HIS:ND1	2.47	0.43
23:C:503:CLA:H93	23:C:507:CLA:H43	2.01	0.43
6:F:27:ALA:HB1	33:F:101:HEM:HAC	2.00	0.43
1:A:308:ASP:HB3	1:A:314:ILE:HD11	2.00	0.43
28:A:414:PL9:H411	6:F:18:VAL:HG13	2.00	0.43
23:C:502:CLA:HBB2	23:C:510:CLA:H151	2.01	0.43
4:D:312:GLU:HB2	13:O:159:PRO:HG3	2.01	0.43
1:A:259:ILE:HD12	28:A:414:PL9:H253	2.01	0.42
2:B:298:LEU:HD23	2:B:402:TYR:CZ	2.54	0.42
2:B:321:LYS:NZ	2:B:363:PHE:O	2.51	0.42
23:B:603:CLA:H41	23:B:603:CLA:H61	1.76	0.42
3:C:318:LEU:HD22	3:C:351:PHE:HE1	1.84	0.42
26:A:412:SQD:H362	25:K:101:BCR:H291	2.01	0.42
17:Y:22:LEU:O	17:Y:26:ALA:N	2.46	0.42
1:A:61:ASP:HB3	1:A:63:ILE:HG12	2.00	0.42
1:A:126:TYR:CZ	24:A:408:PHO:HBA1	2.54	0.42
1:A:170:ASP:OD2	3:C:357:ARG:NH1	2.52	0.42
2:B:340:TRP:HE1	2:B:428:GLU:HB3	1.84	0.42
23:B:608:CLA:H42	27:B:622:LMG:H301	2.01	0.42
3:C:134:ILE:HD12	19:Z:28:ALA:HB2	2.00	0.42
3:C:324:LEU:HB3	15:U:32:ILE:HD13	2.00	0.42
4:D:48:TRP:NE1	4:D:173:PHE:O	2.40	0.42
9:J:12:ILE:HA	9:J:15:THR:HG22	2.00	0.42
15:U:79:LEU:HA	15:U:79:LEU:HD23	1.78	0.42
16:V:46:THR:OG1	16:V:52:LEU:O	2.30	0.42
1:A:68:SER:N	4:D:312:GLU:O	2.44	0.42
2:B:57:ARG:NH2	2:B:334:ASP:OD1	2.50	0.42
2:B:70:GLY:HA2	2:B:178:VAL:HG11	2.02	0.42
2:B:256:MET:HG3	2:B:448:ARG:HG3	2.01	0.42
23:B:611:CLA:H111	23:B:611:CLA:H72	1.84	0.42
4:D:199:MET:HB3	28:D:405:PL9:H272	2.01	0.42
3:C:240:ILE:HD13	3:C:240:ILE:HA	1.93	0.42
9:J:11:TRP:CD1	10:K:42:ALA:HA	2.55	0.42
4:D:162:LEU:HD11	30:H:102:DGD:HA32	2.01	0.42
2:B:289:GLN:HA	2:B:292:LEU:HB2	2.02	0.42
25:C:515:BCR:H15C	25:C:515:BCR:H351	1.86	0.42
15:U:21:TYR:HA	15:U:26:ASP:HB2	2.00	0.42
4:D:148:ALA:HB2	4:D:276:VAL:HG13	2.01	0.42
4:D:171:PRO:HB3	4:D:181:PHE:CG	2.55	0.42
7:H:35:MET:SD	34:H:101:RRX:H5	2.60	0.42
24:A:409:PHO:H161	24:A:409:PHO:H122	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:GLU:O	7:H:12:ARG:NH1	2.52	0.41
4:D:22:LEU:HD23	4:D:22:LEU:HA	1.89	0.41
1:A:130:GLN:NE2	24:A:408:PHO:OBD	2.41	0.41
28:A:414:PL9:H302	4:D:45:LEU:HD13	2.02	0.41
2:B:55:MET:HE2	2:B:55:MET:HB3	1.87	0.41
2:B:368:VAL:HG21	2:B:422:ARG:HG2	2.02	0.41
3:C:152:LYS:H	3:C:152:LYS:HG2	1.65	0.41
3:C:281:MET:HE2	3:C:281:MET:HB3	1.97	0.41
10:K:41:ALA:HB2	25:K:101:BCR:H272	2.01	0.41
23:A:407:CLA:HMB1	24:A:409:PHO:H121	2.02	0.41
25:B:620:BCR:H15C	25:B:620:BCR:H351	1.93	0.41
1:A:184:ILE:HG23	1:A:328:MET:SD	2.60	0.41
3:C:46:SER:HB2	3:C:140:LEU:H	1.84	0.41
3:C:243:ILE:O	3:C:247:GLY:N	2.53	0.41
23:C:510:CLA:HBC3	23:C:510:CLA:H192	2.01	0.41
30:C:517:DGD:HBT1	30:C:517:DGD:HBH1	1.80	0.41
25:K:102:BCR:H20C	25:K:102:BCR:H361	1.89	0.41
23:A:406:CLA:HHC	23:A:406:CLA:HBB1	2.03	0.41
2:B:30:VAL:HG22	23:B:614:CLA:C3C	2.49	0.41
28:D:405:PL9:H352	11:L:30:LEU:HD22	2.02	0.41
10:K:17:ILE:HD13	10:K:17:ILE:HA	1.98	0.41
13:O:52:VAL:HG22	13:O:233:VAL:HG22	2.02	0.41
2:B:249:ALA:HB2	23:B:605:CLA:HHD	2.03	0.41
23:B:602:CLA:H162	23:B:602:CLA:H203	1.86	0.41
23:B:605:CLA:H41	23:B:605:CLA:H62	1.60	0.41
3:C:43:ILE:O	3:C:151:TRP:NE1	2.41	0.41
23:C:509:CLA:H93	23:C:509:CLA:H111	1.91	0.41
16:V:4:THR:HG23	16:V:6:GLU:H	1.84	0.41
1:A:61:ASP:OD2	1:A:333:GLU:CG	2.66	0.41
1:A:137:LEU:HA	3:C:469:MET:HE1	2.03	0.41
1:A:269:ARG:HE	4:D:243:THR:HG1	1.64	0.41
1:A:269:ARG:NH2	4:D:223:PHE:O	2.42	0.41
5:E:11:SER:O	5:E:15:THR:OG1	2.39	0.41
5:E:67:THR:H	5:E:75:GLN:HE22	1.67	0.41
32:L:101:LHG:HC62	32:L:101:LHG:H242	1.77	0.41
32:L:101:LHG:HC11	32:L:101:LHG:HC61	2.02	0.41
1:A:59:ASP:HA	1:A:66:PRO:HA	2.02	0.41
1:A:131:TRP:CZ3	23:C:505:CLA:HAA2	2.56	0.41
2:B:71:VAL:HG21	2:B:96:VAL:HG21	2.03	0.41
4:D:110:LEU:HD23	4:D:110:LEU:HA	1.87	0.41
1:A:304:HIS:CD2	1:A:313:VAL:HG21	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ASN:HB3	3:C:412:THR:HG22	2.03	0.41
25:A:411:BCR:H20C	25:A:411:BCR:H361	1.96	0.41
2:B:7:ARG:O	2:B:10:THR:OG1	2.34	0.41
23:B:606:CLA:H41	23:B:606:CLA:H62	1.79	0.41
25:B:618:BCR:H15C	25:B:618:BCR:H351	1.79	0.41
3:C:263:ALA:HB1	25:C:515:BCR:HC22	2.02	0.41
23:C:503:CLA:H51	23:C:503:CLA:H8	1.85	0.41
28:D:405:PL9:H28	28:D:405:PL9:H322	1.86	0.41
13:O:153:THR:HA	13:O:190:PHE:HE2	1.85	0.41
13:O:205:ASP:O	13:O:209:GLY:N	2.54	0.41
1:A:41:LEU:HD23	1:A:41:LEU:HA	1.92	0.41
1:A:166:GLY:HA3	3:C:358:PHE:CE1	2.56	0.41
1:A:183:MET:HE3	23:A:406:CLA:HAC1	2.03	0.41
2:B:242:ILE:HA	2:B:245:VAL:HG22	2.02	0.41
2:B:341:LYS:HD2	2:B:429:ILE:HG22	2.03	0.41
13:O:104:GLN:N	13:O:120:PHE:O	2.43	0.41
1:A:120:LEU:HD22	1:A:155:PHE:HD1	1.86	0.40
26:A:412:SQD:H351	26:A:412:SQD:H382	1.88	0.40
2:B:334:ASP:OD1	2:B:334:ASP:N	2.54	0.40
2:B:383:PHE:CZ	13:O:167:GLY:HA2	2.56	0.40
23:B:616:CLA:H172	7:H:7:LEU:HD21	2.03	0.40
25:B:618:BCR:H11C	25:B:618:BCR:H341	1.81	0.40
23:C:501:CLA:ND	23:C:503:CLA:H52	2.35	0.40
4:D:88:SER:O	4:D:167:TRP:NE1	2.34	0.40
1:A:91:LEU:HD11	1:A:163:ILE:HA	2.03	0.40
26:A:412:SQD:H301	26:A:412:SQD:H332	1.81	0.40
2:B:382:PRO:HG2	2:B:385:ARG:HG2	2.01	0.40
3:C:164:HIS:ND1	23:C:507:CLA:OBD	2.38	0.40
4:D:136:VAL:HG23	4:D:138:VAL:HG13	2.03	0.40
5:E:26:THR:HG22	20:R:15:ALA:HB1	2.03	0.40
16:V:80:THR:HB	16:V:84:GLY:HA2	2.04	0.40
17:Y:46:LEU:HD23	17:Y:46:LEU:HA	1.92	0.40
2:B:364:GLU:HG3	4:D:296:TYR:CZ	2.56	0.40
3:C:362:ARG:HA	3:C:370:ARG:NH2	2.36	0.40
2:B:42:LEU:HD13	2:B:94:GLU:HG3	2.02	0.40
4:D:296:TYR:OH	4:D:326:ARG:NH1	2.36	0.40
10:K:35:LEU:HD12	10:K:38:VAL:HB	2.04	0.40
1:A:131:TRP:CZ2	3:C:449:ARG:HD2	2.56	0.40
23:C:503:CLA:HBC1	23:C:509:CLA:H12	2.03	0.40
4:D:156:VAL:HG22	4:D:286:VAL:HG11	2.04	0.40
5:E:14:ILE:O	5:E:20:TRP:NE1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:36:LEU:O	5:E:40:THR:OG1	2.30	0.40
15:U:67:LEU:HD12	15:U:67:LEU:HA	1.95	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 PDB entries followed by that with respect to all EM entries.

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	332/334 (99%)	323 (97%)	9 (3%)	0	100	100
2	B	502/504 (100%)	484 (96%)	18 (4%)	0	100	100
3	C	449/451 (100%)	435 (97%)	14 (3%)	0	100	100
4	D	339/341 (99%)	326 (96%)	13 (4%)	0	100	100
5	E	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
6	F	32/45 (71%)	32 (100%)	0	0	100	100
7	H	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
8	I	30/38 (79%)	28 (93%)	2 (7%)	0	100	100
9	J	34/40 (85%)	34 (100%)	0	0	100	100
10	K	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	L	28/37 (76%)	28 (100%)	0	0	100	100
12	M	28/30 (93%)	25 (89%)	3 (11%)	0	100	100
13	O	166/244 (68%)	156 (94%)	10 (6%)	0	100	100
14	T	25/30 (83%)	23 (92%)	2 (8%)	0	100	100
15	U	74/104 (71%)	71 (96%)	3 (4%)	0	100	100
16	V	131/163 (80%)	126 (96%)	5 (4%)	0	100	100
17	Y	25/30 (83%)	25 (100%)	0	0	100	100
18	X	36/40 (90%)	35 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Z	53/62 (86%)	52 (98%)	1 (2%)	0	100	100
20	R	32/34 (94%)	31 (97%)	1 (3%)	0	100	100
All	All	2489/2710 (92%)	2403 (96%)	86 (4%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	262/269 (97%)	259 (99%)	3 (1%)	65	85
2	B	379/402 (94%)	378 (100%)	1 (0%)	86	94
3	C	340/352 (97%)	340 (100%)	0	100	100
4	D	267/275 (97%)	265 (99%)	2 (1%)	76	90
5	E	63/73 (86%)	62 (98%)	1 (2%)	55	81
6	F	27/39 (69%)	27 (100%)	0	100	100
7	H	50/53 (94%)	50 (100%)	0	100	100
8	I	27/34 (79%)	27 (100%)	0	100	100
9	J	23/28 (82%)	23 (100%)	0	100	100
10	K	26/30 (87%)	25 (96%)	1 (4%)	29	61
11	L	27/35 (77%)	27 (100%)	0	100	100
12	M	24/27 (89%)	24 (100%)	0	100	100
13	O	139/207 (67%)	138 (99%)	1 (1%)	76	90
14	T	22/26 (85%)	22 (100%)	0	100	100
15	U	60/89 (67%)	60 (100%)	0	100	100
16	V	105/138 (76%)	104 (99%)	1 (1%)	68	86
17	Y	17/23 (74%)	17 (100%)	0	100	100
18	X	28/33 (85%)	28 (100%)	0	100	100
19	Z	40/52 (77%)	40 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	R	6/29 (21%)	6 (100%)	0	100	100
All	All	1932/2214 (87%)	1922 (100%)	10 (0%)	78	92

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	ILE
1	A	313	VAL
1	A	343	LEU
2	B	334	ASP
4	D	293[A]	LEU
4	D	293[B]	LEU
5	E	5	THR
10	K	25	LEU
13	O	75	THR
16	V	42	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	304	HIS
2	B	179	GLN
2	B	216	HIS
2	B	223	GLN
2	B	285	ASN
2	B	289	GLN
2	B	331	ASN
3	C	28	GLN
3	C	311	GLN
3	C	415	ASN
4	D	142	ASN
4	D	186	GLN
5	E	58	GLN
5	E	75	GLN
5	E	82	GLN
8	I	31	ASN
13	O	17	ASN
13	O	176	GLN
13	O	219	GLN
15	U	71	GLN

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Mol	Chain	Res	Type
16	V	68	ASN
16	V	86	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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
14	FME	T	1	14	3,4,10	0.94	0	2,4,11	1.09	0
4	HSK	D	336[A]	-	9,10,12	6.29	2 (22%)	6,12,16	0.93	0
4	HSK	D	336[B]	-	9,11,12	2.45	2 (22%)	6,14,16	1.14	0
8	FME	I	1	8	8,9,10	0.69	0	7,9,11	1.37	1 (14%)

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
14	FME	T	1	14	-	0/0/2/11	-
4	HSK	D	336[A]	-	-	0/5/6/8	0/1/1/1
4	HSK	D	336[B]	-	-	0/5/6/8	0/1/1/1
8	FME	I	1	8	-	0/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	336[A]	HSK	OM-ND1	-18.41	1.14	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	336[B]	HSK	OM-ND1	-6.20	1.30	1.38
4	D	336[A]	HSK	CD2-CG	3.04	1.41	1.36
4	D	336[B]	HSK	CD2-CG	2.86	1.40	1.36

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	I	1	FME	O-C-CA	-2.46	118.33	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	336[A]	HSK	1	0
4	D	336[B]	HSK	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 67 ligands modelled in this entry, 1 is monoatomic and 1 is unknown - leaving 65 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	$\# Z > 2$
31	BCT	D	401	22	2,3,3	0.56	0	2,3,3	1.71	1 (50%)
23	CLA	C	506	3	61,65,73	2.16	19 (31%)	73,103,113	2.85	29 (39%)
27	LMG	A	413	-	38,38,55	1.07	2 (5%)	46,46,63	1.37	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	B	612	2	69,73,73	2.02	21 (30%)	83,113,113	3.29	30 (36%)
25	BCR	A	411	-	41,41,41	1.15	1 (2%)	56,56,56	1.78	15 (26%)
33	HEM	F	101	5,6	50,50,50	1.62	8 (16%)	66,82,82	1.71	15 (22%)
23	CLA	B	605	2	58,62,73	2.16	18 (31%)	69,99,113	2.99	33 (47%)
32	LHG	D	408	-	48,48,48	0.93	2 (4%)	51,54,54	0.99	2 (3%)
25	BCR	D	404	-	29,29,41	0.65	0	37,37,56	1.74	8 (21%)
23	CLA	B	610	2	60,64,73	2.11	19 (31%)	72,102,113	3.00	33 (45%)
23	CLA	B	611	36	69,73,73	1.98	19 (27%)	83,113,113	2.90	32 (38%)
27	LMG	D	411	-	24,24,55	1.13	2 (8%)	32,32,63	1.43	6 (18%)
24	PHO	A	409	-	58,69,69	2.72	17 (29%)	56,99,99	3.08	20 (35%)
25	BCR	K	101	-	41,41,41	1.30	2 (4%)	56,56,56	2.23	22 (39%)
23	CLA	B	607	2	59,63,73	2.12	19 (32%)	71,101,113	3.07	28 (39%)
23	CLA	D	402	4	63,67,73	2.05	18 (28%)	73,104,113	3.03	35 (47%)
30	DGD	C	516	-	42,42,67	1.03	2 (4%)	56,56,81	1.38	7 (12%)
23	CLA	C	507	36	69,73,73	1.93	18 (26%)	83,113,113	3.00	28 (33%)
23	CLA	B	604	2	65,69,73	2.03	18 (27%)	78,108,113	2.84	30 (38%)
32	LHG	D	410	-	32,32,48	1.11	2 (6%)	35,38,54	1.22	3 (8%)
34	RRX	H	101	-	42,42,42	5.13	18 (42%)	57,58,58	5.04	32 (56%)
35	HEC	V	201	16	50,50,50	1.79	10 (20%)	68,82,82	1.86	16 (23%)
23	CLA	B	608	36	55,59,73	2.24	19 (34%)	66,96,113	2.94	30 (45%)
23	CLA	B	616	2	69,73,73	1.97	20 (28%)	83,113,113	2.90	29 (34%)
23	CLA	B	606	2	69,73,73	1.96	19 (27%)	83,113,113	2.90	32 (38%)
30	DGD	H	102	-	51,51,67	0.97	2 (3%)	65,65,81	1.39	10 (15%)
23	CLA	C	509	3	69,73,73	1.96	19 (27%)	83,113,113	2.84	32 (38%)
28	PL9	A	414	-	51,51,55	0.64	2 (3%)	63,64,69	1.69	21 (33%)
28	PL9	D	405	-	43,43,55	0.71	1 (2%)	53,54,69	1.76	15 (28%)
23	CLA	A	405	1	61,65,73	2.13	19 (31%)	73,103,113	2.91	31 (42%)
23	CLA	C	511	3	69,73,73	1.96	19 (27%)	83,113,113	2.74	31 (37%)
25	BCR	B	620	-	41,41,41	1.13	1 (2%)	56,56,56	1.87	15 (26%)
23	CLA	C	503	3	69,73,73	1.95	17 (24%)	83,113,113	2.84	30 (36%)
23	CLA	C	513	3	49,53,73	2.43	21 (42%)	59,89,113	3.39	29 (49%)
23	CLA	D	403	4	49,53,73	2.40	21 (42%)	59,89,113	3.32	29 (49%)
25	BCR	K	102	-	41,41,41	1.25	2 (4%)	56,56,56	1.82	16 (28%)
25	BCR	C	514	-	41,41,41	1.20	2 (4%)	56,56,56	1.85	15 (26%)
23	CLA	B	615	2	55,59,73	2.23	20 (36%)	66,96,113	3.06	31 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	CLA	A	407	36	58,62,73	2.18	19 (32%)	69,99,113	3.10	30 (43%)
26	SQD	D	407	-	23,24,54	1.21	2 (8%)	30,33,65	2.06	9 (30%)
23	CLA	C	505	3	69,73,73	1.98	20 (28%)	83,113,113	2.80	32 (38%)
23	CLA	A	406	36	55,59,73	2.24	18 (32%)	66,96,113	3.35	29 (43%)
23	CLA	C	510	3	69,73,73	1.97	19 (27%)	83,113,113	2.84	30 (36%)
23	CLA	C	502	3	66,70,73	1.99	19 (28%)	79,109,113	2.86	29 (36%)
23	CLA	C	508	3	56,60,73	2.20	19 (33%)	67,97,113	3.05	30 (44%)
21	OEX	A	401	36,3,1	0,14,14	-	-	-	-	-
27	LMG	B	622	-	39,39,55	1.05	2 (5%)	47,47,63	1.53	9 (19%)
24	PHO	A	408	-	58,69,69	2.62	15 (25%)	56,99,99	3.02	17 (30%)
26	SQD	A	412	-	53,54,54	1.00	3 (5%)	62,65,65	1.60	8 (12%)
23	CLA	B	602	36	69,73,73	2.04	20 (28%)	83,113,113	2.81	29 (34%)
30	DGD	C	518	-	51,51,67	0.97	2 (3%)	65,65,81	0.98	3 (4%)
32	LHG	D	409	-	31,31,48	1.10	2 (6%)	34,37,54	1.17	2 (5%)
23	CLA	B	609	2	55,59,73	2.28	18 (32%)	66,96,113	2.99	29 (43%)
25	BCR	B	618	-	41,41,41	1.15	1 (2%)	56,56,56	1.90	12 (21%)
30	DGD	C	517	-	50,50,67	0.91	2 (4%)	64,64,81	1.36	8 (12%)
25	BCR	C	515	-	41,41,41	1.19	2 (4%)	56,56,56	1.77	15 (26%)
23	CLA	C	501	3	69,73,73	2.01	18 (26%)	83,113,113	2.90	31 (37%)
23	CLA	B	603	2	56,60,73	2.27	18 (32%)	67,97,113	3.22	32 (47%)
23	CLA	B	614	2	58,62,73	2.13	19 (32%)	69,99,113	3.04	27 (39%)
23	CLA	C	512	3	57,61,73	2.15	19 (33%)	68,98,113	3.20	28 (41%)
23	CLA	B	617	2	49,53,73	2.35	19 (38%)	59,89,113	3.23	28 (47%)
32	LHG	L	101	-	39,39,48	1.01	2 (5%)	42,45,54	1.18	4 (9%)
23	CLA	C	504	36	54,58,73	2.31	20 (37%)	65,95,113	3.12	31 (47%)
23	CLA	A	410	1	49,53,73	2.34	18 (36%)	59,89,113	3.26	26 (44%)
23	CLA	B	613	2	69,73,73	2.33	22 (31%)	83,113,113	2.76	32 (38%)

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
23	CLA	C	506	3	-	9/30/106/115	-
27	LMG	A	413	-	-	13/33/53/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	B	612	2	-	9/39/115/115	-
25	BCR	A	411	-	-	7/29/63/63	0/2/2/2
33	HEM	F	101	5,6	-	8/14/54/54	-
23	CLA	B	605	2	-	9/26/102/115	-
32	LHG	D	408	-	-	20/53/53/53	-
25	BCR	D	404	-	-	7/23/40/63	0/1/1/2
23	CLA	B	610	2	-	11/29/105/115	-
23	CLA	B	611	36	-	13/39/115/115	-
27	LMG	D	411	-	-	6/18/38/70	0/1/1/1
24	PHO	A	409	-	-	9/37/103/103	0/5/6/6
25	BCR	K	101	-	-	13/29/63/63	0/2/2/2
23	CLA	B	607	2	-	5/27/103/115	-
23	CLA	D	402	4	-	8/30/106/115	-
30	DGD	C	516	-	-	10/30/70/95	0/2/2/2
23	CLA	C	507	36	-	10/39/115/115	-
23	CLA	B	604	2	-	15/35/111/115	-
32	LHG	D	410	-	-	13/37/37/53	-
34	RRX	H	101	-	-	16/29/65/65	0/2/2/2
23	CLA	B	608	36	-	12/23/99/115	-
23	CLA	B	616	2	-	14/39/115/115	-
23	CLA	B	606	2	-	12/39/115/115	-
30	DGD	H	102	-	-	13/39/79/95	0/2/2/2
23	CLA	C	509	3	-	7/39/115/115	-
28	PL9	A	414	-	-	13/49/69/73	0/1/1/1
28	PL9	D	405	-	-	9/39/59/73	0/1/1/1
23	CLA	A	405	1	-	6/30/106/115	-
23	CLA	C	511	3	-	15/39/115/115	-
25	BCR	B	620	-	-	7/29/63/63	0/2/2/2
23	CLA	C	503	3	-	10/39/115/115	-
23	CLA	C	513	3	-	4/15/91/115	-
23	CLA	D	403	4	-	5/15/91/115	-
25	BCR	K	102	-	-	7/29/63/63	0/2/2/2
25	BCR	C	514	-	-	5/29/63/63	0/2/2/2
23	CLA	B	615	2	-	13/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	CLA	A	407	36	-	5/26/102/115	-
26	SQD	D	407	-	-	5/16/36/69	0/1/1/1
23	CLA	C	505	3	-	20/39/115/115	-
23	CLA	A	406	36	-	5/23/99/115	-
23	CLA	C	510	3	-	19/39/115/115	-
23	CLA	C	502	3	-	6/36/112/115	-
23	CLA	C	508	3	-	7/24/100/115	-
27	LMG	B	622	-	-	9/34/54/70	0/1/1/1
24	PHO	A	408	-	-	8/37/103/103	0/5/6/6
26	SQD	A	412	-	-	19/49/69/69	0/1/1/1
23	CLA	B	602	36	-	15/39/115/115	-
30	DGD	C	518	-	-	16/39/79/95	0/2/2/2
32	LHG	D	409	-	-	14/36/36/53	-
23	CLA	B	609	2	-	9/23/99/115	-
25	BCR	B	618	-	-	4/29/63/63	0/2/2/2
30	DGD	C	517	-	-	14/38/78/95	0/2/2/2
25	BCR	C	515	-	-	7/29/63/63	0/2/2/2
23	CLA	C	501	3	-	11/39/115/115	-
23	CLA	B	613	2	-	14/39/115/115	-
23	CLA	B	603	2	-	8/24/100/115	-
23	CLA	B	614	2	-	7/26/102/115	-
23	CLA	C	512	3	-	8/25/101/115	-
23	CLA	B	617	2	-	2/15/91/115	-
32	LHG	L	101	-	-	19/44/44/53	-
23	CLA	C	504	36	-	4/21/97/115	-
23	CLA	A	410	1	-	6/15/91/115	-
35	HEC	V	201	16	1/1/3/7	6/14/54/54	-

All (777) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	H	101	RRX	C21-C22	13.64	1.53	1.35
34	H	101	RRX	C17-C18	13.45	1.53	1.35
34	H	101	RRX	C10-C9	12.90	1.52	1.35
34	H	101	RRX	C14-C13	12.77	1.52	1.35
34	H	101	RRX	C26-C25	12.47	1.56	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	H	101	RRX	C5-C6	11.40	1.54	1.34
24	A	409	PHO	C1D-C2D	8.05	1.48	1.39
24	A	409	PHO	C1B-C2B	8.00	1.48	1.39
24	A	408	PHO	C1D-C2D	7.90	1.48	1.39
24	A	408	PHO	C1B-C2B	7.48	1.47	1.39
23	B	613	CLA	MG-NA	6.99	2.22	2.06
24	A	409	PHO	C3B-C2B	6.61	1.49	1.40
24	A	408	PHO	C3B-C4B	6.60	1.49	1.41
25	K	101	BCR	C23-C22	-6.45	1.32	1.45
24	A	409	PHO	C3B-C4B	6.29	1.48	1.41
23	B	613	CLA	MG-NC	-6.23	1.91	2.06
25	K	102	BCR	C23-C22	-6.17	1.32	1.45
24	A	408	PHO	C3B-C2B	5.99	1.48	1.40
24	A	409	PHO	C3C-C2C	5.71	1.48	1.36
25	C	515	BCR	C23-C22	-5.67	1.33	1.45
25	B	618	BCR	C23-C22	-5.63	1.33	1.45
25	C	514	BCR	C23-C22	-5.62	1.33	1.45
25	A	411	BCR	C23-C22	-5.59	1.33	1.45
25	B	620	BCR	C23-C22	-5.51	1.34	1.45
24	A	408	PHO	C4D-CHA	5.50	1.48	1.39
23	D	403	CLA	C3C-C2C	5.47	1.48	1.36
23	B	613	CLA	MG-ND	-5.43	1.95	2.05
23	B	609	CLA	C3C-C2C	5.41	1.48	1.36
24	A	409	PHO	C4D-CHA	5.41	1.48	1.39
23	C	512	CLA	C3C-C2C	5.41	1.48	1.36
23	B	603	CLA	C3C-C2C	5.38	1.48	1.36
23	B	610	CLA	O2D-CGD	5.32	1.46	1.33
23	B	605	CLA	C3C-C2C	5.28	1.48	1.36
23	C	513	CLA	C3C-C2C	5.28	1.47	1.36
23	B	611	CLA	C3C-C2C	5.27	1.47	1.36
24	A	408	PHO	C3C-C2C	5.27	1.47	1.36
23	C	506	CLA	C3C-C2C	5.26	1.47	1.36
23	C	511	CLA	C3C-C2C	5.22	1.47	1.36
23	A	407	CLA	C3C-C2C	5.22	1.47	1.36
23	A	410	CLA	C3C-C2C	5.20	1.47	1.36
23	B	604	CLA	C3C-C2C	5.19	1.47	1.36
23	B	612	CLA	CHC-C1C	5.19	1.49	1.38
23	B	608	CLA	C3C-C2C	5.18	1.47	1.36
23	A	406	CLA	C3C-C2C	5.16	1.47	1.36
23	A	405	CLA	C3C-C2C	5.16	1.47	1.36
33	F	101	HEM	FE-NB	5.14	2.10	1.94
23	B	607	CLA	C3C-C2C	5.14	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	C3C-C2C	5.13	1.47	1.36
23	C	507	CLA	C3C-C2C	5.13	1.47	1.36
23	C	510	CLA	C3C-C2C	5.09	1.47	1.36
23	C	513	CLA	O2D-CGD	5.09	1.45	1.33
24	A	409	PHO	O2D-CGD	5.06	1.45	1.33
23	C	503	CLA	C3C-C2C	5.06	1.47	1.36
23	A	406	CLA	C1D-ND	5.06	1.44	1.37
23	B	616	CLA	C3C-C2C	5.05	1.47	1.36
23	C	501	CLA	C1D-ND	5.02	1.44	1.37
23	A	406	CLA	O2D-CGD	5.01	1.45	1.33
23	C	504	CLA	C3C-C2C	5.01	1.47	1.36
23	C	505	CLA	C3C-C2C	5.00	1.47	1.36
23	B	609	CLA	O2D-CGD	5.00	1.45	1.33
23	B	613	CLA	O2D-CGD	5.00	1.45	1.33
23	C	504	CLA	O2D-CGD	4.99	1.45	1.33
23	C	513	CLA	CHC-C1C	4.99	1.48	1.38
23	C	509	CLA	C3C-C2C	4.98	1.47	1.36
23	B	607	CLA	O2D-CGD	4.97	1.45	1.33
23	B	605	CLA	O2D-CGD	4.97	1.45	1.33
23	D	402	CLA	C1B-NB	-4.94	1.31	1.37
23	B	603	CLA	O2D-CGD	4.94	1.45	1.33
23	C	501	CLA	C3C-C2C	4.94	1.47	1.36
23	B	614	CLA	C3C-C2C	4.93	1.47	1.36
23	C	509	CLA	O2D-CGD	4.93	1.45	1.33
35	V	201	HEC	FE-NB	4.92	2.10	1.94
23	C	501	CLA	O2D-CGD	4.91	1.45	1.33
23	B	615	CLA	O2D-CGD	4.90	1.45	1.33
23	D	402	CLA	C3C-C2C	4.89	1.47	1.36
23	B	604	CLA	C1B-NB	-4.89	1.31	1.37
23	B	606	CLA	O2D-CGD	4.89	1.45	1.33
23	C	503	CLA	C1D-ND	4.89	1.43	1.37
23	C	508	CLA	C3C-C2C	4.88	1.47	1.36
23	B	603	CLA	C1D-ND	4.88	1.43	1.37
23	B	610	CLA	C3C-C2C	4.87	1.47	1.36
23	B	602	CLA	O2D-CGD	4.86	1.45	1.33
23	C	506	CLA	O2D-CGD	4.86	1.45	1.33
23	B	603	CLA	CHC-C1C	4.85	1.48	1.38
23	B	608	CLA	O2D-CGD	4.85	1.45	1.33
23	B	612	CLA	C3C-C2C	4.85	1.47	1.36
24	A	409	PHO	C3D-C2D	4.84	1.48	1.39
23	C	506	CLA	C1D-ND	4.83	1.43	1.37
23	B	617	CLA	O2D-CGD	4.83	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	504	CLA	CHD-C1D	4.82	1.47	1.38
23	C	508	CLA	O2D-CGD	4.82	1.45	1.33
23	B	609	CLA	C1B-NB	-4.82	1.31	1.37
23	C	512	CLA	CHC-C1C	4.81	1.48	1.38
23	B	609	CLA	C1D-ND	4.78	1.43	1.37
23	B	615	CLA	C3C-C2C	4.77	1.46	1.36
23	C	505	CLA	C1B-NB	-4.77	1.31	1.37
23	B	615	CLA	O2A-CGA	4.76	1.47	1.33
23	C	502	CLA	O2D-CGD	4.76	1.44	1.33
23	A	410	CLA	CHC-C1C	4.76	1.48	1.38
23	C	505	CLA	O2D-CGD	4.75	1.44	1.33
23	B	613	CLA	MG-NB	4.75	2.15	2.05
23	C	510	CLA	O2D-CGD	4.75	1.44	1.33
23	A	407	CLA	C1D-ND	4.73	1.43	1.37
23	B	610	CLA	C1D-ND	4.73	1.43	1.37
23	D	402	CLA	CHC-C1C	4.73	1.48	1.38
23	C	512	CLA	O2D-CGD	4.71	1.44	1.33
23	A	405	CLA	C1B-NB	-4.71	1.32	1.37
23	D	402	CLA	O2D-CGD	4.70	1.44	1.33
23	B	606	CLA	C3C-C2C	4.69	1.46	1.36
23	C	503	CLA	O2D-CGD	4.69	1.44	1.33
23	C	510	CLA	C1D-ND	4.69	1.43	1.37
23	C	504	CLA	C1D-ND	4.66	1.43	1.37
23	B	616	CLA	O2D-CGD	4.66	1.44	1.33
23	C	511	CLA	O2D-CGD	4.65	1.44	1.33
23	B	604	CLA	O2D-CGD	4.65	1.44	1.33
24	A	408	PHO	C3D-C2D	4.62	1.47	1.39
23	C	508	CLA	C1B-NB	-4.62	1.32	1.37
23	B	602	CLA	C1D-ND	4.62	1.43	1.37
23	B	611	CLA	O2D-CGD	4.60	1.44	1.33
23	D	403	CLA	O2D-CGD	4.60	1.44	1.33
23	D	403	CLA	C1D-ND	4.60	1.43	1.37
23	B	613	CLA	C3C-C2C	4.59	1.46	1.36
23	B	614	CLA	O2D-CGD	4.58	1.44	1.33
23	B	608	CLA	C1D-ND	4.58	1.43	1.37
23	B	608	CLA	C1B-NB	-4.58	1.32	1.37
23	C	513	CLA	C1D-ND	4.57	1.43	1.37
23	B	616	CLA	C1D-ND	4.57	1.43	1.37
23	C	502	CLA	C3C-C2C	4.56	1.46	1.36
23	C	503	CLA	CHC-C1C	4.56	1.47	1.38
24	A	408	PHO	O2D-CGD	4.54	1.44	1.33
23	B	612	CLA	C4B-NB	-4.52	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	603	CLA	O2A-CGA	4.52	1.46	1.33
23	B	614	CLA	C1D-ND	4.51	1.43	1.37
23	A	407	CLA	O2D-CGD	4.51	1.44	1.33
23	C	507	CLA	O2D-CGD	4.51	1.44	1.33
23	A	410	CLA	O2A-CGA	4.50	1.45	1.30
23	A	405	CLA	C4B-NB	-4.49	1.32	1.37
23	B	602	CLA	CHC-C1C	4.48	1.47	1.38
23	B	617	CLA	C3C-C2C	4.48	1.46	1.36
23	B	612	CLA	O2D-CGD	4.47	1.44	1.33
23	B	617	CLA	O2A-CGA	4.47	1.45	1.30
23	C	501	CLA	CHC-C1C	4.47	1.47	1.38
23	C	511	CLA	CHC-C1C	4.45	1.47	1.38
23	C	508	CLA	C1D-ND	4.45	1.43	1.37
23	C	513	CLA	O2A-CGA	4.45	1.45	1.30
30	C	518	DGD	O1G-C1A	4.44	1.46	1.33
23	A	410	CLA	O2D-CGD	4.44	1.44	1.33
23	C	510	CLA	CHC-C1C	4.43	1.47	1.38
23	D	403	CLA	O2A-CGA	4.43	1.45	1.30
23	B	605	CLA	C1B-NB	-4.43	1.32	1.37
23	B	617	CLA	C1B-NB	-4.42	1.32	1.37
23	B	607	CLA	CHC-C1C	4.42	1.47	1.38
23	C	503	CLA	C1B-NB	-4.41	1.32	1.37
23	B	609	CLA	CHD-C1D	4.41	1.46	1.38
23	D	403	CLA	CHC-C1C	4.40	1.47	1.38
23	A	405	CLA	CHC-C1C	4.40	1.47	1.38
23	A	405	CLA	CHD-C1D	4.40	1.46	1.38
23	B	604	CLA	CHC-C1C	4.39	1.47	1.38
23	B	608	CLA	O2A-CGA	4.39	1.46	1.33
23	C	504	CLA	C1B-NB	-4.39	1.32	1.37
23	C	502	CLA	C1D-ND	4.37	1.43	1.37
23	B	614	CLA	C1B-NB	-4.36	1.32	1.37
23	C	504	CLA	CHD-C4C	4.36	1.49	1.39
23	B	613	CLA	C1B-NB	-4.35	1.32	1.37
23	B	606	CLA	C1D-ND	4.35	1.43	1.37
27	B	622	LMG	O8-C28	4.34	1.46	1.33
23	C	501	CLA	CHD-C1D	4.33	1.46	1.38
23	B	611	CLA	C1D-ND	4.33	1.43	1.37
23	B	615	CLA	C1B-NB	-4.33	1.32	1.37
23	B	602	CLA	CHD-C1D	4.32	1.46	1.38
23	B	609	CLA	CHC-C1C	4.31	1.47	1.38
23	B	610	CLA	O2A-CGA	4.31	1.45	1.33
23	C	506	CLA	C1B-NB	-4.31	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	509	CLA	O2A-CGA	4.29	1.45	1.33
23	B	606	CLA	O2A-CGA	4.28	1.45	1.33
26	D	407	SQD	O48-C23	4.28	1.45	1.33
23	C	502	CLA	C1B-NB	-4.28	1.32	1.37
23	C	505	CLA	O2A-CGA	4.27	1.45	1.33
23	B	604	CLA	O2A-CGA	4.27	1.45	1.33
23	B	612	CLA	CHC-C4B	4.26	1.49	1.39
23	C	509	CLA	C1D-ND	4.26	1.43	1.37
30	H	102	DGD	O1G-C1A	4.26	1.45	1.33
23	A	405	CLA	O2D-CGD	4.26	1.43	1.33
23	B	611	CLA	CHC-C1C	4.26	1.47	1.38
23	C	508	CLA	C4B-NB	-4.25	1.32	1.37
23	A	407	CLA	C1B-NB	-4.25	1.32	1.37
23	B	615	CLA	CHC-C1C	4.25	1.47	1.38
23	A	410	CLA	C1D-ND	4.25	1.43	1.37
23	B	602	CLA	O2A-CGA	4.24	1.45	1.33
23	C	501	CLA	CHD-C4C	4.24	1.48	1.39
23	C	504	CLA	CHC-C1C	4.24	1.47	1.38
23	C	511	CLA	C1B-NB	-4.24	1.32	1.37
23	C	512	CLA	O2A-CGA	4.24	1.45	1.33
23	C	506	CLA	CHC-C1C	4.23	1.47	1.38
23	B	603	CLA	CHD-C1D	4.23	1.46	1.38
23	A	406	CLA	C1B-NB	-4.23	1.32	1.37
23	B	616	CLA	CHC-C1C	4.23	1.47	1.38
23	B	615	CLA	C4B-NB	-4.23	1.32	1.37
23	A	406	CLA	O2A-CGA	4.22	1.45	1.33
23	B	611	CLA	C1B-NB	-4.22	1.32	1.37
23	C	507	CLA	C1D-ND	4.21	1.43	1.37
23	C	502	CLA	C4B-NB	-4.20	1.32	1.37
23	C	502	CLA	CHC-C1C	4.19	1.47	1.38
23	B	617	CLA	C1D-ND	4.19	1.42	1.37
27	A	413	LMG	O7-C10	4.18	1.46	1.34
23	B	616	CLA	O2A-CGA	4.18	1.45	1.33
35	V	201	HEC	CBC-CAC	-4.17	1.32	1.51
30	C	518	DGD	O2G-C1B	4.17	1.46	1.34
23	C	506	CLA	O2A-CGA	4.17	1.45	1.33
23	B	605	CLA	C1D-ND	4.17	1.42	1.37
23	C	506	CLA	CHD-C1D	4.16	1.46	1.38
23	A	407	CLA	CHD-C1D	4.14	1.46	1.38
24	A	409	PHO	OBD-CAD	4.14	1.28	1.22
32	D	408	LHG	O8-C23	4.14	1.45	1.33
23	C	503	CLA	O2A-CGA	4.14	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	614	CLA	CHC-C1C	4.14	1.46	1.38
23	B	607	CLA	C1B-NB	-4.14	1.32	1.37
23	C	507	CLA	C1B-NB	-4.14	1.32	1.37
23	B	611	CLA	O2A-CGA	4.14	1.45	1.33
23	A	407	CLA	O2A-CGA	4.14	1.45	1.33
32	L	101	LHG	O8-C23	4.13	1.45	1.33
23	C	510	CLA	CHD-C1D	4.13	1.46	1.38
26	A	412	SQD	O48-C23	4.12	1.45	1.33
23	C	511	CLA	O2A-CGA	4.12	1.45	1.33
23	B	614	CLA	C4B-NB	-4.11	1.32	1.37
35	V	201	HEC	CBB-CAB	-4.11	1.33	1.51
23	B	606	CLA	CHC-C1C	4.10	1.46	1.38
30	H	102	DGD	O2G-C1B	4.09	1.45	1.34
23	B	615	CLA	CHD-C1D	4.09	1.46	1.38
23	D	402	CLA	O2A-CGA	4.09	1.45	1.33
23	B	608	CLA	CHD-C1D	4.09	1.46	1.38
23	C	507	CLA	O2A-CGA	4.09	1.45	1.33
30	C	517	DGD	O1G-C1A	4.08	1.45	1.33
27	D	411	LMG	O7-C10	4.08	1.45	1.34
30	C	516	DGD	O1G-C1A	4.08	1.45	1.33
23	C	507	CLA	C4B-NB	-4.08	1.32	1.37
23	B	607	CLA	C1D-ND	4.07	1.42	1.37
23	C	505	CLA	C1D-ND	4.06	1.42	1.37
32	D	410	LHG	O7-C7	4.05	1.45	1.34
23	C	508	CLA	O2A-CGA	4.05	1.45	1.33
23	B	614	CLA	O2A-CGA	4.05	1.45	1.33
23	B	615	CLA	C1D-ND	4.05	1.42	1.37
23	B	605	CLA	C4B-NB	-4.05	1.32	1.37
23	B	605	CLA	CHD-C1D	4.04	1.46	1.38
23	B	603	CLA	CHD-C4C	4.04	1.48	1.39
23	C	508	CLA	C3D-C2D	4.04	1.50	1.39
27	A	413	LMG	O8-C28	4.03	1.45	1.33
33	F	101	HEM	FE-NC	4.02	2.08	1.95
23	B	613	CLA	CHC-C1C	4.02	1.46	1.38
23	C	505	CLA	CHD-C1D	4.01	1.46	1.38
23	C	509	CLA	CHC-C1C	4.01	1.46	1.38
23	A	407	CLA	CHC-C1C	4.01	1.46	1.38
23	C	509	CLA	CHD-C1D	4.01	1.46	1.38
23	B	610	CLA	CHC-C1C	4.01	1.46	1.38
23	B	612	CLA	C1D-ND	4.00	1.42	1.37
23	D	403	CLA	CHD-C1D	4.00	1.46	1.38
23	B	610	CLA	C3D-C2D	4.00	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	602	CLA	C1B-NB	-4.00	1.32	1.37
23	B	605	CLA	O2A-CGA	3.99	1.45	1.33
23	B	606	CLA	C1B-NB	-3.99	1.32	1.37
23	A	406	CLA	CHC-C1C	3.98	1.46	1.38
23	C	507	CLA	CHD-C1D	3.98	1.46	1.38
35	V	201	HEC	C1D-ND	-3.97	1.33	1.40
23	B	609	CLA	O2A-CGA	3.97	1.44	1.33
23	B	610	CLA	C1B-NB	-3.97	1.32	1.37
23	C	504	CLA	O2A-CGA	3.96	1.44	1.33
24	A	408	PHO	OBD-CAD	3.96	1.27	1.22
30	C	517	DGD	O2G-C1B	3.95	1.45	1.34
23	C	507	CLA	CHC-C1C	3.95	1.46	1.38
23	C	510	CLA	O2A-CGA	3.94	1.44	1.33
30	C	516	DGD	O2G-C1B	3.94	1.45	1.34
23	B	617	CLA	CHD-C1D	3.94	1.46	1.38
35	V	201	HEC	FE-NC	3.94	2.08	1.95
23	C	505	CLA	CHC-C1C	3.93	1.46	1.38
23	C	510	CLA	C1B-NB	-3.93	1.33	1.37
23	C	513	CLA	CHD-C1D	3.92	1.46	1.38
23	C	509	CLA	C1B-NB	-3.92	1.33	1.37
23	D	403	CLA	C1B-NB	-3.92	1.33	1.37
23	B	617	CLA	CHC-C1C	3.92	1.46	1.38
23	C	506	CLA	CHD-C4C	3.91	1.48	1.39
23	D	403	CLA	CHD-C4C	3.91	1.48	1.39
23	C	512	CLA	C1B-NB	-3.91	1.33	1.37
23	A	407	CLA	CHD-C4C	3.91	1.48	1.39
23	B	609	CLA	CHD-C4C	3.90	1.48	1.39
23	A	410	CLA	CHD-C1D	3.90	1.46	1.38
23	B	617	CLA	C1C-NC	-3.90	1.32	1.37
32	L	101	LHG	O7-C7	3.89	1.45	1.34
32	D	409	LHG	O8-C23	3.88	1.44	1.33
23	B	602	CLA	CHD-C4C	3.88	1.48	1.39
23	B	617	CLA	C3D-C2D	3.87	1.49	1.39
23	D	402	CLA	CHC-C4B	3.87	1.48	1.39
23	C	502	CLA	O2A-CGA	3.87	1.44	1.33
23	B	602	CLA	C4B-NB	-3.87	1.33	1.37
23	B	603	CLA	CHC-C4B	3.86	1.48	1.39
32	D	409	LHG	O7-C7	3.86	1.45	1.34
24	A	409	PHO	O2A-CGA	3.86	1.44	1.33
23	B	604	CLA	CHD-C1D	3.85	1.45	1.38
24	A	408	PHO	C3A-C2A	-3.85	1.51	1.54
23	B	608	CLA	CHD-C4C	3.85	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	405	CLA	C1D-ND	3.85	1.42	1.37
23	B	604	CLA	C1D-ND	3.85	1.42	1.37
33	F	101	HEM	C1B-NB	-3.84	1.33	1.40
23	C	513	CLA	C1B-NB	-3.84	1.33	1.37
23	C	506	CLA	C3D-C2D	3.84	1.49	1.39
23	B	607	CLA	CHD-C1D	3.84	1.45	1.38
23	C	511	CLA	C1D-ND	3.83	1.42	1.37
23	B	605	CLA	CHC-C1C	3.83	1.46	1.38
23	A	406	CLA	CHD-C4C	3.83	1.48	1.39
23	C	513	CLA	C3D-C2D	3.83	1.49	1.39
23	C	513	CLA	CHC-C4B	3.83	1.48	1.39
23	B	608	CLA	C3D-C2D	3.82	1.49	1.39
23	C	504	CLA	C3D-C2D	3.82	1.49	1.39
23	C	506	CLA	OBD-CAD	3.82	1.29	1.22
27	B	622	LMG	O7-C10	3.82	1.45	1.34
23	C	507	CLA	CHD-C4C	3.82	1.47	1.39
23	C	508	CLA	CHC-C1C	3.81	1.46	1.38
23	B	616	CLA	C1B-NB	-3.81	1.33	1.37
23	B	608	CLA	CHC-C1C	3.81	1.46	1.38
23	C	502	CLA	CHD-C1D	3.80	1.45	1.38
23	C	509	CLA	CHD-C4C	3.80	1.47	1.39
23	B	606	CLA	CHC-C4B	3.79	1.47	1.39
32	D	408	LHG	O7-C7	3.78	1.45	1.34
23	C	510	CLA	CHD-C4C	3.78	1.47	1.39
23	C	512	CLA	CHC-C4B	3.77	1.47	1.39
23	B	612	CLA	C1B-C2B	3.77	1.52	1.43
23	C	512	CLA	C1D-ND	3.77	1.42	1.37
23	B	602	CLA	CHC-C4B	3.77	1.47	1.39
23	C	505	CLA	CHD-C4C	3.77	1.47	1.39
23	C	513	CLA	C4B-NB	-3.76	1.33	1.37
23	B	607	CLA	O2A-CGA	3.76	1.44	1.33
26	A	412	SQD	O47-C7	3.75	1.44	1.34
23	B	604	CLA	CHD-C4C	3.74	1.47	1.39
24	A	408	PHO	O2A-CGA	3.74	1.44	1.33
23	A	405	CLA	O2A-CGA	3.73	1.44	1.33
23	B	608	CLA	OBD-CAD	3.72	1.28	1.22
33	F	101	HEM	C4D-ND	-3.72	1.33	1.40
23	C	510	CLA	CHC-C4B	3.72	1.47	1.39
23	C	501	CLA	O2A-CGA	3.72	1.44	1.33
23	A	405	CLA	CHD-C4C	3.71	1.47	1.39
32	D	410	LHG	O8-C23	3.71	1.44	1.33
23	A	410	CLA	CHD-C4C	3.71	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	610	CLA	CHD-C1D	3.69	1.45	1.38
23	A	410	CLA	C1B-NB	-3.69	1.33	1.37
23	B	612	CLA	OBD-CAD	3.69	1.28	1.22
23	C	508	CLA	CHD-C1D	3.69	1.45	1.38
23	C	513	CLA	CHD-C4C	3.69	1.47	1.39
23	C	512	CLA	CHD-C4C	3.69	1.47	1.39
23	C	511	CLA	CHD-C1D	3.69	1.45	1.38
23	B	612	CLA	O2A-CGA	3.68	1.44	1.33
23	C	503	CLA	CHD-C4C	3.67	1.47	1.39
23	B	604	CLA	C4B-NB	-3.67	1.33	1.37
23	B	605	CLA	CHD-C4C	3.67	1.47	1.39
23	B	616	CLA	C3D-C2D	3.67	1.49	1.39
23	B	613	CLA	O2A-CGA	3.66	1.44	1.33
23	C	505	CLA	C4B-NB	-3.66	1.33	1.37
23	B	606	CLA	CHD-C4C	3.65	1.47	1.39
23	B	603	CLA	C1B-NB	-3.65	1.33	1.37
23	B	606	CLA	CHD-C1D	3.65	1.45	1.38
23	D	403	CLA	CHC-C4B	3.64	1.47	1.39
23	C	511	CLA	CHD-C4C	3.63	1.47	1.39
23	B	614	CLA	CHD-C4C	3.62	1.47	1.39
23	B	611	CLA	C4B-NB	-3.61	1.33	1.37
23	A	410	CLA	C3D-C2D	3.61	1.49	1.39
23	B	615	CLA	CHD-C4C	3.61	1.47	1.39
23	C	503	CLA	CHD-C1D	3.60	1.45	1.38
23	A	406	CLA	CHD-C1D	3.60	1.45	1.38
23	C	501	CLA	OBD-CAD	3.60	1.28	1.22
23	B	611	CLA	CHD-C1D	3.60	1.45	1.38
23	B	607	CLA	C3D-C2D	3.59	1.48	1.39
23	B	603	CLA	OBD-CAD	3.59	1.28	1.22
23	B	617	CLA	OBD-CAD	3.59	1.28	1.22
23	B	611	CLA	CHC-C4B	3.59	1.47	1.39
23	C	512	CLA	C3D-C2D	3.59	1.48	1.39
23	B	616	CLA	C4B-NB	-3.58	1.33	1.37
23	B	602	CLA	C3D-C2D	3.58	1.48	1.39
23	C	503	CLA	CHC-C4B	3.58	1.47	1.39
23	C	509	CLA	C4B-NB	-3.57	1.33	1.37
23	B	611	CLA	C3D-C2D	3.57	1.48	1.39
23	B	617	CLA	C4B-NB	-3.56	1.33	1.37
23	A	407	CLA	C4B-NB	-3.55	1.33	1.37
24	A	409	PHO	C3A-C2A	-3.55	1.51	1.54
23	C	502	CLA	CHD-C4C	3.55	1.47	1.39
23	B	602	CLA	OBD-CAD	3.54	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	409	PHO	CHA-CBD	-3.53	1.47	1.51
23	B	609	CLA	C3D-C2D	3.53	1.48	1.39
23	B	614	CLA	C3D-C2D	3.53	1.48	1.39
23	B	616	CLA	CHD-C4C	3.50	1.47	1.39
23	C	501	CLA	C3D-C2D	3.50	1.48	1.39
23	A	410	CLA	CHC-C4B	3.50	1.47	1.39
23	C	501	CLA	C1B-NB	-3.50	1.33	1.37
23	C	501	CLA	CHC-C4B	3.50	1.47	1.39
23	A	407	CLA	OBD-CAD	3.50	1.28	1.22
23	B	612	CLA	CHB-C1B	3.50	1.47	1.39
23	C	504	CLA	C4B-NB	-3.49	1.33	1.37
23	B	616	CLA	CHD-C1D	3.49	1.45	1.38
23	A	410	CLA	C4B-NB	-3.48	1.33	1.37
23	B	614	CLA	CHD-C1D	3.48	1.45	1.38
23	B	610	CLA	C4B-NB	-3.48	1.33	1.37
23	A	410	CLA	OBD-CAD	3.47	1.28	1.22
23	B	616	CLA	OBD-CAD	3.47	1.28	1.22
23	D	402	CLA	CHD-C4C	3.46	1.47	1.39
23	B	606	CLA	C3D-C2D	3.46	1.48	1.39
23	B	611	CLA	CHD-C4C	3.45	1.47	1.39
23	C	502	CLA	OBD-CAD	3.44	1.28	1.22
23	B	611	CLA	CHB-C1B	3.44	1.47	1.39
23	B	603	CLA	C3D-C2D	3.43	1.48	1.39
23	B	613	CLA	C4B-NB	-3.43	1.33	1.37
23	B	607	CLA	C4B-NB	-3.43	1.33	1.37
23	B	606	CLA	C4B-NB	-3.43	1.33	1.37
23	B	610	CLA	CHD-C4C	3.43	1.47	1.39
23	D	403	CLA	CHB-C1B	3.42	1.47	1.39
23	C	502	CLA	C3D-C2D	3.42	1.48	1.39
23	C	503	CLA	C3B-C4B	3.42	1.50	1.42
23	B	607	CLA	CHD-C4C	3.41	1.47	1.39
23	B	604	CLA	OBD-CAD	3.41	1.28	1.22
23	B	607	CLA	OBD-CAD	3.41	1.28	1.22
23	D	402	CLA	C4B-NB	-3.41	1.33	1.37
23	C	512	CLA	CHD-C1D	3.40	1.45	1.38
23	D	403	CLA	C3D-C2D	3.40	1.48	1.39
23	A	407	CLA	CHB-C1B	3.40	1.47	1.39
23	C	511	CLA	CHC-C4B	3.40	1.47	1.39
23	B	612	CLA	C3D-C2D	3.39	1.48	1.39
23	B	613	CLA	CHB-C1B	3.39	1.47	1.39
23	C	511	CLA	OBD-CAD	3.39	1.28	1.22
23	A	406	CLA	CHC-C4B	3.39	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	406	CLA	C3D-C2D	3.39	1.48	1.39
23	C	508	CLA	OBD-CAD	3.37	1.28	1.22
23	D	403	CLA	C4B-NB	-3.37	1.33	1.37
23	B	608	CLA	C4B-NB	-3.37	1.33	1.37
23	A	407	CLA	C3D-C2D	3.36	1.48	1.39
23	B	607	CLA	CHC-C4B	3.34	1.46	1.39
23	C	511	CLA	C4B-NB	-3.34	1.33	1.37
23	C	506	CLA	C4B-NB	-3.34	1.33	1.37
23	A	406	CLA	OBD-CAD	3.33	1.28	1.22
23	C	507	CLA	CHC-C4B	3.32	1.46	1.39
23	C	513	CLA	OBD-CAD	3.32	1.28	1.22
23	C	507	CLA	C3D-C2D	3.31	1.48	1.39
23	B	611	CLA	OBD-CAD	3.31	1.28	1.22
23	B	610	CLA	CHB-C1B	3.31	1.46	1.39
23	B	615	CLA	C3D-C2D	3.30	1.48	1.39
23	C	508	CLA	C1C-NC	-3.30	1.32	1.37
24	A	408	PHO	C1D-ND	-3.30	1.32	1.38
23	C	507	CLA	OBD-CAD	3.29	1.28	1.22
23	C	510	CLA	OBD-CAD	3.29	1.28	1.22
23	B	616	CLA	CHC-C4B	3.28	1.46	1.39
23	D	402	CLA	CHD-C1D	3.28	1.44	1.38
23	B	609	CLA	CHC-C4B	3.28	1.46	1.39
23	C	511	CLA	CHB-C1B	3.28	1.46	1.39
35	V	201	HEC	C4B-NB	-3.27	1.34	1.40
23	C	505	CLA	CHC-C4B	3.26	1.46	1.39
23	B	605	CLA	CHB-C1B	3.25	1.46	1.39
23	B	613	CLA	CHC-C4B	3.25	1.46	1.39
23	C	505	CLA	OBD-CAD	3.24	1.28	1.22
23	D	402	CLA	C1D-ND	3.24	1.41	1.37
23	B	609	CLA	OBD-CAD	3.23	1.28	1.22
23	A	407	CLA	CHC-C4B	3.23	1.46	1.39
23	B	609	CLA	C4B-NB	-3.22	1.33	1.37
23	B	617	CLA	CHD-C4C	3.22	1.46	1.39
23	C	501	CLA	C4B-NB	-3.22	1.33	1.37
23	C	502	CLA	CHB-C1B	3.21	1.46	1.39
23	C	509	CLA	OBD-CAD	3.21	1.28	1.22
23	B	615	CLA	CHC-C4B	3.21	1.46	1.39
23	B	614	CLA	CHC-C4B	3.21	1.46	1.39
23	B	606	CLA	CHB-C1B	3.21	1.46	1.39
23	D	403	CLA	OBD-CAD	3.21	1.28	1.22
23	B	604	CLA	CHC-C4B	3.21	1.46	1.39
23	A	405	CLA	C3D-C2D	3.21	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	C3D-C2D	3.21	1.47	1.39
23	B	607	CLA	CHB-C1B	3.20	1.46	1.39
23	C	510	CLA	CHB-C1B	3.20	1.46	1.39
23	B	604	CLA	C3D-C2D	3.20	1.47	1.39
23	B	610	CLA	OBD-CAD	3.20	1.28	1.22
23	C	508	CLA	CHD-C4C	3.19	1.46	1.39
23	C	504	CLA	OBD-CAD	3.19	1.28	1.22
34	H	101	RRX	C15-C14	3.19	1.53	1.43
23	B	605	CLA	OBD-CAD	3.18	1.28	1.22
23	A	405	CLA	CHC-C4B	3.18	1.46	1.39
34	H	101	RRX	C19-C18	3.18	1.52	1.45
24	A	409	PHO	C4B-NB	-3.18	1.32	1.38
34	H	101	RRX	C16-C17	3.17	1.53	1.43
23	A	406	CLA	CHB-C1B	3.17	1.46	1.39
23	B	614	CLA	CHB-C1B	3.17	1.46	1.39
23	B	605	CLA	C1C-NC	-3.16	1.33	1.37
34	H	101	RRX	C8-C9	3.15	1.52	1.45
23	B	608	CLA	CHB-C1B	3.15	1.46	1.39
23	C	513	CLA	C3B-C4B	3.13	1.50	1.42
34	H	101	RRX	C20-C21	3.13	1.53	1.43
23	B	613	CLA	C3D-C2D	3.13	1.47	1.39
23	B	613	CLA	OBD-CAD	3.13	1.27	1.22
23	B	603	CLA	C3B-C4B	3.12	1.50	1.42
23	B	617	CLA	C3B-C4B	3.12	1.50	1.42
23	B	603	CLA	C4B-NB	-3.11	1.34	1.37
33	F	101	HEM	C1C-C2C	-3.11	1.39	1.45
23	D	403	CLA	C3B-C4B	3.11	1.50	1.42
23	C	502	CLA	C1C-NC	-3.10	1.33	1.37
23	B	606	CLA	C3B-C4B	3.10	1.50	1.42
23	C	512	CLA	CHB-C1B	3.10	1.46	1.39
23	C	509	CLA	CHC-C4B	3.10	1.46	1.39
23	C	501	CLA	CHB-C1B	3.09	1.46	1.39
23	B	606	CLA	OBD-CAD	3.09	1.27	1.22
23	D	402	CLA	OBD-CAD	3.09	1.27	1.22
23	C	504	CLA	CHC-C4B	3.08	1.46	1.39
23	C	506	CLA	CHB-C1B	3.07	1.46	1.39
23	C	505	CLA	C3D-C2D	3.07	1.47	1.39
23	A	405	CLA	CHB-C1B	3.06	1.46	1.39
23	A	406	CLA	C3B-C4B	3.06	1.49	1.42
34	H	101	RRX	C11-C10	3.06	1.52	1.43
23	C	503	CLA	C3D-C2D	3.05	1.47	1.39
23	B	602	CLA	C3B-C4B	3.05	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	512	CLA	C3B-C4B	3.04	1.49	1.42
23	A	406	CLA	C4B-NB	-3.03	1.34	1.37
23	C	503	CLA	CHB-C1B	3.03	1.46	1.39
23	D	402	CLA	C3D-C2D	3.03	1.47	1.39
23	D	402	CLA	C3D-C4D	-3.03	1.37	1.44
23	C	506	CLA	CHC-C4B	3.03	1.46	1.39
34	H	101	RRX	C12-C13	3.02	1.52	1.45
23	B	617	CLA	CHC-C4B	3.02	1.46	1.39
23	C	504	CLA	CHB-C1B	3.01	1.46	1.39
23	B	615	CLA	CHB-C1B	3.01	1.46	1.39
23	C	509	CLA	C3D-C2D	3.01	1.47	1.39
23	B	602	CLA	CHB-C1B	3.01	1.46	1.39
23	B	609	CLA	C3B-C4B	3.01	1.49	1.42
23	B	612	CLA	C3B-C2B	3.00	1.51	1.41
23	B	612	CLA	CHD-C4C	3.00	1.46	1.39
23	B	611	CLA	C3B-C4B	3.00	1.49	1.42
23	C	512	CLA	C4B-NB	-2.99	1.34	1.37
34	H	101	RRX	C23-C22	2.99	1.52	1.45
23	B	612	CLA	CHD-C1D	2.99	1.44	1.38
23	C	508	CLA	CHB-C1B	2.99	1.46	1.39
23	C	510	CLA	C4B-NB	-2.98	1.34	1.37
23	B	612	CLA	C3B-C4B	2.97	1.49	1.42
26	D	407	SQD	C6-S	-2.97	1.66	1.77
23	C	501	CLA	C3B-C4B	2.96	1.49	1.42
23	B	605	CLA	C3D-C4D	-2.95	1.37	1.44
23	C	509	CLA	C3D-C4D	-2.95	1.37	1.44
23	B	616	CLA	CHB-C1B	2.95	1.46	1.39
23	A	410	CLA	CHB-C1B	2.95	1.46	1.39
23	D	402	CLA	C3B-C4B	2.94	1.49	1.42
23	A	405	CLA	C3D-C4D	-2.94	1.37	1.44
26	A	412	SQD	C6-S	-2.94	1.66	1.77
23	B	604	CLA	CHB-C1B	2.93	1.46	1.39
23	C	510	CLA	C3D-C2D	2.93	1.47	1.39
23	A	407	CLA	C3B-C4B	2.92	1.49	1.42
23	C	512	CLA	OBD-CAD	2.90	1.27	1.22
23	C	505	CLA	CHB-C1B	2.90	1.45	1.39
23	B	613	CLA	CHD-C1D	2.89	1.44	1.38
23	C	508	CLA	CHC-C4B	2.89	1.45	1.39
24	A	408	PHO	C4B-NB	-2.87	1.33	1.38
23	D	402	CLA	CHB-C1B	2.87	1.45	1.39
34	H	101	RRX	C24-C25	2.86	1.55	1.45
23	B	616	CLA	C3B-C4B	2.85	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	615	CLA	C3D-C4D	-2.85	1.37	1.44
23	C	509	CLA	C1C-NC	-2.85	1.33	1.37
23	C	503	CLA	C4B-NB	-2.84	1.34	1.37
23	C	509	CLA	CHB-C1B	2.84	1.45	1.39
23	B	613	CLA	CHD-C4C	2.83	1.45	1.39
23	B	609	CLA	CHB-C1B	2.82	1.45	1.39
23	C	513	CLA	CHB-C1B	2.82	1.45	1.39
23	B	603	CLA	CHB-C1B	2.82	1.45	1.39
23	C	510	CLA	C3B-C4B	2.80	1.49	1.42
23	B	610	CLA	CHC-C4B	2.80	1.45	1.39
23	C	503	CLA	C3D-C4D	-2.78	1.37	1.44
23	B	613	CLA	C1D-ND	2.77	1.41	1.37
23	B	605	CLA	CHC-C4B	2.77	1.45	1.39
23	C	510	CLA	C3D-C4D	-2.76	1.37	1.44
23	A	407	CLA	C3D-C4D	-2.76	1.37	1.44
23	C	504	CLA	C4C-C3C	2.75	1.49	1.45
34	H	101	RRX	C7-C6	2.75	1.54	1.45
24	A	409	PHO	C1B-NB	-2.75	1.33	1.38
23	C	502	CLA	CHC-C4B	2.73	1.45	1.39
23	B	615	CLA	OBD-CAD	2.71	1.27	1.22
23	A	405	CLA	C1C-NC	-2.69	1.33	1.37
23	B	610	CLA	C3B-C4B	2.69	1.49	1.42
23	B	611	CLA	C1C-NC	-2.69	1.33	1.37
23	B	609	CLA	C3D-C4D	-2.69	1.38	1.44
23	B	613	CLA	C1C-NC	-2.69	1.33	1.37
23	B	604	CLA	C3D-C4D	-2.69	1.38	1.44
23	B	614	CLA	OBD-CAD	2.68	1.27	1.22
23	B	612	CLA	C1B-NB	-2.67	1.34	1.37
23	A	406	CLA	C3D-C4D	-2.67	1.38	1.44
23	C	509	CLA	C3B-C4B	2.66	1.49	1.42
23	C	507	CLA	CHB-C1B	2.66	1.45	1.39
23	C	506	CLA	C1C-NC	-2.65	1.33	1.37
23	B	609	CLA	C4D-CHA	2.65	1.47	1.38
23	A	410	CLA	C3B-C4B	2.63	1.48	1.42
23	C	505	CLA	C3B-C4B	2.63	1.48	1.42
23	B	602	CLA	C4D-CHA	2.63	1.47	1.38
24	A	408	PHO	C1B-NB	-2.62	1.33	1.38
23	B	617	CLA	CHB-C1B	2.62	1.45	1.39
23	B	617	CLA	C4D-CHA	2.62	1.47	1.38
23	B	612	CLA	CMB-C2B	2.62	1.56	1.50
23	B	608	CLA	CHC-C4B	2.62	1.45	1.39
23	C	506	CLA	C4D-CHA	2.61	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	A	410	CLA	C3D-C4D	-2.61	1.38	1.44
23	C	506	CLA	C3B-C4B	2.61	1.48	1.42
23	C	504	CLA	C4D-CHA	2.60	1.47	1.38
23	A	406	CLA	C1C-NC	-2.60	1.33	1.37
23	B	612	CLA	C1C-NC	-2.60	1.33	1.37
23	B	608	CLA	C4D-CHA	2.59	1.47	1.38
23	B	616	CLA	C4D-CHA	2.58	1.47	1.38
23	B	608	CLA	C1C-NC	-2.58	1.34	1.37
23	B	606	CLA	C3D-C4D	-2.57	1.38	1.44
23	B	603	CLA	C3D-C4D	-2.56	1.38	1.44
23	B	613	CLA	C3B-C4B	2.56	1.48	1.42
23	C	502	CLA	C4D-CHA	2.55	1.47	1.38
23	B	605	CLA	C1B-C2B	2.55	1.49	1.43
23	B	605	CLA	C3D-C2D	2.55	1.46	1.39
23	B	616	CLA	C3D-C4D	-2.55	1.38	1.44
23	B	615	CLA	C4D-CHA	2.54	1.47	1.38
23	C	505	CLA	C3D-C4D	-2.54	1.38	1.44
23	C	503	CLA	C4D-CHA	2.54	1.47	1.38
25	K	101	BCR	C21-C22	-2.53	1.32	1.35
23	B	614	CLA	C3D-C4D	-2.52	1.38	1.44
23	C	509	CLA	C4D-CHA	2.52	1.47	1.38
23	C	508	CLA	C4D-CHA	2.52	1.47	1.38
23	C	511	CLA	C3D-C4D	-2.52	1.38	1.44
23	C	511	CLA	C3B-C4B	2.51	1.48	1.42
23	B	614	CLA	C4D-CHA	2.50	1.47	1.38
23	C	507	CLA	C4D-CHA	2.50	1.47	1.38
23	B	603	CLA	C1C-C2C	2.50	1.49	1.44
23	B	611	CLA	C3D-C4D	-2.50	1.38	1.44
23	C	502	CLA	C1B-C2B	2.50	1.49	1.43
23	C	508	CLA	C3B-C4B	2.50	1.48	1.42
23	B	610	CLA	C4D-CHA	2.49	1.47	1.38
23	D	403	CLA	C3D-C4D	-2.48	1.38	1.44
23	C	513	CLA	C4D-CHA	2.48	1.47	1.38
23	C	511	CLA	C4D-CHA	2.48	1.47	1.38
23	C	504	CLA	C3D-C4D	-2.48	1.38	1.44
23	C	512	CLA	C1C-C2C	2.48	1.49	1.44
23	B	608	CLA	C4C-C3C	2.47	1.49	1.45
23	C	512	CLA	C4D-CHA	2.47	1.47	1.38
23	B	604	CLA	C3B-C4B	2.46	1.48	1.42
34	H	101	RRX	C38-C26	2.46	1.55	1.50
23	C	507	CLA	C3D-C4D	-2.46	1.38	1.44
23	B	606	CLA	C4D-CHA	2.45	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	511	CLA	C1B-C2B	2.45	1.49	1.43
23	B	607	CLA	C1B-C2B	2.44	1.49	1.43
23	A	410	CLA	C4D-CHA	2.44	1.47	1.38
23	B	602	CLA	C3D-C4D	-2.43	1.38	1.44
23	C	513	CLA	C1C-C2C	2.43	1.49	1.44
23	B	615	CLA	C3B-C4B	2.43	1.48	1.42
23	C	513	CLA	C3D-C4D	-2.43	1.38	1.44
23	B	607	CLA	C3B-C4B	2.43	1.48	1.42
23	C	505	CLA	C4C-C3C	2.42	1.49	1.45
23	C	501	CLA	C4C-C3C	2.42	1.49	1.45
23	B	616	CLA	C1C-NC	-2.42	1.34	1.37
35	V	201	HEC	C4D-ND	-2.42	1.33	1.38
23	B	613	CLA	C3D-C4D	-2.42	1.38	1.44
27	D	411	LMG	O8-C28	2.41	1.45	1.33
23	C	501	CLA	C1B-C2B	2.41	1.48	1.43
23	B	606	CLA	C1B-C2B	2.40	1.48	1.43
23	B	617	CLA	C1B-C2B	2.40	1.48	1.43
23	B	607	CLA	C4D-CHA	2.39	1.46	1.38
35	V	201	HEC	C4A-C3A	-2.39	1.40	1.45
28	A	414	PL9	C6-C5	2.38	1.47	1.35
35	V	201	HEC	C1B-NB	-2.38	1.33	1.38
23	B	605	CLA	C4C-C3C	2.38	1.49	1.45
24	A	409	PHO	C1D-ND	-2.38	1.34	1.38
23	A	410	CLA	C1C-C2C	2.38	1.49	1.44
23	B	607	CLA	C1C-NC	-2.37	1.34	1.37
23	C	501	CLA	C3D-C4D	-2.37	1.38	1.44
23	A	407	CLA	C1C-NC	-2.37	1.34	1.37
23	B	616	CLA	C1B-C2B	2.37	1.48	1.43
23	B	604	CLA	CHB-C4A	-2.37	1.32	1.37
23	B	610	CLA	C1B-C2B	2.36	1.48	1.43
23	C	502	CLA	C3D-C4D	-2.36	1.38	1.44
23	A	406	CLA	C1B-C2B	2.36	1.48	1.43
23	B	602	CLA	C1C-C2C	2.36	1.49	1.44
23	B	613	CLA	CMA-C3A	-2.36	1.48	1.53
23	B	603	CLA	C4D-CHA	2.35	1.46	1.38
23	B	607	CLA	C3D-C4D	-2.35	1.38	1.44
23	B	611	CLA	C4D-CHA	2.35	1.46	1.38
23	A	405	CLA	OBD-CAD	2.35	1.26	1.22
23	D	402	CLA	C1C-NC	-2.34	1.34	1.37
23	D	403	CLA	C4D-CHA	2.34	1.46	1.38
23	B	608	CLA	C3B-C4B	2.34	1.48	1.42
23	B	610	CLA	C3D-C4D	-2.34	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	513	CLA	C3B-C2B	2.33	1.49	1.41
23	B	615	CLA	C1C-NC	-2.33	1.34	1.37
23	C	501	CLA	C4D-CHA	2.32	1.46	1.38
35	V	201	HEC	C1A-C2A	-2.32	1.41	1.45
23	C	508	CLA	C3D-C4D	-2.32	1.38	1.44
23	C	512	CLA	C3D-C4D	-2.32	1.38	1.44
23	D	402	CLA	CHB-C4A	-2.31	1.32	1.37
23	C	506	CLA	C3D-C4D	-2.31	1.39	1.44
23	B	603	CLA	CHB-C4A	-2.31	1.32	1.37
23	A	405	CLA	C4D-CHA	2.30	1.46	1.38
23	B	605	CLA	C4D-CHA	2.30	1.46	1.38
24	A	408	PHO	C3D-C4D	-2.30	1.38	1.41
23	B	610	CLA	C1C-NC	-2.30	1.34	1.37
23	B	614	CLA	C1C-NC	-2.29	1.34	1.37
33	F	101	HEM	C3C-C4C	-2.29	1.42	1.46
23	D	403	CLA	C4C-C3C	2.29	1.49	1.45
23	A	407	CLA	C4D-CHA	2.29	1.46	1.38
23	C	505	CLA	C1C-NC	-2.29	1.34	1.37
23	C	502	CLA	C3B-C4B	2.29	1.48	1.42
23	C	505	CLA	C4D-CHA	2.28	1.46	1.38
23	B	617	CLA	C3D-C4D	-2.28	1.39	1.44
23	B	604	CLA	C4D-CHA	2.27	1.46	1.38
23	C	507	CLA	C1B-C2B	2.27	1.48	1.43
23	C	505	CLA	CHB-C4A	-2.27	1.32	1.37
23	A	406	CLA	C4D-CHA	2.27	1.46	1.38
23	C	512	CLA	C1B-C2B	2.27	1.48	1.43
23	B	612	CLA	C4D-CHA	2.27	1.46	1.38
23	B	608	CLA	C3D-C4D	-2.27	1.39	1.44
23	B	614	CLA	C3B-C4B	2.26	1.48	1.42
28	D	405	PL9	C6-C5	2.26	1.47	1.35
23	C	506	CLA	C4C-C3C	2.26	1.48	1.45
23	B	609	CLA	CHB-C4A	-2.26	1.32	1.37
23	B	609	CLA	C4C-C3C	2.26	1.48	1.45
23	C	510	CLA	C4D-CHA	2.25	1.46	1.38
23	B	617	CLA	CMC-C2C	-2.25	1.46	1.50
23	B	614	CLA	C3B-C2B	2.25	1.48	1.41
23	D	403	CLA	C1B-C2B	2.24	1.48	1.43
23	C	511	CLA	C1C-NC	-2.24	1.34	1.37
23	C	504	CLA	C3B-C2B	2.23	1.48	1.41
34	H	101	RRX	C33-C5	2.23	1.54	1.50
23	B	614	CLA	C1B-C2B	2.23	1.48	1.43
33	F	101	HEM	C1D-ND	-2.22	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	503	CLA	OBD-CAD	2.21	1.26	1.22
23	C	509	CLA	C1B-C2B	2.21	1.48	1.43
25	C	514	BCR	C17-C18	-2.21	1.32	1.35
23	C	513	CLA	CHB-C4A	-2.21	1.32	1.37
23	A	410	CLA	CHB-C4A	-2.20	1.32	1.37
23	C	504	CLA	CHB-C4A	-2.20	1.32	1.37
25	C	515	BCR	C10-C9	-2.20	1.32	1.35
23	C	510	CLA	C1C-NC	-2.19	1.34	1.37
23	B	606	CLA	C1C-C2C	2.19	1.48	1.44
23	C	513	CLA	C4C-C3C	2.19	1.48	1.45
23	B	615	CLA	C1B-C2B	2.19	1.48	1.43
23	A	405	CLA	C3B-C2B	2.19	1.48	1.41
23	D	403	CLA	C3B-C2B	2.18	1.48	1.41
23	B	612	CLA	C3D-C4D	-2.18	1.39	1.44
23	C	508	CLA	C3B-C2B	2.16	1.48	1.41
23	B	602	CLA	CHB-C4A	-2.16	1.32	1.37
23	D	402	CLA	C4D-CHA	2.16	1.46	1.38
33	F	101	HEM	C4B-NB	-2.15	1.34	1.38
23	C	510	CLA	CHB-C4A	-2.15	1.32	1.37
23	B	611	CLA	C1B-C2B	2.15	1.48	1.43
23	B	611	CLA	C1C-C2C	2.14	1.48	1.44
23	A	405	CLA	C3B-C4B	2.14	1.47	1.42
23	D	403	CLA	C1C-NC	-2.14	1.34	1.37
23	C	513	CLA	C1C-NC	-2.13	1.34	1.37
23	B	604	CLA	C4C-C3C	2.13	1.48	1.45
23	B	613	CLA	C4D-CHA	2.13	1.46	1.38
23	C	511	CLA	C1C-C2C	2.13	1.48	1.44
23	B	602	CLA	C4C-C3C	2.13	1.48	1.45
23	B	606	CLA	C1C-NC	-2.11	1.34	1.37
24	A	409	PHO	C3D-C4D	-2.11	1.38	1.41
23	A	407	CLA	C4C-C3C	2.11	1.48	1.45
23	C	506	CLA	CHB-C4A	-2.10	1.32	1.37
23	C	508	CLA	CHB-C4A	-2.10	1.32	1.37
23	B	615	CLA	C3B-C2B	2.10	1.48	1.41
23	B	607	CLA	C4C-C3C	2.10	1.48	1.45
23	C	507	CLA	C3B-C4B	2.10	1.47	1.42
23	B	612	CLA	C1C-C2C	2.09	1.48	1.44
23	C	505	CLA	C3B-C2B	2.08	1.48	1.41
23	C	510	CLA	C1B-C2B	2.08	1.48	1.43
23	C	512	CLA	C1C-NC	-2.06	1.34	1.37
23	B	602	CLA	C1B-C2B	2.05	1.48	1.43
23	C	504	CLA	C3B-C4B	2.05	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	616	CLA	C1C-C2C	2.04	1.48	1.44
23	C	503	CLA	C1B-C2B	2.04	1.48	1.43
23	C	504	CLA	C1C-NC	-2.04	1.34	1.37
23	B	610	CLA	C1C-C2C	2.04	1.48	1.44
23	B	616	CLA	CHB-C4A	-2.04	1.32	1.37
28	A	414	PL9	C2-C3	2.03	1.40	1.34
23	C	507	CLA	C3B-C2B	2.03	1.48	1.41
23	C	509	CLA	C4C-C3C	2.03	1.48	1.45
24	A	409	PHO	CBD-CAD	-2.03	1.46	1.53
25	K	102	BCR	C21-C22	-2.03	1.33	1.35
23	B	615	CLA	C4C-C3C	2.03	1.48	1.45
23	C	502	CLA	C1A-CHA	2.02	1.51	1.43
23	D	403	CLA	C1C-C2C	2.02	1.48	1.44
23	A	407	CLA	C3B-C2B	2.01	1.48	1.41
23	A	405	CLA	C1B-C2B	2.00	1.48	1.43
23	B	608	CLA	C1A-CHA	2.00	1.51	1.43

All (1387) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	408	PHO	C2D-C1D-ND	12.42	118.10	109.53
24	A	409	PHO	C2D-C1D-ND	11.81	117.68	109.53
23	B	612	CLA	C2B-C1B-NB	11.50	117.94	110.23
34	H	101	RRX	C33-C5-C6	-11.40	111.73	124.53
23	B	612	CLA	C1D-ND-C4D	-11.38	98.25	106.33
23	B	612	CLA	C2D-C1D-ND	10.83	118.08	110.10
34	H	101	RRX	C16-C17-C18	-10.50	112.33	127.31
23	B	613	CLA	C1D-ND-C4D	-10.40	98.95	106.33
23	A	406	CLA	C1D-ND-C4D	-10.34	98.99	106.33
23	C	512	CLA	C1D-ND-C4D	-10.13	99.14	106.33
34	H	101	RRX	C35-C13-C14	-10.04	108.86	122.92
34	H	101	RRX	C11-C10-C9	-9.98	113.07	127.31
23	C	513	CLA	C2B-C1B-NB	9.97	116.92	110.23
34	H	101	RRX	C38-C26-C25	-9.91	113.41	124.53
23	C	512	CLA	C2D-C1D-ND	9.89	117.39	110.10
23	D	403	CLA	C1D-ND-C4D	-9.74	99.42	106.33
23	A	407	CLA	C1D-ND-C4D	-9.69	99.45	106.33
23	C	513	CLA	C1D-ND-C4D	-9.66	99.47	106.33
34	H	101	RRX	C15-C14-C13	-9.54	113.69	127.31
23	B	616	CLA	C1D-ND-C4D	-9.41	99.65	106.33
23	C	503	CLA	C1D-ND-C4D	-9.35	99.70	106.33
23	B	606	CLA	C1D-ND-C4D	-9.28	99.74	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	C2B-C1B-NB	9.22	116.41	110.23
23	B	602	CLA	C2B-C1B-NB	9.19	116.39	110.23
23	C	502	CLA	C1D-ND-C4D	-9.15	99.84	106.33
23	B	611	CLA	C1D-ND-C4D	-9.15	99.84	106.33
23	A	410	CLA	C1D-ND-C4D	-9.14	99.84	106.33
23	C	501	CLA	C1D-ND-C4D	-9.13	99.85	106.33
23	D	402	CLA	C1D-ND-C4D	-9.10	99.87	106.33
23	C	507	CLA	C1D-ND-C4D	-9.09	99.88	106.33
23	B	603	CLA	C1D-ND-C4D	-9.07	99.89	106.33
23	B	610	CLA	C1D-ND-C4D	-9.07	99.90	106.33
23	C	510	CLA	C1D-ND-C4D	-9.06	99.90	106.33
23	B	613	CLA	C2D-C1D-ND	9.06	116.78	110.10
23	A	406	CLA	C2D-C1D-ND	9.05	116.78	110.10
23	C	511	CLA	C1D-ND-C4D	-9.04	99.91	106.33
23	C	513	CLA	C2D-C1D-ND	8.96	116.71	110.10
23	B	607	CLA	C1D-ND-C4D	-8.95	99.98	106.33
23	B	614	CLA	C1D-ND-C4D	-8.91	100.01	106.33
23	B	616	CLA	C2D-C1D-ND	8.90	116.66	110.10
23	B	614	CLA	C2D-C1D-ND	8.85	116.63	110.10
23	C	507	CLA	C2B-C1B-NB	8.84	116.16	110.23
23	B	616	CLA	C2B-C1B-NB	8.81	116.14	110.23
23	C	512	CLA	C2B-C1B-NB	8.79	116.12	110.23
23	B	605	CLA	CMD-C2D-C1D	8.74	140.12	124.71
23	B	603	CLA	C2B-C1B-NB	8.73	116.09	110.23
23	C	508	CLA	C2D-C1D-ND	8.71	116.52	110.10
23	C	508	CLA	C1D-ND-C4D	-8.66	100.18	106.33
23	C	506	CLA	C1D-ND-C4D	-8.62	100.21	106.33
23	C	501	CLA	C2B-C1B-NB	8.62	116.01	110.23
23	B	609	CLA	C1D-ND-C4D	-8.61	100.22	106.33
23	B	602	CLA	C1D-ND-C4D	-8.54	100.27	106.33
23	B	612	CLA	C3B-C2B-C1B	-8.53	96.86	107.16
23	B	615	CLA	C1D-ND-C4D	-8.52	100.28	106.33
23	C	510	CLA	CMD-C2D-C1D	8.51	139.71	124.71
34	H	101	RRX	C36-C18-C17	-8.46	111.07	122.92
23	D	403	CLA	C2B-C1B-NB	8.45	115.90	110.23
23	C	507	CLA	C2D-C1D-ND	8.43	116.32	110.10
23	B	617	CLA	C1D-ND-C4D	-8.40	100.36	106.33
23	B	610	CLA	C2D-C1D-ND	8.40	116.29	110.10
34	H	101	RRX	C23-C22-C21	-8.39	106.06	118.94
23	C	503	CLA	C2B-C1B-NB	8.38	115.85	110.23
23	B	611	CLA	C2D-C1D-ND	8.32	116.23	110.10
23	B	611	CLA	C2B-C1B-NB	8.30	115.80	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	604	CLA	C1D-ND-C4D	-8.28	100.45	106.33
23	C	503	CLA	C2D-C1D-ND	8.26	116.19	110.10
23	C	504	CLA	C1D-ND-C4D	-8.21	100.50	106.33
23	B	607	CLA	C2D-C1D-ND	8.17	116.13	110.10
23	B	617	CLA	C2B-C1B-NB	8.16	115.70	110.23
23	C	505	CLA	C1D-ND-C4D	-8.15	100.54	106.33
23	A	405	CLA	C1D-ND-C4D	-8.15	100.55	106.33
23	C	509	CLA	C1D-ND-C4D	-8.14	100.56	106.33
23	A	410	CLA	C2B-C1B-NB	8.13	115.68	110.23
23	B	606	CLA	C2D-C1D-ND	8.11	116.08	110.10
23	D	403	CLA	C2D-C1D-ND	8.07	116.05	110.10
23	B	608	CLA	C1D-ND-C4D	-8.02	100.64	106.33
23	B	615	CLA	C2B-C1B-NB	8.00	115.60	110.23
34	H	101	RRX	C37-C22-C21	-8.00	111.72	122.92
23	C	504	CLA	C2B-C1B-NB	7.98	115.58	110.23
23	A	405	CLA	C2B-C1B-NB	7.98	115.58	110.23
23	C	502	CLA	C2D-C1D-ND	7.97	115.98	110.10
23	B	612	CLA	CHD-C4C-C3C	-7.95	113.15	124.84
23	C	511	CLA	C2D-C1D-ND	7.94	115.96	110.10
23	C	509	CLA	C2B-C1B-NB	7.93	115.55	110.23
23	A	407	CLA	C2D-C1D-ND	7.92	115.94	110.10
23	B	617	CLA	C2D-C1D-ND	7.91	115.93	110.10
23	B	609	CLA	C2B-C1B-NB	7.90	115.53	110.23
23	A	410	CLA	C2D-C1D-ND	7.85	115.89	110.10
23	C	509	CLA	CMD-C2D-C1D	7.85	138.55	124.71
23	B	605	CLA	C1D-ND-C4D	-7.85	100.76	106.33
23	A	406	CLA	C2B-C1B-NB	7.84	115.48	110.23
24	A	409	PHO	O2D-CGD-CBD	7.78	120.86	111.00
34	H	101	RRX	C1-C6-C5	-7.75	111.70	122.61
23	A	407	CLA	CMD-C2D-C1D	7.74	138.36	124.71
23	D	402	CLA	C2B-C1B-NB	7.72	115.41	110.23
23	C	506	CLA	C2D-C1D-ND	7.64	115.74	110.10
23	C	501	CLA	CMD-C2D-C1D	7.57	138.05	124.71
34	H	101	RRX	C34-C9-C10	-7.54	112.36	122.92
23	B	604	CLA	C2B-C1B-NB	7.53	115.28	110.23
23	C	503	CLA	CMD-C2D-C1D	7.51	137.95	124.71
23	B	614	CLA	C2B-C1B-NB	7.51	115.27	110.23
23	D	402	CLA	C2D-C1D-ND	7.48	115.61	110.10
23	C	511	CLA	C2B-C1B-NB	7.44	115.22	110.23
23	B	603	CLA	C2D-C1D-ND	7.43	115.58	110.10
23	B	602	CLA	C2D-C1D-ND	7.42	115.57	110.10
23	C	510	CLA	C2B-C1B-NB	7.41	115.20	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	H	101	RRX	C20-C21-C22	-7.39	116.77	127.31
23	C	502	CLA	C2B-C1B-NB	7.39	115.18	110.23
34	H	101	RRX	C34-C9-C8	-7.36	106.48	118.08
23	C	507	CLA	CMD-C2D-C1D	7.36	137.68	124.71
24	A	408	PHO	C2B-C1B-NB	7.33	114.59	109.53
23	B	606	CLA	C2B-C1B-NB	7.29	115.12	110.23
23	A	406	CLA	CMD-C2D-C1D	7.29	137.56	124.71
23	B	603	CLA	CMD-C2D-C1D	7.29	137.56	124.71
24	A	409	PHO	C2B-C1B-NB	7.26	114.54	109.53
24	A	408	PHO	C4D-ND-C1D	-7.23	101.47	108.83
23	B	608	CLA	C2D-C1D-ND	7.18	115.39	110.10
23	C	506	CLA	C2B-C1B-NB	7.17	115.04	110.23
24	A	409	PHO	C4D-ND-C1D	-7.17	101.54	108.83
23	A	406	CLA	CHD-C1D-ND	-7.16	117.88	124.45
23	D	403	CLA	CMD-C2D-C1D	7.15	137.31	124.71
23	C	501	CLA	C2D-C1D-ND	7.13	115.36	110.10
23	C	508	CLA	C2B-C1B-NB	7.11	115.00	110.23
23	B	607	CLA	C2B-C1B-NB	7.07	114.97	110.23
23	B	604	CLA	C2D-C1D-ND	7.07	115.31	110.10
23	A	405	CLA	CMD-C2D-C1D	7.05	137.14	124.71
23	B	610	CLA	C2B-C1B-NB	7.04	114.95	110.23
34	H	101	RRX	C4-C5-C6	-6.97	112.61	122.73
23	C	507	CLA	CHD-C1D-ND	-6.97	118.05	124.45
23	B	615	CLA	C2D-C1D-ND	6.91	115.20	110.10
23	B	613	CLA	CHD-C4C-C3C	-6.91	114.68	124.84
24	A	408	PHO	O2D-CGD-CBD	6.91	119.75	111.00
23	C	501	CLA	CHD-C1D-ND	-6.91	118.11	124.45
23	B	609	CLA	C2D-C1D-ND	6.89	115.18	110.10
23	A	407	CLA	C2B-C1B-NB	6.88	114.85	110.23
23	C	510	CLA	C2D-C1D-ND	6.88	115.18	110.10
23	B	607	CLA	CMD-C2D-C1D	6.88	136.84	124.71
23	B	602	CLA	CMD-C2D-C1D	6.81	136.72	124.71
23	C	504	CLA	CHD-C1D-ND	-6.77	118.24	124.45
23	B	606	CLA	CMD-C2D-C1D	6.76	136.63	124.71
23	D	402	CLA	CMD-C2D-C1D	6.74	136.59	124.71
23	C	505	CLA	CMD-C2D-C1D	6.73	136.57	124.71
23	C	505	CLA	O2D-CGD-CBD	6.68	123.14	111.27
23	A	406	CLA	CHD-C4C-C3C	-6.67	115.03	124.84
23	C	504	CLA	C2D-C1D-ND	6.67	115.02	110.10
24	A	408	PHO	C1C-C2C-C3C	-6.62	103.11	108.61
23	B	607	CLA	CHD-C1D-ND	-6.60	118.39	124.45
26	A	412	SQD	O6-C1-C2	6.60	118.60	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	H	101	RRX	C19-C18-C17	-6.59	108.83	118.94
23	B	613	CLA	O2D-CGD-CBD	6.58	122.96	111.27
23	C	504	CLA	CMD-C2D-C1D	6.56	136.28	124.71
23	B	603	CLA	CHD-C1D-ND	-6.51	118.47	124.45
23	D	402	CLA	C4A-NA-C1A	-6.49	103.79	106.71
23	B	611	CLA	CHD-C4C-C3C	-6.48	115.31	124.84
23	A	407	CLA	CHD-C1D-ND	-6.48	118.50	124.45
23	B	614	CLA	CMD-C2D-C1D	6.48	136.13	124.71
23	B	609	CLA	CMD-C2D-C1D	6.48	136.13	124.71
23	D	403	CLA	CHD-C1D-ND	-6.47	118.51	124.45
23	C	511	CLA	CMD-C2D-C1D	6.43	136.05	124.71
23	B	616	CLA	CHD-C1D-ND	-6.39	118.58	124.45
23	B	615	CLA	CMD-C2D-C1D	6.38	135.96	124.71
23	B	616	CLA	CMD-C2D-C1D	6.38	135.96	124.71
23	B	608	CLA	C2B-C1B-NB	6.38	114.51	110.23
23	B	610	CLA	CHD-C4C-C3C	-6.34	115.52	124.84
23	C	509	CLA	C2D-C1D-ND	6.31	114.75	110.10
23	C	506	CLA	CMD-C2D-C1D	6.29	135.81	124.71
23	B	606	CLA	CHD-C1D-ND	-6.29	118.67	124.45
23	B	604	CLA	CMD-C2D-C1D	6.28	135.78	124.71
34	H	101	RRX	C12-C13-C14	-6.28	109.30	118.94
23	A	405	CLA	C2D-C1D-ND	6.26	114.72	110.10
23	C	513	CLA	CHD-C1D-ND	-6.24	118.72	124.45
23	B	608	CLA	C2C-C1C-NC	6.21	115.79	109.97
23	C	505	CLA	C2C-C1C-NC	6.20	115.78	109.97
23	C	508	CLA	CHD-C4C-C3C	-6.17	115.78	124.84
23	B	604	CLA	O2D-CGD-CBD	6.14	122.17	111.27
23	B	605	CLA	C2C-C1C-NC	6.13	115.71	109.97
23	A	407	CLA	C2C-C1C-NC	6.12	115.70	109.97
23	B	614	CLA	CHD-C4C-C3C	-6.08	115.90	124.84
23	C	512	CLA	O2D-CGD-CBD	6.08	122.07	111.27
23	B	608	CLA	CMD-C2D-C1D	6.07	135.42	124.71
23	D	402	CLA	CHD-C4C-C3C	-6.05	115.95	124.84
23	C	510	CLA	CHD-C1D-ND	-6.05	118.90	124.45
23	B	617	CLA	O2D-CGD-CBD	6.04	122.00	111.27
23	C	512	CLA	CHD-C4C-C3C	-6.03	115.97	124.84
23	B	604	CLA	C4A-NA-C1A	-6.03	104.00	106.71
23	C	507	CLA	O2D-CGD-CBD	6.03	121.98	111.27
23	B	602	CLA	CHD-C1D-ND	-6.01	118.93	124.45
23	A	410	CLA	CMD-C2D-C1D	6.01	135.30	124.71
23	B	607	CLA	O2D-CGD-CBD	6.00	121.93	111.27
23	C	513	CLA	CMD-C2D-C1D	5.98	135.24	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	410	CLA	CHD-C4C-C3C	-5.97	116.07	124.84
23	C	509	CLA	C2C-C1C-NC	5.96	115.55	109.97
23	B	611	CLA	CMD-C2D-C1D	5.96	135.21	124.71
23	B	611	CLA	O2D-CGD-CBD	5.94	121.83	111.27
23	C	507	CLA	C3B-C2B-C1B	-5.94	99.99	107.16
23	C	506	CLA	CHD-C1D-ND	-5.93	119.01	124.45
23	C	508	CLA	O2D-CGD-CBD	5.90	121.74	111.27
25	K	101	BCR	C3-C4-C5	-5.89	103.57	114.08
23	C	511	CLA	CHD-C4C-C3C	-5.88	116.20	124.84
23	C	507	CLA	CHD-C4C-C3C	-5.87	116.20	124.84
23	C	502	CLA	CHD-C4C-C3C	-5.87	116.21	124.84
23	C	509	CLA	CHD-C1D-ND	-5.87	119.06	124.45
23	B	606	CLA	O2D-CGD-CBD	5.87	121.70	111.27
23	C	503	CLA	CHD-C1D-ND	-5.87	119.06	124.45
34	H	101	RRX	C37-C22-C23	-5.86	108.84	118.08
23	B	616	CLA	CHD-C4C-C3C	-5.85	116.25	124.84
23	C	506	CLA	C2C-C1C-NC	5.84	115.45	109.97
23	C	513	CLA	C3B-C2B-C1B	-5.82	100.14	107.16
23	B	603	CLA	C4A-NA-C1A	-5.82	104.09	106.71
23	C	510	CLA	CHD-C4C-C3C	-5.80	116.32	124.84
23	C	512	CLA	CHD-C1D-ND	-5.77	119.15	124.45
23	A	410	CLA	CHD-C1D-ND	-5.76	119.16	124.45
23	C	505	CLA	C2D-C1D-ND	5.75	114.34	110.10
23	B	611	CLA	C2C-C1C-NC	5.73	115.34	109.97
23	C	502	CLA	CMD-C2D-C1D	5.71	134.78	124.71
23	C	513	CLA	CHD-C4C-C3C	-5.71	116.45	124.84
23	A	406	CLA	C2C-C1C-NC	5.70	115.31	109.97
23	B	609	CLA	C2C-C1C-NC	5.70	115.31	109.97
23	C	507	CLA	C2C-C1C-NC	5.66	115.28	109.97
23	C	501	CLA	O2D-CGD-CBD	5.66	121.33	111.27
23	B	608	CLA	CHD-C1D-ND	-5.66	119.25	124.45
25	B	618	BCR	C3-C4-C5	-5.65	103.98	114.08
23	C	503	CLA	CHD-C4C-C3C	-5.64	116.55	124.84
23	C	504	CLA	O2D-CGD-CBD	5.63	121.28	111.27
23	B	608	CLA	O2D-CGD-CBD	5.63	121.28	111.27
23	C	509	CLA	O2D-CGD-CBD	5.63	121.28	111.27
23	C	504	CLA	C2C-C1C-NC	5.63	115.25	109.97
23	B	614	CLA	CHD-C1D-ND	-5.63	119.28	124.45
23	B	602	CLA	O2D-CGD-CBD	5.61	121.24	111.27
34	H	101	RRX	C35-C13-C12	-5.61	109.24	118.08
23	B	603	CLA	O2D-CGD-CBD	5.60	121.23	111.27
23	B	609	CLA	CHD-C1D-ND	-5.60	119.31	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	603	CLA	CHD-C4C-C3C	-5.59	116.62	124.84
24	A	409	PHO	C1C-C2C-C3C	-5.59	103.96	108.61
23	B	615	CLA	CHD-C4C-C3C	-5.57	116.65	124.84
23	B	605	CLA	C2B-C1B-NB	5.56	113.96	110.23
23	B	606	CLA	CHD-C4C-C3C	-5.54	116.70	124.84
23	A	405	CLA	C4A-NA-C1A	-5.51	104.23	106.71
23	A	405	CLA	CHD-C1D-ND	-5.50	119.40	124.45
23	B	602	CLA	CHD-C4C-C3C	-5.50	116.76	124.84
23	B	617	CLA	CHD-C4C-C3C	-5.49	116.76	124.84
23	B	610	CLA	C2C-C1C-NC	5.49	115.12	109.97
24	A	409	PHO	C3D-C4D-ND	5.46	115.17	107.72
23	C	501	CLA	C2C-C1C-NC	5.45	115.08	109.97
23	C	510	CLA	O2D-CGD-CBD	5.44	120.93	111.27
23	B	612	CLA	CHB-C1B-NB	-5.42	118.52	124.26
34	H	101	RRX	C36-C18-C19	-5.41	109.55	118.08
23	A	405	CLA	CHD-C4C-C3C	-5.41	116.89	124.84
24	A	409	PHO	C1A-C2A-C3A	-5.41	97.69	102.84
24	A	408	PHO	C3D-C4D-ND	5.40	115.09	107.72
23	B	613	CLA	C2B-C1B-NB	5.40	113.85	110.23
23	B	606	CLA	C2C-C1C-NC	5.40	115.03	109.97
23	A	405	CLA	CAA-C2A-C3A	-5.39	98.01	112.78
23	B	602	CLA	C3B-C2B-C1B	-5.39	100.66	107.16
23	B	614	CLA	C3D-C2D-C1D	-5.37	98.51	105.83
23	B	605	CLA	O2D-CGD-CBD	5.36	120.79	111.27
23	B	616	CLA	C2C-C1C-NC	5.33	114.96	109.97
23	D	403	CLA	C2C-C1C-NC	5.33	114.96	109.97
23	A	406	CLA	C3D-C2D-C1D	-5.32	98.57	105.83
23	B	607	CLA	C2C-C1C-NC	5.31	114.94	109.97
23	A	406	CLA	C1C-C2C-C3C	-5.29	101.39	106.96
23	C	511	CLA	CHD-C1D-ND	-5.29	119.60	124.45
23	D	403	CLA	CHD-C4C-C3C	-5.28	117.08	124.84
23	B	614	CLA	C2C-C1C-NC	5.26	114.90	109.97
23	C	502	CLA	CHD-C1D-ND	-5.25	119.63	124.45
23	B	607	CLA	CHD-C4C-C3C	-5.24	117.13	124.84
23	A	410	CLA	C3B-C2B-C1B	-5.23	100.84	107.16
23	C	504	CLA	C4A-NA-C1A	-5.23	104.35	106.71
23	D	402	CLA	CHD-C1D-ND	-5.20	119.67	124.45
23	C	506	CLA	CHD-C4C-C3C	-5.20	117.20	124.84
23	B	616	CLA	C3B-C2B-C1B	-5.19	100.90	107.16
23	B	612	CLA	C3D-C2D-C1D	-5.18	98.76	105.83
23	B	616	CLA	C3D-C2D-C1D	-5.17	98.78	105.83
23	C	512	CLA	C3B-C2B-C1B	-5.17	100.92	107.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	503	CLA	C3D-C2D-C1D	-5.16	98.80	105.83
23	B	605	CLA	C2D-C1D-ND	5.15	113.90	110.10
23	B	613	CLA	C3C-C4C-NC	5.12	116.32	110.57
23	C	509	CLA	CHD-C4C-C3C	-5.11	117.33	124.84
23	B	604	CLA	C2C-C1C-NC	5.10	114.75	109.97
23	C	507	CLA	C3D-C2D-C1D	-5.10	98.87	105.83
23	C	502	CLA	C2C-C1C-NC	5.09	114.74	109.97
23	B	604	CLA	CHD-C4C-C3C	-5.08	117.38	124.84
23	C	505	CLA	CHD-C4C-C3C	-5.06	117.41	124.84
23	B	615	CLA	C2C-C1C-NC	5.05	114.70	109.97
23	C	508	CLA	C3D-C2D-C1D	-5.05	98.94	105.83
23	A	407	CLA	O2D-CGD-CBD	5.05	120.24	111.27
23	B	603	CLA	C3B-C2B-C1B	-5.04	101.08	107.16
23	C	501	CLA	C3B-C2B-C1B	-5.04	101.08	107.16
23	B	615	CLA	C3B-C2B-C1B	-5.03	101.08	107.16
23	C	512	CLA	C3D-C2D-C1D	-5.03	98.96	105.83
23	C	513	CLA	C3D-C2D-C1D	-5.02	98.97	105.83
23	C	511	CLA	C2C-C1C-NC	5.02	114.68	109.97
23	A	407	CLA	CHD-C4C-C3C	-5.01	117.47	124.84
23	C	509	CLA	CMB-C2B-C1B	4.99	132.98	125.37
23	B	615	CLA	CHD-C1D-ND	-4.99	119.87	124.45
23	B	605	CLA	CHD-C1D-ND	-4.96	119.90	124.45
23	B	612	CLA	CHD-C1D-ND	-4.96	119.90	124.45
23	B	609	CLA	C4A-NA-C1A	-4.95	104.48	106.71
23	B	612	CLA	CMD-C2D-C1D	4.95	133.43	124.71
23	B	609	CLA	CHD-C4C-C3C	-4.95	117.57	124.84
23	D	402	CLA	O2D-CGD-CBD	4.94	120.05	111.27
23	A	405	CLA	C3B-C2B-C1B	-4.94	101.20	107.16
23	C	505	CLA	C3B-C2B-C1B	-4.92	101.22	107.16
23	C	507	CLA	C1C-C2C-C3C	-4.92	101.79	106.96
23	B	612	CLA	C3C-C4C-NC	4.91	116.07	110.57
23	B	615	CLA	O2D-CGD-CBD	4.91	119.99	111.27
23	C	508	CLA	C2C-C1C-NC	4.89	114.56	109.97
23	B	604	CLA	CHD-C1D-ND	-4.89	119.96	124.45
23	D	402	CLA	CAA-C2A-C3A	-4.88	99.41	112.78
23	D	403	CLA	C3B-C2B-C1B	-4.87	101.28	107.16
23	B	605	CLA	CHD-C4C-C3C	-4.87	117.68	124.84
23	B	611	CLA	C3B-C2B-C1B	-4.87	101.28	107.16
25	A	411	BCR	C16-C17-C18	-4.86	120.37	127.31
23	B	617	CLA	C4C-C3C-C2C	-4.86	99.82	106.90
23	A	407	CLA	C3D-C2D-C1D	-4.86	99.20	105.83
23	B	611	CLA	CHD-C1D-ND	-4.85	120.00	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	617	CLA	C1D-CHD-C4C	-4.85	115.60	126.06
23	B	614	CLA	C3B-C2B-C1B	-4.83	101.33	107.16
23	C	502	CLA	CMB-C2B-C1B	4.83	132.72	125.37
27	B	622	LMG	O7-C10-C11	4.83	121.91	111.50
23	B	602	CLA	C2C-C1C-NC	4.82	114.49	109.97
23	C	508	CLA	CHD-C1D-ND	-4.82	120.03	124.45
25	A	411	BCR	C15-C14-C13	-4.81	120.44	127.31
23	C	510	CLA	C2C-C1C-NC	4.81	114.48	109.97
23	B	610	CLA	CMD-C2D-C1D	4.80	133.17	124.71
23	C	502	CLA	O2D-CGD-CBD	4.79	119.78	111.27
23	C	509	CLA	C3B-C2B-C1B	-4.78	101.39	107.16
27	A	413	LMG	O7-C10-C11	4.78	121.79	111.50
23	C	508	CLA	CMD-C2D-C1D	4.77	133.13	124.71
23	C	503	CLA	C2C-C1C-NC	4.77	114.44	109.97
23	C	504	CLA	CAC-C3C-C4C	4.77	131.00	124.81
23	B	616	CLA	O2D-CGD-CBD	4.76	119.73	111.27
23	B	611	CLA	C3D-C2D-C1D	-4.75	99.35	105.83
30	C	516	DGD	O2G-C1B-C2B	4.74	121.72	111.50
25	K	101	BCR	C28-C27-C26	-4.74	105.61	114.08
23	B	608	CLA	C3B-C4B-NB	4.74	114.91	110.52
23	B	606	CLA	C3D-C2D-C1D	-4.73	99.37	105.83
23	B	612	CLA	C1D-CHD-C4C	-4.73	115.86	126.06
23	A	405	CLA	C2C-C1C-NC	4.72	114.39	109.97
33	F	101	HEM	CHC-C4B-NB	4.70	129.52	124.42
23	B	606	CLA	C3B-C2B-C1B	-4.69	101.50	107.16
23	C	511	CLA	C3B-C2B-C1B	-4.68	101.51	107.16
23	A	410	CLA	O2D-CGD-CBD	4.68	119.58	111.27
23	B	608	CLA	CHD-C4C-C3C	-4.68	117.97	124.84
23	C	502	CLA	C3B-C2B-C1B	-4.66	101.53	107.16
23	A	410	CLA	C4A-NA-C1A	-4.66	104.61	106.71
23	C	512	CLA	CMD-C2D-C1D	4.66	132.92	124.71
23	B	611	CLA	C3C-C4C-NC	4.66	115.79	110.57
23	B	607	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
23	D	403	CLA	C3D-C2D-C1D	-4.64	99.49	105.83
23	C	510	CLA	C3B-C2B-C1B	-4.64	101.56	107.16
26	A	412	SQD	O8-S-C6	4.62	113.11	105.74
23	D	403	CLA	C4A-NA-C1A	-4.61	104.63	106.71
23	C	512	CLA	C2C-C1C-NC	4.60	114.28	109.97
23	C	506	CLA	C3D-C2D-C1D	-4.60	99.56	105.83
23	A	410	CLA	C2C-C1C-NC	4.60	114.28	109.97
23	B	613	CLA	C3D-C4D-ND	4.58	117.65	110.24
25	B	620	BCR	C16-C17-C18	-4.58	120.78	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	C4A-NA-C1A	-4.57	104.65	106.71
25	C	515	BCR	C15-C14-C13	-4.57	120.79	127.31
23	B	612	CLA	C3D-C4D-ND	4.56	117.62	110.24
23	A	410	CLA	C3D-C2D-C1D	-4.56	99.60	105.83
23	B	611	CLA	C4A-NA-C1A	-4.56	104.66	106.71
23	C	501	CLA	C3D-C4D-ND	4.55	117.60	110.24
23	B	610	CLA	CHD-C1D-ND	-4.54	120.28	124.45
23	C	501	CLA	CHD-C4C-C3C	-4.54	118.16	124.84
25	K	102	BCR	C28-C27-C26	-4.54	105.97	114.08
23	B	617	CLA	CAC-C3C-C4C	4.53	130.69	124.81
23	B	610	CLA	C3D-C2D-C1D	-4.53	99.65	105.83
25	B	618	BCR	C15-C14-C13	-4.53	120.85	127.31
23	C	510	CLA	CMB-C2B-C1B	4.52	132.25	125.37
23	A	407	CLA	C1C-C2C-C3C	-4.52	102.21	106.96
23	C	505	CLA	CHD-C1D-ND	-4.51	120.31	124.45
23	C	511	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
23	A	407	CLA	C3D-C4D-ND	4.51	117.53	110.24
23	B	602	CLA	C3D-C2D-C1D	-4.51	99.68	105.83
23	D	403	CLA	C3D-C4D-ND	4.50	117.52	110.24
35	V	201	HEC	CHB-C1B-NB	4.50	129.31	124.42
23	B	607	CLA	C3B-C2B-C1B	-4.50	101.73	107.16
23	C	504	CLA	C3B-C2B-C1B	-4.49	101.75	107.16
23	C	508	CLA	C3B-C4B-NB	4.48	114.67	110.52
23	C	510	CLA	C4A-NA-C1A	-4.48	104.69	106.71
23	C	503	CLA	C4A-NA-C1A	-4.48	104.69	106.71
23	B	617	CLA	C2C-C1C-NC	4.46	114.15	109.97
25	B	620	BCR	C20-C21-C22	-4.46	120.94	127.31
23	B	613	CLA	C2C-C1C-NC	4.46	114.15	109.97
23	B	603	CLA	C3D-C2D-C1D	-4.45	99.76	105.83
25	K	101	BCR	C15-C14-C13	-4.44	120.97	127.31
25	C	514	BCR	C15-C14-C13	-4.44	120.97	127.31
23	C	512	CLA	C4A-NA-C1A	-4.44	104.71	106.71
23	B	617	CLA	C3C-C4C-NC	4.43	115.53	110.57
25	K	102	BCR	C15-C14-C13	-4.42	121.00	127.31
23	A	406	CLA	C3D-C4D-ND	4.42	117.39	110.24
23	B	612	CLA	O2D-CGD-CBD	4.42	119.12	111.27
23	B	609	CLA	O2D-CGD-CBD	4.41	119.11	111.27
23	A	410	CLA	CAA-C2A-C3A	-4.40	100.73	112.78
23	A	410	CLA	C3D-C4D-ND	4.39	117.33	110.24
23	C	513	CLA	C2C-C1C-NC	4.39	114.08	109.97
23	B	613	CLA	C1D-CHD-C4C	-4.38	116.60	126.06
23	B	602	CLA	C4A-NA-C1A	-4.37	104.74	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	620	BCR	C28-C27-C26	-4.37	106.28	114.08
23	C	508	CLA	C1D-CHD-C4C	-4.36	116.65	126.06
23	B	617	CLA	C3B-C2B-C1B	-4.36	101.90	107.16
32	D	409	LHG	O7-C7-C8	4.36	120.89	111.50
23	B	603	CLA	C2C-C1C-NC	4.35	114.05	109.97
23	C	502	CLA	C3D-C2D-C1D	-4.35	99.90	105.83
27	B	622	LMG	C4-C3-C2	4.33	118.38	110.82
23	B	610	CLA	C1D-CHD-C4C	-4.33	116.72	126.06
23	B	606	CLA	C3D-C4D-ND	4.33	117.24	110.24
23	A	406	CLA	C3B-C2B-C1B	-4.33	101.94	107.16
23	B	607	CLA	C3C-C4C-NC	4.33	115.43	110.57
23	C	501	CLA	C3D-C2D-C1D	-4.32	99.93	105.83
23	B	608	CLA	C3D-C2D-C1D	-4.32	99.94	105.83
35	V	201	HEC	C4B-NB-C1B	4.31	109.53	105.07
23	C	503	CLA	O2D-CGD-CBD	4.31	118.93	111.27
23	B	603	CLA	C3D-C4D-ND	4.30	117.20	110.24
23	B	604	CLA	C3B-C2B-C1B	-4.30	101.98	107.16
23	D	402	CLA	C3B-C2B-C1B	-4.29	101.98	107.16
23	B	603	CLA	CAA-C2A-C3A	-4.29	101.03	112.78
34	H	101	RRX	C7-C6-C5	-4.29	111.08	121.46
23	C	506	CLA	O2D-CGD-CBD	4.28	118.86	111.27
25	B	618	BCR	C11-C10-C9	-4.27	121.21	127.31
35	V	201	HEC	C4C-NC-C1C	4.27	109.53	105.35
23	C	513	CLA	C3D-C4D-ND	4.27	117.14	110.24
23	C	512	CLA	C3D-C4D-ND	4.27	117.14	110.24
28	D	405	PL9	C7-C8-C9	-4.26	119.70	126.79
23	D	402	CLA	C3D-C4D-ND	4.26	117.12	110.24
23	C	501	CLA	C1-C2-C3	-4.26	118.68	126.04
26	D	407	SQD	C1-O5-C5	4.26	122.04	113.69
26	D	407	SQD	O6-C1-C2	4.25	114.94	108.30
23	C	503	CLA	C3B-C2B-C1B	-4.25	102.04	107.16
23	C	511	CLA	C3C-C4C-NC	4.24	115.33	110.57
23	C	504	CLA	C3D-C4D-ND	4.24	117.09	110.24
23	C	501	CLA	C1C-C2C-C3C	-4.23	102.51	106.96
23	A	406	CLA	CHD-C4C-NC	4.22	130.86	124.20
34	H	101	RRX	C8-C9-C10	-4.22	112.47	118.94
23	C	508	CLA	C3C-C4C-NC	4.22	115.30	110.57
25	B	618	BCR	C16-C17-C18	-4.22	121.29	127.31
23	C	510	CLA	C3D-C2D-C1D	-4.22	100.08	105.83
23	B	616	CLA	C3C-C4C-NC	4.21	115.29	110.57
23	C	505	CLA	C3D-C4D-ND	4.21	117.05	110.24
23	B	605	CLA	O2A-CGA-CBA	4.21	125.11	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	C3D-C2D-C1D	-4.21	100.09	105.83
23	A	406	CLA	O2D-CGD-CBD	4.20	118.74	111.27
23	C	510	CLA	C3D-C4D-ND	4.19	117.02	110.24
23	C	502	CLA	C1D-CHD-C4C	-4.19	117.02	126.06
26	A	412	SQD	O47-C7-C8	4.19	120.53	111.50
23	C	504	CLA	C3B-C4B-NB	4.18	114.39	110.52
23	B	609	CLA	C3D-C4D-ND	4.17	116.98	110.24
23	B	606	CLA	C4A-NA-C1A	-4.17	104.83	106.71
23	B	610	CLA	C3D-C4D-ND	4.17	116.98	110.24
25	D	404	BCR	C7-C8-C9	-4.16	119.95	126.23
23	B	614	CLA	C1D-CHD-C4C	-4.16	117.08	126.06
23	C	507	CLA	C1D-CHD-C4C	-4.16	117.08	126.06
23	B	605	CLA	C3B-C4B-NB	4.15	114.37	110.52
23	A	405	CLA	C3D-C4D-ND	4.15	116.95	110.24
23	C	502	CLA	C3D-C4D-ND	4.14	116.94	110.24
23	B	606	CLA	C1C-C2C-C3C	-4.14	102.61	106.96
25	K	101	BCR	C10-C11-C12	-4.13	110.32	123.22
23	B	612	CLA	CHD-C4C-NC	4.13	130.71	124.20
23	C	506	CLA	C3D-C4D-ND	4.13	116.91	110.24
23	B	617	CLA	C3D-C2D-C1D	-4.12	100.20	105.83
23	C	502	CLA	C3C-C4C-NC	4.12	115.19	110.57
30	C	517	DGD	O2G-C1B-C2B	4.12	120.38	111.50
25	B	618	BCR	C7-C8-C9	-4.12	120.01	126.23
23	D	403	CLA	O2D-CGD-CBD	4.11	118.58	111.27
23	C	503	CLA	C1D-CHD-C4C	-4.11	117.19	126.06
23	C	502	CLA	C3B-C4B-NB	4.11	114.33	110.52
23	C	511	CLA	C3D-C4D-ND	4.11	116.88	110.24
23	C	513	CLA	O2D-CGD-CBD	4.10	118.56	111.27
23	C	509	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
23	B	611	CLA	C3D-C4D-ND	4.10	116.86	110.24
23	A	405	CLA	C3B-C4B-NB	4.10	114.31	110.52
23	B	609	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
23	C	505	CLA	C1C-C2C-C3C	-4.10	102.65	106.96
23	B	617	CLA	CMD-C2D-C1D	4.09	131.93	124.71
23	B	611	CLA	C1D-CHD-C4C	-4.09	117.23	126.06
23	C	509	CLA	C3D-C2D-C1D	-4.09	100.25	105.83
23	B	612	CLA	C4C-C3C-C2C	-4.08	100.96	106.90
35	V	201	HEC	CHA-C4D-ND	4.07	128.84	124.42
23	B	615	CLA	C3D-C4D-ND	4.07	116.83	110.24
23	A	406	CLA	C1D-CHD-C4C	-4.07	117.29	126.06
23	B	604	CLA	O2A-CGA-CBA	4.07	124.67	111.91
23	C	504	CLA	C3D-C2D-C1D	-4.06	100.29	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	407	CLA	C4A-NA-C1A	-4.05	104.88	106.71
23	B	607	CLA	C3D-C4D-ND	4.05	116.79	110.24
23	B	610	CLA	C3C-C4C-NC	4.05	115.11	110.57
30	C	517	DGD	O1G-C1A-C2A	4.04	121.98	111.38
23	A	410	CLA	C3C-C4C-NC	4.04	115.10	110.57
23	D	402	CLA	C3C-C4C-NC	4.03	115.09	110.57
23	B	604	CLA	C3D-C2D-C1D	-4.02	100.34	105.83
23	B	605	CLA	CMD-C2D-C3D	-4.01	118.40	127.61
23	A	407	CLA	C3B-C2B-C1B	-4.00	102.33	107.16
23	B	608	CLA	C3D-C4D-ND	4.00	116.71	110.24
23	B	610	CLA	C3B-C2B-C1B	-4.00	102.34	107.16
23	C	508	CLA	C3D-C4D-ND	3.99	116.70	110.24
23	A	405	CLA	C1D-CHD-C4C	-3.99	117.45	126.06
23	B	614	CLA	C1C-C2C-C3C	-3.99	102.76	106.96
23	B	616	CLA	C3D-C4D-ND	3.99	116.69	110.24
23	B	605	CLA	C3C-C4C-NC	3.99	115.04	110.57
23	C	512	CLA	C3C-C4C-NC	3.98	115.03	110.57
23	B	606	CLA	CAC-C3C-C4C	3.98	129.97	124.81
23	D	402	CLA	C3D-C2D-C1D	-3.98	100.40	105.83
23	B	602	CLA	C3D-C4D-ND	3.98	116.67	110.24
23	B	606	CLA	CMC-C2C-C1C	3.98	131.09	125.04
23	B	615	CLA	C3C-C4C-NC	3.98	115.03	110.57
23	B	615	CLA	C1D-CHD-C4C	-3.97	117.49	126.06
23	B	606	CLA	CMB-C2B-C1B	3.97	131.41	125.37
25	K	101	BCR	C21-C20-C19	-3.97	110.83	123.22
23	C	503	CLA	C3C-C4C-NC	3.97	115.02	110.57
23	B	605	CLA	C3B-C2B-C1B	-3.96	102.38	107.16
23	B	615	CLA	C3D-C2D-C1D	-3.96	100.43	105.83
23	C	507	CLA	C4A-NA-C1A	-3.96	104.93	106.71
23	D	402	CLA	C2C-C1C-NC	3.96	113.68	109.97
23	B	610	CLA	C3B-C4B-NB	3.95	114.18	110.52
23	B	617	CLA	C3D-C4D-ND	3.95	116.63	110.24
23	B	605	CLA	C1D-CHD-C4C	-3.94	117.55	126.06
35	V	201	HEC	CHC-C4B-NB	3.94	129.24	124.37
23	B	615	CLA	C4A-NA-C1A	-3.94	104.94	106.71
23	C	507	CLA	C3D-C4D-ND	3.94	116.61	110.24
23	B	604	CLA	C3D-C4D-ND	3.94	116.61	110.24
23	B	610	CLA	C1C-C2C-C3C	-3.94	102.82	106.96
24	A	409	PHO	CAA-CBA-CGA	-3.93	101.78	113.25
23	C	503	CLA	CBC-CAC-C3C	-3.92	101.62	112.43
23	C	509	CLA	C3D-C4D-ND	3.92	116.57	110.24
23	C	510	CLA	C1C-C2C-C3C	-3.90	102.85	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	C1D-CHD-C4C	-3.90	117.64	126.06
23	B	611	CLA	C1C-C2C-C3C	-3.89	102.87	106.96
25	K	102	BCR	C7-C8-C9	-3.89	120.36	126.23
23	C	501	CLA	CAC-C3C-C4C	3.88	129.85	124.81
24	A	408	PHO	CMB-C2B-C3B	3.88	131.94	124.68
23	B	617	CLA	C3B-C4B-NB	3.87	114.11	110.52
23	C	513	CLA	C3C-C4C-NC	3.87	114.91	110.57
23	C	511	CLA	O2D-CGD-CBD	3.86	118.13	111.27
23	B	605	CLA	C3D-C4D-ND	3.85	116.47	110.24
26	D	407	SQD	O5-C5-C4	3.85	116.69	109.69
27	A	413	LMG	C1-O6-C5	3.84	121.23	113.69
23	C	504	CLA	CHD-C4C-C3C	-3.84	119.20	124.84
23	A	405	CLA	C3D-C2D-C1D	-3.83	100.60	105.83
23	B	608	CLA	CHC-C1C-C2C	-3.82	116.11	126.73
23	B	614	CLA	C3B-C4B-NB	3.82	114.06	110.52
23	C	505	CLA	C3B-C4B-NB	3.82	114.06	110.52
32	D	408	LHG	O7-C7-C8	3.81	119.72	111.50
24	A	409	PHO	C4A-C3A-C2A	-3.81	99.21	102.84
26	D	407	SQD	C44-O6-C1	-3.81	107.53	113.84
23	C	502	CLA	C1-C2-C3	-3.81	119.46	126.04
23	C	505	CLA	C3C-C4C-NC	3.80	114.84	110.57
23	B	605	CLA	CMB-C2B-C1B	3.80	131.16	125.37
23	C	506	CLA	C3C-C4C-NC	3.80	114.83	110.57
23	C	508	CLA	C3B-C2B-C1B	-3.80	102.58	107.16
23	B	604	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
23	C	509	CLA	C1D-CHD-C4C	-3.80	117.87	126.06
23	B	613	CLA	C4C-C3C-C2C	-3.80	101.36	106.90
33	F	101	HEM	CHD-C1D-ND	3.79	128.54	124.42
23	C	508	CLA	C4C-C3C-C2C	-3.79	101.37	106.90
30	C	518	DGD	O2G-C1B-C2B	3.79	119.68	111.50
23	C	505	CLA	C1D-CHD-C4C	-3.79	117.89	126.06
23	C	512	CLA	C1C-C2C-C3C	-3.79	102.98	106.96
23	C	505	CLA	C4A-NA-C1A	-3.77	105.01	106.71
28	D	405	PL9	C10-C9-C11	3.76	121.59	115.27
23	B	605	CLA	C4C-C3C-C2C	-3.75	101.43	106.90
23	B	606	CLA	C3C-C4C-NC	3.75	114.78	110.57
25	A	411	BCR	C20-C21-C22	-3.75	121.96	127.31
23	C	503	CLA	C3D-C4D-ND	3.74	116.30	110.24
23	C	511	CLA	C1D-CHD-C4C	-3.73	118.02	126.06
23	B	609	CLA	C3B-C2B-C1B	-3.72	102.67	107.16
23	B	605	CLA	CHC-C1C-C2C	-3.72	116.39	126.73
32	L	101	LHG	O7-C7-C8	3.72	119.52	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	610	CLA	C4-C3-C5	3.72	121.52	115.27
34	H	101	RRX	C24-C25-C26	-3.72	112.46	121.46
32	D	410	LHG	O7-C7-C8	3.71	119.51	111.50
23	B	613	CLA	CMB-C2B-C1B	3.71	131.02	125.37
24	A	408	PHO	C4-C3-C5	3.70	121.50	115.27
25	C	514	BCR	C16-C17-C18	-3.70	122.03	127.31
23	C	506	CLA	C3B-C2B-C1B	-3.70	102.70	107.16
23	B	602	CLA	C3C-C4C-NC	3.69	114.71	110.57
23	B	614	CLA	C3D-C4D-ND	3.68	116.20	110.24
23	B	604	CLA	CAA-C2A-C3A	-3.68	102.70	112.78
23	A	407	CLA	C1D-CHD-C4C	-3.68	118.13	126.06
23	B	617	CLA	CHC-C1C-C2C	-3.67	116.52	126.73
23	C	502	CLA	C4C-C3C-C2C	-3.67	101.54	106.90
23	B	609	CLA	C1D-CHD-C4C	-3.67	118.13	126.06
23	B	607	CLA	CMB-C2B-C1B	3.67	130.96	125.37
23	B	614	CLA	O2D-CGD-CBD	3.66	117.78	111.27
23	B	614	CLA	C4A-NA-C1A	-3.65	105.06	106.71
23	C	504	CLA	C1C-C2C-C3C	-3.65	103.11	106.96
23	D	403	CLA	C1C-C2C-C3C	-3.65	103.12	106.96
24	A	409	PHO	CMB-C2B-C3B	3.64	131.49	124.68
23	B	607	CLA	C4A-NA-C1A	-3.63	105.07	106.71
23	C	506	CLA	CHC-C1C-C2C	-3.63	116.65	126.73
35	V	201	HEC	C1D-ND-C4D	3.63	108.82	105.07
25	C	515	BCR	C15-C16-C17	-3.61	116.08	123.47
25	K	102	BCR	C21-C20-C19	-3.61	111.96	123.22
23	B	615	CLA	CAC-C3C-C4C	3.60	129.49	124.81
23	D	403	CLA	C3C-C4C-NC	3.60	114.61	110.57
23	B	610	CLA	O2D-CGD-CBD	3.60	117.67	111.27
34	H	101	RRX	C23-C24-C25	-3.60	117.10	127.20
30	H	102	DGD	C4D-C3D-C2D	3.60	117.10	110.82
23	A	410	CLA	C1D-CHD-C4C	-3.59	118.31	126.06
23	B	608	CLA	C1C-C2C-C3C	-3.59	103.18	106.96
23	B	615	CLA	C3B-C4B-NB	3.59	113.85	110.52
30	H	102	DGD	O2G-C1B-C2B	3.59	119.23	111.50
23	C	513	CLA	C1D-CHD-C4C	-3.59	118.32	126.06
23	B	604	CLA	C3C-C4C-NC	3.58	114.59	110.57
23	A	405	CLA	C3C-C4C-NC	3.58	114.59	110.57
23	B	616	CLA	C4A-NA-C1A	-3.58	105.10	106.71
23	C	506	CLA	C3B-C4B-NB	3.58	113.83	110.52
23	B	612	CLA	CHB-C4A-NA	3.57	129.45	124.51
25	K	101	BCR	C16-C17-C18	-3.57	122.21	127.31
28	A	414	PL9	C10-C9-C11	3.57	121.28	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	501	CLA	C4A-NA-C1A	-3.56	105.11	106.71
33	F	101	HEM	CHD-C4C-NC	3.54	128.27	124.44
23	B	603	CLA	C3C-C4C-NC	3.54	114.54	110.57
33	F	101	HEM	C4C-NC-C1C	3.54	108.81	105.35
23	B	603	CLA	C1D-CHD-C4C	-3.54	118.42	126.06
23	B	616	CLA	C1C-C2C-C3C	-3.54	103.24	106.96
23	C	506	CLA	C1C-C2C-C3C	-3.53	103.24	106.96
23	B	616	CLA	C1D-CHD-C4C	-3.53	118.45	126.06
23	B	602	CLA	C1D-CHD-C4C	-3.53	118.45	126.06
23	B	615	CLA	C4-C3-C5	3.52	120.01	115.98
23	B	614	CLA	C3C-C4C-NC	3.52	114.52	110.57
23	B	610	CLA	CMB-C2B-C1B	3.52	130.73	125.37
25	C	514	BCR	C15-C16-C17	-3.52	116.27	123.47
27	D	411	LMG	O7-C10-C11	3.51	120.60	110.80
23	B	607	CLA	C3B-C4B-NB	3.51	113.77	110.52
23	B	617	CLA	CHD-C1D-ND	-3.50	121.23	124.45
23	D	402	CLA	C1D-CHD-C4C	-3.50	118.50	126.06
23	B	604	CLA	C1C-C2C-C3C	-3.50	103.28	106.96
25	C	515	BCR	C20-C21-C22	-3.49	122.32	127.31
25	K	101	BCR	C24-C23-C22	-3.49	120.96	126.23
25	B	620	BCR	C15-C14-C13	-3.49	122.33	127.31
23	C	502	CLA	CHC-C1C-C2C	-3.49	117.03	126.73
23	C	505	CLA	O2D-CGD-O1D	-3.49	117.02	123.84
23	B	610	CLA	CMC-C2C-C1C	3.49	130.35	125.04
23	B	602	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
25	C	514	BCR	C7-C8-C9	-3.48	120.98	126.23
23	B	608	CLA	C1D-CHD-C4C	-3.48	118.56	126.06
23	B	603	CLA	C1C-C2C-C3C	-3.48	103.30	106.96
33	F	101	HEM	C1B-NB-C4B	3.47	108.66	105.07
23	C	508	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
34	H	101	RRX	C30-C25-C26	-3.46	117.74	122.61
23	C	507	CLA	CHD-C4C-NC	3.46	129.66	124.20
23	B	610	CLA	O2A-CGA-CBA	3.46	122.76	111.91
25	K	102	BCR	C10-C11-C12	-3.45	112.44	123.22
23	C	506	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
23	C	512	CLA	C1D-CHD-C4C	-3.45	118.61	126.06
23	C	504	CLA	CHC-C1C-C2C	-3.45	117.14	126.73
23	A	405	CLA	CAC-C3C-C4C	3.45	129.28	124.81
23	B	606	CLA	C1D-CHD-C4C	-3.45	118.62	126.06
23	B	611	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
24	A	408	PHO	C4A-C3A-C2A	-3.44	99.56	102.84
30	H	102	DGD	O6E-C5E-C4E	3.44	115.95	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	607	CLA	CAA-C2A-C3A	-3.44	103.36	112.78
23	C	501	CLA	C1D-CHD-C4C	-3.44	118.64	126.06
23	B	604	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
23	C	509	CLA	C3C-C4C-NC	3.42	114.41	110.57
23	A	405	CLA	C4C-C3C-C2C	-3.42	101.91	106.90
23	B	607	CLA	C1C-C2C-C3C	-3.42	103.36	106.96
23	C	507	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
28	D	405	PL9	C53-C6-C1	3.41	121.95	114.99
23	B	614	CLA	CHD-C4C-NC	3.41	129.57	124.20
23	C	504	CLA	C1D-CHD-C4C	-3.40	118.72	126.06
23	B	608	CLA	C3C-C4C-NC	3.40	114.38	110.57
23	D	403	CLA	C1D-CHD-C4C	-3.40	118.73	126.06
23	B	607	CLA	C4C-C3C-C2C	-3.39	101.95	106.90
23	B	609	CLA	C3C-C4C-NC	3.39	114.38	110.57
23	C	511	CLA	C1C-C2C-C3C	-3.39	103.39	106.96
23	B	613	CLA	C3B-C2B-C1B	-3.39	103.07	107.16
23	C	509	CLA	CHC-C1C-C2C	-3.38	117.33	126.73
23	B	613	CLA	C3D-C2D-C1D	-3.38	101.21	105.83
34	H	101	RRX	C33-C5-C4	-3.38	107.12	113.62
23	A	410	CLA	C1C-C2C-C3C	-3.38	103.40	106.96
23	B	616	CLA	C3B-C4B-NB	3.37	113.65	110.52
23	B	617	CLA	CHC-C1C-NC	3.37	129.32	124.20
26	D	407	SQD	C3-C4-C5	3.37	116.26	110.24
23	B	605	CLA	C1-C2-C3	-3.37	120.21	126.04
23	B	615	CLA	CAA-C2A-C3A	-3.37	103.56	112.78
25	D	404	BCR	C3-C4-C5	-3.36	108.07	114.08
25	C	514	BCR	C11-C10-C9	-3.36	122.51	127.31
23	C	507	CLA	CBC-CAC-C3C	-3.36	103.18	112.43
33	F	101	HEM	C4D-ND-C1D	3.36	108.54	105.07
23	B	611	CLA	C4C-C3C-C2C	-3.36	102.01	106.90
23	C	510	CLA	CHD-C4C-NC	3.36	129.49	124.20
23	B	617	CLA	O2D-CGD-O1D	-3.35	117.28	123.84
35	V	201	HEC	CHA-C1A-NA	3.35	128.06	124.44
26	D	407	SQD	O7-S-C6	3.35	110.92	106.94
23	A	406	CLA	C3B-C4B-NB	3.34	113.61	110.52
23	A	406	CLA	CBC-CAC-C3C	-3.34	103.23	112.43
23	B	609	CLA	C4-C3-C5	3.33	119.80	115.98
23	C	510	CLA	CAA-C2A-C3A	-3.33	103.65	112.78
23	C	511	CLA	C3B-C4B-NB	3.32	113.60	110.52
23	B	607	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
23	B	611	CLA	CAA-C2A-C3A	-3.32	103.69	112.78
23	C	506	CLA	C4C-C3C-C2C	-3.32	102.06	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	406	CLA	CAC-C3C-C2C	3.31	133.20	127.53
23	B	612	CLA	CMB-C2B-C1B	3.31	130.42	125.37
30	H	102	DGD	C3E-C4E-C5E	3.31	116.14	110.24
23	A	406	CLA	C1-C2-C3	-3.31	120.32	126.04
23	B	609	CLA	CHC-C1C-C2C	-3.31	117.55	126.73
25	B	620	BCR	C16-C15-C14	-3.30	116.72	123.47
25	K	101	BCR	C15-C16-C17	-3.30	116.72	123.47
23	A	407	CLA	CHC-C1C-C2C	-3.29	117.60	126.73
23	C	505	CLA	CHC-C1C-C2C	-3.28	117.61	126.73
23	C	511	CLA	C4C-C3C-C2C	-3.28	102.12	106.90
23	B	607	CLA	C1D-CHD-C4C	-3.28	118.99	126.06
23	C	509	CLA	CHB-C1B-NB	-3.27	120.79	124.26
23	B	610	CLA	CHD-C4C-NC	3.27	129.36	124.20
23	B	603	CLA	CMB-C2B-C1B	3.27	130.36	125.37
25	B	620	BCR	C11-C10-C9	-3.26	122.65	127.31
23	A	407	CLA	CBC-CAC-C3C	-3.26	103.44	112.43
23	B	609	CLA	C3B-C4B-NB	3.25	113.53	110.52
23	B	613	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
23	C	502	CLA	CHB-C1B-NB	-3.24	120.82	124.26
23	A	406	CLA	CHC-C1C-C2C	-3.24	117.74	126.73
23	C	510	CLA	C3C-C4C-NC	3.23	114.19	110.57
30	C	516	DGD	C1D-O6D-C5D	3.22	120.02	113.69
23	B	612	CLA	C4-C3-C5	3.22	120.69	115.27
23	C	502	CLA	CHB-C4A-NA	3.22	128.97	124.51
23	B	616	CLA	C4C-C3C-C2C	-3.22	102.20	106.90
23	C	502	CLA	CAC-C3C-C4C	3.22	128.98	124.81
23	C	510	CLA	CMD-C2D-C3D	-3.22	120.22	127.61
23	B	605	CLA	C1C-C2C-C3C	-3.21	103.58	106.96
25	K	101	BCR	C23-C22-C21	-3.21	114.02	118.94
23	B	608	CLA	C4-C3-C5	3.21	119.65	115.98
23	C	513	CLA	C4C-C3C-C2C	-3.21	102.22	106.90
23	D	402	CLA	C4C-C3C-C2C	-3.20	102.23	106.90
23	C	501	CLA	C3B-C4B-NB	3.20	113.49	110.52
23	B	615	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
23	C	509	CLA	CHB-C4A-NA	3.20	128.94	124.51
23	C	501	CLA	CBC-CAC-C3C	-3.20	103.61	112.43
23	B	605	CLA	C3D-C2D-C1D	-3.20	101.46	105.83
23	B	614	CLA	C1-C2-C3	-3.20	120.51	126.04
34	H	101	RRX	C8-C7-C6	-3.19	118.24	127.20
23	B	615	CLA	C4C-C3C-C2C	-3.19	102.25	106.90
27	D	411	LMG	C9-C8-C7	-3.19	104.25	111.79
25	B	620	BCR	C24-C23-C22	-3.18	121.43	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	C3C-C4C-NC	3.18	114.14	110.57
25	K	101	BCR	C37-C22-C23	3.18	123.09	118.08
25	K	102	BCR	C20-C21-C22	-3.18	122.78	127.31
23	C	509	CLA	O2D-CGD-O1D	-3.18	117.63	123.84
23	C	503	CLA	CAC-C3C-C4C	3.17	128.93	124.81
23	A	405	CLA	O2D-CGD-CBD	3.17	116.90	111.27
23	C	506	CLA	C4A-NA-C1A	-3.17	105.28	106.71
23	C	501	CLA	CHC-C1C-C2C	-3.16	117.94	126.73
23	C	503	CLA	C1C-C2C-C3C	-3.16	103.63	106.96
23	B	615	CLA	O2A-CGA-CBA	3.16	121.83	111.91
23	B	611	CLA	O2A-CGA-CBA	3.16	121.82	111.91
23	A	406	CLA	C3C-C4C-NC	3.16	114.11	110.57
23	C	513	CLA	C1C-C2C-C3C	-3.15	103.64	106.96
23	D	402	CLA	O2A-CGA-CBA	3.15	121.79	111.91
23	B	610	CLA	CMA-C3A-C4A	-3.15	103.31	111.77
23	A	410	CLA	CMB-C2B-C1B	3.15	130.16	125.37
23	C	507	CLA	CHC-C1C-C2C	-3.15	117.99	126.73
23	C	504	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
23	B	608	CLA	C4C-C3C-C2C	-3.14	102.31	106.90
23	C	511	CLA	CAA-CBA-CGA	-3.14	104.06	113.25
23	A	407	CLA	C3C-C4C-NC	3.14	114.09	110.57
23	B	608	CLA	C3B-C2B-C1B	-3.14	103.37	107.16
34	H	101	RRX	C40-C30-C25	-3.13	105.22	110.30
23	D	402	CLA	CAC-C3C-C4C	3.13	128.87	124.81
23	B	610	CLA	C4A-NA-C1A	-3.13	105.30	106.71
23	C	508	CLA	CAC-C3C-C4C	3.13	128.87	124.81
23	B	617	CLA	CAA-C2A-C3A	-3.12	104.23	112.78
23	B	607	CLA	C4-C3-C5	3.12	120.52	115.27
23	B	602	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
23	C	508	CLA	CHC-C1C-C2C	-3.11	118.10	126.73
23	B	617	CLA	C4A-NA-C1A	-3.11	105.31	106.71
24	A	408	PHO	C6-C5-C3	-3.10	105.32	113.45
23	C	509	CLA	C4A-NA-C1A	-3.10	105.31	106.71
23	B	606	CLA	CAA-C2A-C3A	-3.10	104.28	112.78
23	B	604	CLA	CHC-C1C-C2C	-3.10	118.12	126.73
25	D	404	BCR	C15-C14-C13	-3.10	122.89	127.31
23	B	616	CLA	CMB-C2B-C1B	3.09	130.08	125.37
25	C	514	BCR	C37-C22-C23	3.09	122.94	118.08
23	B	604	CLA	CAC-C3C-C4C	3.09	128.82	124.81
23	A	405	CLA	CHC-C1C-C2C	-3.08	118.16	126.73
23	C	503	CLA	C4C-C3C-C2C	-3.08	102.40	106.90
25	D	404	BCR	C11-C10-C9	-3.08	122.92	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	513	CLA	CHB-C4A-NA	3.07	128.76	124.51
23	B	608	CLA	CAC-C3C-C4C	3.07	128.79	124.81
32	L	101	LHG	O8-C23-C24	3.06	121.52	111.91
23	D	403	CLA	CAC-C3C-C4C	3.06	128.78	124.81
23	B	610	CLA	CBC-CAC-C3C	-3.06	103.99	112.43
23	B	602	CLA	CAC-C3C-C4C	3.06	128.78	124.81
25	C	514	BCR	C20-C21-C22	-3.05	122.95	127.31
23	C	512	CLA	C1-C2-C3	-3.05	120.77	126.04
24	A	409	PHO	C4-C3-C5	3.05	120.39	115.27
23	B	613	CLA	CHD-C4C-NC	3.04	129.00	124.20
23	A	407	CLA	C4-C3-C5	3.04	120.39	115.27
23	C	501	CLA	CAA-C2A-C3A	-3.04	104.45	112.78
28	A	414	PL9	C53-C6-C1	3.04	121.21	114.99
23	C	512	CLA	CHD-C4C-NC	3.04	128.99	124.20
25	A	411	BCR	C15-C16-C17	-3.04	117.25	123.47
24	A	409	PHO	O2D-CGD-O1D	-3.03	117.91	123.84
23	B	606	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
23	B	603	CLA	C4-C3-C5	3.02	120.36	115.27
25	C	515	BCR	C10-C11-C12	-3.02	113.78	123.22
23	A	410	CLA	C4C-C3C-C2C	-3.02	102.50	106.90
23	C	511	CLA	C4A-NA-C1A	-3.02	105.35	106.71
23	C	506	CLA	CAC-C3C-C4C	3.01	128.72	124.81
23	D	402	CLA	CHD-C4C-NC	3.01	128.95	124.20
23	D	402	CLA	CMC-C2C-C1C	3.01	129.62	125.04
23	C	511	CLA	CMB-C2B-C1B	3.00	129.94	125.37
23	C	505	CLA	CAC-C3C-C4C	3.00	128.70	124.81
23	B	614	CLA	CHC-C1C-C2C	-3.00	118.40	126.73
23	B	617	CLA	CMB-C2B-C1B	3.00	129.93	125.37
23	D	403	CLA	C4C-C3C-C2C	-3.00	102.53	106.90
23	D	403	CLA	C3B-C4B-NB	2.99	113.29	110.52
25	K	101	BCR	C33-C5-C6	-2.99	121.17	124.53
23	C	505	CLA	CAA-C2A-C3A	-2.99	104.60	112.78
23	C	501	CLA	CMC-C2C-C1C	2.98	129.58	125.04
23	B	607	CLA	CHB-C4A-NA	2.98	128.64	124.51
23	C	505	CLA	C3D-C2D-C1D	-2.98	101.76	105.83
23	B	605	CLA	C4A-NA-C1A	-2.98	105.37	106.71
23	D	402	CLA	C1C-C2C-C3C	-2.98	103.83	106.96
23	C	508	CLA	CHD-C4C-NC	2.98	128.90	124.20
23	B	611	CLA	CHD-C4C-NC	2.98	128.90	124.20
23	D	402	CLA	CBC-CAC-C3C	-2.98	104.22	112.43
23	B	614	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
23	B	610	CLA	CAC-C3C-C4C	2.97	128.67	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	613	CLA	C4-C3-C5	2.97	120.26	115.27
23	B	604	CLA	O2A-CGA-O1A	-2.96	116.11	123.59
26	A	412	SQD	O5-C1-C2	-2.96	104.08	110.35
23	B	605	CLA	CAA-C2A-C3A	-2.96	104.67	112.78
28	A	414	PL9	C32-C33-C34	-2.96	120.54	127.66
23	D	403	CLA	CHC-C1C-C2C	-2.96	118.52	126.73
23	D	403	CLA	CAA-C2A-C3A	-2.95	104.69	112.78
23	C	511	CLA	CHC-C1C-C2C	-2.95	118.53	126.73
23	C	505	CLA	CBC-CAC-C3C	-2.95	104.29	112.43
25	C	514	BCR	C16-C15-C14	-2.95	117.43	123.47
23	C	507	CLA	C3B-C4B-NB	2.95	113.25	110.52
23	B	604	CLA	C4C-C3C-C2C	-2.95	102.60	106.90
23	B	612	CLA	CMC-C2C-C1C	2.95	129.53	125.04
23	B	613	CLA	CHB-C4A-NA	2.94	128.58	124.51
26	D	407	SQD	O48-C23-C24	2.94	121.13	111.91
33	F	101	HEM	CHB-C1B-NB	2.94	128.00	124.37
23	A	410	CLA	CHD-C4C-NC	2.94	128.83	124.20
23	B	603	CLA	CHD-C4C-NC	2.94	128.83	124.20
23	B	607	CLA	O2A-CGA-CBA	2.94	121.12	111.91
23	C	501	CLA	CMB-C2B-C1B	2.93	129.84	125.37
23	A	406	CLA	CAA-C2A-C3A	-2.93	104.74	112.78
23	B	617	CLA	CHC-C4B-NB	-2.93	121.15	124.26
23	C	509	CLA	C3B-C4B-NB	2.93	113.23	110.52
23	C	509	CLA	CBC-CAC-C3C	-2.93	104.36	112.43
25	C	514	BCR	C21-C20-C19	-2.93	114.08	123.22
23	B	609	CLA	CAC-C3C-C4C	2.92	128.60	124.81
23	B	606	CLA	O2A-CGA-CBA	2.92	121.06	111.91
23	A	410	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
23	B	613	CLA	CMA-C3A-C4A	-2.91	103.94	111.77
23	C	503	CLA	CHC-C4B-NB	-2.91	121.17	124.26
34	H	101	RRX	C38-C26-C27	-2.91	108.96	114.36
23	A	407	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
23	B	615	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
25	C	515	BCR	C11-C10-C9	-2.91	123.16	127.31
23	B	610	CLA	CED-O2D-CGD	2.91	122.51	115.94
26	A	412	SQD	C45-O47-C7	-2.90	110.64	117.79
30	C	516	DGD	O6D-C5D-C4D	2.90	114.97	109.69
23	B	615	CLA	CHC-C1C-C2C	-2.90	118.67	126.73
23	B	602	CLA	CAA-C2A-C3A	-2.90	104.83	112.78
23	B	610	CLA	CHB-C4A-NA	2.90	128.53	124.51
25	D	404	BCR	C21-C20-C19	-2.90	117.43	124.67
25	K	102	BCR	C11-C10-C9	-2.90	123.17	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	D	405	PL9	C12-C13-C14	-2.90	120.69	127.66
23	B	610	CLA	CHC-C1C-C2C	-2.90	118.69	126.73
23	C	504	CLA	CAA-C2A-C3A	-2.90	104.85	112.78
23	C	508	CLA	CAA-C2A-C3A	-2.90	104.85	112.78
23	C	503	CLA	CHC-C1C-C2C	-2.89	118.69	126.73
23	C	505	CLA	C4C-C3C-C2C	-2.89	102.68	106.90
23	B	608	CLA	C4A-NA-C1A	-2.89	105.41	106.71
23	D	402	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
35	V	201	HEC	CAD-CBD-CGD	2.88	119.81	113.60
23	C	511	CLA	CAA-C2A-C1A	2.88	121.42	111.97
25	C	515	BCR	C16-C17-C18	-2.88	123.20	127.31
23	C	512	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
35	V	201	HEC	CBB-CAB-C3B	2.88	120.37	112.43
23	B	602	CLA	C4C-C3C-C2C	-2.88	102.70	106.90
23	C	504	CLA	C1-C2-C3	-2.87	122.10	126.75
24	A	409	PHO	C6-C5-C3	-2.87	105.94	113.45
23	C	507	CLA	O2A-CGA-CBA	2.86	120.89	111.91
23	B	616	CLA	CAC-C3C-C4C	2.86	128.52	124.81
23	B	616	CLA	CHC-C1C-C2C	-2.85	118.80	126.73
23	C	506	CLA	CHB-C4A-NA	2.85	128.46	124.51
23	C	513	CLA	CMB-C2B-C3B	2.85	133.50	126.59
23	C	507	CLA	C4-C3-C5	2.85	120.07	115.27
23	B	605	CLA	CHB-C1B-NB	-2.85	121.24	124.26
23	C	508	CLA	C4A-NA-C1A	-2.85	105.43	106.71
23	B	613	CLA	CHD-C1D-ND	-2.84	121.84	124.45
35	V	201	HEC	CHB-C1B-C2B	-2.84	120.54	124.98
23	B	612	CLA	CMA-C3A-C4A	-2.84	104.13	111.77
23	B	612	CLA	CBC-CAC-C3C	-2.84	104.61	112.43
23	A	407	CLA	C1-C2-C3	-2.84	121.14	126.04
30	H	102	DGD	C4E-C3E-C2E	2.84	115.78	110.82
23	B	604	CLA	C1-C2-C3	-2.84	121.14	126.04
23	C	510	CLA	O2A-CGA-CBA	2.83	120.80	111.91
23	B	616	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
28	D	405	PL9	C7-C3-C4	-2.83	114.58	116.88
23	C	512	CLA	CMB-C2B-C1B	2.83	129.68	125.37
27	D	411	LMG	O6-C5-C4	2.82	114.82	109.69
25	A	411	BCR	C3-C4-C5	-2.82	109.04	114.08
34	H	101	RRX	C16-C15-C14	-2.82	117.70	123.47
23	D	402	CLA	C6-C5-C3	-2.82	106.06	113.45
30	H	102	DGD	O1G-C1A-C2A	2.82	120.75	111.91
23	C	513	CLA	CHD-C4C-NC	2.81	128.64	124.20
30	C	517	DGD	C2G-O2G-C1B	-2.81	110.87	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	407	CLA	CAA-C2A-C3A	-2.81	105.08	112.78
23	B	607	CLA	CHC-C1C-C2C	-2.81	118.94	126.73
23	A	405	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
23	B	607	CLA	CAC-C3C-C4C	2.80	128.45	124.81
23	B	610	CLA	C4C-C3C-C2C	-2.80	102.81	106.90
25	C	515	BCR	C32-C1-C6	2.80	114.84	110.30
23	C	503	CLA	C3B-C4B-NB	2.80	113.11	110.52
23	A	407	CLA	C3B-C4B-NB	2.80	113.11	110.52
23	B	610	CLA	CGD-CBD-CAD	-2.80	101.68	110.73
23	B	616	CLA	CHB-C4A-NA	2.80	128.38	124.51
27	B	622	LMG	C3-C4-C5	2.80	115.23	110.24
23	C	505	CLA	O2A-CGA-CBA	2.80	120.68	111.91
23	C	509	CLA	CMD-C2D-C3D	-2.79	121.19	127.61
35	V	201	HEC	C3C-C4C-NC	-2.79	107.03	110.15
23	C	506	CLA	CMB-C2B-C1B	2.79	129.62	125.37
23	B	603	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
23	C	509	CLA	C4C-C3C-C2C	-2.79	102.83	106.90
23	C	502	CLA	CHD-C4C-NC	2.79	128.60	124.20
33	F	101	HEM	C4A-NA-C1A	2.79	108.08	105.35
23	C	510	CLA	CBC-CAC-C3C	-2.78	104.76	112.43
23	C	510	CLA	C1-C2-C3	-2.78	121.23	126.04
25	K	101	BCR	C23-C24-C25	-2.78	119.40	127.20
32	L	101	LHG	C6-C5-C4	-2.77	105.23	111.79
25	C	514	BCR	C10-C11-C12	-2.77	114.56	123.22
28	D	405	PL9	C30-C29-C31	2.76	119.92	115.27
23	C	501	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
30	C	517	DGD	C3G-O3G-C1D	-2.76	108.34	113.74
23	B	612	CLA	C3B-C4B-NB	2.76	113.08	110.52
23	C	510	CLA	CHC-C1C-C2C	-2.76	119.07	126.73
23	C	504	CLA	C3C-C4C-NC	2.76	113.66	110.57
23	C	502	CLA	CBC-CAC-C3C	-2.75	104.84	112.43
23	C	512	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
23	B	602	CLA	CHD-C4C-NC	2.75	128.53	124.20
23	B	611	CLA	CHC-C1C-C2C	-2.75	119.10	126.73
23	B	602	CLA	CMC-C2C-C1C	2.75	129.22	125.04
23	B	606	CLA	CHD-C4C-NC	2.74	128.53	124.20
34	H	101	RRX	C11-C12-C13	-2.74	118.71	126.42
28	D	405	PL9	C22-C23-C24	-2.74	121.06	127.66
23	B	606	CLA	C1-C2-C3	-2.74	121.30	126.04
23	A	405	CLA	CHD-C4C-NC	2.74	128.52	124.20
35	V	201	HEC	C3B-C4B-NB	-2.74	107.12	110.17
25	C	515	BCR	C37-C22-C23	2.74	122.39	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	613	CLA	C1-C2-C3	-2.73	121.31	126.04
23	C	513	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
23	C	509	CLA	CAC-C3C-C4C	2.73	128.35	124.81
32	D	410	LHG	O8-C23-C24	2.73	120.47	111.91
23	C	509	CLA	CMA-C3A-C4A	-2.73	104.44	111.77
34	H	101	RRX	C27-C26-C25	-2.72	114.78	120.85
23	C	502	CLA	O2A-C1-C2	2.72	115.78	108.64
23	B	602	CLA	O2A-CGA-CBA	2.72	120.44	111.91
23	C	501	CLA	C3C-C4C-NC	2.72	113.62	110.57
23	B	608	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
25	K	101	BCR	C8-C9-C10	-2.71	114.78	118.94
23	B	611	CLA	C3B-C4B-NB	2.71	113.03	110.52
23	B	613	CLA	CMA-C3A-C2A	-2.71	102.89	113.83
23	B	613	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
23	B	602	CLA	CHC-C1C-C2C	-2.71	119.22	126.73
23	C	511	CLA	CHD-C4C-NC	2.70	128.46	124.20
28	A	414	PL9	C45-C44-C46	2.70	119.07	115.98
25	B	620	BCR	C10-C11-C12	-2.70	114.78	123.22
26	A	412	SQD	O48-C23-C24	2.70	120.38	111.91
23	B	616	CLA	CHD-C4C-NC	2.70	128.46	124.20
23	B	606	CLA	CHC-C1C-C2C	-2.70	119.23	126.73
24	A	408	PHO	O2A-C1-C2	-2.70	101.55	108.64
23	C	501	CLA	CHB-C4A-NA	2.69	128.24	124.51
28	A	414	PL9	C20-C19-C21	2.69	119.80	115.27
23	B	617	CLA	CBC-CAC-C3C	-2.69	105.01	112.43
23	A	407	CLA	CHD-C4C-NC	2.68	128.43	124.20
23	A	405	CLA	CMB-C2B-C3B	2.68	133.09	126.59
28	A	414	PL9	C42-C43-C44	-2.68	121.21	127.66
23	C	503	CLA	CHD-C4C-NC	2.68	128.43	124.20
23	B	603	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
23	B	614	CLA	CMC-C2C-C1C	2.68	129.12	125.04
23	B	607	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
23	B	614	CLA	O2A-CGA-CBA	2.67	120.29	111.91
30	H	102	DGD	C1D-C2D-C3D	2.67	115.55	110.00
23	C	511	CLA	CAC-C3C-C4C	2.67	128.27	124.81
23	C	502	CLA	O2A-CGA-CBA	2.66	120.27	111.91
23	B	610	CLA	CAA-C2A-C3A	-2.66	105.49	112.78
25	B	620	BCR	C7-C8-C9	-2.66	122.21	126.23
23	C	513	CLA	CMA-C3A-C4A	-2.66	104.62	111.77
23	B	615	CLA	CHB-C4A-NA	2.66	128.19	124.51
28	A	414	PL9	C30-C29-C31	2.66	119.74	115.27
23	B	614	CLA	CAA-C2A-C3A	-2.65	105.53	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	507	CLA	C1-C2-C3	-2.65	121.47	126.04
23	B	608	CLA	CMB-C2B-C1B	2.65	129.40	125.37
23	B	609	CLA	C4C-C3C-C2C	-2.65	103.04	106.90
23	C	508	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
23	B	604	CLA	C3B-C4B-NB	2.64	112.97	110.52
23	C	502	CLA	CHC-C1C-NC	2.64	128.21	124.20
23	B	614	CLA	C4C-C3C-C2C	-2.64	103.05	106.90
28	A	414	PL9	C22-C23-C24	-2.64	121.30	127.66
25	B	618	BCR	C21-C20-C19	-2.64	114.98	123.22
28	A	414	PL9	C37-C38-C39	-2.64	121.31	127.66
23	B	604	CLA	C4-C3-C5	2.64	119.71	115.27
23	C	512	CLA	CHC-C1C-C2C	-2.64	119.41	126.73
23	B	613	CLA	CMD-C2D-C1D	2.63	129.35	124.71
23	C	511	CLA	C1-C2-C3	-2.63	121.49	126.04
23	A	407	CLA	CAC-C3C-C4C	2.63	128.22	124.81
23	B	613	CLA	CHC-C1C-C2C	-2.63	119.43	126.73
28	A	414	PL9	C15-C14-C16	2.63	119.69	115.27
25	C	515	BCR	C21-C20-C19	-2.63	115.02	123.22
23	A	406	CLA	CMB-C2B-C1B	2.62	129.36	125.37
25	C	514	BCR	C36-C18-C19	2.62	122.21	118.08
28	A	414	PL9	C37-C36-C34	-2.62	104.36	112.98
32	D	409	LHG	O8-C23-C24	2.62	120.13	111.91
23	C	502	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
23	B	615	CLA	CMC-C2C-C1C	2.62	129.03	125.04
28	D	405	PL9	C32-C33-C34	-2.62	121.36	127.66
23	B	617	CLA	CHB-C4A-NA	2.62	128.13	124.51
23	B	615	CLA	CHD-C4C-NC	2.61	128.32	124.20
23	C	505	CLA	C1-O2A-CGA	2.61	123.30	116.44
23	A	410	CLA	CHC-C1C-C2C	-2.61	119.47	126.73
23	B	616	CLA	C1-C2-C3	-2.61	121.53	126.04
23	C	509	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
25	B	618	BCR	C20-C21-C22	-2.60	123.60	127.31
23	C	504	CLA	C4C-C3C-C2C	-2.60	103.11	106.90
23	D	403	CLA	CHD-C4C-NC	2.60	128.29	124.20
28	A	414	PL9	C7-C3-C4	2.59	118.98	116.88
28	D	405	PL9	C15-C14-C16	2.59	119.63	115.27
27	D	411	LMG	C7-O1-C1	-2.59	108.68	113.74
23	B	605	CLA	CHB-C4A-NA	2.59	128.09	124.51
23	B	608	CLA	CHB-C4A-NA	2.59	128.09	124.51
23	B	602	CLA	C3B-C4B-NB	2.59	112.92	110.52
25	D	404	BCR	C10-C11-C12	-2.59	115.14	123.22
25	K	101	BCR	C7-C8-C9	-2.58	122.33	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	505	CLA	CMD-C2D-C3D	-2.58	121.67	127.61
23	B	603	CLA	CHC-C1C-C2C	-2.58	119.56	126.73
23	B	602	CLA	C4-C3-C5	2.58	119.61	115.27
23	B	602	CLA	CHB-C4A-NA	2.58	128.08	124.51
23	C	509	CLA	CHD-C4C-NC	2.58	128.26	124.20
24	A	409	PHO	CMA-C3A-C4A	-2.58	108.74	114.38
23	B	603	CLA	O2A-CGA-CBA	2.57	119.99	111.91
23	C	507	CLA	CMB-C2B-C1B	2.57	129.29	125.37
23	B	613	CLA	CAC-C3C-C4C	2.57	128.15	124.81
23	D	403	CLA	CHB-C4A-NA	2.57	128.07	124.51
23	B	608	CLA	CHC-C1C-NC	2.57	128.10	124.20
30	H	102	DGD	C3D-C4D-C5D	2.57	114.82	110.24
23	C	511	CLA	CHB-C4A-NA	2.57	128.06	124.51
23	B	606	CLA	C4C-C3C-C2C	-2.57	103.16	106.90
26	A	412	SQD	C1-C2-C3	-2.57	104.65	110.00
23	A	410	CLA	CMC-C2C-C1C	2.56	128.94	125.04
23	C	506	CLA	CAA-C2A-C3A	-2.56	105.77	112.78
23	C	509	CLA	O2A-CGA-CBA	2.55	119.92	111.91
23	D	402	CLA	CHB-C1B-C2B	-2.55	120.02	127.24
23	A	406	CLA	O1D-CGD-CBD	-2.55	119.26	124.48
23	B	602	CLA	CBC-CAC-C3C	-2.55	105.39	112.43
23	C	511	CLA	O2A-CGA-CBA	2.55	119.91	111.91
25	B	618	BCR	C37-C22-C23	2.55	122.09	118.08
25	A	411	BCR	C10-C11-C12	-2.55	115.27	123.22
23	C	501	CLA	CHD-C4C-NC	2.55	128.22	124.20
28	A	414	PL9	C8-C7-C3	2.55	119.17	111.98
23	B	605	CLA	C4-C3-C5	2.55	119.55	115.27
23	B	603	CLA	CMC-C2C-C1C	2.54	128.91	125.04
23	B	615	CLA	C1-O2A-CGA	2.54	123.11	116.44
23	B	612	CLA	C2C-C1C-NC	2.54	112.35	109.97
23	B	612	CLA	CAC-C3C-C4C	2.54	128.10	124.81
23	B	616	CLA	C4-C3-C5	2.53	119.53	115.27
25	K	101	BCR	C16-C15-C14	-2.53	118.28	123.47
23	A	410	CLA	CAC-C3C-C4C	2.53	128.10	124.81
26	D	407	SQD	C1-C2-C3	-2.53	104.72	110.00
23	C	513	CLA	CHB-C1B-C2B	-2.53	120.09	127.24
23	B	612	CLA	CMB-C2B-C3B	2.53	132.71	126.59
23	C	503	CLA	C4-C3-C5	2.52	119.52	115.27
23	B	610	CLA	CHB-C1B-NB	-2.52	121.59	124.26
23	C	508	CLA	O2A-CGA-CBA	2.52	119.81	111.91
35	V	201	HEC	CHD-C1D-ND	2.52	127.48	124.37
23	C	512	CLA	CAA-C2A-C3A	-2.52	105.89	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	504	CLA	O2A-CGA-CBA	2.51	119.80	111.91
23	B	611	CLA	CMB-C2B-C1B	2.51	129.20	125.37
28	A	414	PL9	C17-C18-C19	-2.51	121.61	127.66
23	B	603	CLA	CAC-C3C-C4C	2.51	128.07	124.81
27	B	622	LMG	O8-C28-C29	2.51	119.79	111.91
24	A	409	PHO	C1-C2-C3	-2.51	121.70	126.04
23	C	504	CLA	CMA-C3A-C4A	-2.51	105.03	111.77
25	A	411	BCR	C21-C20-C19	-2.51	115.40	123.22
23	C	513	CLA	CBC-CAC-C3C	-2.50	105.53	112.43
24	A	409	PHO	O2A-CGA-CBA	2.50	119.75	111.91
23	B	603	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	K	101	BCR	C34-C9-C8	2.50	122.01	118.08
25	A	411	BCR	C31-C1-C6	-2.49	106.25	110.30
23	C	510	CLA	C4C-C3C-C2C	-2.49	103.26	106.90
23	C	508	CLA	O2A-CGA-O1A	-2.49	117.30	123.59
23	C	513	CLA	CHC-C1C-C2C	-2.49	119.81	126.73
30	C	517	DGD	C4D-C3D-C2D	2.49	115.17	110.82
33	F	101	HEM	CHA-C4D-ND	2.49	127.44	124.37
23	D	403	CLA	CMB-C2B-C1B	2.49	129.16	125.37
28	D	405	PL9	C35-C34-C36	2.49	119.45	115.27
23	B	609	CLA	CBC-CAC-C3C	-2.49	105.58	112.43
23	C	503	CLA	CMC-C2C-C1C	2.48	128.82	125.04
23	B	613	CLA	C3B-C4B-NB	2.48	112.82	110.52
24	A	408	PHO	CBA-CAA-C2A	-2.47	106.59	113.81
23	B	609	CLA	CHC-C4B-NB	-2.47	121.64	124.26
23	B	605	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
23	C	502	CLA	CAA-C2A-C3A	-2.46	106.04	112.78
23	C	512	CLA	O1D-CGD-CBD	-2.46	119.45	124.48
23	A	407	CLA	C4C-C3C-C2C	-2.46	103.31	106.90
25	C	514	BCR	C8-C9-C10	-2.46	115.17	118.94
27	B	622	LMG	O6-C5-C4	2.46	114.16	109.69
23	C	508	CLA	CHB-C4A-NA	2.46	127.91	124.51
25	K	102	BCR	C16-C17-C18	-2.45	123.81	127.31
23	B	613	CLA	O2A-CGA-CBA	2.45	119.60	111.91
23	C	512	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	B	605	CLA	CAC-C3C-C4C	2.45	127.99	124.81
23	C	507	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	C	515	BCR	C23-C24-C25	-2.45	120.32	127.20
35	V	201	HEC	CHD-C4C-NC	2.45	128.35	123.85
23	B	611	CLA	C1-C2-C3	-2.45	121.81	126.04
23	C	504	CLA	C5-C3-C4	2.45	120.01	114.60
24	A	408	PHO	O2D-CGD-O1D	-2.44	119.06	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	609	CLA	CHD-C4C-NC	2.44	128.05	124.20
25	C	515	BCR	C34-C9-C8	2.44	121.92	118.08
23	C	506	CLA	CHC-C1C-NC	2.44	127.90	124.20
23	C	503	CLA	O2A-CGA-CBA	2.43	119.54	111.91
23	C	501	CLA	CMD-C2D-C3D	-2.43	122.02	127.61
33	F	101	HEM	CBD-CAD-C3D	-2.43	105.87	112.63
27	B	622	LMG	O7-C10-O9	-2.43	117.83	123.70
23	B	604	CLA	CHD-C4C-NC	2.43	128.03	124.20
28	D	405	PL9	C17-C18-C19	-2.43	121.81	127.66
28	D	405	PL9	C20-C19-C21	2.43	119.36	115.27
23	D	402	CLA	CAA-CBA-CGA	-2.43	106.16	113.25
23	B	605	CLA	CHC-C1C-NC	2.43	127.89	124.20
23	C	512	CLA	CMC-C2C-C1C	2.42	128.73	125.04
23	B	606	CLA	C1-O2A-CGA	2.42	122.80	116.44
25	D	404	BCR	C2-C1-C6	2.42	114.21	110.48
25	A	411	BCR	C34-C9-C8	2.42	121.89	118.08
28	A	414	PL9	C40-C39-C41	2.42	119.34	115.27
23	C	508	CLA	CMB-C2B-C3B	2.42	132.44	126.59
33	F	101	HEM	CAD-CBD-CGD	2.42	118.81	113.60
23	B	615	CLA	CBC-CAC-C3C	-2.42	105.77	112.43
23	A	406	CLA	CED-O2D-CGD	2.41	121.40	115.94
23	B	613	CLA	C6-C7-C8	-2.41	108.12	115.92
23	B	613	CLA	O1D-CGD-CBD	-2.41	119.56	124.48
23	B	611	CLA	CHB-C4A-NA	2.41	127.84	124.51
23	C	512	CLA	C3B-C4B-NB	2.41	112.75	110.52
23	B	606	CLA	C6-C7-C8	-2.41	108.14	115.92
23	A	405	CLA	CMA-C3A-C2A	-2.41	104.12	113.83
23	A	410	CLA	CHB-C4A-NA	2.40	127.83	124.51
33	F	101	HEM	C2A-C1A-NA	-2.40	107.47	110.15
23	C	504	CLA	CMB-C2B-C3B	2.40	132.39	126.59
23	B	603	CLA	C1-O2A-CGA	2.40	122.73	116.44
23	B	605	CLA	O1D-CGD-CBD	-2.40	119.58	124.48
23	B	616	CLA	CAA-C2A-C3A	-2.39	106.23	112.78
25	K	102	BCR	C16-C15-C14	-2.39	118.58	123.47
23	C	506	CLA	CED-O2D-CGD	2.39	121.34	115.94
23	C	506	CLA	CHD-C4C-NC	2.39	127.97	124.20
25	K	102	BCR	C23-C24-C25	-2.39	120.50	127.20
23	A	406	CLA	CHB-C4A-NA	2.38	127.81	124.51
27	B	622	LMG	C8-O7-C10	-2.38	111.92	117.79
23	C	504	CLA	CHB-C4A-NA	2.38	127.81	124.51
32	D	408	LHG	O8-C23-C24	2.38	119.38	111.91
23	C	505	CLA	C1-C2-C3	-2.38	121.93	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	608	CLA	CBC-CAC-C3C	-2.38	105.87	112.43
31	D	401	BCT	O3-C-O1	2.38	125.71	119.55
28	A	414	PL9	C27-C28-C29	-2.38	121.94	127.66
26	A	412	SQD	O47-C7-O49	-2.38	117.96	123.70
23	C	510	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
23	A	410	CLA	CBC-CAC-C3C	-2.37	105.91	112.43
23	D	402	CLA	O2A-CGA-O1A	-2.37	117.62	123.59
23	C	509	CLA	CAA-C2A-C3A	-2.36	106.31	112.78
25	B	620	BCR	C33-C5-C6	-2.36	121.87	124.53
23	B	616	CLA	O2A-CGA-O1A	-2.36	117.63	123.59
25	B	620	BCR	C29-C30-C25	2.36	114.12	110.48
23	B	602	CLA	CHB-C1B-C2B	-2.36	120.57	127.24
28	A	414	PL9	O1-C4-C3	2.36	123.32	120.72
23	D	402	CLA	CHC-C1C-C2C	-2.36	120.17	126.73
25	C	514	BCR	C3-C4-C5	-2.36	109.87	114.08
23	C	513	CLA	CAC-C3C-C4C	2.36	127.87	124.81
25	K	101	BCR	C31-C1-C6	-2.36	106.48	110.30
23	B	603	CLA	CHB-C1B-C2B	-2.35	120.59	127.24
25	B	620	BCR	C35-C13-C12	2.35	121.78	118.08
23	C	503	CLA	CMB-C2B-C1B	2.34	128.94	125.37
23	A	405	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
23	B	612	CLA	O2A-CGA-CBA	2.34	119.25	111.91
23	C	508	CLA	C4-C3-C5	2.34	119.21	115.27
23	B	616	CLA	CHB-C1B-NB	-2.34	121.78	124.26
23	B	605	CLA	CED-O2D-CGD	2.33	121.22	115.94
25	K	101	BCR	C38-C26-C27	2.32	118.08	113.62
23	C	506	CLA	O2A-CGA-CBA	2.32	119.19	111.91
23	B	613	CLA	CMC-C2C-C1C	2.32	128.57	125.04
30	C	516	DGD	O6E-C5E-C6E	2.32	112.20	106.44
25	C	515	BCR	C36-C18-C19	2.32	121.73	118.08
23	B	612	CLA	O2A-CGA-O1A	-2.31	117.76	123.59
23	B	611	CLA	CAA-CBA-CGA	-2.31	106.51	113.25
35	V	201	HEC	CBC-CAC-C3C	2.30	118.78	112.43
23	A	406	CLA	C4A-NA-C1A	-2.30	105.67	106.71
23	A	405	CLA	CAA-C2A-C1A	-2.30	104.42	111.97
27	A	413	LMG	C8-O7-C10	-2.30	112.12	117.79
23	A	406	CLA	CHC-C4B-NB	-2.30	121.82	124.26
25	A	411	BCR	C2-C1-C6	2.30	114.02	110.48
23	B	617	CLA	CHB-C1B-NB	-2.30	121.82	124.26
23	C	503	CLA	CHB-C4A-NA	2.30	127.69	124.51
25	K	101	BCR	C11-C10-C9	-2.29	124.04	127.31
27	A	413	LMG	O8-C28-C29	2.29	119.10	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	607	CLA	CMA-C3A-C2A	-2.29	104.59	113.83
23	B	604	CLA	CHB-C1B-C2B	-2.29	120.78	127.24
25	K	101	BCR	C33-C5-C4	2.29	118.01	113.62
23	B	611	CLA	C4-C3-C5	2.28	119.11	115.27
23	B	609	CLA	CHB-C1B-C2B	-2.28	120.79	127.24
23	C	509	CLA	C4-C3-C5	2.28	119.11	115.27
23	C	504	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
23	C	513	CLA	CAA-C2A-C3A	-2.28	106.54	112.78
30	C	517	DGD	O1G-C1A-O1A	-2.28	117.85	123.59
23	B	608	CLA	O2A-CGA-CBA	2.27	119.04	111.91
23	C	505	CLA	O1D-CGD-CBD	-2.27	119.84	124.48
23	A	410	CLA	CHB-C1B-C2B	-2.27	120.83	127.24
30	C	516	DGD	C2G-O2G-C1B	-2.27	112.21	117.79
23	C	511	CLA	CMC-C2C-C1C	2.26	128.49	125.04
23	B	605	CLA	CMC-C2C-C3C	2.26	132.26	126.12
23	B	614	CLA	CAC-C3C-C4C	2.26	127.74	124.81
23	C	510	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
25	B	618	BCR	C31-C1-C6	2.26	113.96	110.30
23	B	602	CLA	O2A-CGA-O1A	-2.26	117.89	123.59
32	D	410	LHG	C6-C5-C4	-2.26	106.45	111.79
30	C	516	DGD	O1G-C1A-C2A	2.25	118.98	111.91
23	A	407	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
23	C	505	CLA	CHD-C4C-NC	2.25	127.75	124.20
25	B	618	BCR	C29-C30-C25	2.25	113.94	110.48
23	D	402	CLA	CMA-C3A-C2A	-2.24	104.78	113.83
23	B	610	CLA	CAA-CBA-CGA	-2.24	106.72	113.25
23	C	506	CLA	C1-C2-C3	-2.24	122.18	126.04
23	C	504	CLA	CHC-C1C-NC	2.24	127.59	124.20
25	K	102	BCR	C31-C1-C6	-2.24	106.67	110.30
23	B	608	CLA	C1-C2-C3	-2.24	122.18	126.04
33	F	101	HEM	CHA-C1A-NA	2.24	127.96	123.85
23	C	511	CLA	CHB-C1B-NB	-2.23	121.89	124.26
30	H	102	DGD	C1E-O6E-C5E	2.23	118.07	113.69
28	D	405	PL9	C2-C3-C4	2.23	121.87	118.80
33	F	101	HEM	CBA-CAA-C2A	-2.23	106.43	112.63
24	A	408	PHO	C1A-C2A-C3A	-2.23	100.72	102.84
23	B	612	CLA	O2D-CGD-O1D	-2.23	119.48	123.84
25	K	102	BCR	C37-C22-C23	2.23	121.59	118.08
23	B	603	CLA	CHC-C4B-NB	-2.23	121.90	124.26
23	C	507	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
23	C	510	CLA	CHB-C1B-C2B	-2.22	120.95	127.24
30	H	102	DGD	C3B-C2B-C1B	-2.22	105.53	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	606	CLA	C4-C3-C5	2.22	119.01	115.27
23	A	407	CLA	O2A-CGA-CBA	2.22	118.87	111.91
23	B	617	CLA	CHD-C4C-NC	2.22	127.69	124.20
23	B	606	CLA	C3B-C4B-NB	2.21	112.57	110.52
23	D	403	CLA	CMA-C3A-C2A	-2.21	104.91	113.83
25	B	618	BCR	C15-C16-C17	-2.21	118.95	123.47
23	C	501	CLA	O2A-CGA-CBA	2.21	118.83	111.91
35	V	201	HEC	CHA-C4D-C3D	-2.20	121.60	124.84
25	B	620	BCR	C40-C30-C25	2.20	113.87	110.30
23	B	612	CLA	CMA-C3A-C2A	-2.20	104.97	113.83
27	A	413	LMG	O6-C5-C4	2.19	113.68	109.69
23	B	609	CLA	O2D-CGD-O1D	-2.19	119.55	123.84
23	C	501	CLA	C4C-C3C-C2C	-2.19	103.70	106.90
23	D	402	CLA	CMA-C3A-C4A	-2.19	105.89	111.77
25	K	101	BCR	C38-C26-C25	-2.19	122.07	124.53
23	B	608	CLA	CHD-C4C-NC	2.19	127.65	124.20
23	C	513	CLA	CED-O2D-CGD	2.18	120.87	115.94
23	C	503	CLA	C1-O2A-CGA	2.18	122.17	116.44
25	K	102	BCR	C15-C16-C17	-2.18	119.01	123.47
28	D	405	PL9	C11-C9-C8	-2.18	116.71	121.12
23	B	615	CLA	CMA-C3A-C4A	-2.18	105.92	111.77
27	B	622	LMG	O3-C3-C4	-2.18	105.32	110.35
23	D	402	CLA	C2A-C1A-CHA	-2.18	120.06	123.86
23	C	513	CLA	C3B-C4B-NB	2.18	112.53	110.52
23	B	609	CLA	CHB-C4A-NA	2.18	127.52	124.51
23	B	605	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
24	A	408	PHO	O1D-CGD-CBD	-2.17	121.12	124.74
32	L	101	LHG	O8-C23-O10	-2.17	118.11	123.59
23	B	606	CLA	CHB-C4A-NA	2.17	127.52	124.51
23	D	402	CLA	CMB-C2B-C3B	2.17	131.84	126.59
24	A	408	PHO	CMA-C3A-C4A	-2.17	109.63	114.38
25	C	515	BCR	C3-C4-C5	-2.17	110.21	114.08
23	B	611	CLA	CHB-C1B-C2B	-2.16	121.12	127.24
30	C	518	DGD	C1G-O1G-C1A	2.16	125.11	117.12
23	C	502	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
28	D	405	PL9	C8-C7-C3	2.16	118.08	111.98
25	B	618	BCR	C11-C12-C13	-2.15	120.36	126.42
23	C	507	CLA	CHB-C1B-C2B	-2.15	121.15	127.24
23	B	604	CLA	CBB-CAB-C3B	-2.15	116.92	127.62
23	B	617	CLA	CMC-C2C-C3C	2.15	131.95	126.12
23	B	603	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
26	D	407	SQD	O9-S-C6	2.15	109.49	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	510	CLA	C2A-C3A-C4A	-2.15	98.40	101.87
23	C	513	CLA	CMC-C2C-C1C	2.15	128.31	125.04
30	C	518	DGD	O1G-C1A-C2A	2.15	118.64	111.91
23	C	506	CLA	O2D-CGD-O1D	-2.14	119.65	123.84
23	C	504	CLA	CMC-C2C-C1C	2.14	128.30	125.04
23	B	606	CLA	CMA-C3A-C2A	-2.14	105.19	113.83
23	A	405	CLA	CHC-C1C-NC	2.14	127.44	124.20
23	C	512	CLA	CBC-CAC-C3C	-2.14	106.54	112.43
23	B	611	CLA	CHC-C4B-NB	-2.13	122.00	124.26
23	C	511	CLA	CBC-CAC-C3C	-2.13	106.56	112.43
24	A	408	PHO	CAA-CBA-CGA	-2.13	107.03	113.25
23	B	603	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
23	C	508	CLA	C1-C2-C3	-2.13	122.36	126.04
24	A	409	PHO	CGD-CBD-CAD	-2.13	103.85	110.73
23	A	405	CLA	CHB-C4A-NA	2.12	127.45	124.51
23	C	507	CLA	CMC-C2C-C1C	2.12	128.27	125.04
23	B	603	CLA	CMA-C3A-C4A	-2.12	106.08	111.77
24	A	409	PHO	O1D-CGD-CBD	-2.12	121.21	124.74
23	C	501	CLA	CHB-C1B-NB	-2.11	122.02	124.26
25	A	411	BCR	C36-C18-C19	2.11	121.40	118.08
23	C	503	CLA	CHA-C1A-NA	-2.11	121.57	126.40
23	B	608	CLA	O1D-CGD-CBD	-2.10	120.18	124.48
23	A	407	CLA	CHB-C4A-NA	2.10	127.42	124.51
23	A	405	CLA	O2A-CGA-CBA	2.10	118.51	111.91
23	A	405	CLA	CHB-C1B-C2B	-2.10	121.30	127.24
34	H	101	RRX	C1-C6-C7	-2.10	109.83	115.78
23	A	407	CLA	CMB-C2B-C1B	2.10	128.57	125.37
25	K	102	BCR	C34-C9-C8	2.09	121.38	118.08
23	B	613	CLA	CHB-C1B-NB	-2.09	122.04	124.26
23	D	403	CLA	CGD-CBD-CAD	-2.09	103.96	110.73
23	C	503	CLA	CHB-C1B-C2B	-2.09	121.33	127.24
25	K	101	BCR	C35-C13-C12	2.09	121.37	118.08
23	C	510	CLA	CHB-C4A-NA	2.09	127.40	124.51
23	C	511	CLA	CAA-C2A-C3A	-2.09	107.06	112.78
25	C	515	BCR	C31-C1-C6	-2.09	106.92	110.30
25	C	514	BCR	C34-C9-C8	2.08	121.36	118.08
28	A	414	PL9	C35-C34-C36	2.08	118.78	115.27
23	A	406	CLA	CMC-C2C-C3C	2.08	131.77	126.12
27	A	413	LMG	O6-C5-C6	2.08	111.61	106.44
23	C	501	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
23	B	615	CLA	CHB-C1B-NB	-2.08	122.05	124.26
23	B	616	CLA	CMC-C2C-C1C	2.08	128.21	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	D	403	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
23	B	612	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
30	C	516	DGD	O2G-C1B-O1B	-2.07	118.69	123.70
23	B	611	CLA	CGD-CBD-CAD	-2.07	104.02	110.73
25	C	515	BCR	C2-C1-C6	2.07	113.67	110.48
23	B	608	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
25	B	620	BCR	C15-C16-C17	-2.07	119.23	123.47
23	C	508	CLA	CHC-C1C-NC	2.07	127.34	124.20
23	C	505	CLA	CHB-C1B-C2B	-2.07	121.39	127.24
23	C	505	CLA	CHB-C4A-NA	2.07	127.37	124.51
25	A	411	BCR	C37-C22-C23	2.07	121.34	118.08
25	K	102	BCR	C3-C2-C1	-2.07	107.21	114.60
30	C	517	DGD	O2G-C1B-O1B	-2.07	118.71	123.70
23	C	505	CLA	C6-C7-C8	-2.07	109.24	115.92
27	D	411	LMG	C1-O6-C5	2.06	117.74	113.69
23	C	510	CLA	CMC-C2C-C1C	2.06	128.18	125.04
28	A	414	PL9	C3-C4-C5	2.06	121.28	118.60
23	B	609	CLA	CHA-C1A-NA	-2.06	121.68	126.40
23	B	615	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
23	C	506	CLA	CBC-CAC-C3C	-2.06	106.76	112.43
23	A	407	CLA	CED-O2D-CGD	2.06	120.59	115.94
23	C	511	CLA	CHA-C1A-NA	-2.05	121.69	126.40
23	D	403	CLA	CMA-C3A-C4A	-2.05	106.25	111.77
24	A	409	PHO	CED-O2D-CGD	2.05	120.58	115.94
25	B	620	BCR	C39-C30-C25	-2.05	106.97	110.30
27	B	622	LMG	C1-C2-C3	2.05	114.27	110.00
27	D	411	LMG	C1-C2-C3	-2.05	105.73	110.00
23	C	505	CLA	CHC-C4B-NB	-2.05	122.09	124.26
23	B	604	CLA	CHA-C1A-NA	-2.05	121.71	126.40
23	B	614	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
23	B	609	CLA	O2A-CGA-CBA	2.04	118.32	111.91
33	F	101	HEM	CHD-C1D-C2D	-2.04	121.79	124.98
23	D	403	CLA	CMC-C2C-C1C	2.04	128.15	125.04
23	A	405	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
30	C	517	DGD	O6D-C1D-O3G	-2.04	105.15	109.97
28	A	414	PL9	C7-C8-C9	-2.04	123.40	126.79
23	C	508	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
25	A	411	BCR	C32-C1-C6	2.04	113.60	110.30
23	D	402	CLA	O2A-C1-C2	2.04	113.99	108.64
23	B	607	CLA	CHD-C4C-NC	2.04	127.41	124.20
25	D	404	BCR	C33-C5-C6	-2.03	122.24	124.53
23	C	504	CLA	CHB-C1B-C2B	-2.03	121.50	127.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	409	PHO	CBC-CAC-C3C	2.03	115.85	112.88
23	D	402	CLA	CHB-C4A-NA	2.03	127.32	124.51
28	A	414	PL9	C25-C24-C26	2.03	118.68	115.27
23	B	604	CLA	C2A-C3A-C4A	-2.03	98.60	101.87
23	B	606	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
25	K	102	BCR	C29-C30-C25	2.03	113.60	110.48
25	A	411	BCR	C11-C10-C9	-2.02	124.42	127.31
23	B	611	CLA	CMC-C2C-C1C	2.02	128.12	125.04
23	B	613	CLA	C2A-C1A-CHA	-2.02	120.32	123.86
23	A	406	CLA	CHB-C1B-NB	-2.02	122.12	124.26
23	B	610	CLA	CHA-C1A-NA	-2.02	121.77	126.40
25	A	411	BCR	C29-C28-C27	-2.02	106.86	111.38
23	B	614	CLA	CHB-C4A-NA	2.02	127.30	124.51
23	B	611	CLA	C6-C7-C8	-2.02	109.40	115.92
23	C	509	CLA	CAA-C2A-C1A	2.01	118.57	111.97
23	A	405	CLA	C4-C3-C5	2.01	118.65	115.27
25	C	514	BCR	C23-C22-C21	-2.01	115.86	118.94
23	D	402	CLA	CMD-C2D-C3D	-2.01	122.99	127.61
23	B	609	CLA	CMA-C3A-C4A	-2.01	106.38	111.77
23	D	403	CLA	CHB-C1B-NB	-2.01	122.13	124.26
23	C	512	CLA	CHB-C1B-NB	-2.01	122.13	124.26

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
35	V	201	HEC	NA

All (630) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	A	405	CLA	CBD-CGD-O2D-CED
23	A	410	CLA	C1A-C2A-CAA-CBA
23	A	410	CLA	C2B-C3B-CAB-CBB
23	A	410	CLA	C4B-C3B-CAB-CBB
23	B	604	CLA	C2B-C3B-CAB-CBB
23	B	604	CLA	C4B-C3B-CAB-CBB
23	B	604	CLA	C2-C3-C5-C6
23	B	604	CLA	C4-C3-C5-C6
23	B	605	CLA	C2-C3-C5-C6
23	B	605	CLA	C4-C3-C5-C6
23	B	607	CLA	C2B-C3B-CAB-CBB
23	B	607	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	B	608	CLA	C1A-C2A-CAA-CBA
23	B	608	CLA	C2-C3-C5-C6
23	B	608	CLA	C4-C3-C5-C6
23	B	611	CLA	CHA-CBD-CGD-O1D
23	B	611	CLA	CHA-CBD-CGD-O2D
23	B	612	CLA	C11-C12-C13-C14
23	B	614	CLA	CBD-CGD-O2D-CED
23	B	615	CLA	CHA-CBD-CGD-O2D
23	B	615	CLA	C2-C3-C5-C6
23	C	501	CLA	C1A-C2A-CAA-CBA
23	C	502	CLA	C2B-C3B-CAB-CBB
23	C	502	CLA	C4B-C3B-CAB-CBB
23	C	503	CLA	CBD-CGD-O2D-CED
23	C	507	CLA	C2-C3-C5-C6
23	C	507	CLA	C4-C3-C5-C6
23	C	508	CLA	CHA-CBD-CGD-O1D
23	C	508	CLA	CHA-CBD-CGD-O2D
23	C	509	CLA	C2-C1-O2A-CGA
23	C	511	CLA	C2B-C3B-CAB-CBB
23	C	511	CLA	C4B-C3B-CAB-CBB
24	A	409	PHO	C3A-C2A-CAA-CBA
25	A	411	BCR	C37-C22-C23-C24
25	B	618	BCR	C17-C18-C19-C20
25	B	618	BCR	C36-C18-C19-C20
25	B	620	BCR	C1-C6-C7-C8
25	B	620	BCR	C11-C12-C13-C14
25	B	620	BCR	C11-C12-C13-C35
25	C	514	BCR	C23-C24-C25-C30
25	C	515	BCR	C23-C24-C25-C30
25	D	404	BCR	C7-C8-C9-C10
25	D	404	BCR	C7-C8-C9-C34
25	K	101	BCR	C7-C8-C9-C10
25	K	101	BCR	C7-C8-C9-C34
25	K	101	BCR	C21-C22-C23-C24
25	K	101	BCR	C37-C22-C23-C24
26	D	407	SQD	C5-C6-S-O7
26	D	407	SQD	C5-C6-S-O8
26	D	407	SQD	C5-C6-S-O9
27	A	413	LMG	C2-C1-O1-C7
27	A	413	LMG	O6-C1-O1-C7
27	A	413	LMG	C11-C10-O7-C8
27	B	622	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
27	D	411	LMG	C11-C10-O7-C8
28	A	414	PL9	C9-C11-C12-C13
28	A	414	PL9	C43-C44-C46-C47
28	A	414	PL9	C45-C44-C46-C47
30	C	516	DGD	C2B-C1B-O2G-C2G
32	D	408	LHG	C3-O3-P-O4
32	D	408	LHG	C3-O3-P-O5
32	D	408	LHG	C3-O3-P-O6
32	D	408	LHG	C4-O6-P-O3
32	D	408	LHG	C4-O6-P-O4
32	D	408	LHG	C4-O6-P-O5
32	D	409	LHG	C3-O3-P-O5
32	D	409	LHG	C4-O6-P-O5
32	D	409	LHG	O10-C23-O8-C6
32	D	409	LHG	C24-C23-O8-C6
32	D	410	LHG	C4-O6-P-O4
32	D	410	LHG	C4-O6-P-O5
32	L	101	LHG	C3-O3-P-O4
32	L	101	LHG	C4-O6-P-O5
32	L	101	LHG	O10-C23-O8-C6
32	L	101	LHG	C24-C23-O8-C6
33	F	101	HEM	C2B-C3B-CAB-CBB
33	F	101	HEM	C4B-C3B-CAB-CBB
33	F	101	HEM	C2C-C3C-CAC-CBC
34	H	101	RRX	C23-C24-C25-C26
34	H	101	RRX	C37-C22-C23-C24
34	H	101	RRX	C21-C22-C23-C24
34	H	101	RRX	C20-C21-C22-C23
34	H	101	RRX	C35-C13-C14-C15
34	H	101	RRX	C11-C12-C13-C35
34	H	101	RRX	C11-C10-C9-C34
34	H	101	RRX	C7-C8-C9-C34
34	H	101	RRX	C5-C6-C7-C8
23	B	614	CLA	O1D-CGD-O2D-CED
23	B	609	CLA	CBD-CGD-O2D-CED
23	B	616	CLA	CBD-CGD-O2D-CED
23	C	513	CLA	CBD-CGD-O2D-CED
23	C	503	CLA	O1D-CGD-O2D-CED
23	A	405	CLA	O1D-CGD-O2D-CED
23	C	506	CLA	CBD-CGD-O2D-CED
23	C	510	CLA	CBD-CGD-O2D-CED
23	C	511	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	C	505	CLA	O1A-CGA-O2A-C1
23	C	509	CLA	O1A-CGA-O2A-C1
27	A	413	LMG	O9-C10-O7-C8
27	B	622	LMG	O9-C10-O7-C8
27	D	411	LMG	O9-C10-O7-C8
30	C	516	DGD	O1B-C1B-O2G-C2G
23	A	407	CLA	C3-C5-C6-C7
23	B	605	CLA	C3-C5-C6-C7
23	B	606	CLA	C3-C5-C6-C7
23	B	616	CLA	C3-C5-C6-C7
23	C	510	CLA	C3-C5-C6-C7
23	B	615	CLA	CBA-CGA-O2A-C1
23	B	603	CLA	C4-C3-C5-C6
28	D	405	PL9	C12-C11-C9-C10
23	B	607	CLA	C2A-CAA-CBA-CGA
23	B	608	CLA	C2A-CAA-CBA-CGA
23	B	611	CLA	C2A-CAA-CBA-CGA
23	C	505	CLA	CBA-CGA-O2A-C1
23	C	509	CLA	CBA-CGA-O2A-C1
23	C	511	CLA	CBA-CGA-O2A-C1
24	A	408	PHO	CBA-CGA-O2A-C1
32	D	410	LHG	C24-C23-O8-C6
23	C	513	CLA	O1D-CGD-O2D-CED
23	B	615	CLA	O1A-CGA-O2A-C1
32	D	410	LHG	O10-C23-O8-C6
30	C	518	DGD	O6E-C5E-C6E-O5E
23	C	508	CLA	CBD-CGD-O2D-CED
23	B	610	CLA	C3-C5-C6-C7
23	C	511	CLA	C3-C5-C6-C7
23	C	512	CLA	CBA-CGA-O2A-C1
24	A	408	PHO	O1A-CGA-O2A-C1
23	B	610	CLA	CBD-CGD-O2D-CED
23	B	615	CLA	CBD-CGD-O2D-CED
23	B	609	CLA	O1D-CGD-O2D-CED
23	C	511	CLA	O1A-CGA-O2A-C1
30	H	102	DGD	O6E-C5E-C6E-O5E
33	F	101	HEM	C3D-CAD-CBD-CGD
30	C	516	DGD	O6D-C5D-C6D-O5D
23	B	616	CLA	O1D-CGD-O2D-CED
27	A	413	LMG	O6-C5-C6-O5
27	D	411	LMG	O6-C5-C6-O5
23	C	512	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
28	A	414	PL9	C19-C21-C22-C23
23	B	606	CLA	CBA-CGA-O2A-C1
23	C	510	CLA	CBA-CGA-O2A-C1
32	D	408	LHG	C24-C23-O8-C6
32	D	409	LHG	C1-C2-C3-O3
32	L	101	LHG	C1-C2-C3-O3
32	D	408	LHG	O10-C23-O8-C6
23	C	507	CLA	CBD-CGD-O2D-CED
25	A	411	BCR	C19-C20-C21-C22
34	H	101	RRX	C9-C10-C11-C12
23	C	505	CLA	C10-C11-C12-C13
23	B	603	CLA	C3-C5-C6-C7
23	B	603	CLA	C2-C3-C5-C6
28	D	405	PL9	C12-C11-C9-C8
23	B	602	CLA	C11-C10-C8-C9
23	B	611	CLA	C14-C13-C15-C16
23	C	506	CLA	O1D-CGD-O2D-CED
23	B	604	CLA	C10-C11-C12-C13
23	B	615	CLA	C2A-CAA-CBA-CGA
25	C	515	BCR	C7-C8-C9-C34
25	K	101	BCR	C11-C12-C13-C35
25	K	102	BCR	C37-C22-C23-C24
34	H	101	RRX	C36-C18-C19-C20
34	H	101	RRX	C11-C12-C13-C14
30	C	516	DGD	C4D-C5D-C6D-O5D
23	C	505	CLA	CBD-CGD-O2D-CED
30	H	102	DGD	C4E-C5E-C6E-O5E
23	C	501	CLA	C13-C15-C16-C17
23	C	510	CLA	C8-C10-C11-C12
24	A	408	PHO	C5-C6-C7-C8
23	C	510	CLA	O1D-CGD-O2D-CED
32	D	408	LHG	C23-C24-C25-C26
23	C	505	CLA	C15-C16-C17-C18
32	L	101	LHG	C7-C8-C9-C10
23	B	602	CLA	C15-C16-C17-C18
23	B	612	CLA	C12-C13-C15-C16
24	A	409	PHO	C3-C5-C6-C7
23	C	511	CLA	O1D-CGD-O2D-CED
27	D	411	LMG	C4-C5-C6-O5
23	B	606	CLA	O1A-CGA-O2A-C1
23	C	510	CLA	O1A-CGA-O2A-C1
30	C	516	DGD	O6E-C1E-O5D-C6D

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Mol	Chain	Res	Type	Atoms
28	D	405	PL9	C34-C36-C37-C38
30	C	518	DGD	C1A-C2A-C3A-C4A
32	D	409	LHG	O2-C2-C3-O3
32	L	101	LHG	O2-C2-C3-O3
30	C	518	DGD	C4E-C5E-C6E-O5E
23	B	614	CLA	C3-C5-C6-C7
23	C	502	CLA	C13-C15-C16-C17
23	C	501	CLA	C5-C6-C7-C8
23	B	613	CLA	CBA-CGA-O2A-C1
32	D	409	LHG	C4-O6-P-O3
32	D	410	LHG	C4-O6-P-O3
32	L	101	LHG	C3-O3-P-O6
23	C	506	CLA	CBA-CGA-O2A-C1
23	B	612	CLA	C10-C11-C12-C13
23	C	501	CLA	C4-C3-C5-C6
26	A	412	SQD	C32-C33-C34-C35
26	A	412	SQD	C8-C7-O47-C45
34	H	101	RRX	C16-C17-C18-C36
23	B	608	CLA	CBA-CGA-O2A-C1
26	A	412	SQD	C33-C34-C35-C36
32	D	408	LHG	C27-C28-C29-C30
32	D	408	LHG	C28-C29-C30-C31
26	A	412	SQD	O49-C7-O47-C45
30	H	102	DGD	C2B-C3B-C4B-C5B
27	A	413	LMG	C11-C12-C13-C14
30	C	518	DGD	C8A-C9A-CAA-CBA
30	H	102	DGD	C7B-C8B-C9B-CAB
30	C	516	DGD	C2E-C1E-O5D-C6D
30	C	517	DGD	C2E-C1E-O5D-C6D
34	H	101	RRX	C16-C17-C18-C19
23	A	407	CLA	C5-C6-C7-C8
30	H	102	DGD	C6B-C7B-C8B-C9B
32	D	408	LHG	C31-C32-C33-C34
23	B	604	CLA	C11-C10-C8-C9
30	H	102	DGD	C9B-CAB-CBB-CCB
32	D	409	LHG	C25-C26-C27-C28
23	C	505	CLA	C2A-CAA-CBA-CGA
25	A	411	BCR	C21-C22-C23-C24
34	H	101	RRX	C7-C8-C9-C10
23	C	509	CLA	C3-C5-C6-C7
30	C	517	DGD	CAB-CBB-CCB-CDB
23	B	605	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
30	C	517	DGD	O6E-C1E-O5D-C6D
23	B	603	CLA	CBD-CGD-O2D-CED
23	C	506	CLA	O1A-CGA-O2A-C1
23	B	608	CLA	C3A-C2A-CAA-CBA
23	D	402	CLA	C3A-C2A-CAA-CBA
30	C	516	DGD	O6E-C5E-C6E-O5E
27	A	413	LMG	C30-C31-C32-C33
30	C	517	DGD	CBB-CCB-CDB-CEB
23	B	613	CLA	O1A-CGA-O2A-C1
25	D	404	BCR	C20-C21-C22-C23
30	H	102	DGD	CCB-CDB-CEB-CFB
32	D	408	LHG	C30-C31-C32-C33
26	A	412	SQD	C31-C32-C33-C34
27	B	622	LMG	C28-C29-C30-C31
23	B	606	CLA	C4-C3-C5-C6
30	C	518	DGD	C1B-C2B-C3B-C4B
30	C	517	DGD	C7B-C8B-C9B-CAB
23	B	605	CLA	C2B-C3B-CAB-CBB
23	B	610	CLA	C2-C1-O2A-CGA
23	C	503	CLA	C8-C10-C11-C12
23	B	608	CLA	O1A-CGA-O2A-C1
25	B	620	BCR	C5-C6-C7-C8
25	C	514	BCR	C23-C24-C25-C26
25	C	515	BCR	C23-C24-C25-C26
25	D	404	BCR	C1-C6-C7-C8
25	D	404	BCR	C5-C6-C7-C8
25	K	101	BCR	C1-C6-C7-C8
25	K	101	BCR	C5-C6-C7-C8
25	K	101	BCR	C23-C24-C25-C26
25	K	101	BCR	C23-C24-C25-C30
23	C	509	CLA	C8-C10-C11-C12
23	B	610	CLA	O1D-CGD-O2D-CED
23	B	602	CLA	C11-C10-C8-C7
23	B	604	CLA	C6-C7-C8-C10
23	B	604	CLA	C11-C10-C8-C7
23	B	616	CLA	C12-C13-C15-C16
23	C	510	CLA	C11-C10-C8-C7
30	C	518	DGD	C2A-C1A-O1G-C1G
23	C	501	CLA	C2A-CAA-CBA-CGA
23	B	612	CLA	C5-C6-C7-C8
30	C	517	DGD	CCB-CDB-CEB-CFB
30	H	102	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
23	C	510	CLA	C16-C17-C18-C20
23	C	508	CLA	O1D-CGD-O2D-CED
33	F	101	HEM	C4C-C3C-CAC-CBC
23	B	612	CLA	C8-C10-C11-C12
23	C	505	CLA	C13-C15-C16-C17
23	B	606	CLA	C2-C3-C5-C6
23	C	501	CLA	C2-C3-C5-C6
23	B	604	CLA	C6-C7-C8-C9
23	B	606	CLA	C11-C12-C13-C14
23	B	616	CLA	C14-C13-C15-C16
23	B	617	CLA	C2A-CAA-CBA-CGA
23	A	406	CLA	C1A-C2A-CAA-CBA
23	A	407	CLA	C1A-C2A-CAA-CBA
23	B	604	CLA	C1A-C2A-CAA-CBA
23	B	605	CLA	C1A-C2A-CAA-CBA
23	B	615	CLA	C1A-C2A-CAA-CBA
23	C	508	CLA	C1A-C2A-CAA-CBA
23	C	511	CLA	C1A-C2A-CAA-CBA
32	D	408	LHG	C11-C10-C9-C8
23	C	501	CLA	C3-C5-C6-C7
23	B	606	CLA	C8-C10-C11-C12
26	A	412	SQD	C24-C23-O48-C46
23	B	616	CLA	C10-C11-C12-C13
27	A	413	LMG	C4-C5-C6-O5
30	C	518	DGD	O1A-C1A-O1G-C1G
30	C	517	DGD	O1G-C1G-C2G-C3G
32	D	410	LHG	C4-C5-C6-O8
23	B	614	CLA	C5-C6-C7-C8
27	B	622	LMG	C13-C14-C15-C16
26	A	412	SQD	O10-C23-O48-C46
28	D	405	PL9	C30-C29-C31-C32
23	C	510	CLA	C16-C17-C18-C19
27	A	413	LMG	C32-C33-C34-C35
26	A	412	SQD	C9-C10-C11-C12
23	C	507	CLA	O1D-CGD-O2D-CED
23	B	602	CLA	C10-C11-C12-C13
23	C	501	CLA	C15-C16-C17-C18
32	D	408	LHG	C9-C10-C11-C12
32	D	410	LHG	C27-C28-C29-C30
23	C	505	CLA	O1D-CGD-O2D-CED
30	H	102	DGD	CBB-CCB-CDB-CEB
23	B	613	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	C	517	DGD	O1G-C1G-C2G-O2G
32	D	410	LHG	O7-C5-C6-O8
30	C	516	DGD	C2A-C1A-O1G-C1G
23	A	405	CLA	C5-C6-C7-C8
24	A	409	PHO	CHA-CBD-CGD-O1D
24	A	409	PHO	CHA-CBD-CGD-O2D
26	A	412	SQD	C34-C35-C36-C37
28	A	414	PL9	C20-C19-C21-C22
28	A	414	PL9	C30-C29-C31-C32
28	D	405	PL9	C15-C14-C16-C17
23	B	606	CLA	C11-C12-C13-C15
23	C	510	CLA	C12-C13-C15-C16
28	A	414	PL9	C18-C19-C21-C22
28	A	414	PL9	C28-C29-C31-C32
23	C	510	CLA	C11-C10-C8-C9
23	C	510	CLA	C14-C13-C15-C16
23	D	403	CLA	CBD-CGD-O2D-CED
23	B	615	CLA	O1D-CGD-O2D-CED
25	K	102	BCR	C11-C12-C13-C35
23	B	611	CLA	C3-C5-C6-C7
30	C	517	DGD	C2B-C1B-O2G-C2G
23	B	608	CLA	C4B-C3B-CAB-CBB
23	C	506	CLA	C4B-C3B-CAB-CBB
23	B	612	CLA	C3-C5-C6-C7
23	C	504	CLA	CBA-CGA-O2A-C1
23	C	510	CLA	C4-C3-C5-C6
28	D	405	PL9	C28-C29-C31-C32
27	B	622	LMG	C4-C5-C6-O5
30	H	102	DGD	C1B-C2B-C3B-C4B
23	B	603	CLA	C3A-C2A-CAA-CBA
23	B	609	CLA	C3A-C2A-CAA-CBA
26	A	412	SQD	C16-C17-C18-C19
32	L	101	LHG	C27-C28-C29-C30
23	B	602	CLA	CBA-CGA-O2A-C1
30	H	102	DGD	O1G-C1G-C2G-C3G
32	D	409	LHG	C4-C5-C6-O8
23	B	613	CLA	C4-C3-C5-C6
28	D	405	PL9	C13-C14-C16-C17
23	A	407	CLA	C6-C7-C8-C9
27	B	622	LMG	C10-C11-C12-C13
23	A	405	CLA	C2A-CAA-CBA-CGA
32	D	408	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
30	C	516	DGD	O1A-C1A-O1G-C1G
32	D	409	LHG	C7-C8-C9-C10
32	L	101	LHG	C10-C11-C12-C13
23	C	506	CLA	C2B-C3B-CAB-CBB
23	C	512	CLA	C2B-C3B-CAB-CBB
24	A	408	PHO	C10-C11-C12-C13
26	A	412	SQD	O6-C44-C45-O47
32	D	409	LHG	O7-C5-C6-O8
30	C	517	DGD	O1B-C1B-O2G-C2G
24	A	408	PHO	C4-C3-C5-C6
23	C	501	CLA	C2-C1-O2A-CGA
24	A	409	PHO	C2-C1-O2A-CGA
23	B	613	CLA	C2-C3-C5-C6
23	C	510	CLA	C2-C3-C5-C6
24	A	408	PHO	C2-C3-C5-C6
23	B	609	CLA	C4-C3-C5-C6
23	B	615	CLA	C4-C3-C5-C6
24	A	409	PHO	C1A-C2A-CAA-CBA
25	A	411	BCR	C1-C6-C7-C8
25	A	411	BCR	C5-C6-C7-C8
25	B	620	BCR	C23-C24-C25-C26
25	C	515	BCR	C5-C6-C7-C8
25	K	102	BCR	C23-C24-C25-C26
25	K	102	BCR	C23-C24-C25-C30
23	B	602	CLA	CAA-CBA-CGA-O2A
25	K	102	BCR	C21-C22-C23-C24
30	C	516	DGD	C1B-C2B-C3B-C4B
32	D	408	LHG	O6-C4-C5-C6
32	D	410	LHG	O2-C2-C3-O3
23	B	612	CLA	C11-C12-C13-C15
23	B	616	CLA	C6-C7-C8-C10
23	C	509	CLA	C6-C7-C8-C10
24	A	409	PHO	C6-C7-C8-C10
34	H	101	RRX	C15-C16-C17-C18
32	L	101	LHG	C9-C10-C11-C12
26	A	412	SQD	C10-C11-C12-C13
32	L	101	LHG	C8-C7-O7-C5
23	B	610	CLA	CBA-CGA-O2A-C1
23	B	606	CLA	CBD-CGD-O2D-CED
23	D	403	CLA	CAD-CBD-CGD-O2D
23	B	604	CLA	C3-C5-C6-C7
23	D	403	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	D	407	SQD	C24-C23-O48-C46
30	C	518	DGD	O6E-C1E-O5D-C6D
26	A	412	SQD	C14-C15-C16-C17
23	A	406	CLA	CHA-CBD-CGD-O1D
23	A	406	CLA	CHA-CBD-CGD-O2D
23	B	602	CLA	CHA-CBD-CGD-O1D
23	B	602	CLA	CHA-CBD-CGD-O2D
23	B	605	CLA	CHA-CBD-CGD-O1D
23	B	605	CLA	CHA-CBD-CGD-O2D
23	B	607	CLA	CHA-CBD-CGD-O1D
23	B	607	CLA	CHA-CBD-CGD-O2D
23	B	610	CLA	CHA-CBD-CGD-O1D
23	B	610	CLA	CHA-CBD-CGD-O2D
23	B	615	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O1D
23	C	503	CLA	CHA-CBD-CGD-O2D
23	C	505	CLA	CHA-CBD-CGD-O1D
23	C	505	CLA	CHA-CBD-CGD-O2D
23	B	602	CLA	O1A-CGA-O2A-C1
23	C	504	CLA	O1A-CGA-O2A-C1
30	H	102	DGD	O1G-C1G-C2G-O2G
23	B	611	CLA	CBA-CGA-O2A-C1
23	B	610	CLA	O1A-CGA-O2A-C1
32	D	410	LHG	C23-C24-C25-C26
28	A	414	PL9	C4-C3-C7-C8
28	D	405	PL9	C4-C3-C7-C8
30	C	518	DGD	O1B-C1B-O2G-C2G
32	L	101	LHG	O9-C7-O7-C5
23	B	616	CLA	C6-C7-C8-C9
23	C	509	CLA	C6-C7-C8-C9
25	C	514	BCR	C11-C12-C13-C35
32	L	101	LHG	C25-C26-C27-C28
23	C	502	CLA	C1A-C2A-CAA-CBA
23	C	504	CLA	C1A-C2A-CAA-CBA
25	D	404	BCR	C9-C10-C11-C12
32	D	409	LHG	C3-O3-P-O6
32	L	101	LHG	C4-O6-P-O3
32	D	408	LHG	C34-C35-C36-C37
23	B	616	CLA	C4-C3-C5-C6
23	B	602	CLA	C4B-C3B-CAB-CBB
23	B	616	CLA	C4B-C3B-CAB-CBB
23	C	501	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	C	505	CLA	C4B-C3B-CAB-CBB
23	C	512	CLA	C4B-C3B-CAB-CBB
23	D	403	CLA	C4B-C3B-CAB-CBB
32	D	409	LHG	C4-O6-P-O4
32	L	101	LHG	C3-O3-P-O5
27	A	413	LMG	C34-C35-C36-C37
23	B	602	CLA	CAD-CBD-CGD-O1D
23	B	605	CLA	CAD-CBD-CGD-O1D
23	B	609	CLA	C2-C3-C5-C6
23	B	610	CLA	CAD-CBD-CGD-O1D
23	B	615	CLA	CAD-CBD-CGD-O1D
23	C	503	CLA	CAD-CBD-CGD-O1D
23	C	505	CLA	CAD-CBD-CGD-O1D
23	C	506	CLA	CAD-CBD-CGD-O1D
32	D	410	LHG	C1-C2-C3-O3
23	B	611	CLA	C6-C7-C8-C10
23	B	611	CLA	C12-C13-C15-C16
23	B	613	CLA	C3A-C2A-CAA-CBA
23	C	506	CLA	C3A-C2A-CAA-CBA
25	B	620	BCR	C9-C10-C11-C12
30	C	518	DGD	C2B-C1B-O2G-C2G
23	A	406	CLA	C2C-C3C-CAC-CBC
23	C	507	CLA	C5-C6-C7-C8
23	B	604	CLA	C2A-CAA-CBA-CGA
23	C	503	CLA	C2A-CAA-CBA-CGA
27	A	413	LMG	O1-C7-C8-C9
27	A	413	LMG	O1-C7-C8-O7
26	D	407	SQD	O10-C23-O48-C46
23	B	614	CLA	C6-C7-C8-C9
23	D	402	CLA	C8-C10-C11-C12
23	B	611	CLA	O1A-CGA-O2A-C1
23	B	612	CLA	C14-C13-C15-C16
23	C	511	CLA	C11-C10-C8-C9
24	A	409	PHO	C6-C7-C8-C9
23	A	405	CLA	C3-C5-C6-C7
32	D	410	LHG	C11-C10-C9-C8
23	C	511	CLA	C15-C16-C17-C18
23	B	611	CLA	C16-C17-C18-C20
23	B	612	CLA	C16-C17-C18-C19
23	B	608	CLA	C2B-C3B-CAB-CBB
23	B	616	CLA	C2B-C3B-CAB-CBB
23	C	505	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	C	507	CLA	C2B-C3B-CAB-CBB
23	B	613	CLA	C13-C15-C16-C17
23	C	510	CLA	C2-C1-O2A-CGA
23	B	604	CLA	CBA-CGA-O2A-C1
25	B	620	BCR	C23-C24-C25-C30
25	C	515	BCR	C1-C6-C7-C8
23	B	616	CLA	C2-C3-C5-C6
24	A	409	PHO	C8-C10-C11-C12
30	C	518	DGD	C2E-C1E-O5D-C6D
32	L	101	LHG	O7-C5-C6-O8
27	D	411	LMG	C7-C8-C9-O8
23	C	511	CLA	C11-C12-C13-C15
23	B	603	CLA	O1D-CGD-O2D-CED
23	C	507	CLA	C4B-C3B-CAB-CBB
23	C	502	CLA	C2-C1-O2A-CGA
23	B	611	CLA	C15-C16-C17-C18
26	A	412	SQD	C23-C24-C25-C26
30	C	517	DGD	O6E-C5E-C6E-O5E
23	C	513	CLA	CAA-CBA-CGA-O2A
23	C	505	CLA	C4-C3-C5-C6
23	B	610	CLA	C6-C7-C8-C9
23	C	505	CLA	C11-C10-C8-C9
24	A	408	PHO	C14-C13-C15-C16
27	B	622	LMG	C33-C34-C35-C36
26	A	412	SQD	O6-C44-C45-C46
32	D	408	LHG	C1-C2-C3-O3
30	C	518	DGD	C7A-C8A-C9A-CAA
30	C	518	DGD	O6D-C1D-O3G-C3G
35	V	201	HEC	CAD-CBD-CGD-O1D
35	V	201	HEC	CAD-CBD-CGD-O2D
23	B	609	CLA	C1A-C2A-CAA-CBA
23	C	503	CLA	C1A-C2A-CAA-CBA
23	B	613	CLA	C6-C7-C8-C10
23	D	402	CLA	C11-C10-C8-C7
23	C	513	CLA	CAA-CBA-CGA-O1A
27	D	411	LMG	O7-C10-C11-C12
25	K	101	BCR	C19-C20-C21-C22
23	C	507	CLA	C8-C10-C11-C12
28	A	414	PL9	C3-C7-C8-C9
23	C	510	CLA	C10-C11-C12-C13
23	C	512	CLA	C4-C3-C5-C6
23	B	602	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	C	501	CLA	C2B-C3B-CAB-CBB
23	D	403	CLA	C2B-C3B-CAB-CBB
30	C	517	DGD	C5B-C6B-C7B-C8B
23	B	602	CLA	C8-C10-C11-C12
25	K	101	BCR	C9-C10-C11-C12
23	B	613	CLA	C8-C10-C11-C12
23	D	402	CLA	C2-C1-O2A-CGA
23	C	505	CLA	C2-C3-C5-C6
23	B	604	CLA	O1A-CGA-O2A-C1
23	C	505	CLA	C11-C12-C13-C14
23	A	410	CLA	C2A-CAA-CBA-CGA
25	A	411	BCR	C23-C24-C25-C30
25	B	618	BCR	C1-C6-C7-C8
25	C	514	BCR	C1-C6-C7-C8
23	C	511	CLA	C8-C10-C11-C12
32	D	408	LHG	C11-C12-C13-C14
25	C	515	BCR	C19-C20-C21-C22
25	K	102	BCR	C19-C20-C21-C22
25	C	515	BCR	C7-C8-C9-C10
25	K	101	BCR	C11-C12-C13-C14
23	B	609	CLA	C2A-CAA-CBA-CGA
32	D	410	LHG	C24-C25-C26-C27
25	D	404	BCR	C13-C14-C15-C16
30	C	518	DGD	C2D-C1D-O3G-C3G
26	A	412	SQD	C15-C16-C17-C18
23	B	606	CLA	C5-C6-C7-C8
23	A	410	CLA	CAA-CBA-CGA-O2A
23	C	512	CLA	C2-C3-C5-C6
23	B	611	CLA	C6-C7-C8-C9
23	B	613	CLA	C6-C7-C8-C9
23	C	511	CLA	C11-C12-C13-C14
23	B	609	CLA	CAA-CBA-CGA-O2A
23	B	606	CLA	CAD-CBD-CGD-O2D
23	C	504	CLA	CAD-CBD-CGD-O2D
23	C	510	CLA	CAD-CBD-CGD-O2D
23	C	512	CLA	CAD-CBD-CGD-O2D
30	C	518	DGD	C6A-C7A-C8A-C9A
26	A	412	SQD	C19-C20-C21-C22
23	C	508	CLA	C4-C3-C5-C6
23	C	508	CLA	C2-C3-C5-C6
32	D	409	LHG	O7-C7-C8-C9
25	C	514	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	A	410	CLA	CAA-CBA-CGA-O1A
23	B	615	CLA	CAA-CBA-CGA-O2A
35	V	201	HEC	C2B-C3B-CAB-CBB
23	D	402	CLA	O2A-C1-C2-C3
23	B	614	CLA	CAA-CBA-CGA-O2A
23	B	604	CLA	CHA-CBD-CGD-O2D
23	B	608	CLA	CHA-CBD-CGD-O1D
23	B	608	CLA	CHA-CBD-CGD-O2D
23	B	616	CLA	CHA-CBD-CGD-O1D
23	B	616	CLA	CHA-CBD-CGD-O2D
23	C	502	CLA	CHA-CBD-CGD-O2D
23	C	506	CLA	CHA-CBD-CGD-O1D
23	C	507	CLA	CHA-CBD-CGD-O1D
23	C	511	CLA	CHA-CBD-CGD-O1D
23	C	511	CLA	CHA-CBD-CGD-O2D
27	A	413	LMG	C13-C14-C15-C16
23	C	503	CLA	C3-C5-C6-C7
27	B	622	LMG	C14-C15-C16-C17
26	A	412	SQD	C26-C27-C28-C29
30	H	102	DGD	O2G-C1B-C2B-C3B
23	C	505	CLA	C11-C10-C8-C7
27	B	622	LMG	O8-C28-C29-C30
23	B	602	CLA	C6-C7-C8-C9
23	D	402	CLA	C11-C10-C8-C9
28	A	414	PL9	C29-C31-C32-C33
23	B	613	CLA	C2A-CAA-CBA-CGA
25	K	101	BCR	C17-C18-C19-C20
23	B	603	CLA	C1A-C2A-CAA-CBA
23	B	613	CLA	C1A-C2A-CAA-CBA
23	C	512	CLA	C1A-C2A-CAA-CBA
23	D	402	CLA	C1A-C2A-CAA-CBA
23	B	614	CLA	CAA-CBA-CGA-O1A
26	A	412	SQD	C30-C31-C32-C33
28	A	414	PL9	C26-C27-C28-C29
28	D	405	PL9	C21-C22-C23-C24
23	C	503	CLA	C2-C1-O2A-CGA
30	C	517	DGD	O1A-C1A-C2A-C3A
32	L	101	LHG	C4-C5-C6-O8
23	B	609	CLA	CAA-CBA-CGA-O1A
23	B	615	CLA	CAA-CBA-CGA-O1A
23	C	510	CLA	CAA-CBA-CGA-O2A
35	V	201	HEC	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
23	B	613	CLA	C15-C16-C17-C18
23	B	603	CLA	C4B-C3B-CAB-CBB
23	B	610	CLA	C4B-C3B-CAB-CBB
23	B	611	CLA	C4B-C3B-CAB-CBB
25	B	618	BCR	C5-C6-C7-C8
33	F	101	HEM	C2A-CAA-CBA-CGA
23	B	602	CLA	CAA-CBA-CGA-O1A
23	A	407	CLA	CAD-CBD-CGD-O1D
23	B	606	CLA	CAD-CBD-CGD-O1D
23	B	608	CLA	CAD-CBD-CGD-O1D
23	B	617	CLA	CAD-CBD-CGD-O1D
23	C	507	CLA	CAD-CBD-CGD-O1D
23	C	510	CLA	CAA-CBA-CGA-O1A
23	D	402	CLA	CAA-CBA-CGA-O2A
23	B	613	CLA	CAA-CBA-CGA-O2A
23	C	505	CLA	CAA-CBA-CGA-O2A
23	A	406	CLA	C4C-C3C-CAC-CBC
33	F	101	HEM	CAD-CBD-CGD-O1D
23	A	405	CLA	C4-C3-C5-C6
24	A	408	PHO	C3A-C2A-CAA-CBA
30	C	517	DGD	O1G-C1A-C2A-C3A
25	K	102	BCR	C7-C8-C9-C10
28	A	414	PL9	C2-C3-C7-C8
35	V	201	HEC	CAA-CBA-CGA-O1A
25	A	411	BCR	C15-C16-C17-C18
30	C	518	DGD	CAA-CBA-CCA-CDA
32	L	101	LHG	C26-C27-C28-C29
23	C	505	CLA	CAA-CBA-CGA-O1A
33	F	101	HEM	CAD-CBD-CGD-O2D
35	V	201	HEC	CAA-CBA-CGA-O2A

There are no ring outliers.

59 monomers are involved in 145 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	D	401	BCT	1	0
23	C	506	CLA	2	0
27	A	413	LMG	1	0
23	B	612	CLA	1	0
25	A	411	BCR	4	0
33	F	101	HEM	4	0
23	B	605	CLA	3	0

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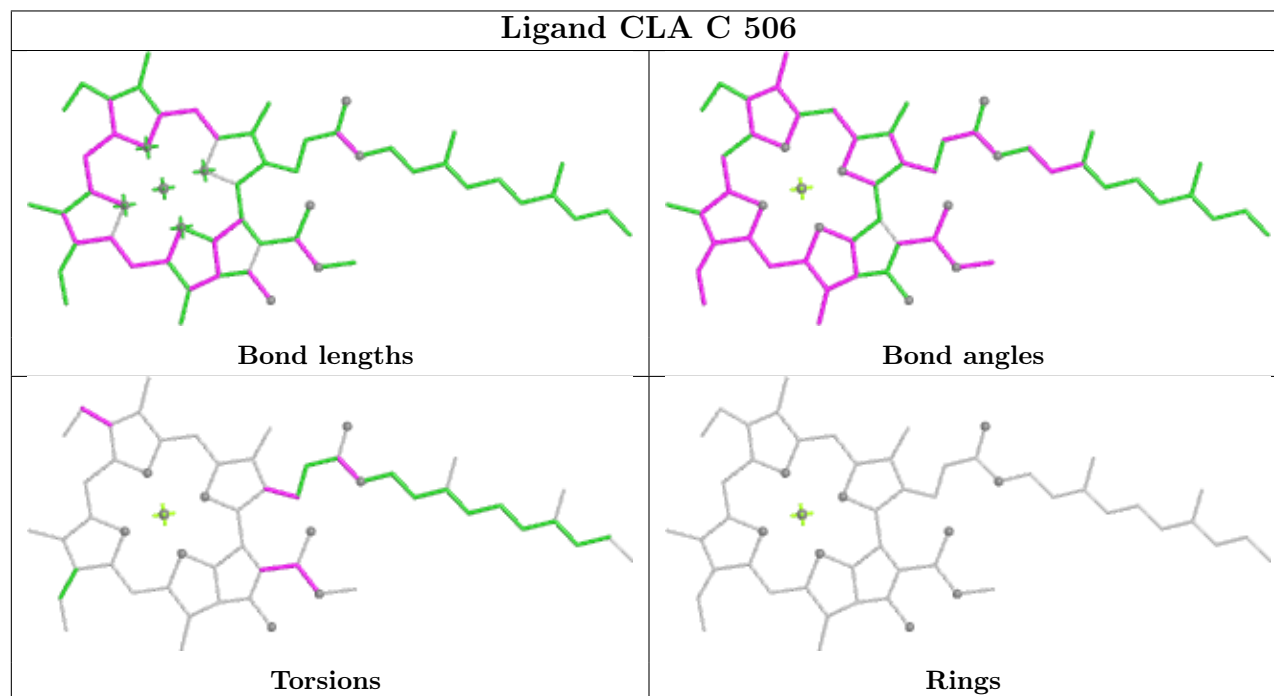
Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	D	408	LHG	2	0
23	B	610	CLA	1	0
23	B	611	CLA	3	0
24	A	409	PHO	5	0
25	K	101	BCR	3	0
23	B	607	CLA	2	0
23	D	402	CLA	4	0
30	C	516	DGD	1	0
23	C	507	CLA	6	0
23	B	604	CLA	2	0
32	D	410	LHG	1	0
34	H	101	RRX	4	0
23	B	608	CLA	1	0
23	B	616	CLA	4	0
23	B	606	CLA	6	0
30	H	102	DGD	3	0
23	C	509	CLA	3	0
28	A	414	PL9	5	0
28	D	405	PL9	4	0
23	A	405	CLA	1	0
23	C	511	CLA	5	0
25	B	620	BCR	3	0
23	C	503	CLA	10	0
25	K	102	BCR	5	0
25	C	514	BCR	1	0
23	A	407	CLA	2	0
26	D	407	SQD	1	0
23	C	505	CLA	3	0
23	A	406	CLA	2	0
23	C	510	CLA	6	0
23	C	502	CLA	4	0
23	C	508	CLA	1	0
21	A	401	OEX	2	0
27	B	622	LMG	2	0
24	A	408	PHO	3	0
26	A	412	SQD	4	0
23	B	602	CLA	2	0
30	C	518	DGD	2	0
32	D	409	LHG	1	0
23	B	609	CLA	2	0
25	B	618	BCR	3	0
30	C	517	DGD	4	0

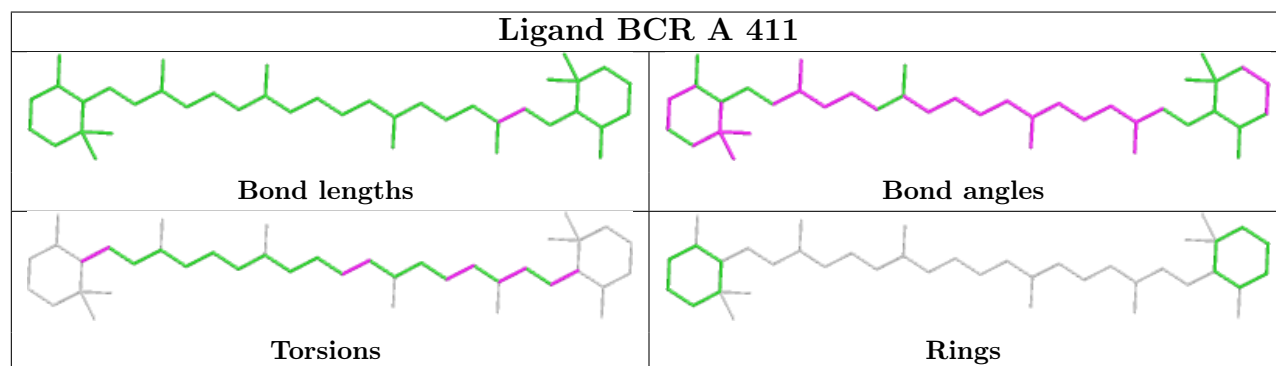
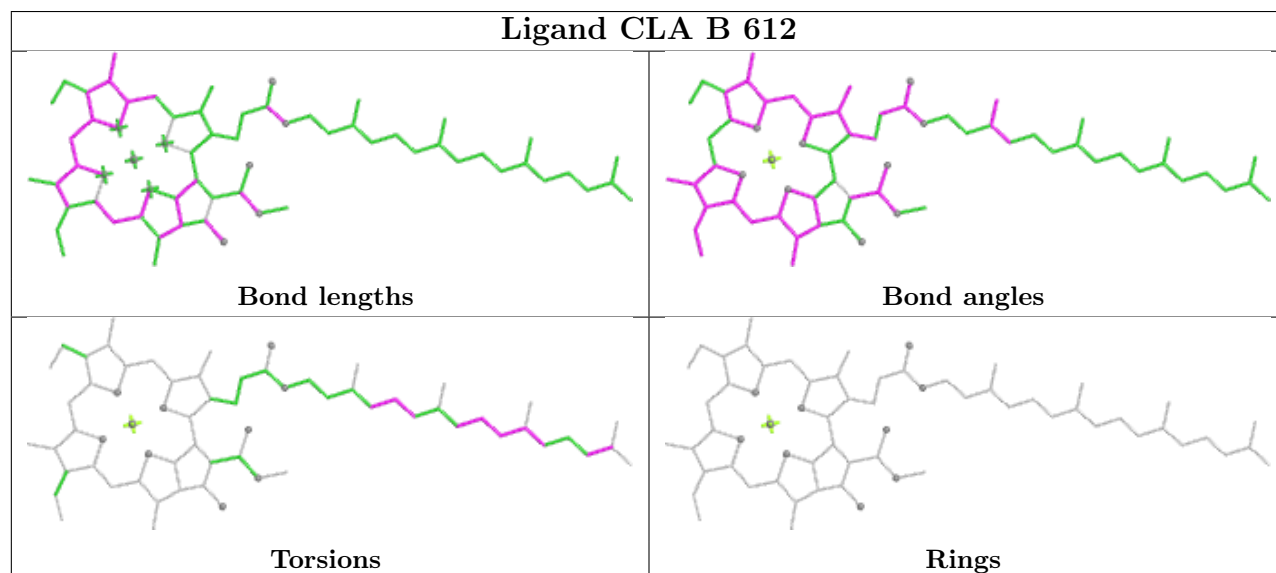
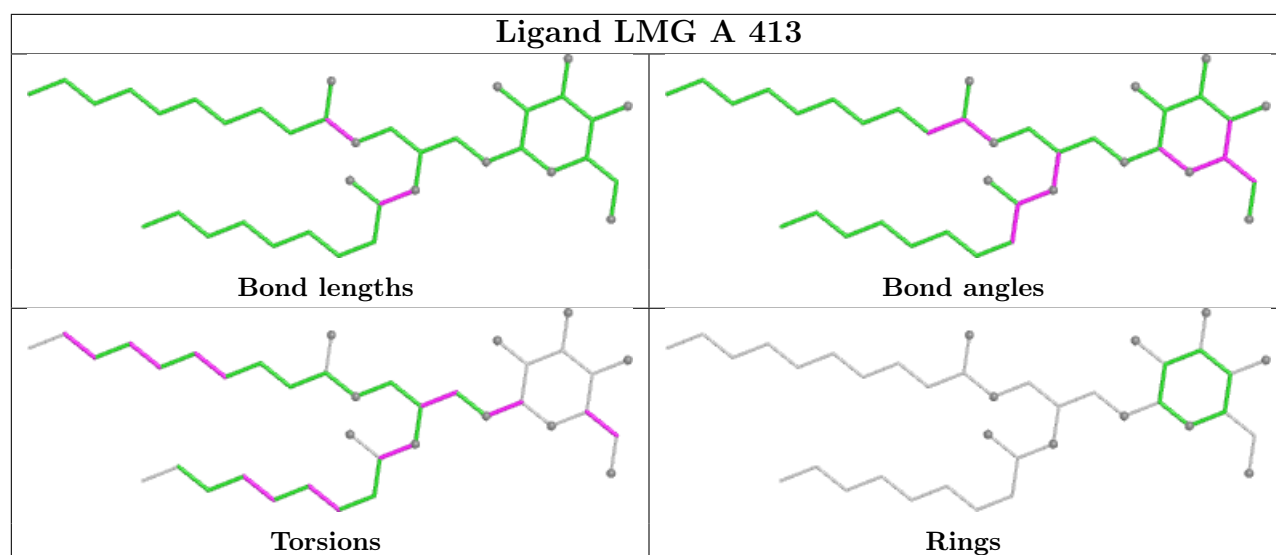
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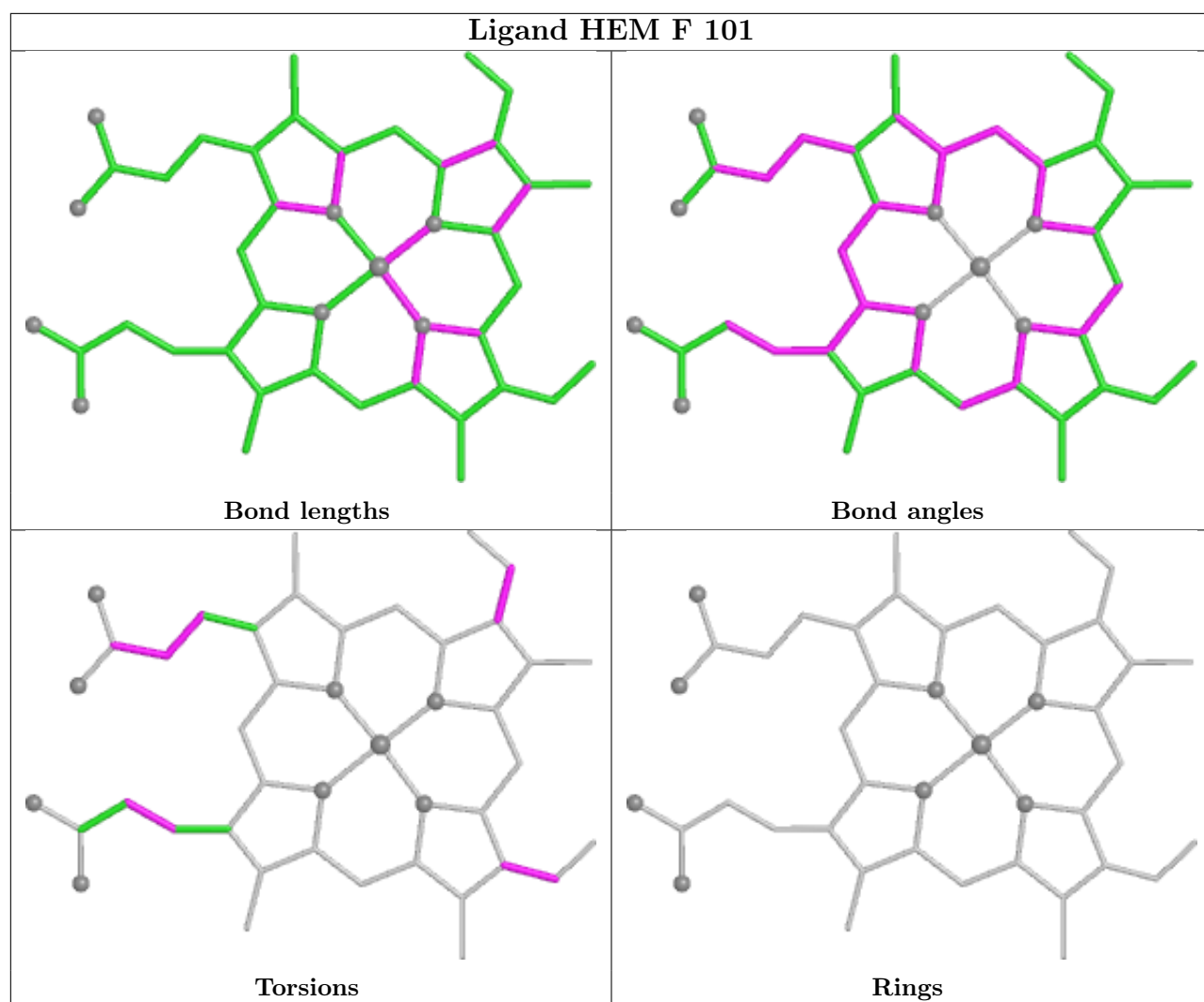
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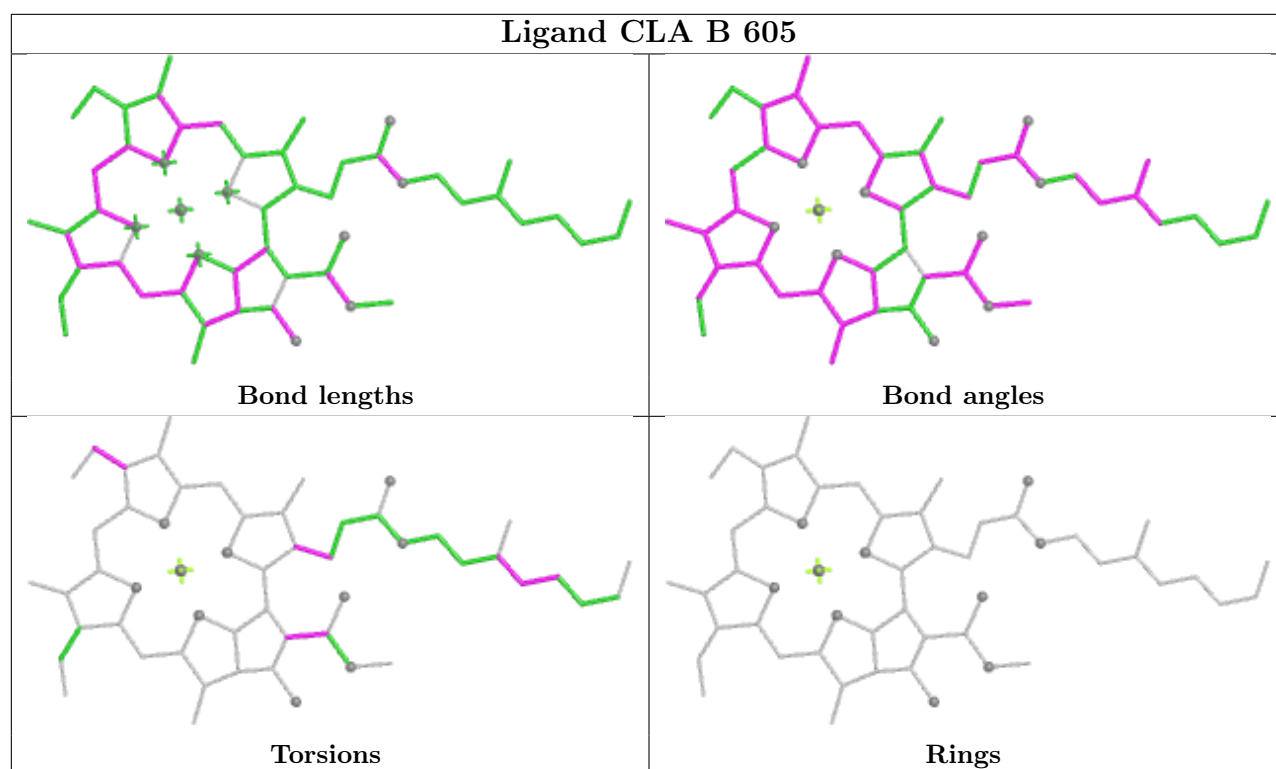
Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	C	515	BCR	3	0
23	C	501	CLA	7	0
23	B	603	CLA	2	0
23	B	614	CLA	4	0
23	C	512	CLA	2	0
23	B	617	CLA	2	0
32	L	101	LHG	5	0
23	C	504	CLA	1	0
23	A	410	CLA	2	0
23	B	613	CLA	4	0

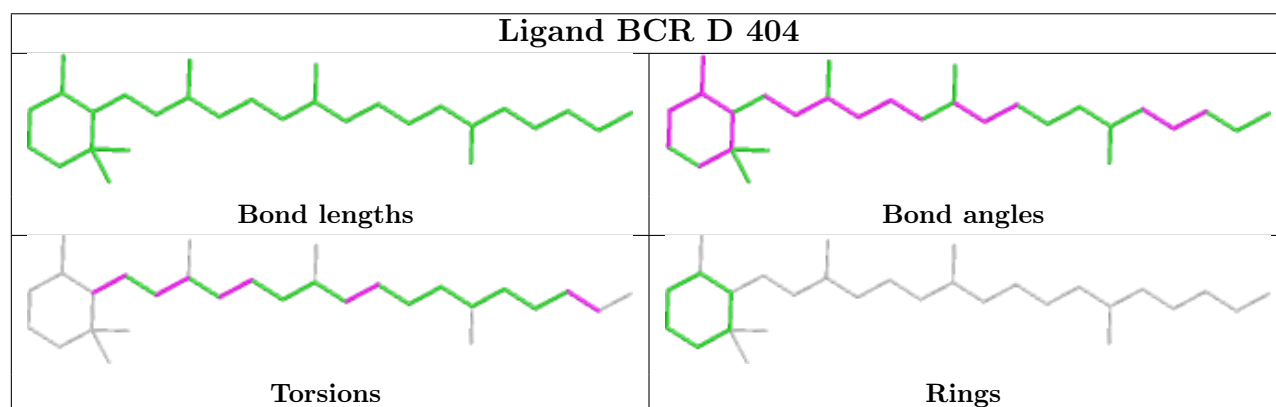
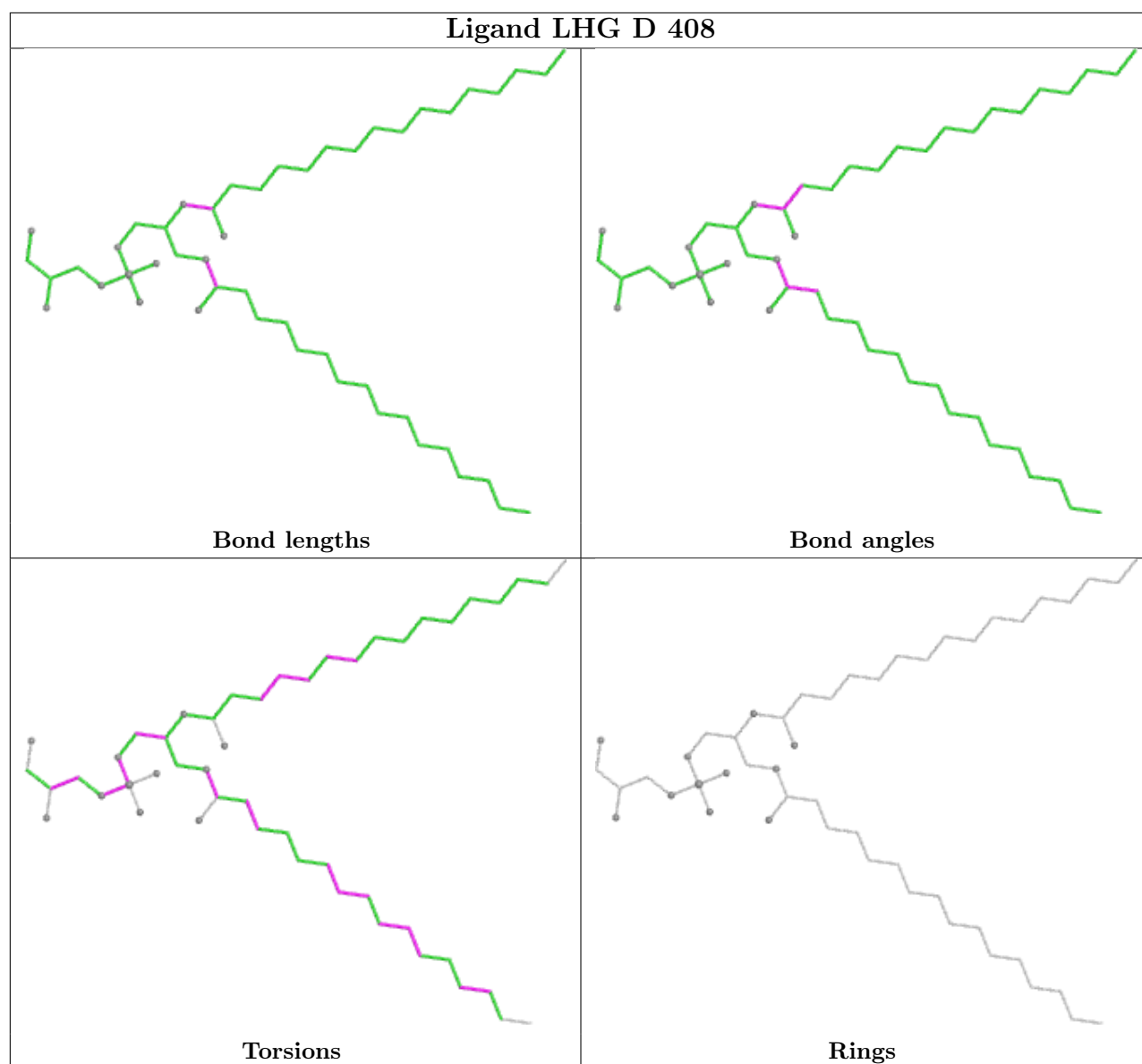
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

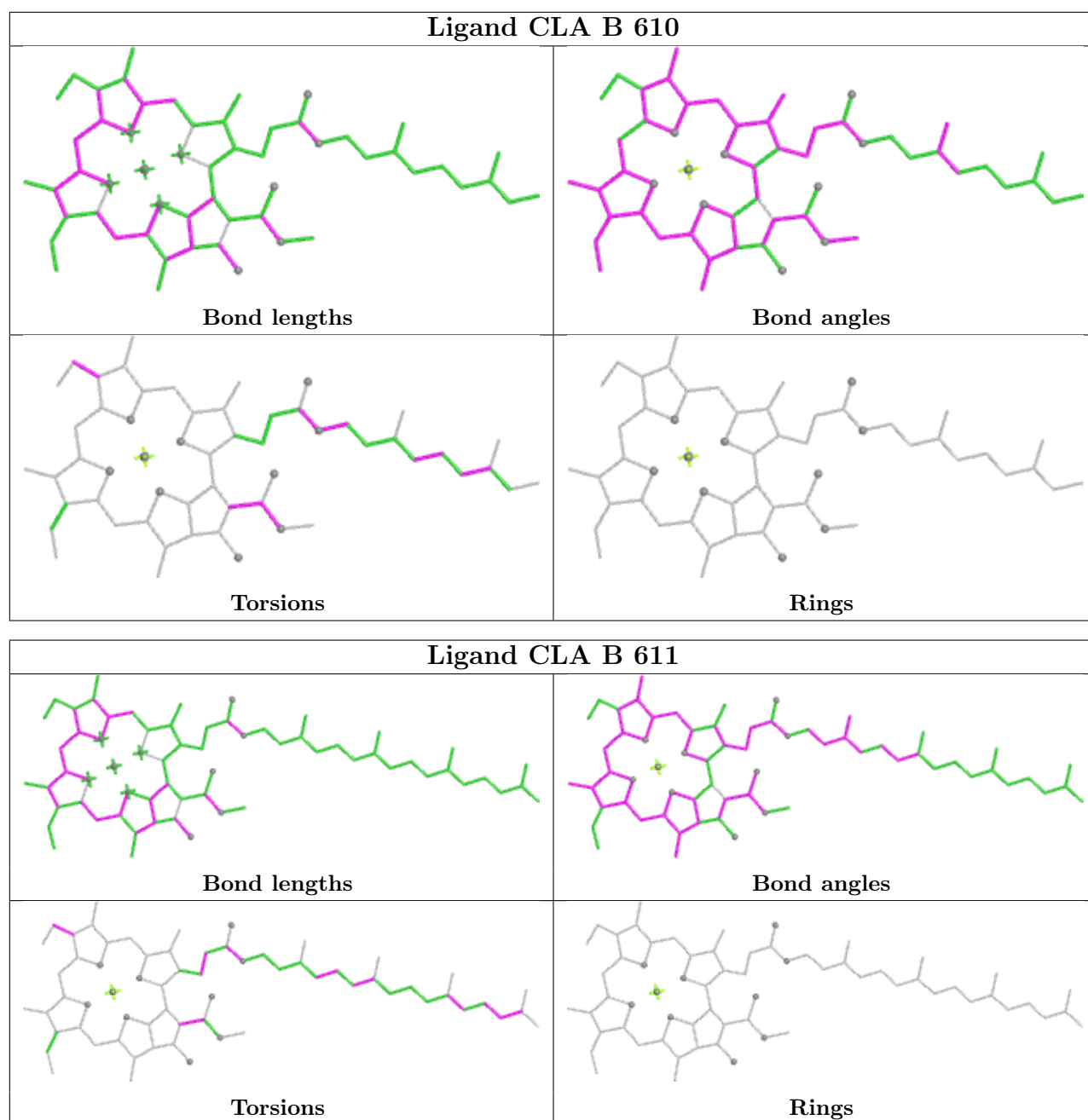


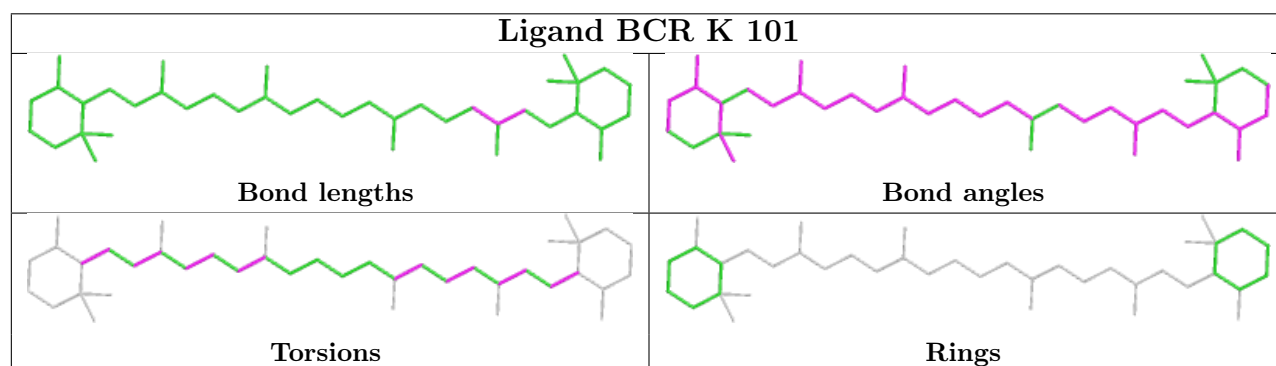
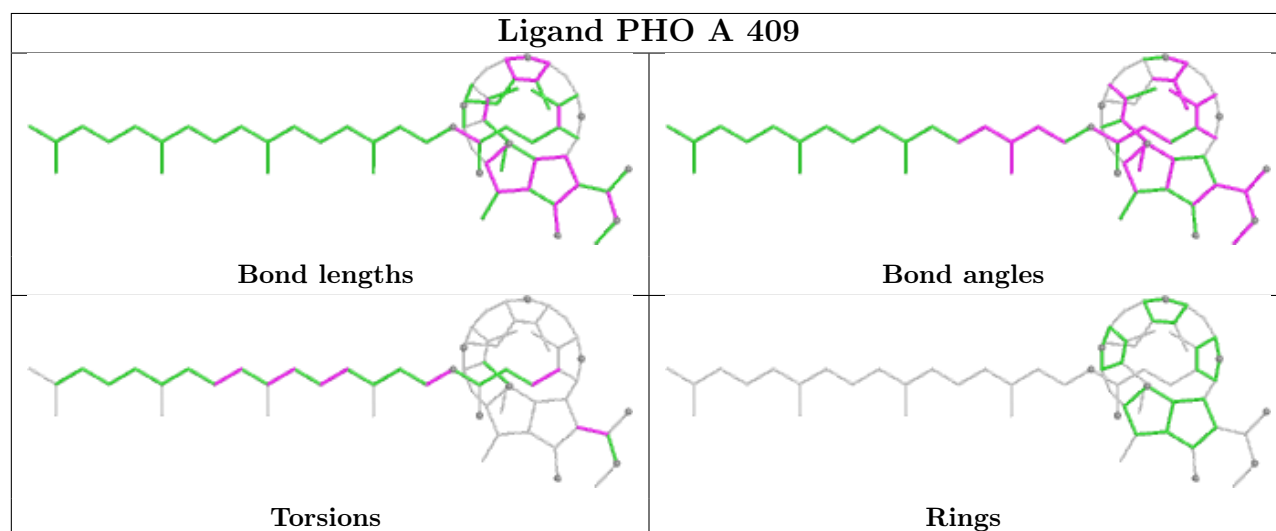
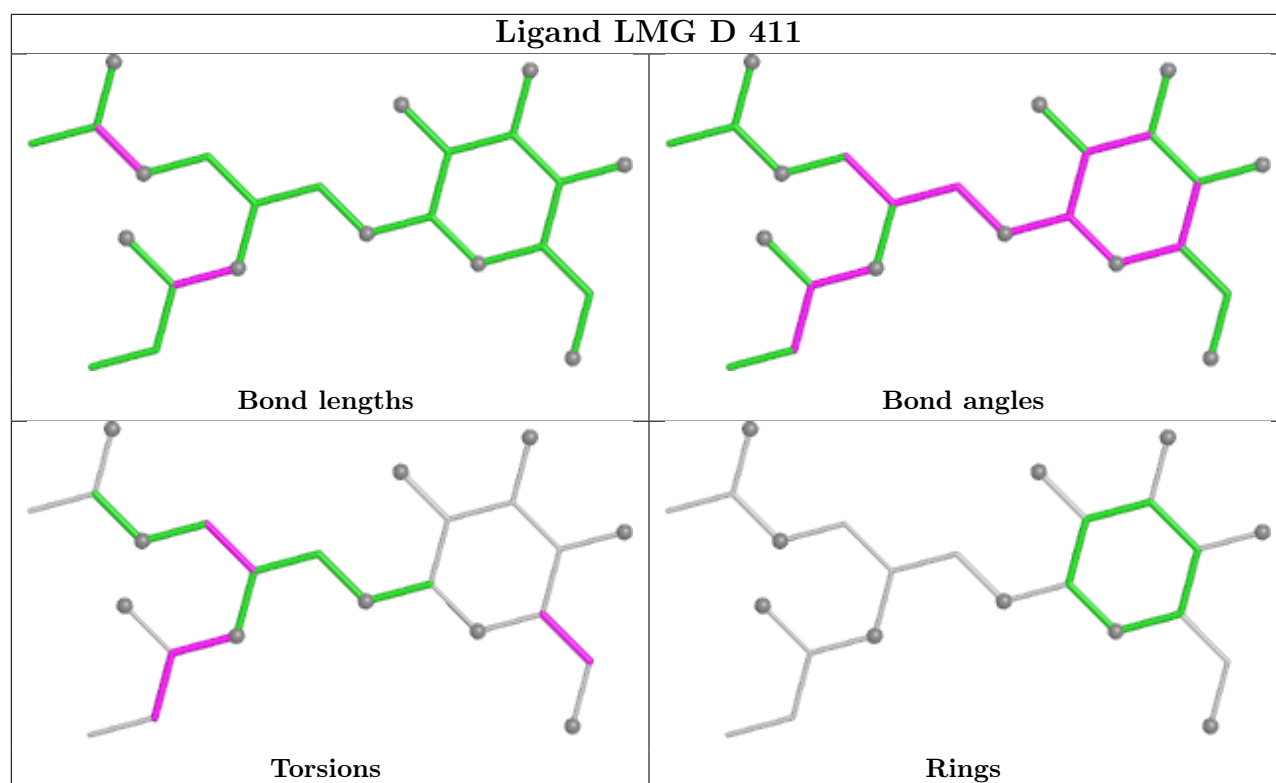




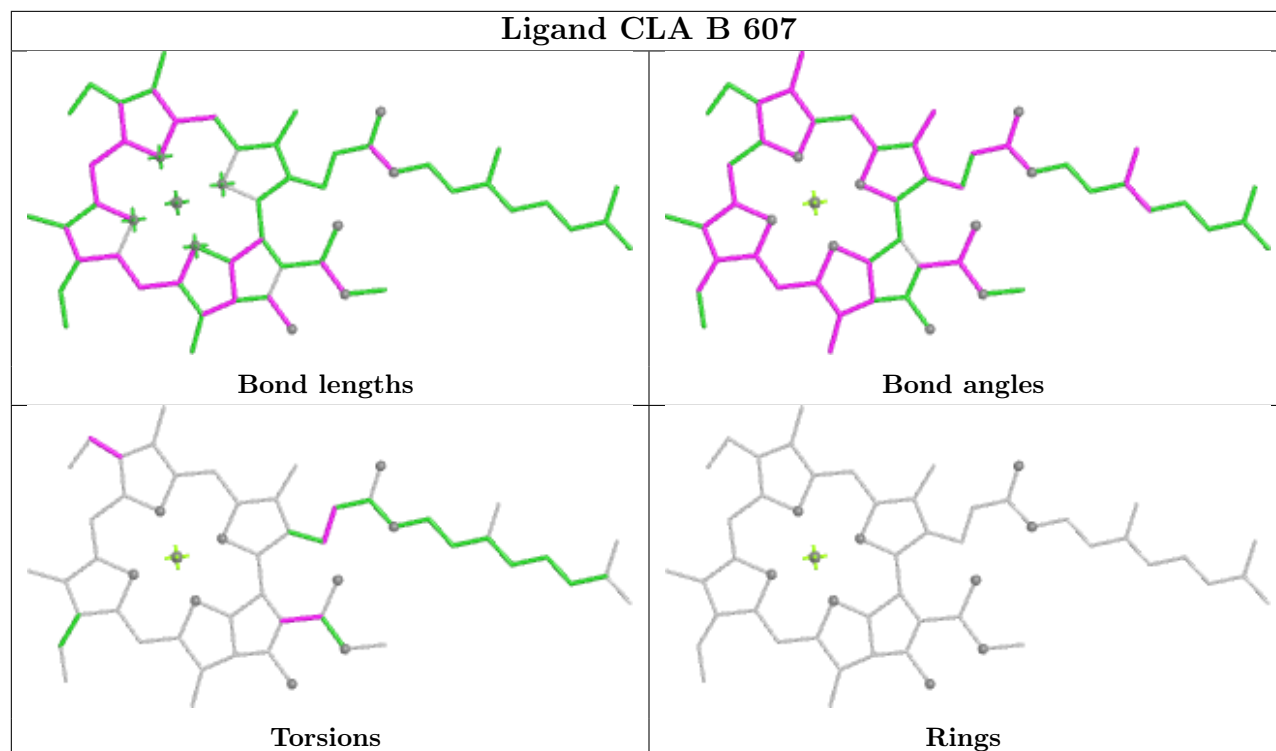




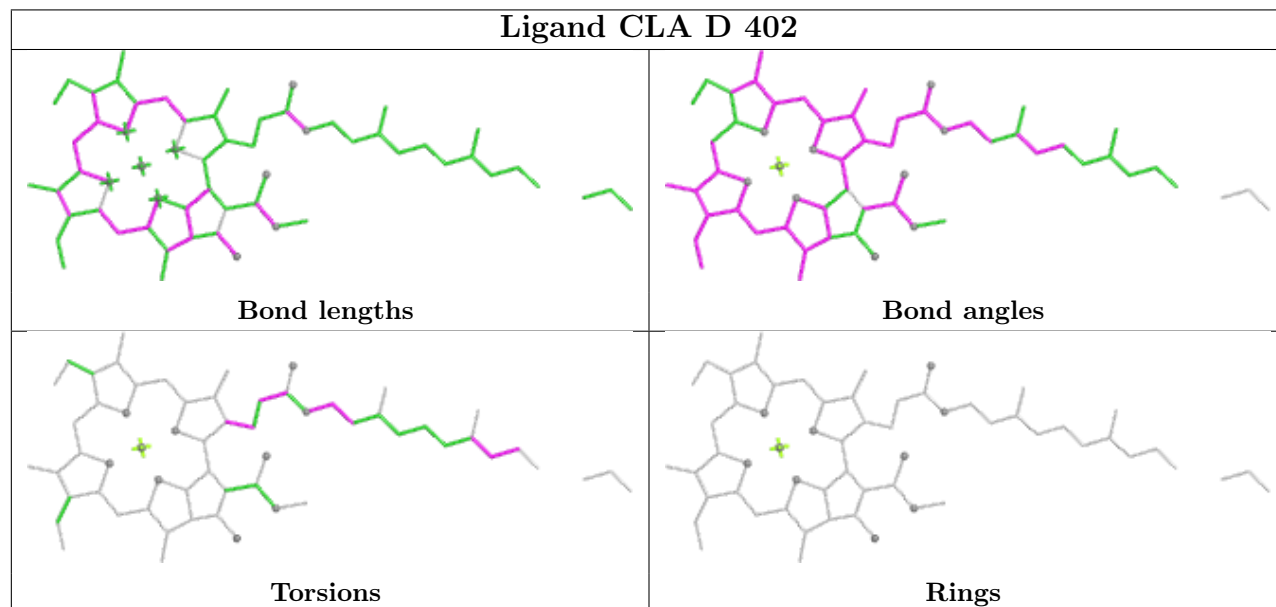


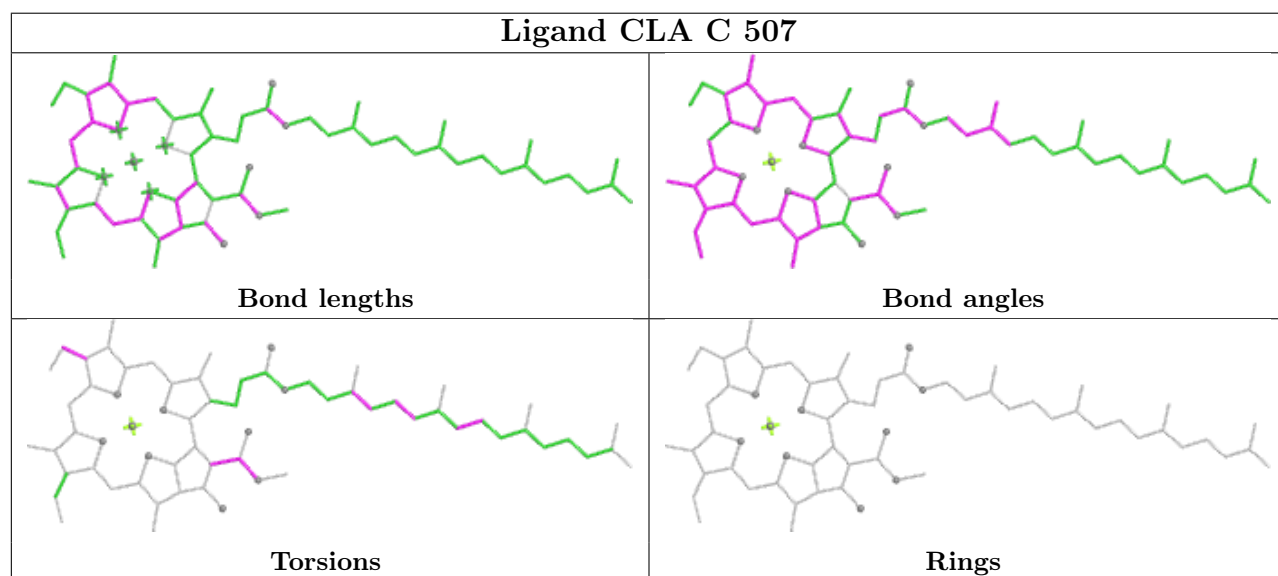
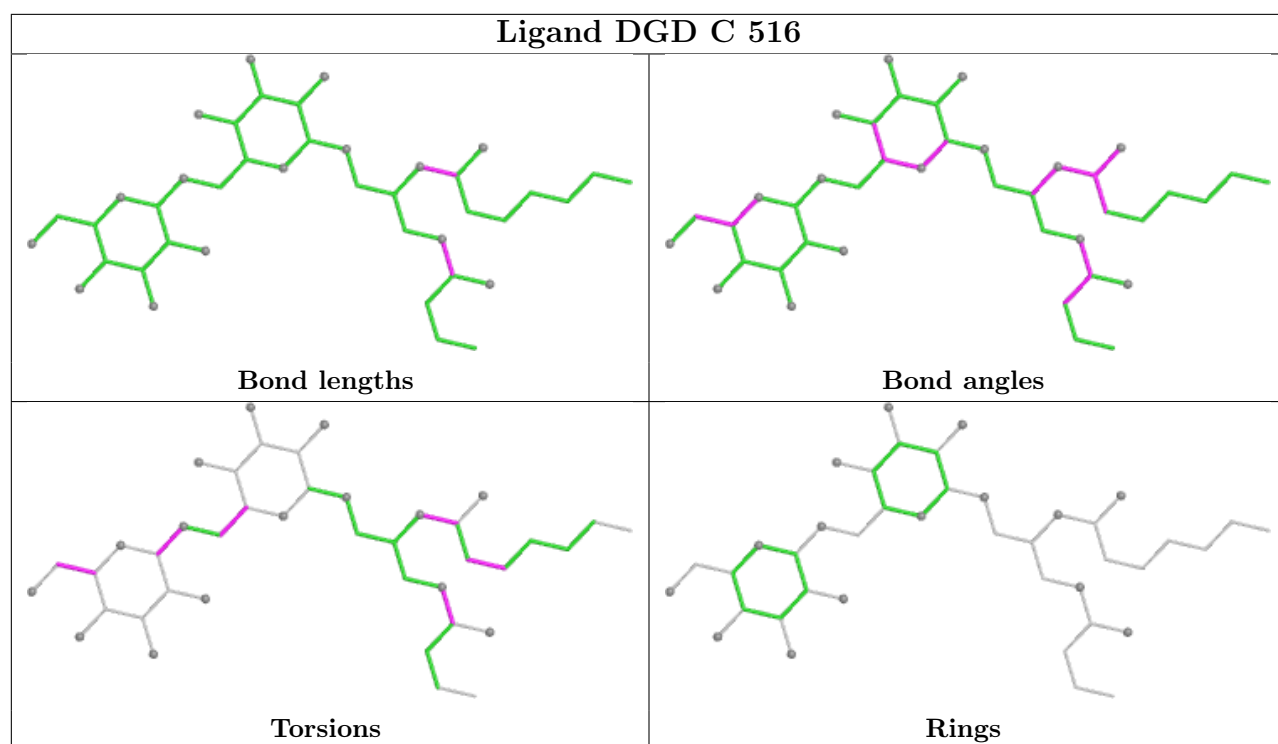


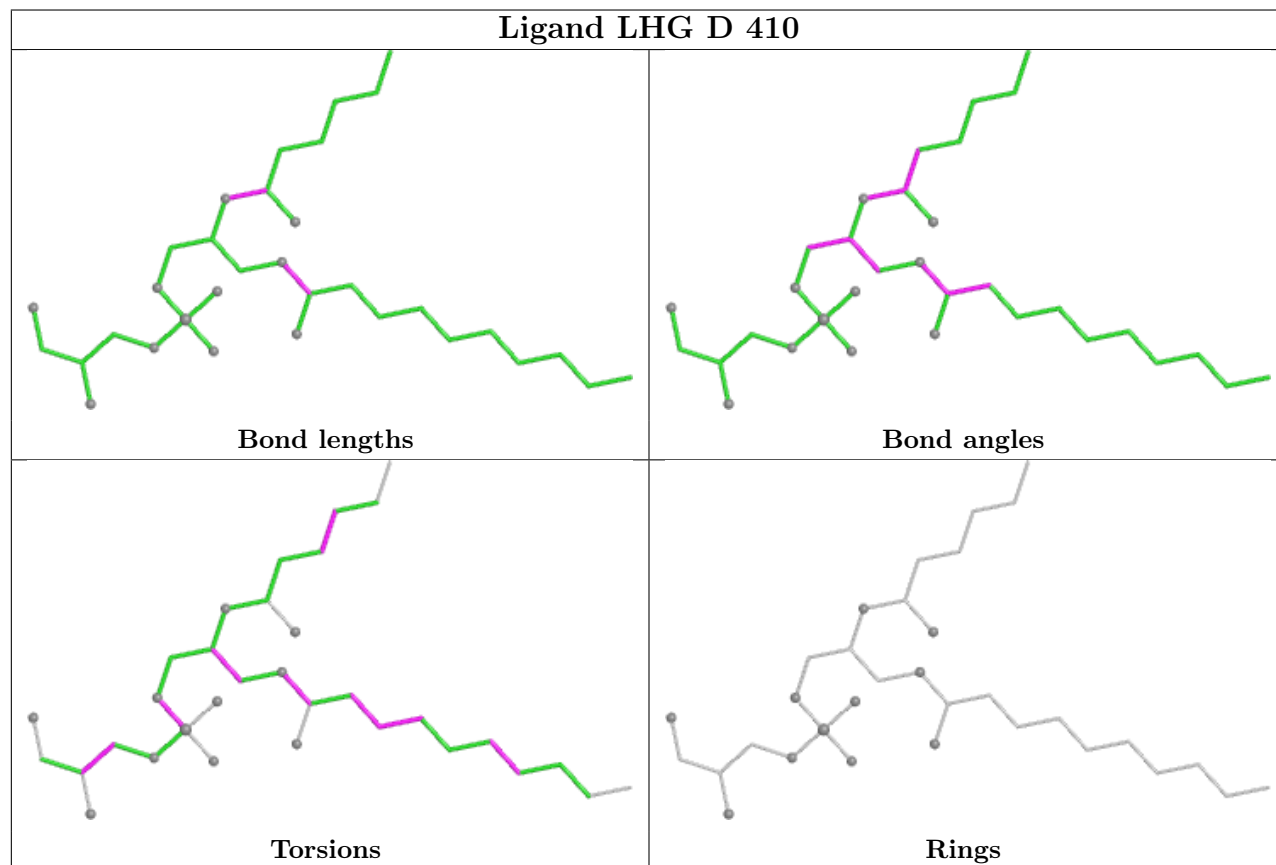
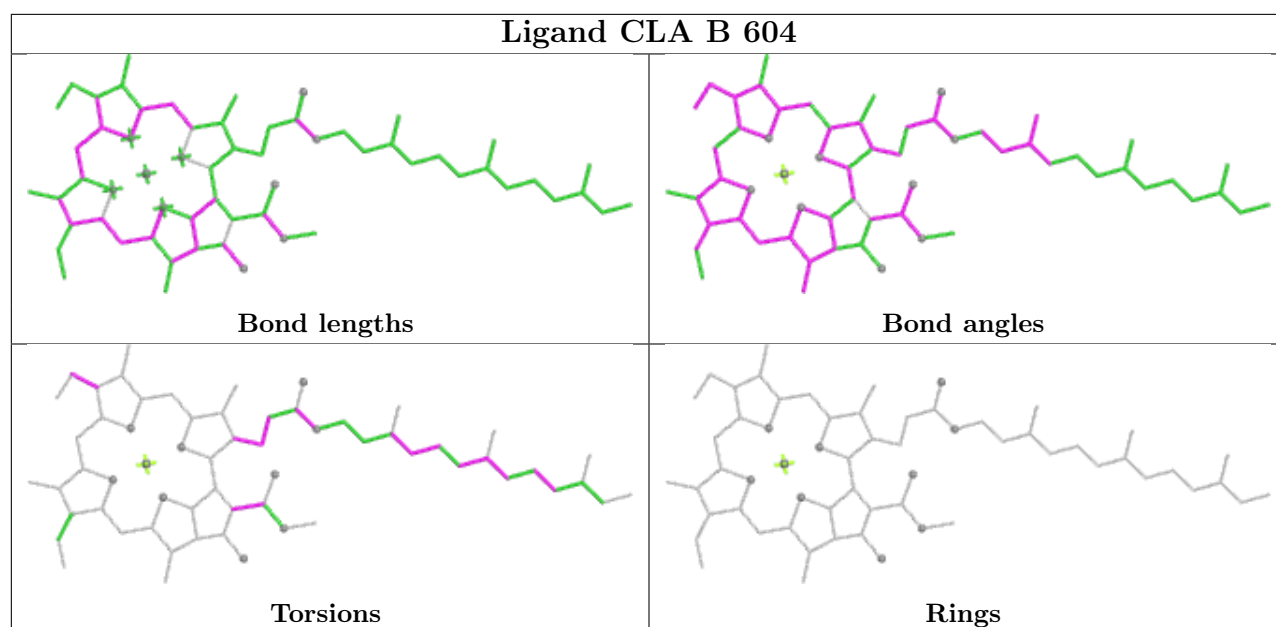
Ligand CLA B 607

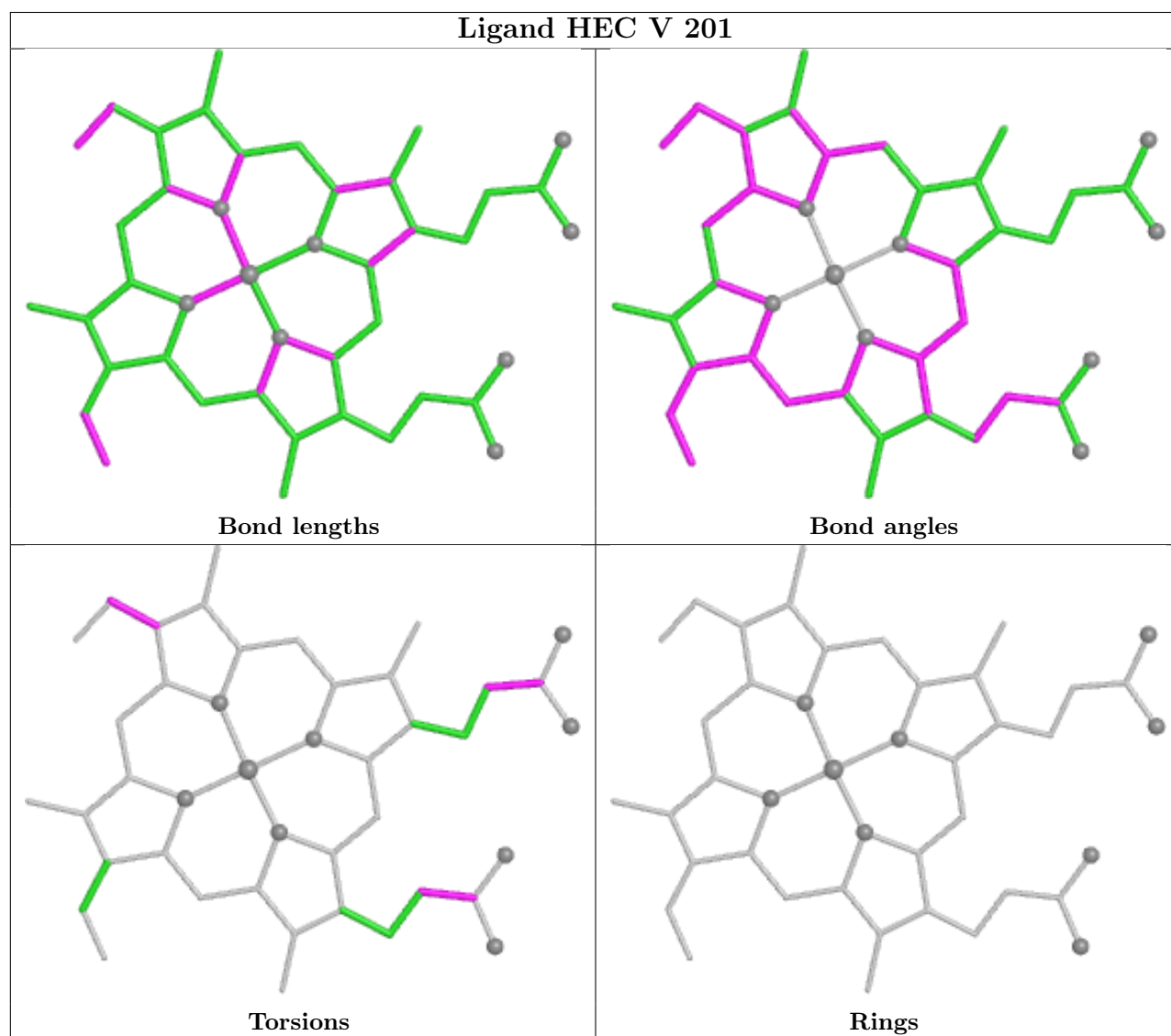
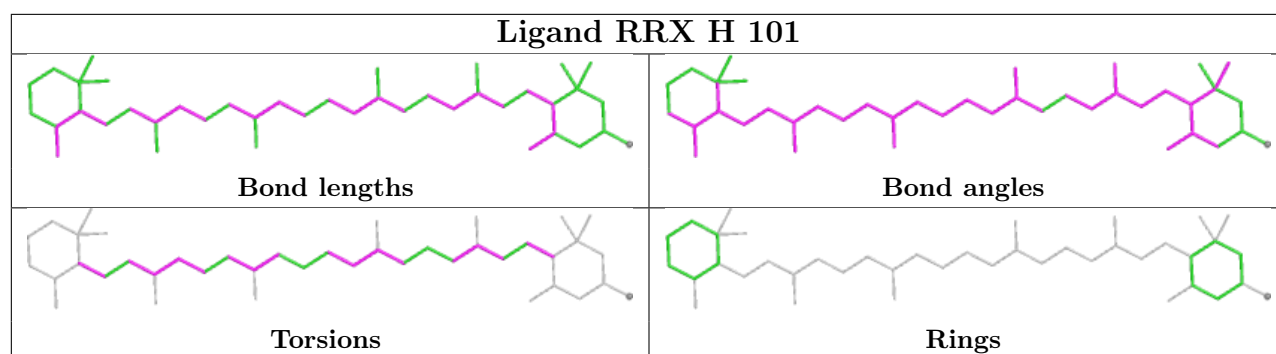


Ligand CLA D 402

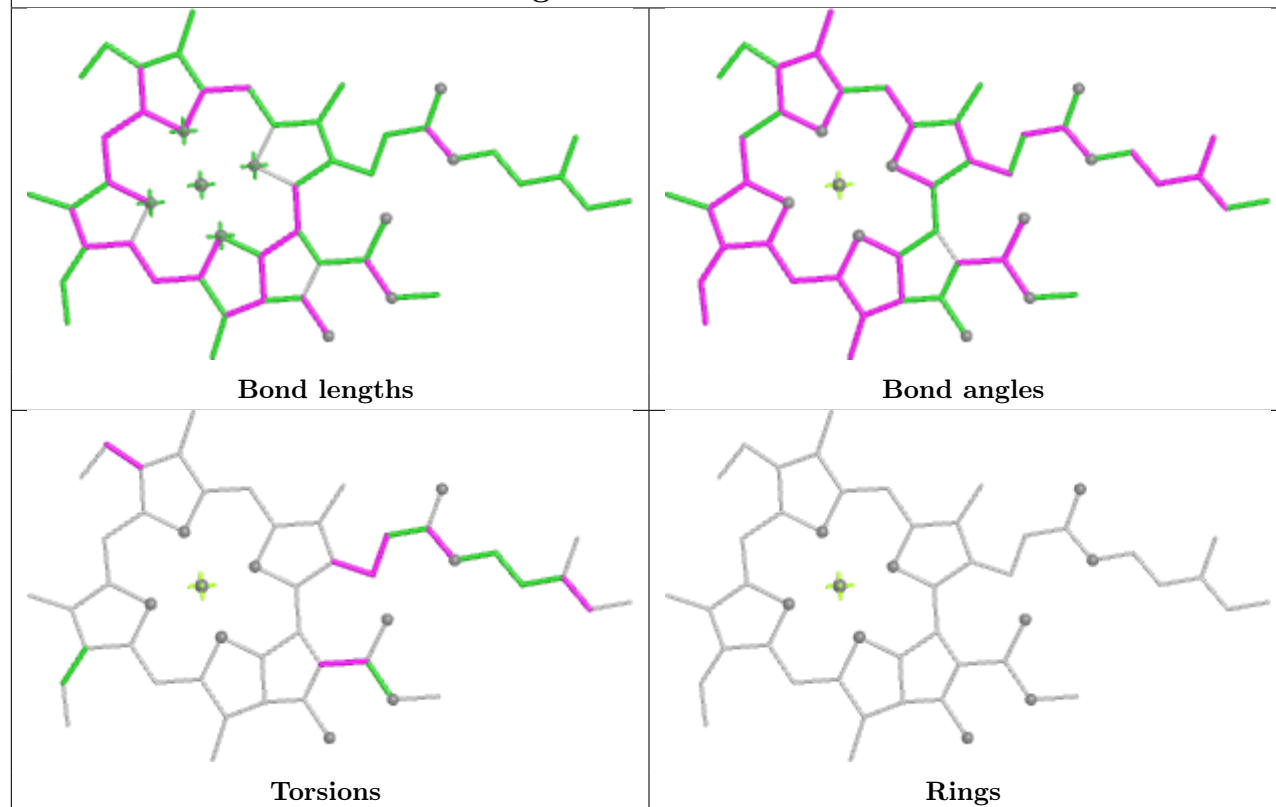




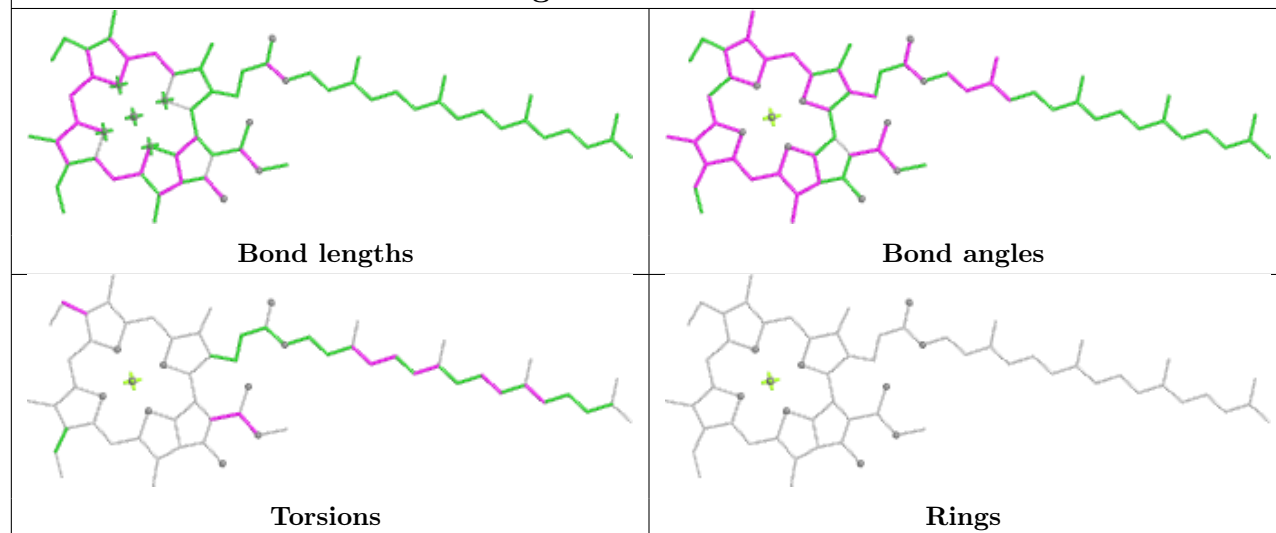


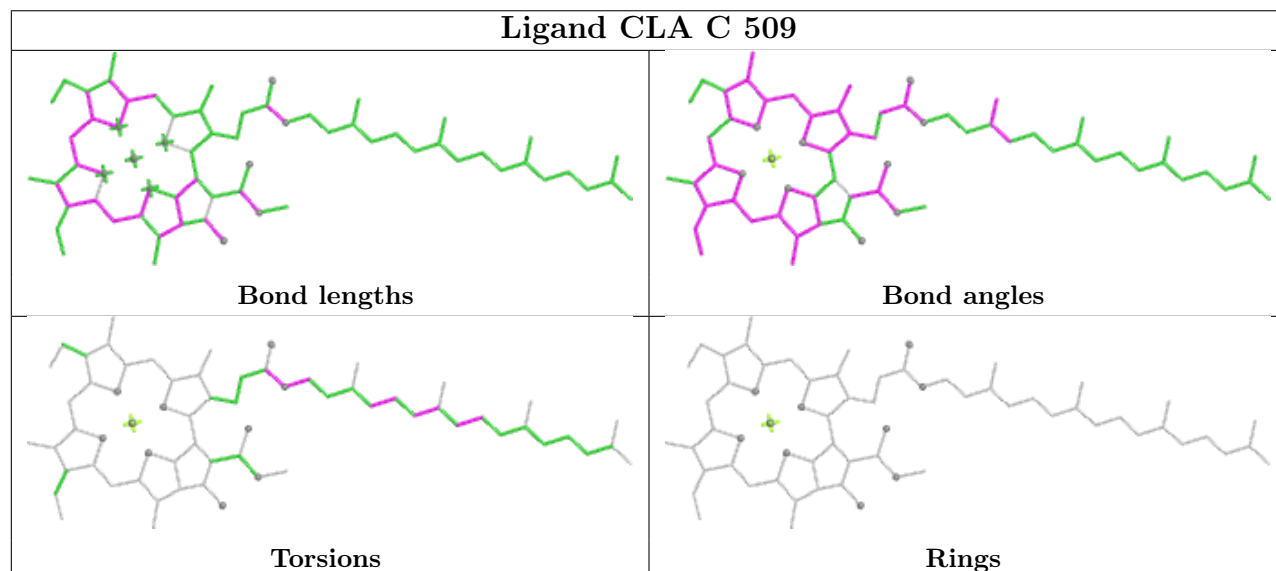
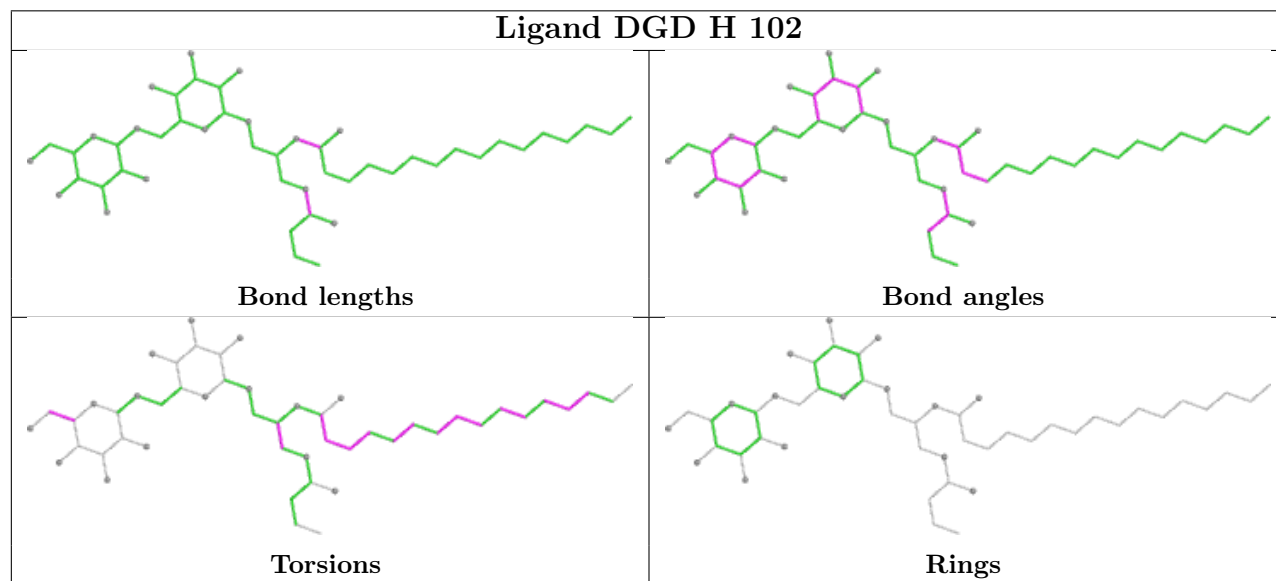
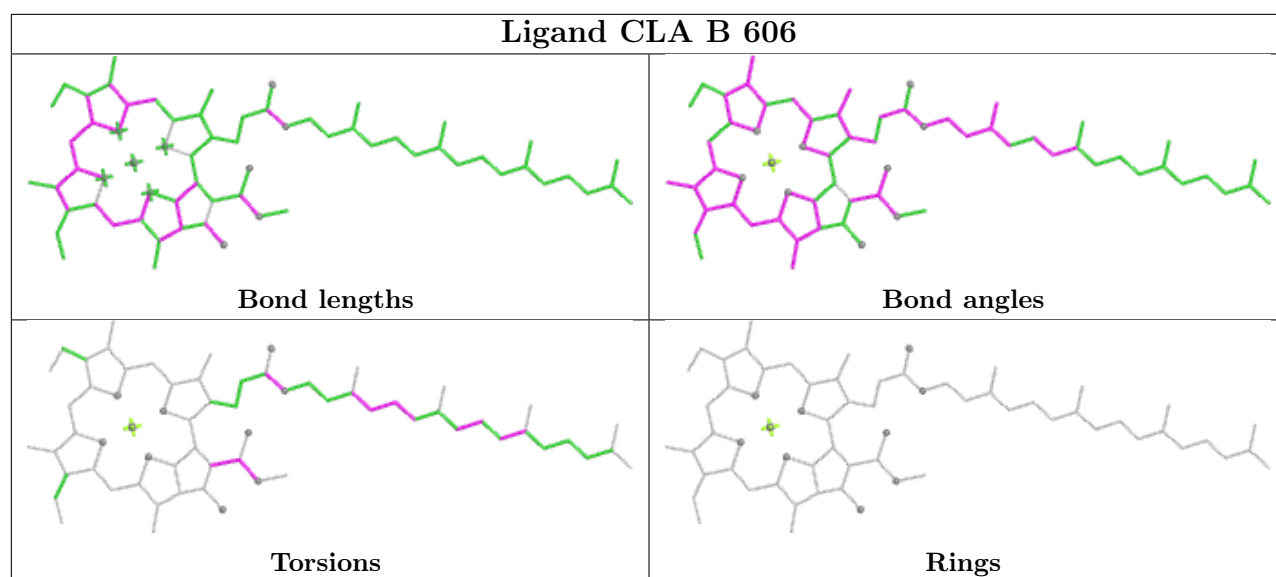


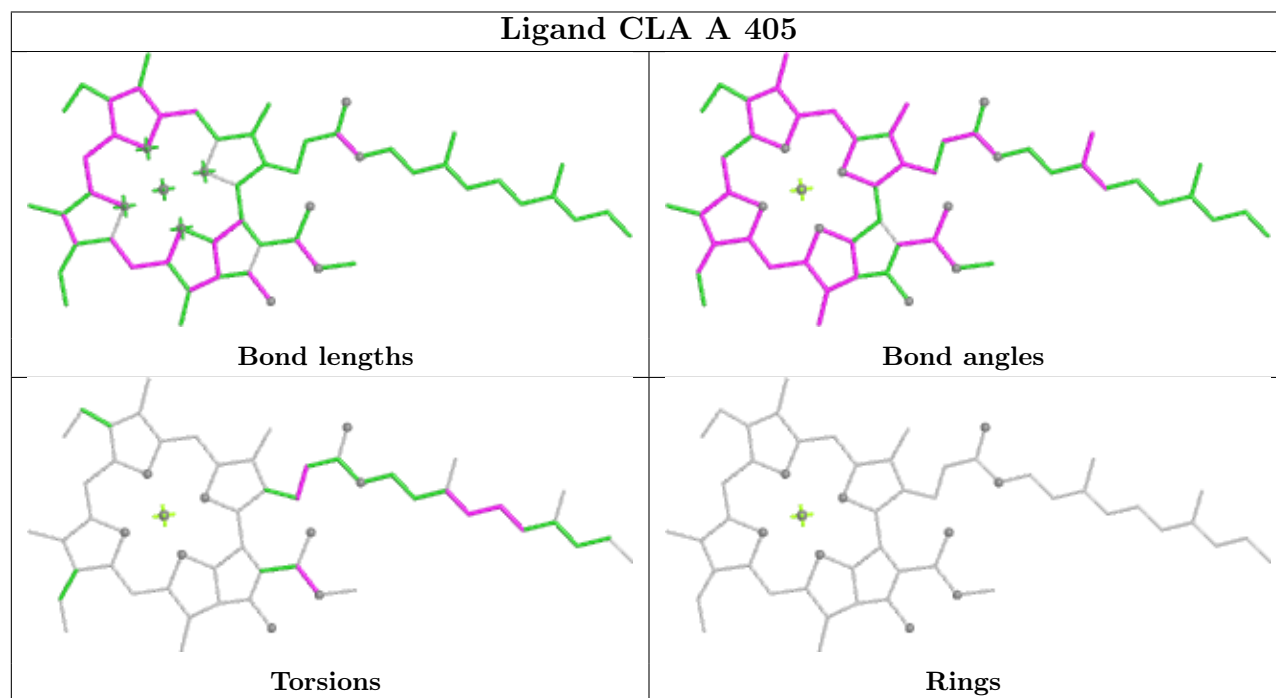
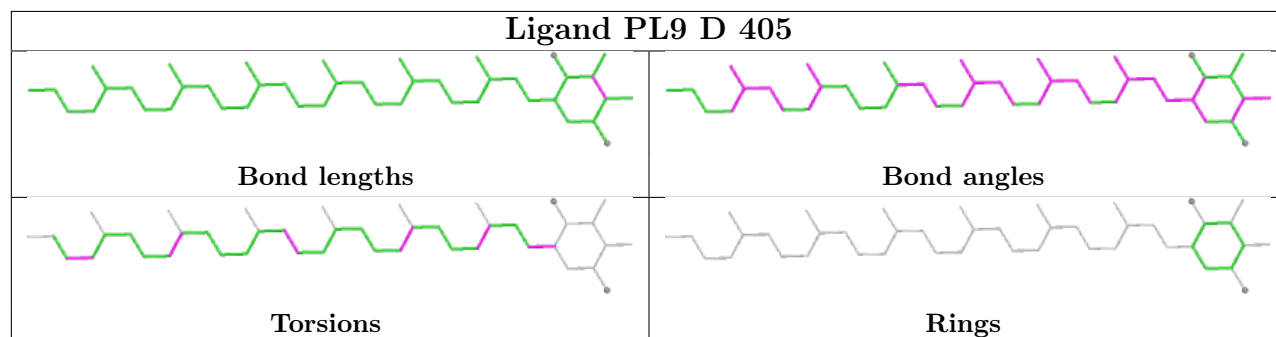
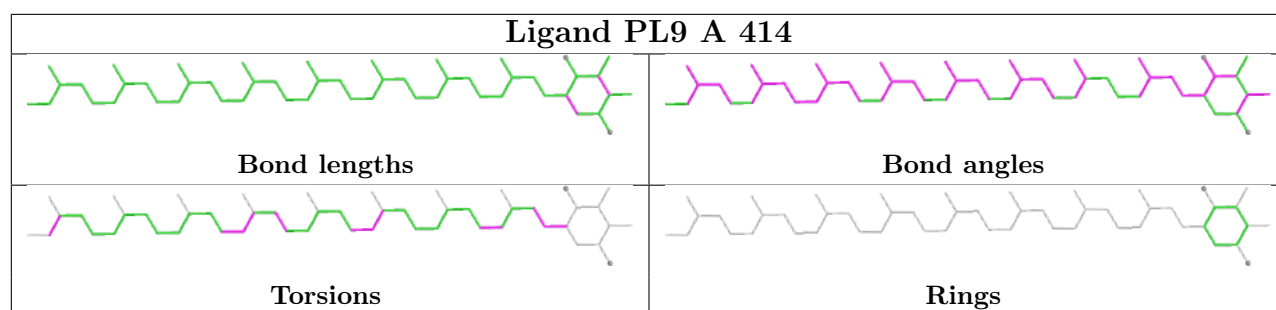
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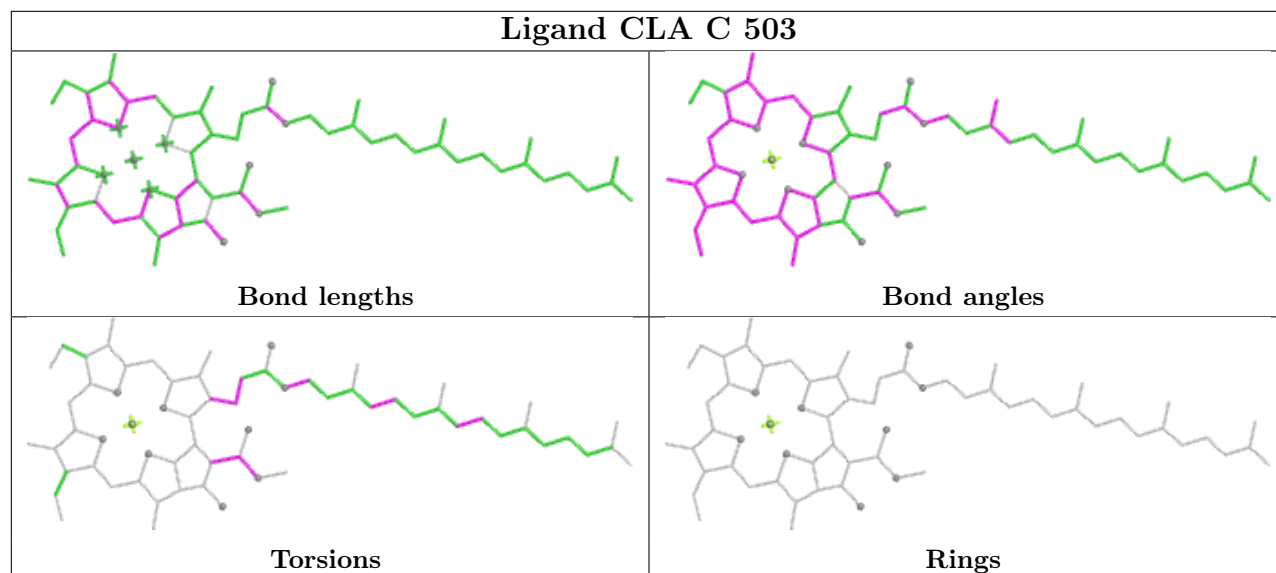
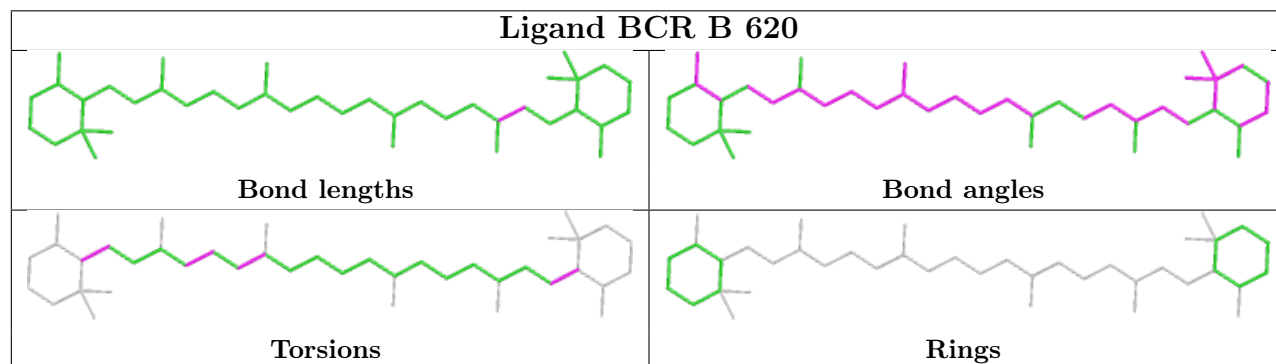
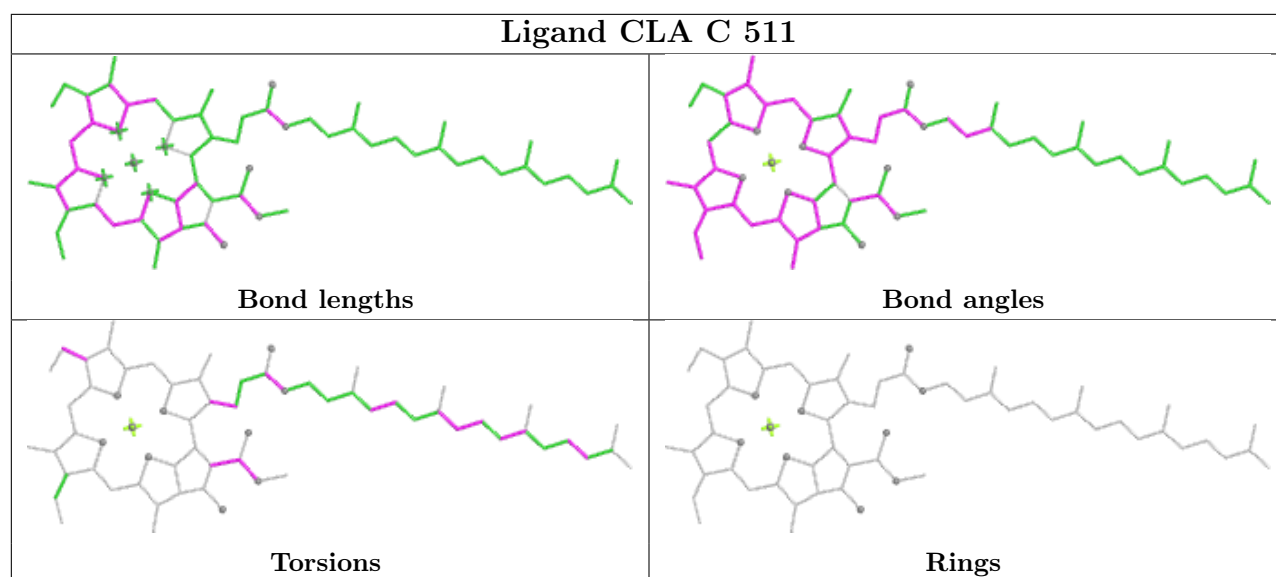


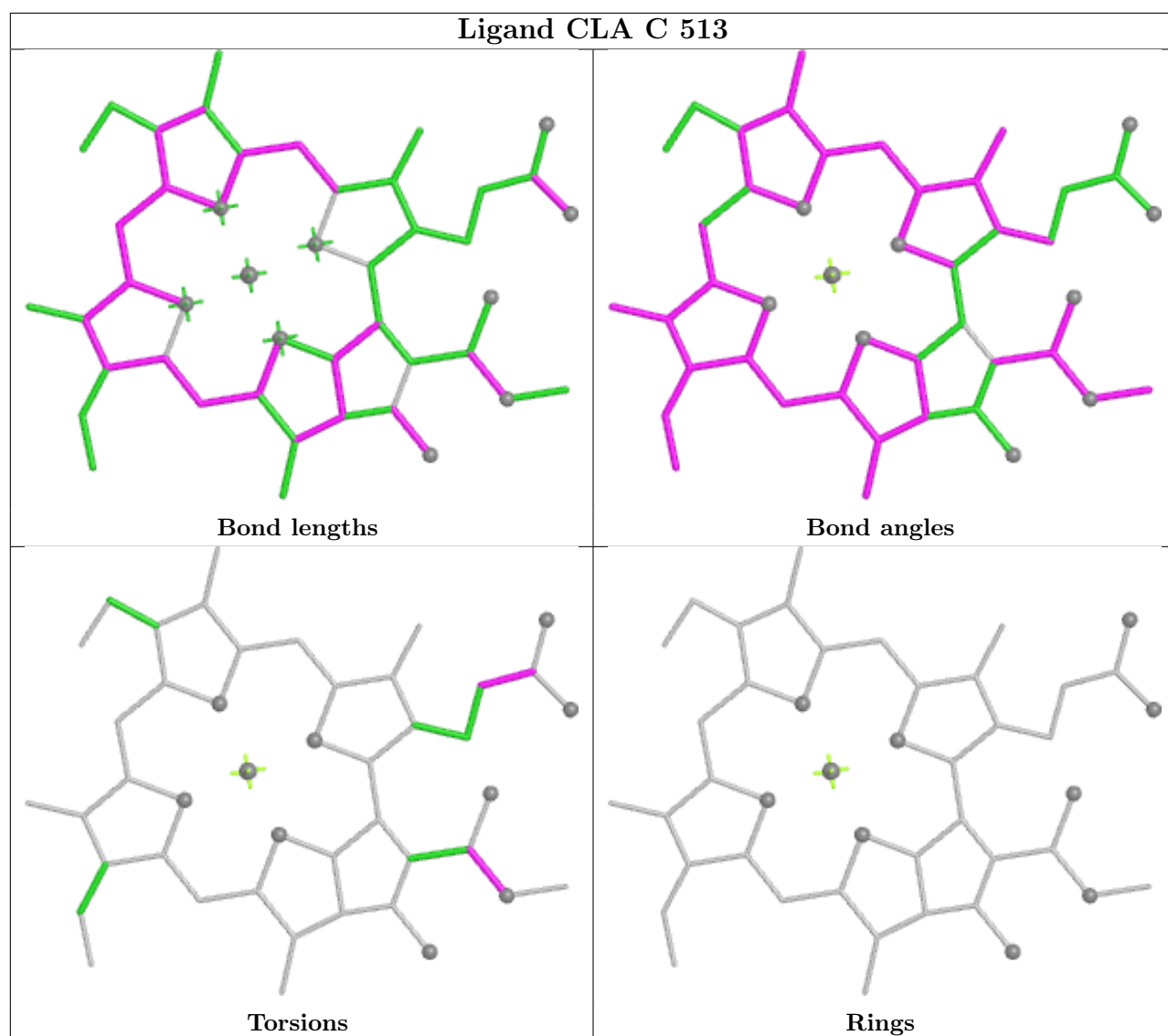
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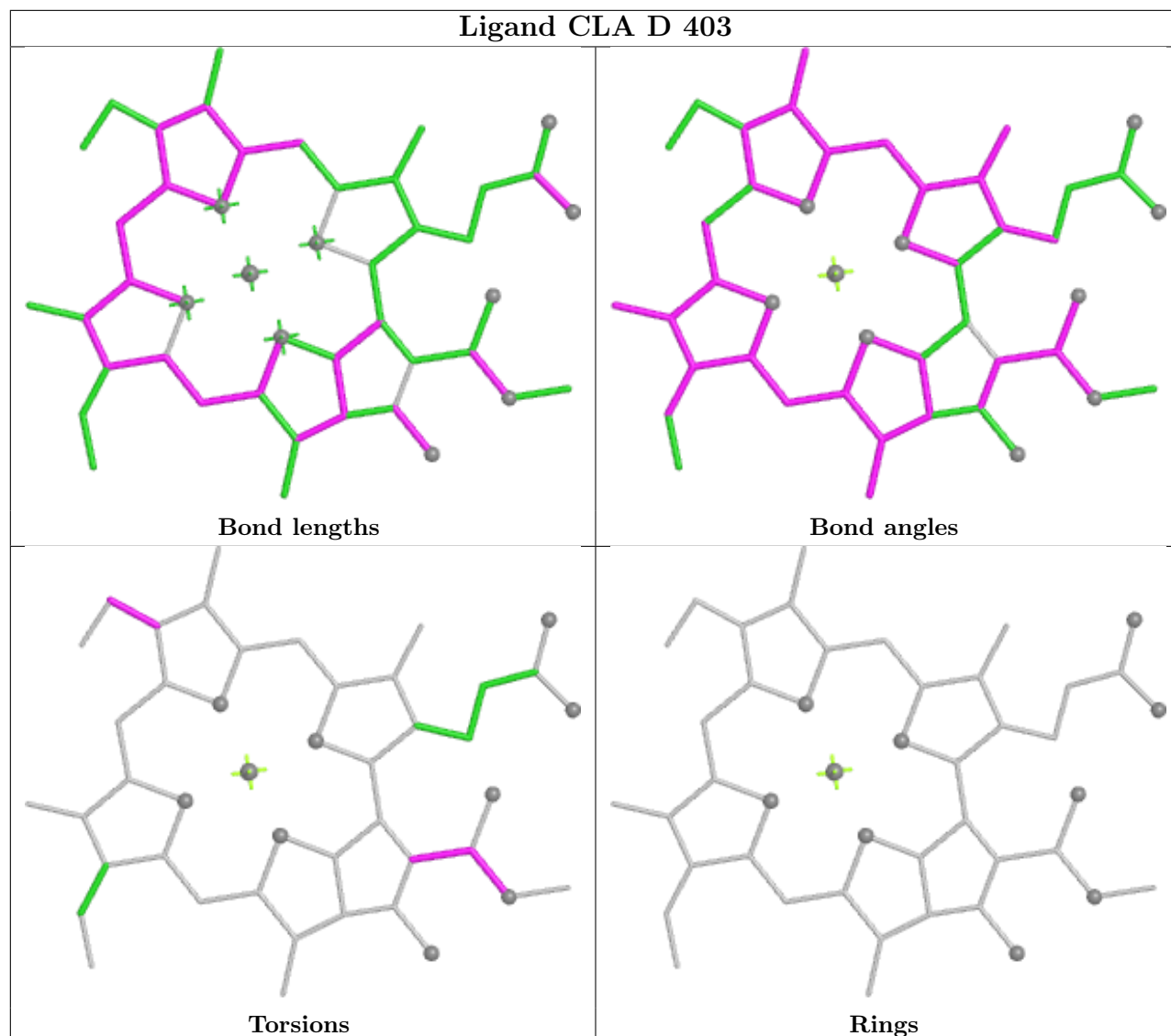




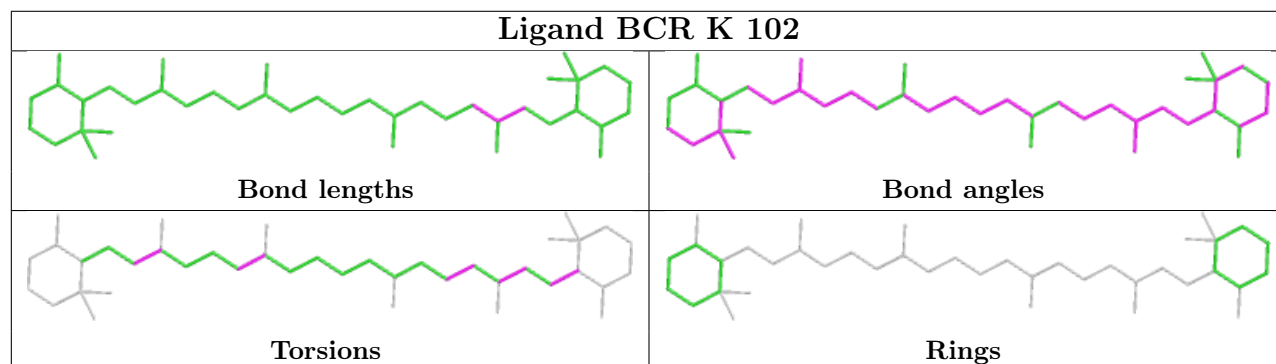


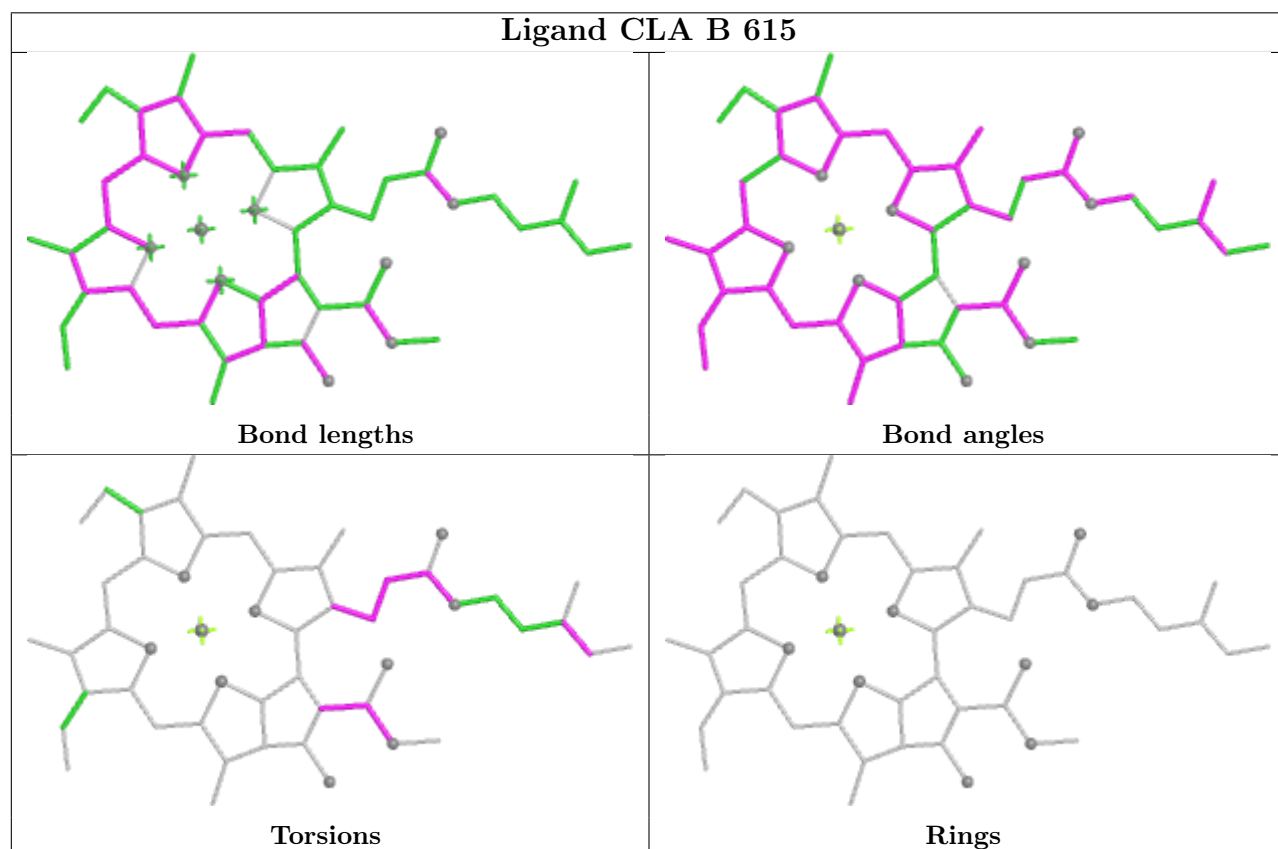
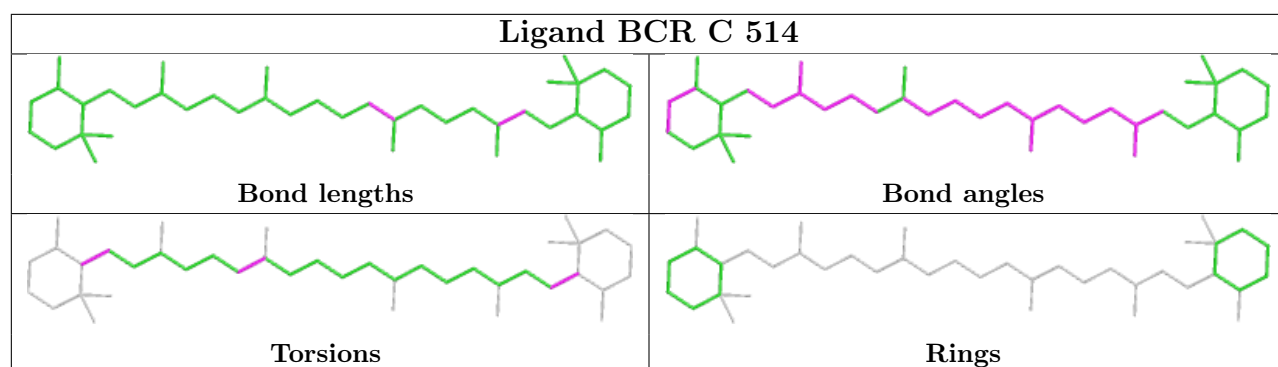


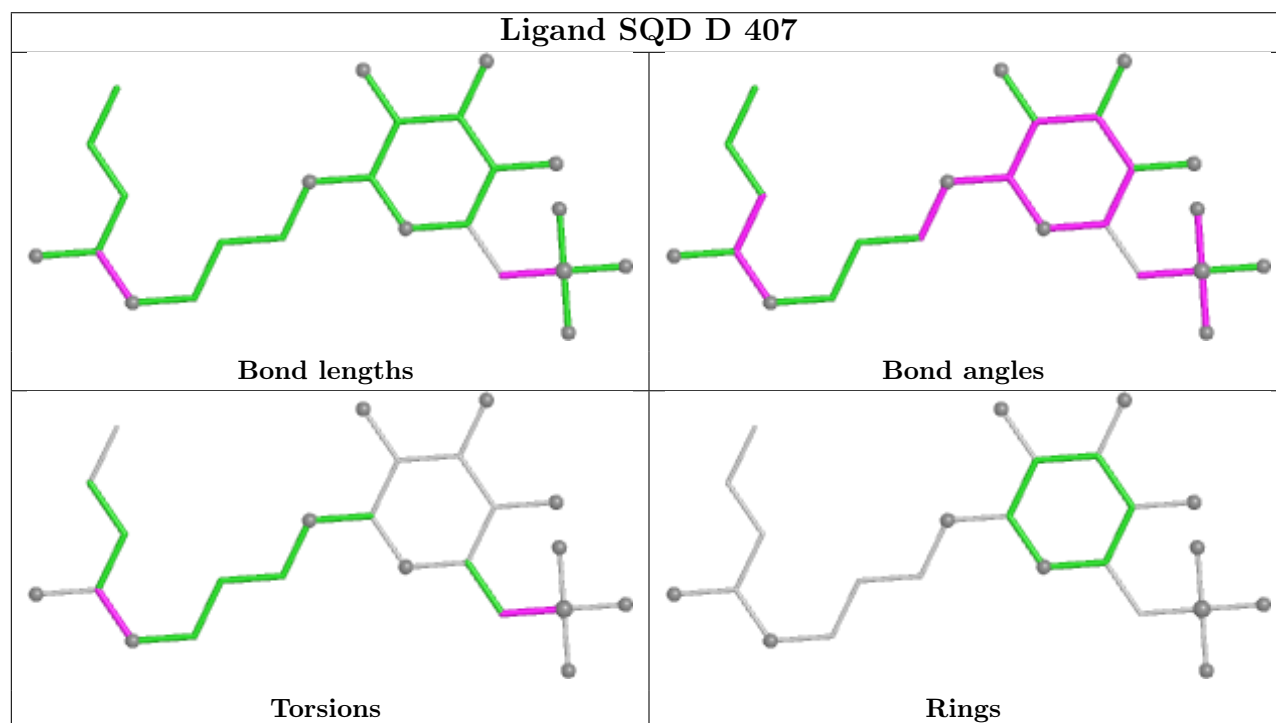
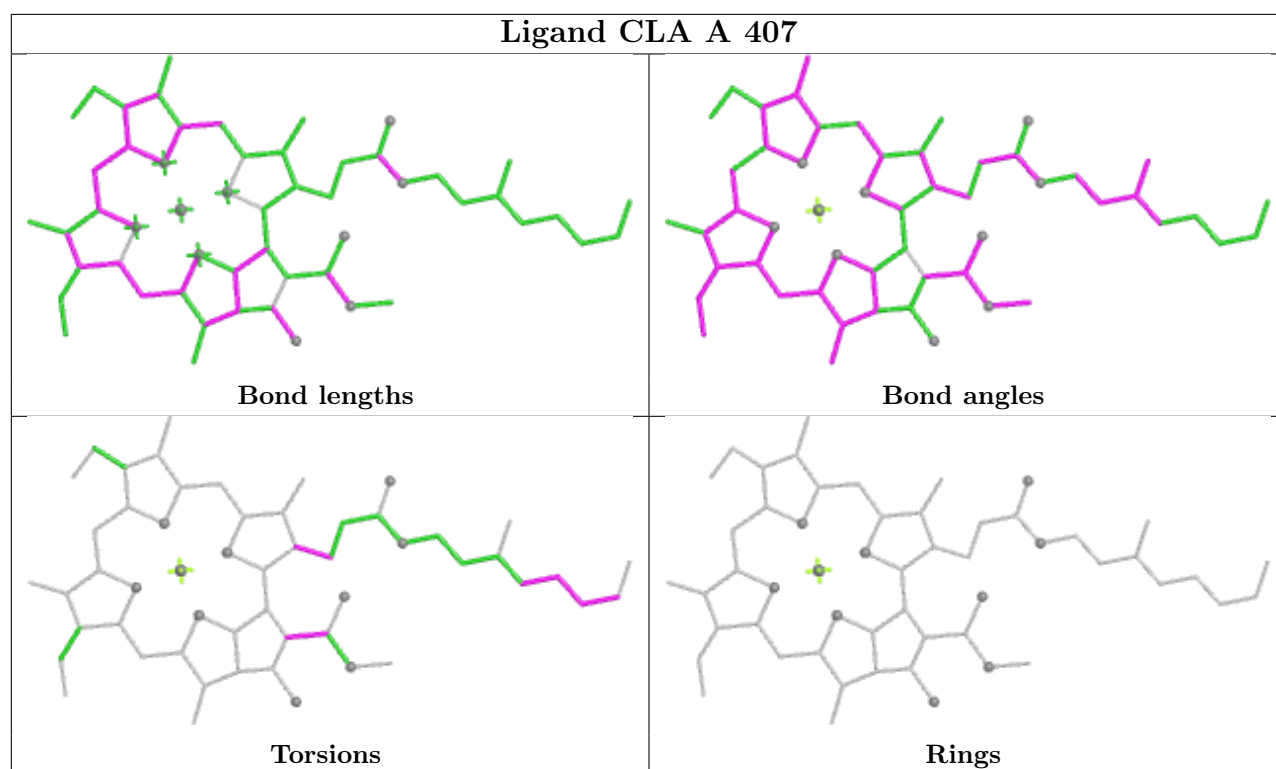
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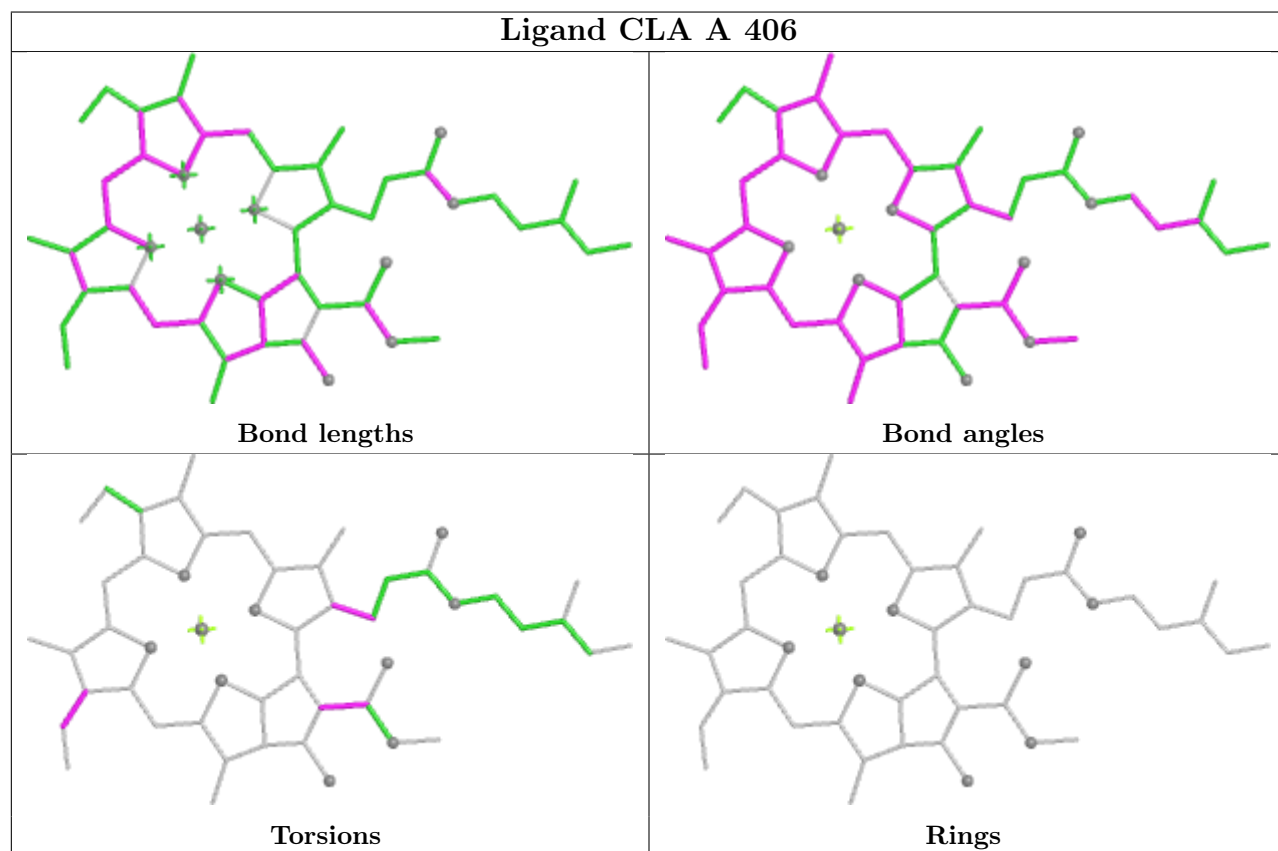
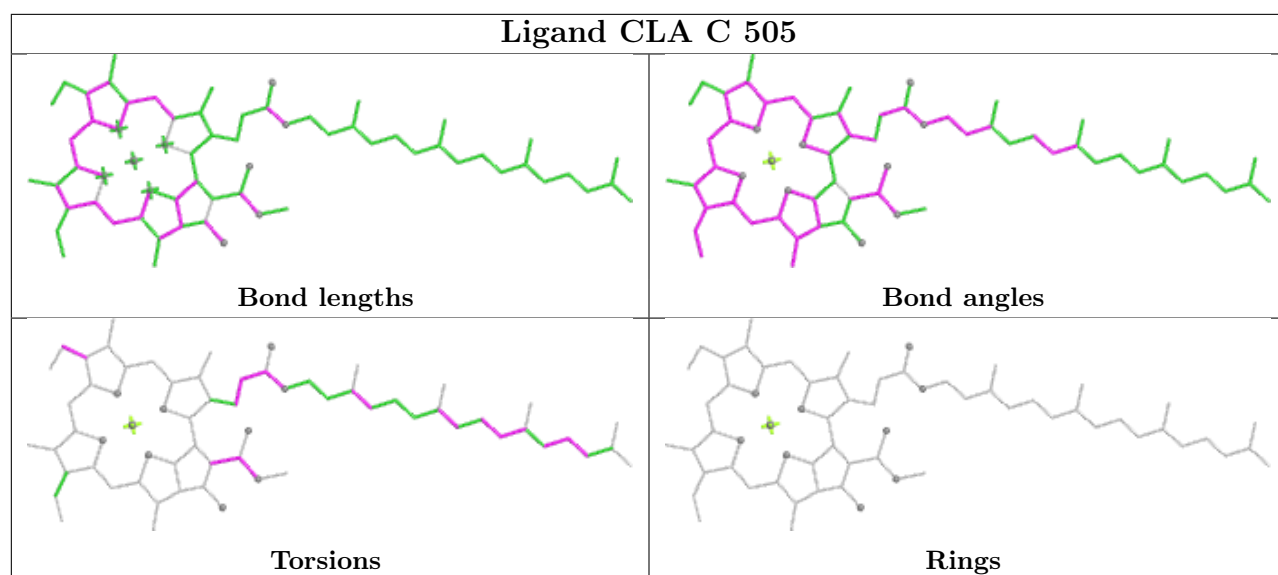


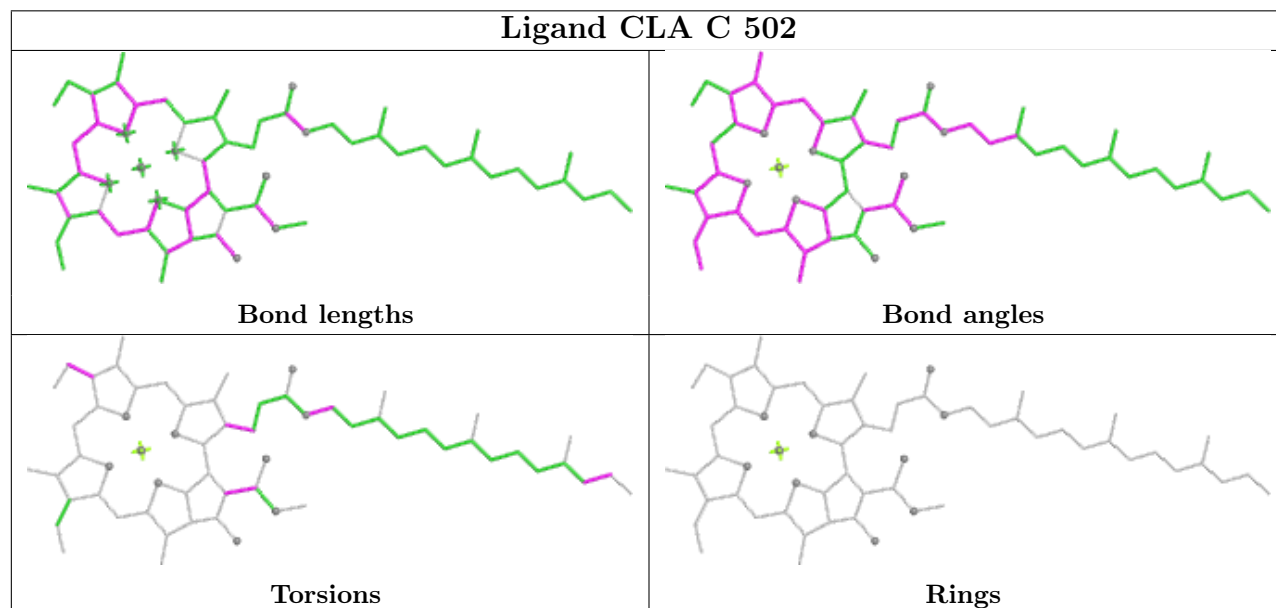
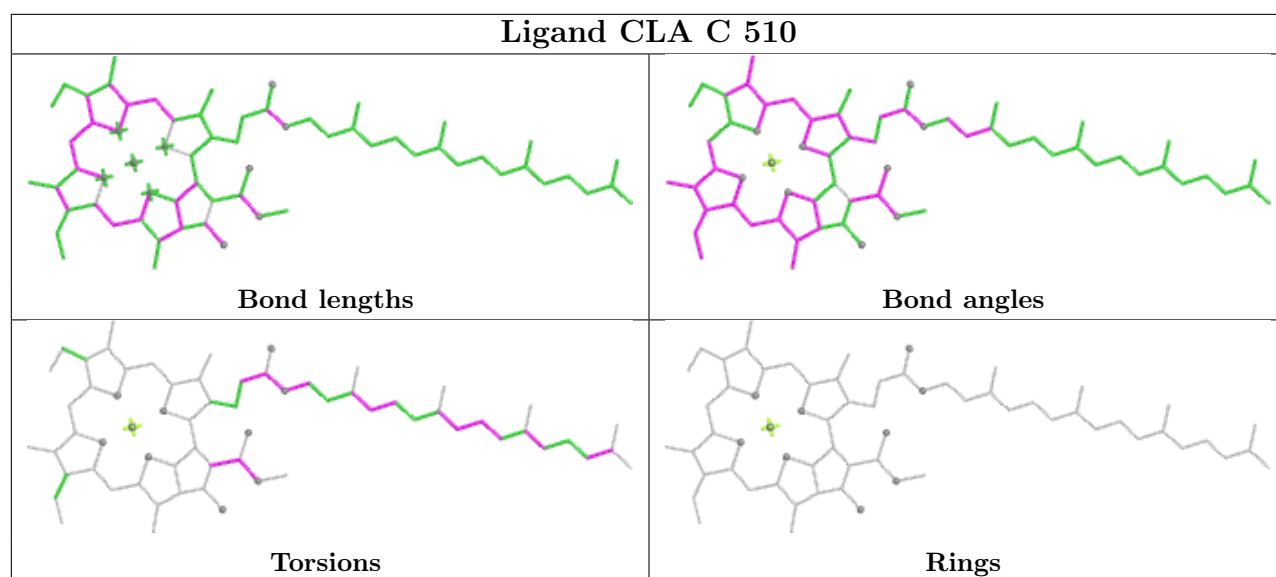
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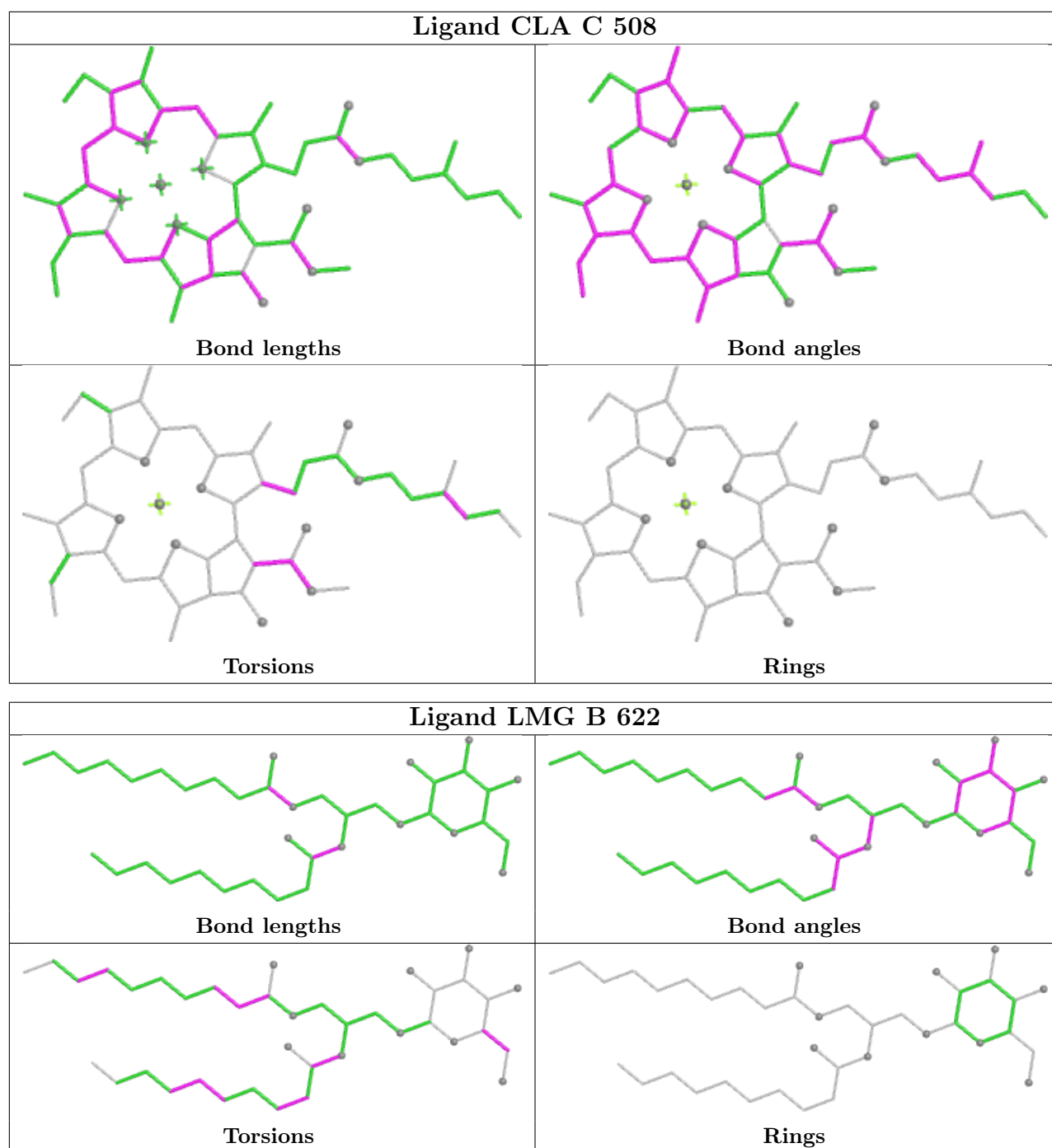


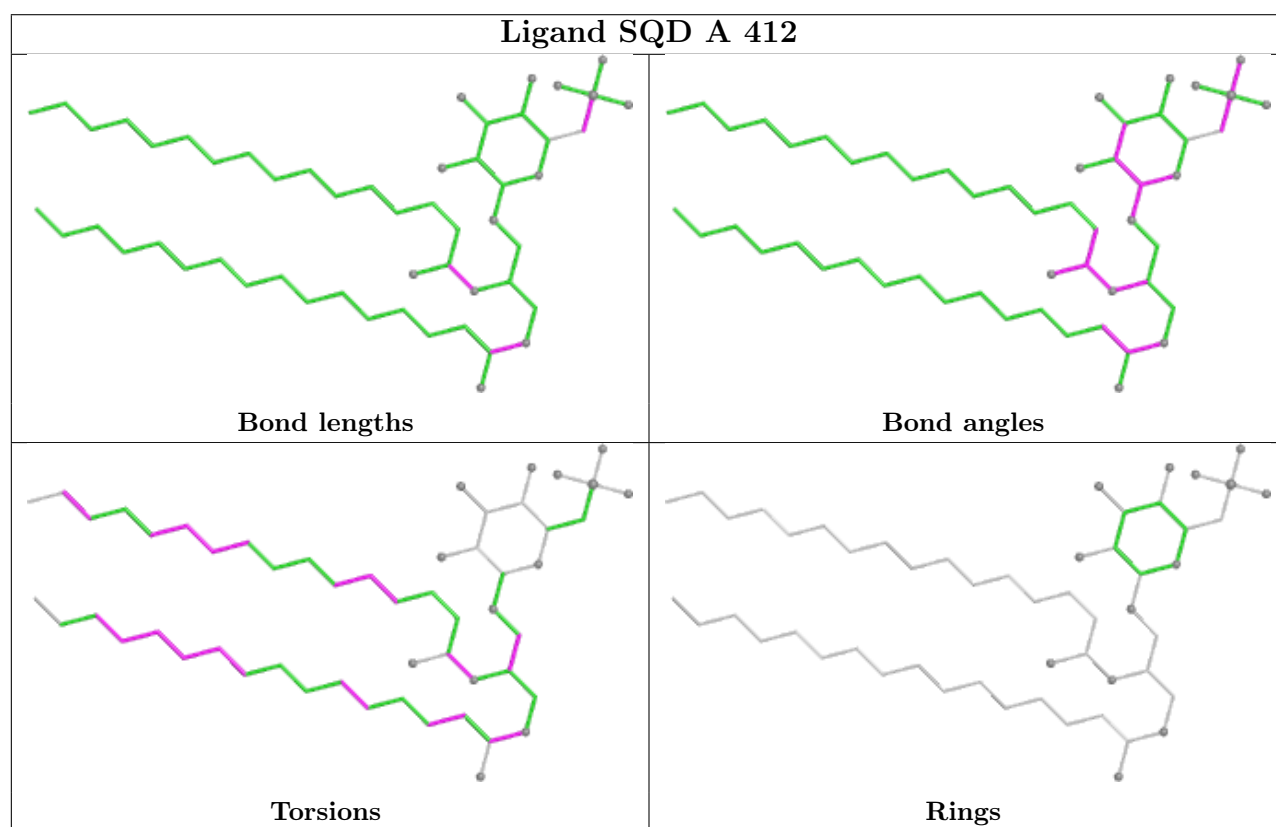
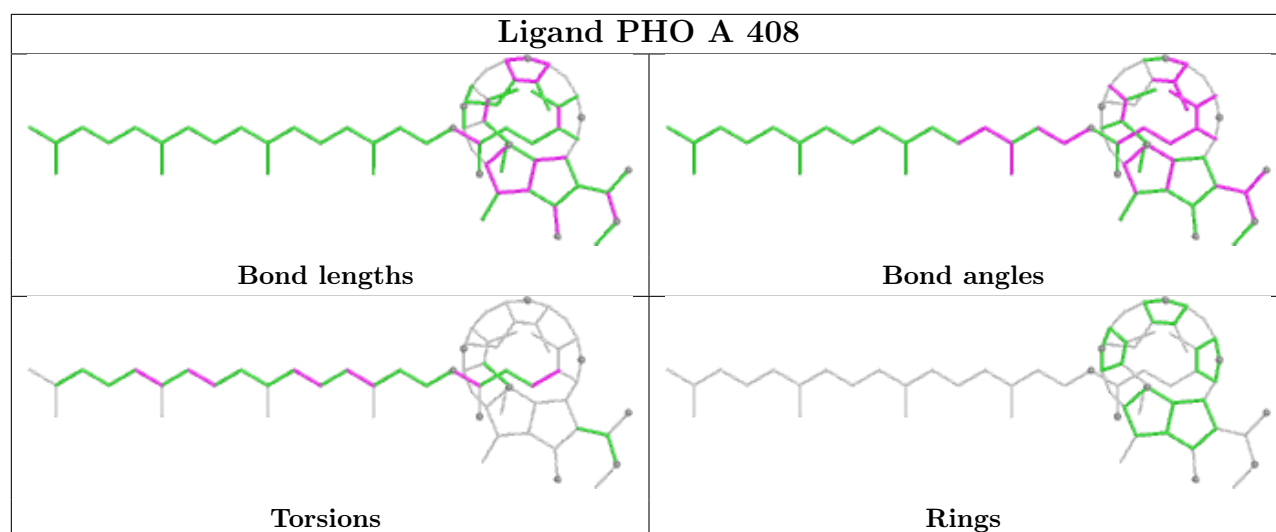


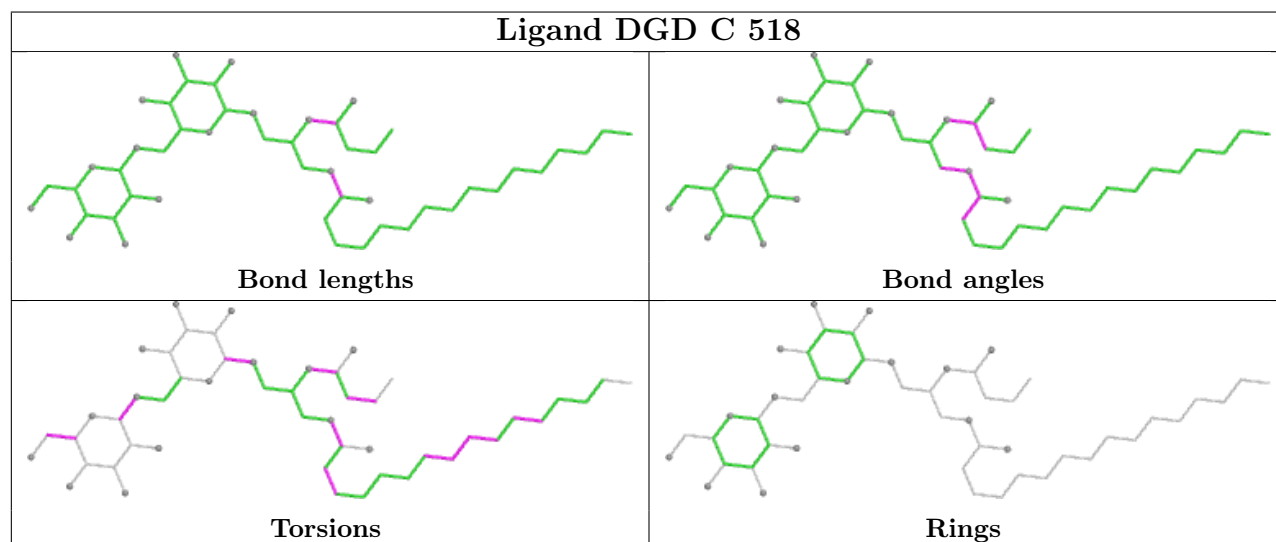
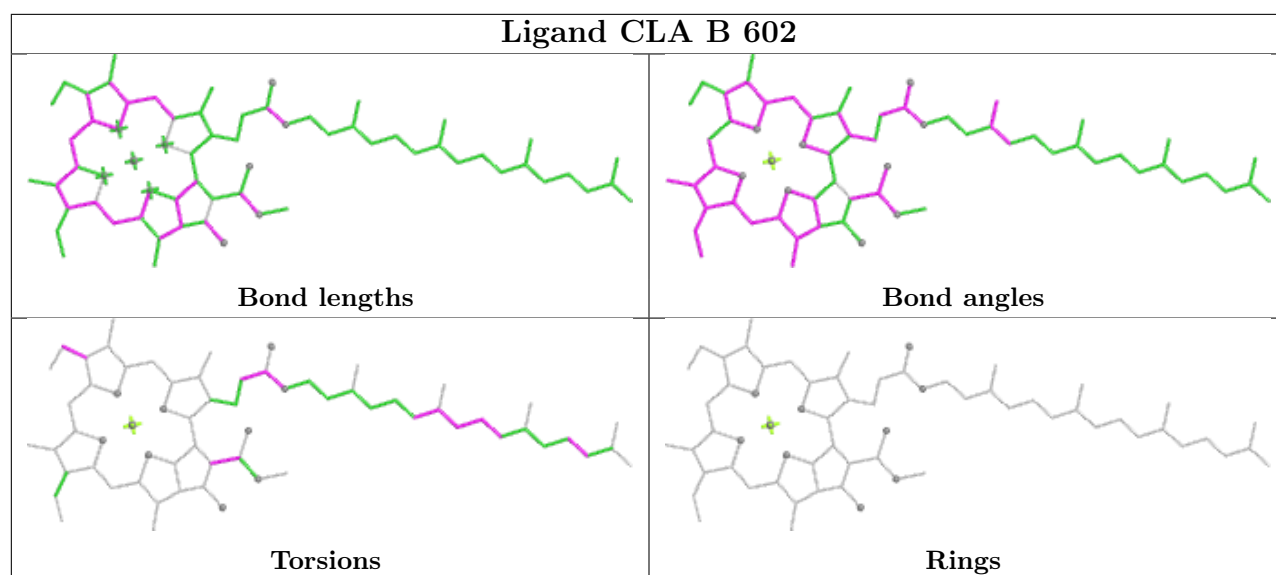


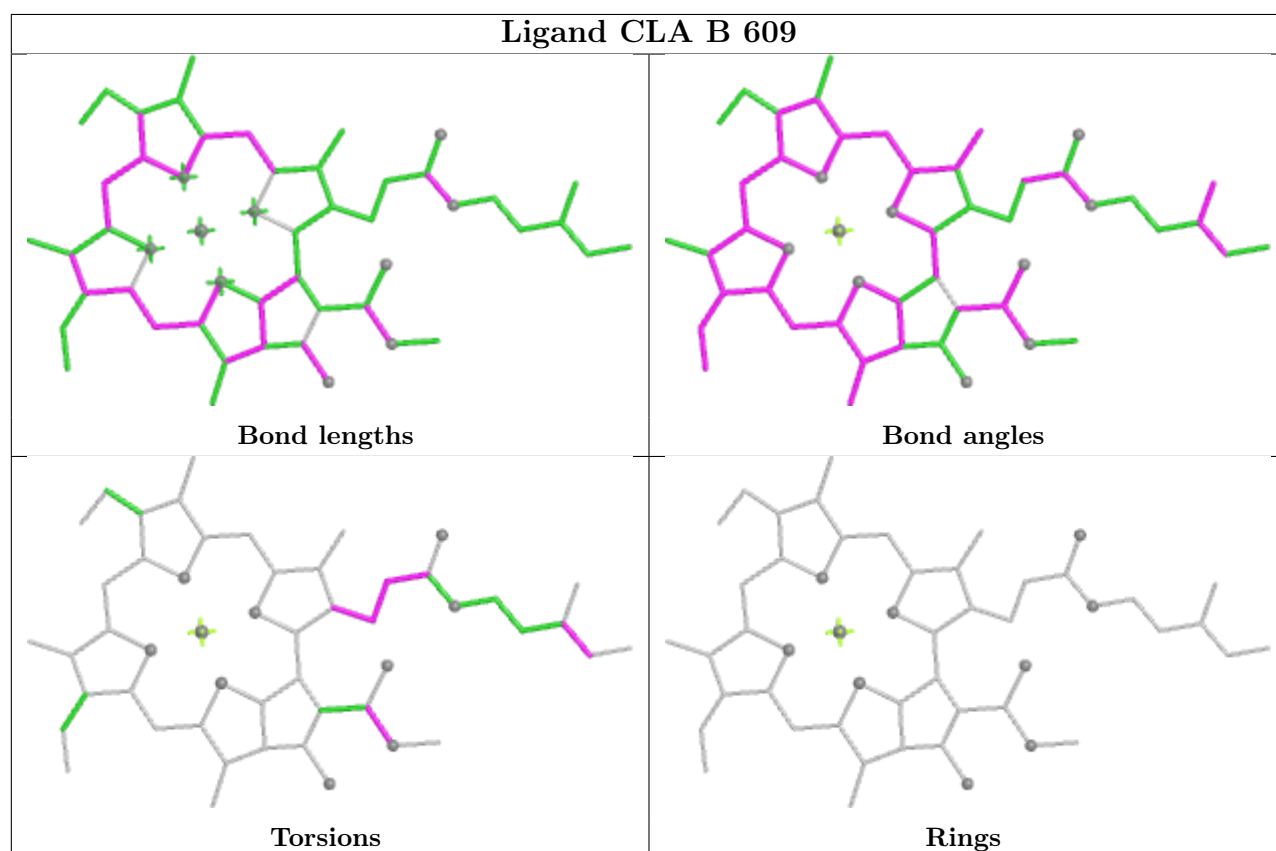
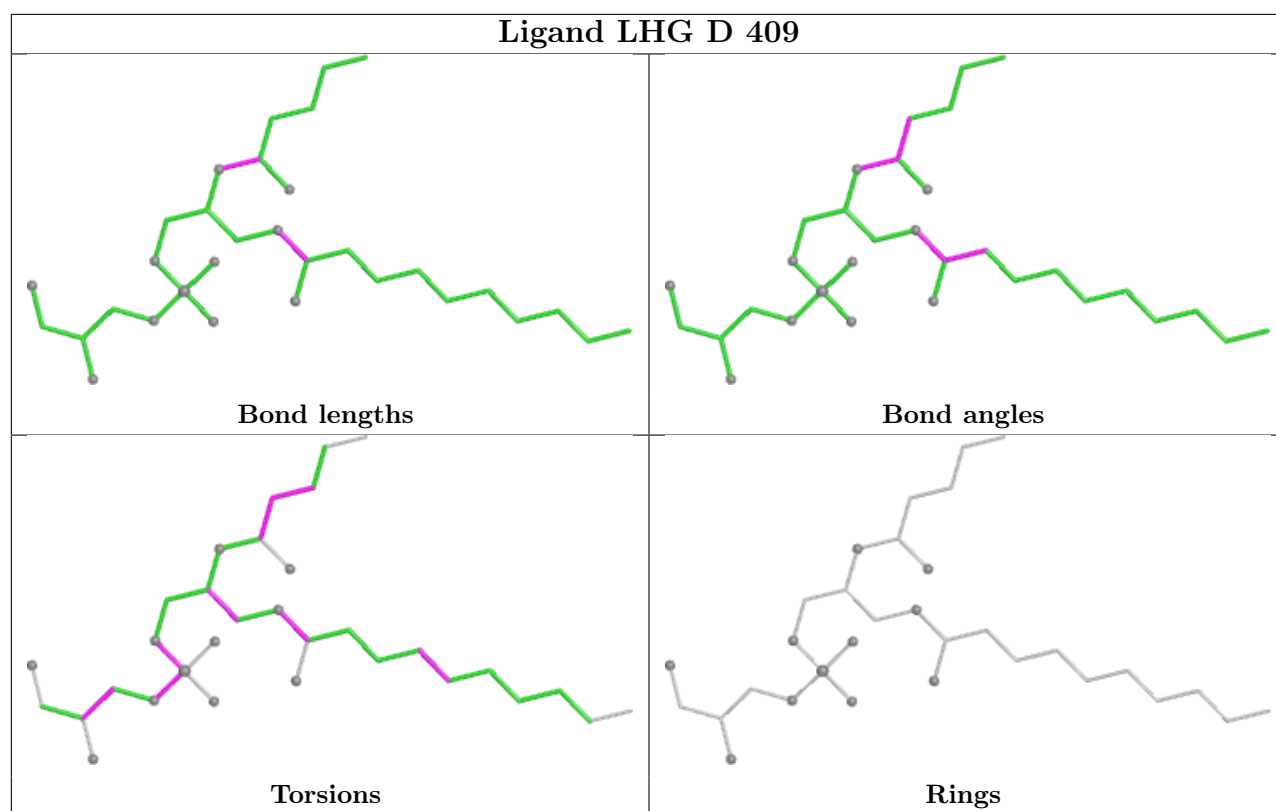


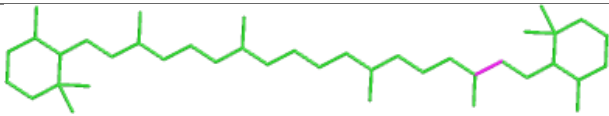
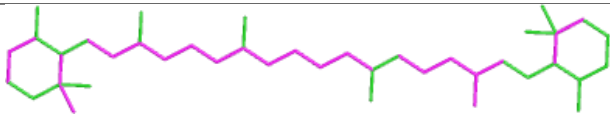
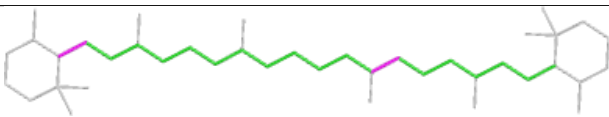
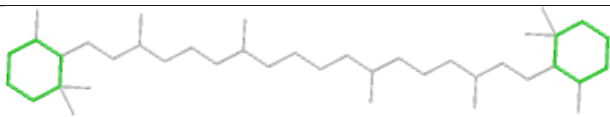


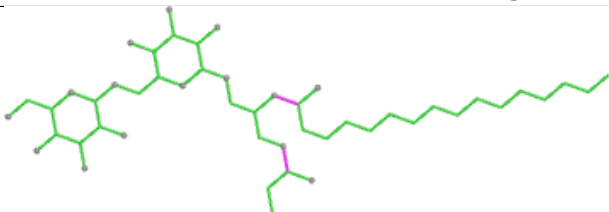
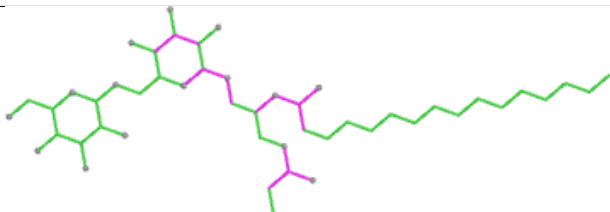
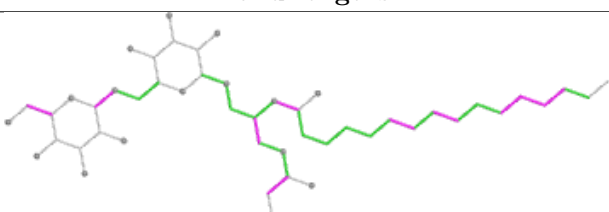
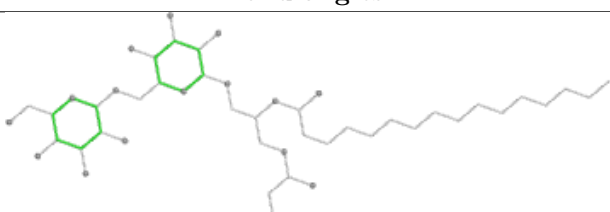


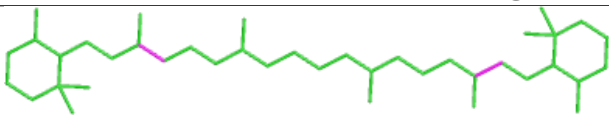
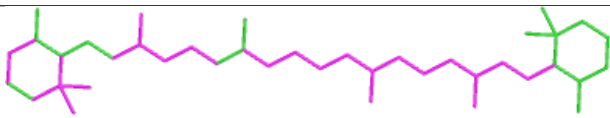
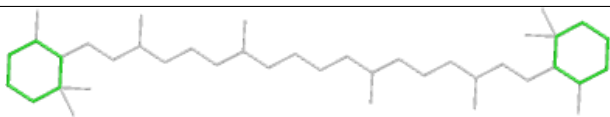


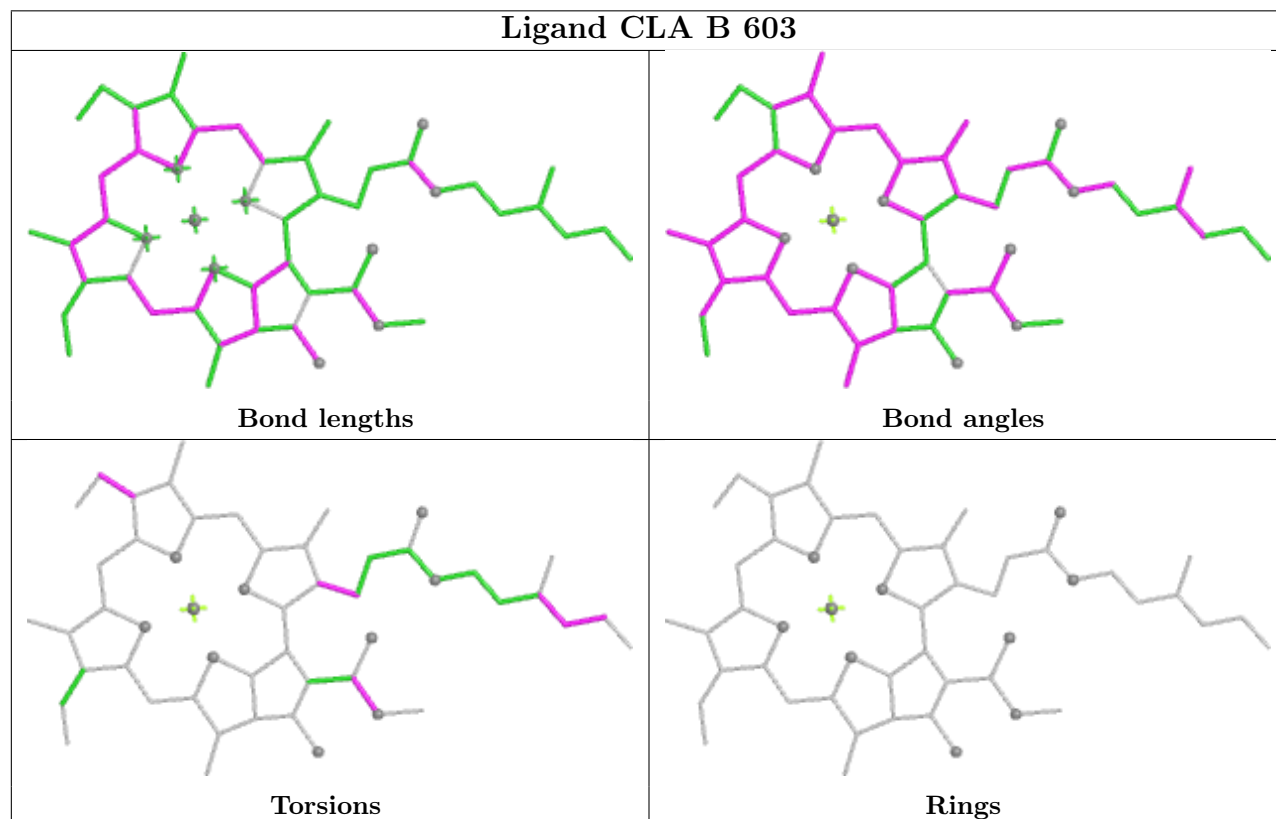
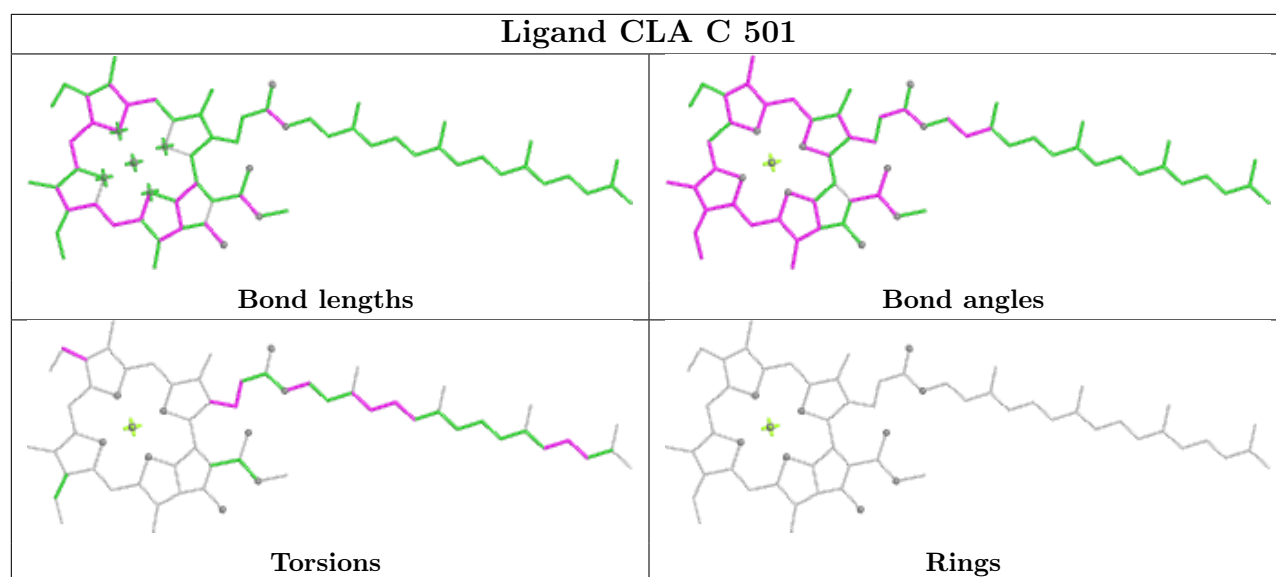




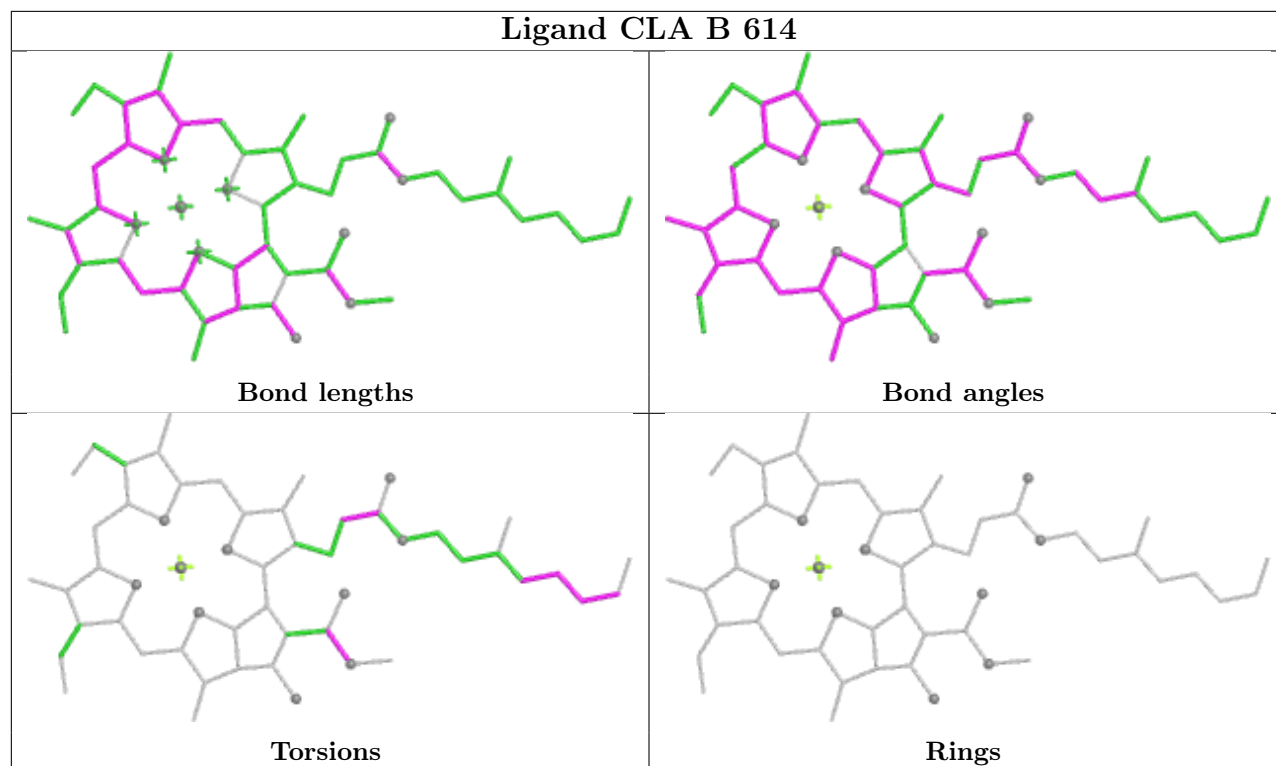
Ligand BCR B 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGD C 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

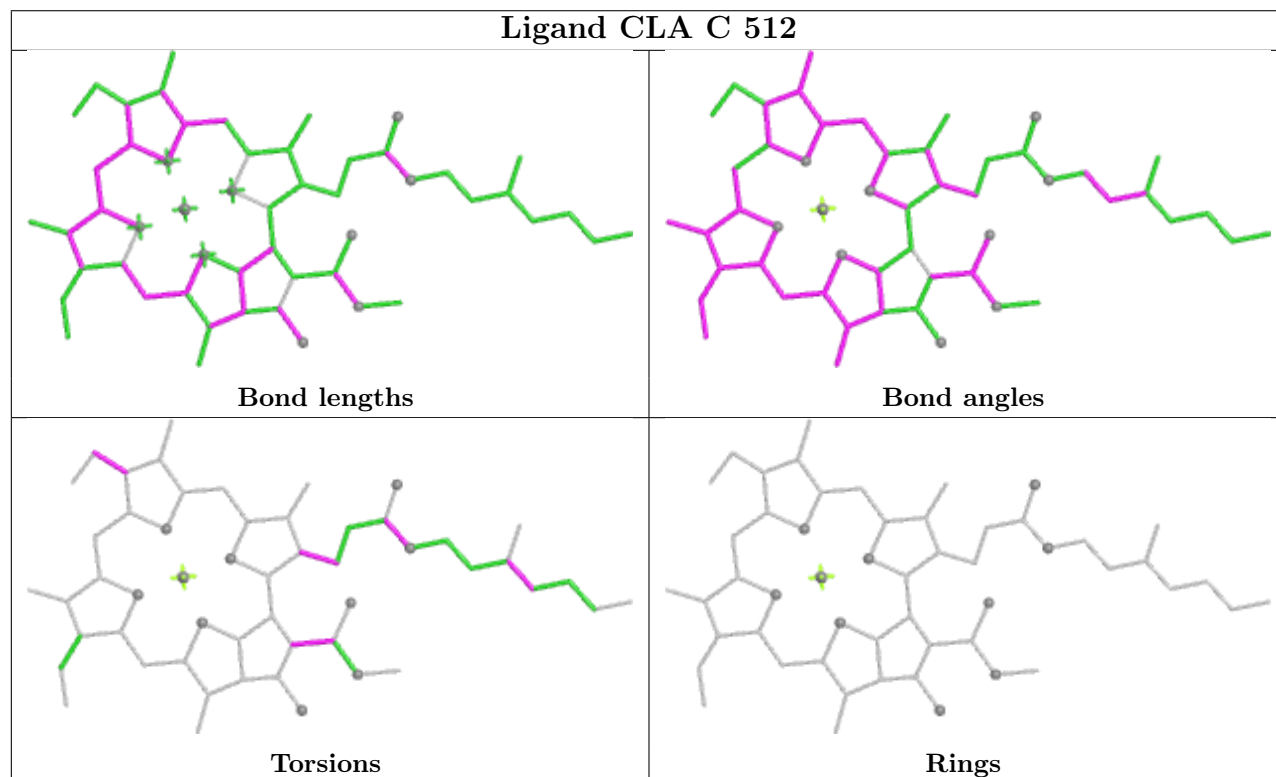
Ligand BCR C 515	
	
Bond lengths	Bond angles
	
Torsions	Rings

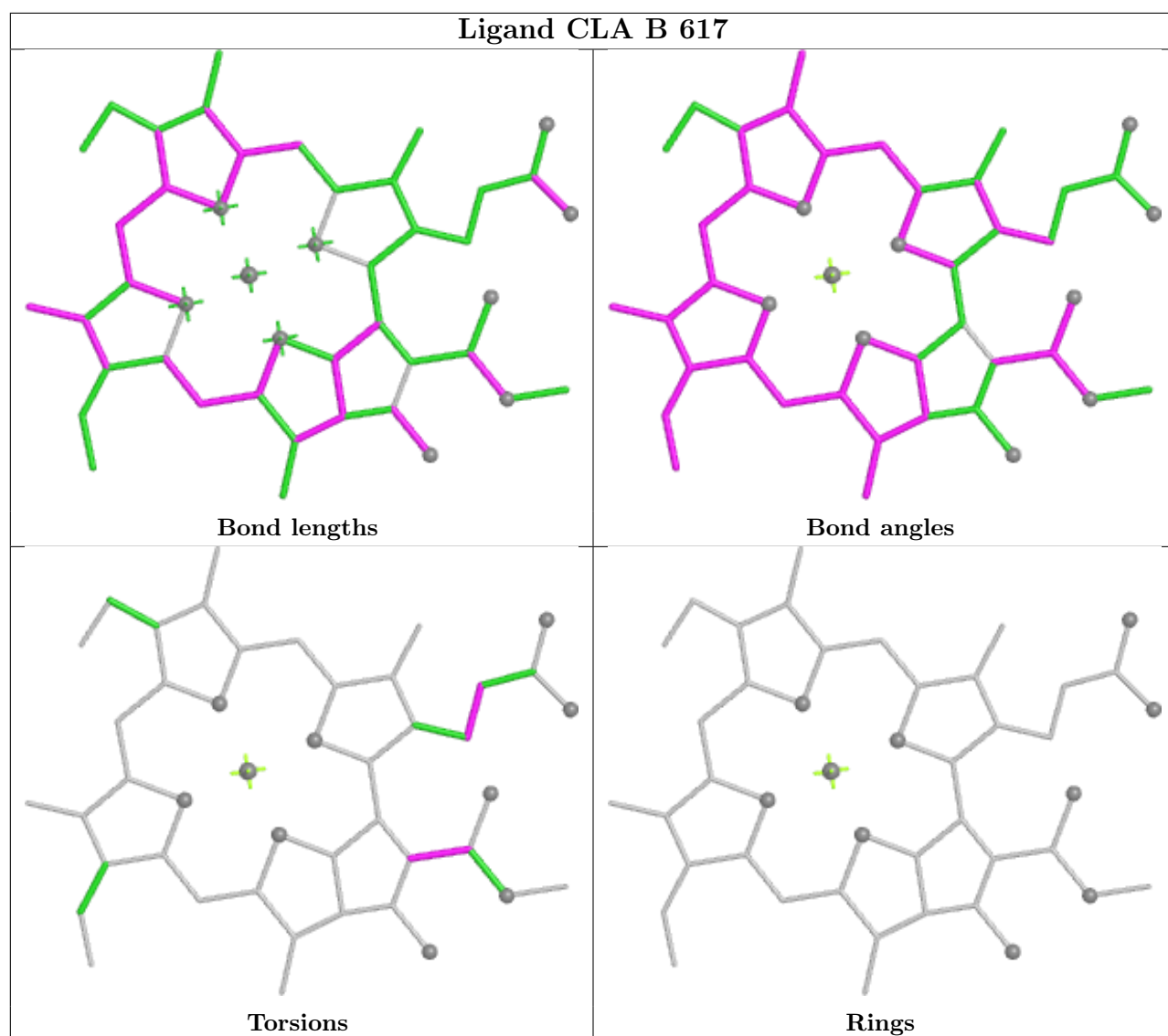


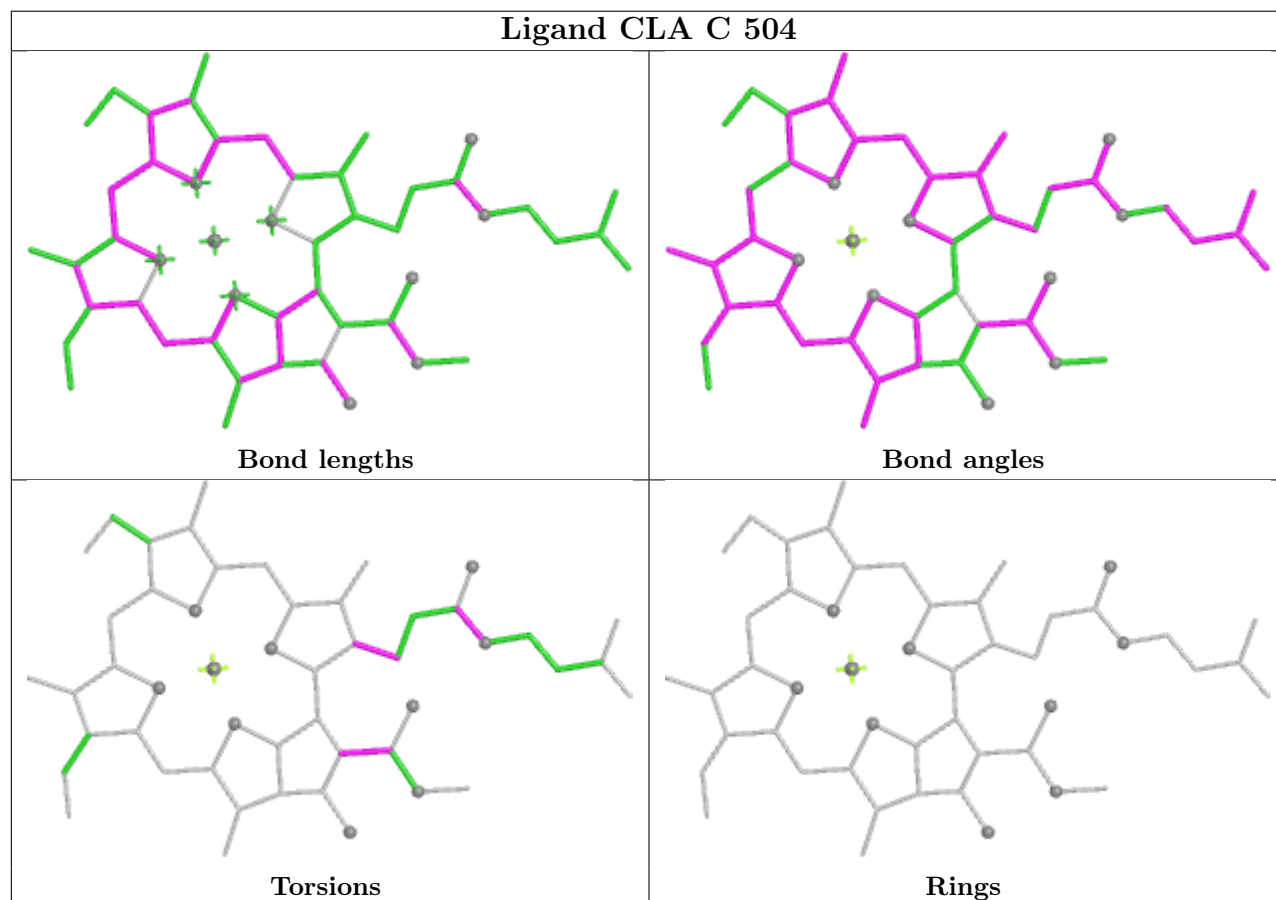
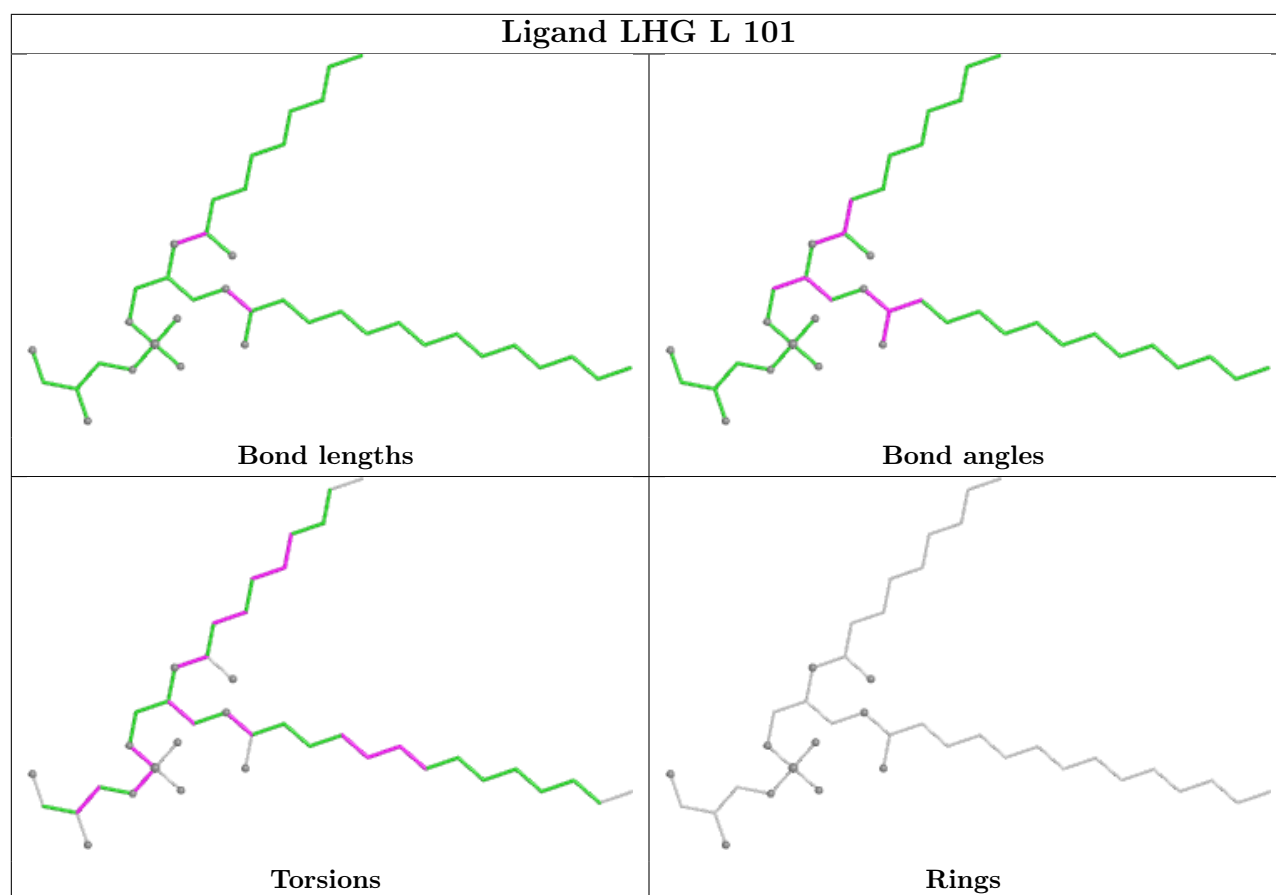
Ligand CLA B 614



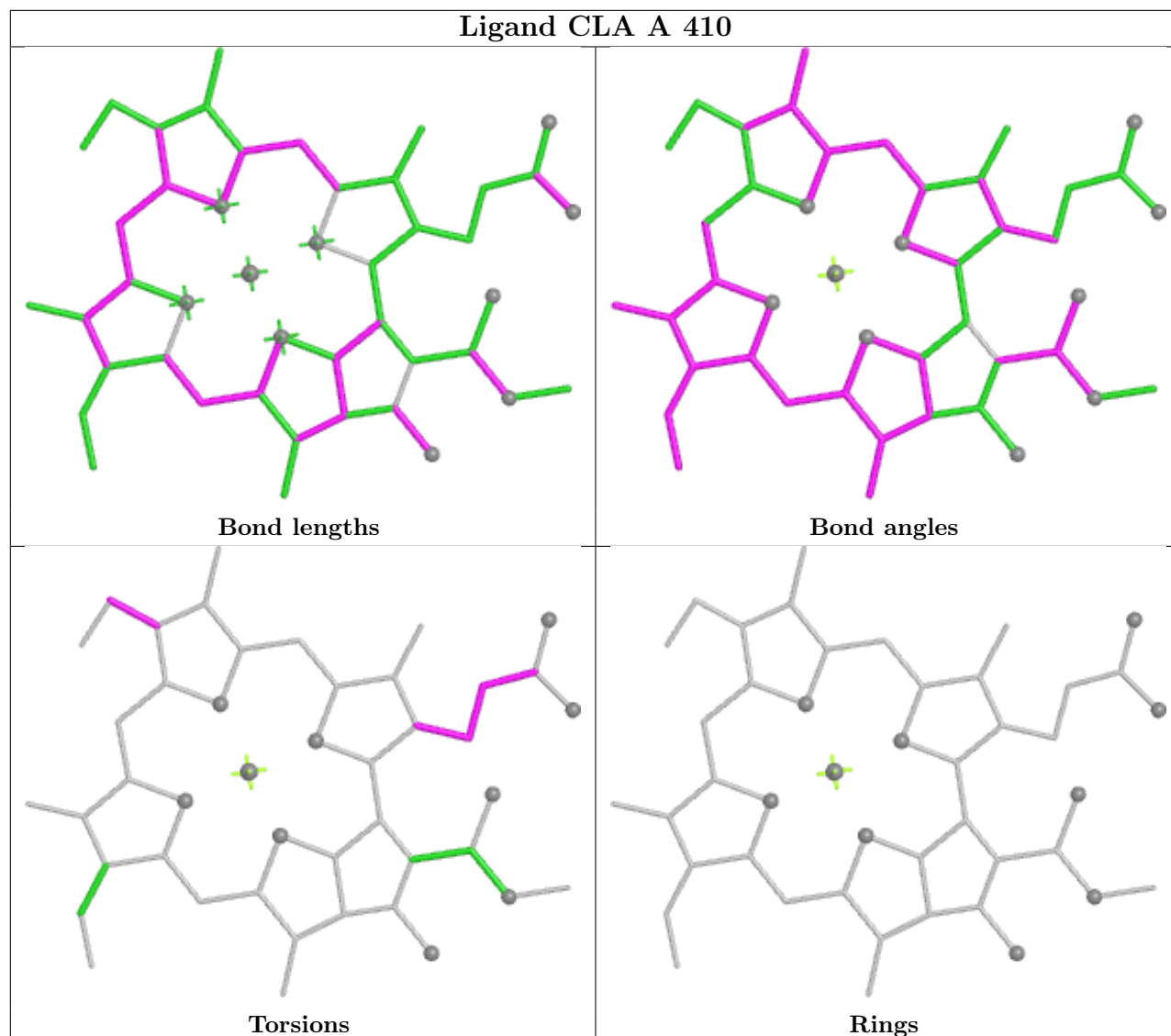
Ligand CLA C 512



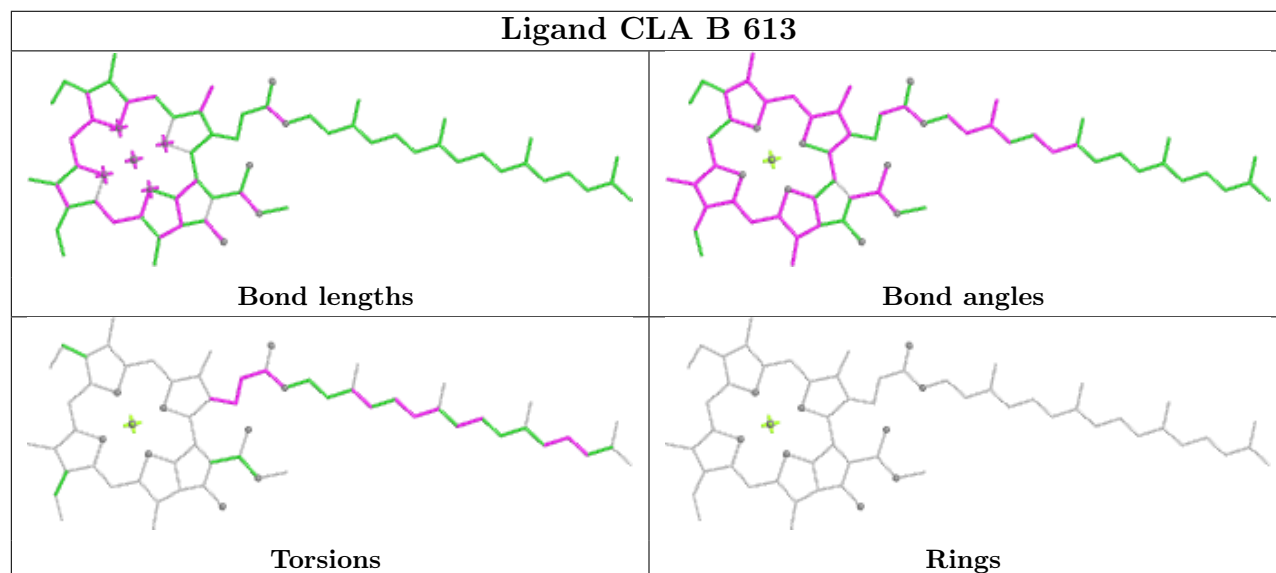




Ligand CLA A 410



Ligand CLA B 613



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

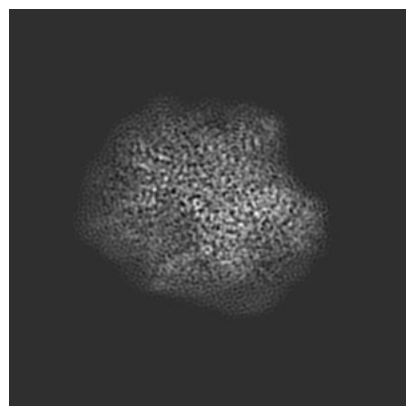
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31062. These allow visual inspection of the internal detail of the map and identification of artifacts.

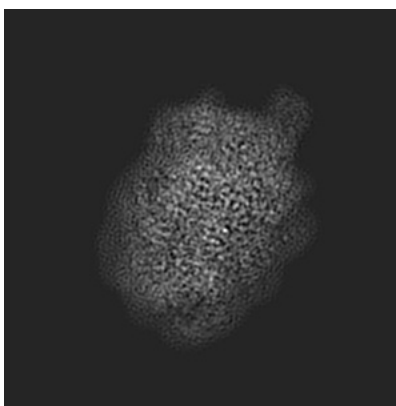
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

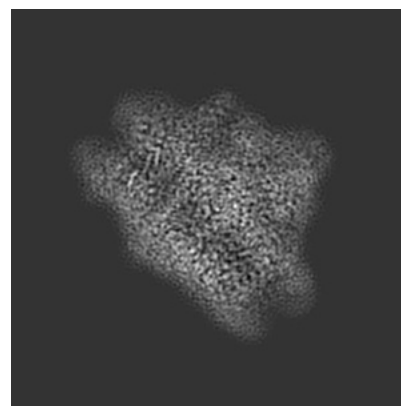
6.1.1 Primary map



X

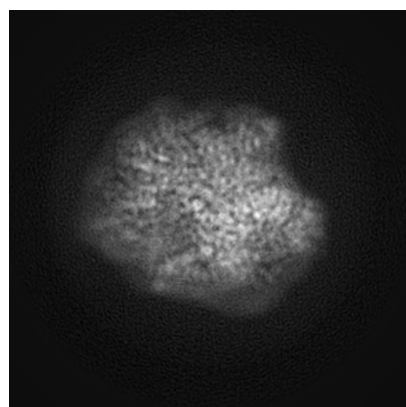


Y

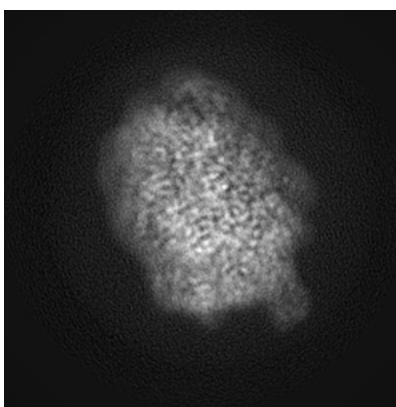


Z

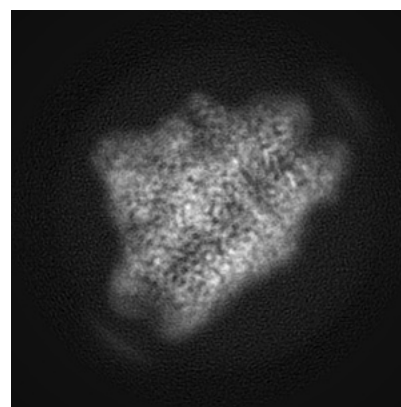
6.1.2 Raw map



X



Y

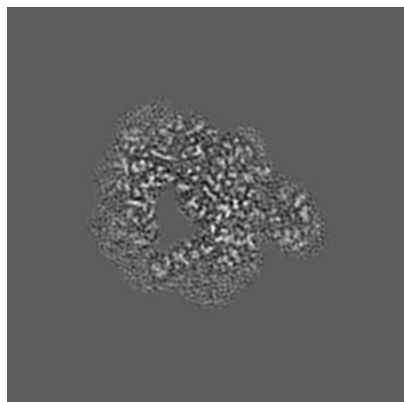


Z

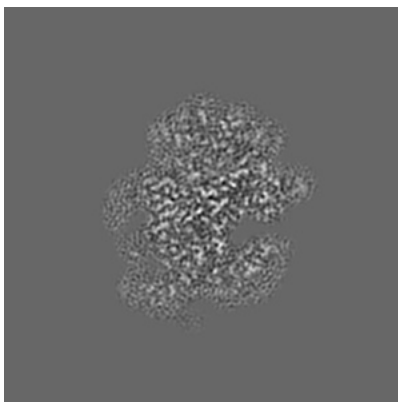
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

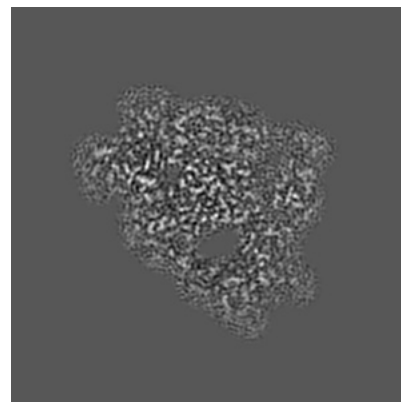
6.2.1 Primary map



X Index: 120

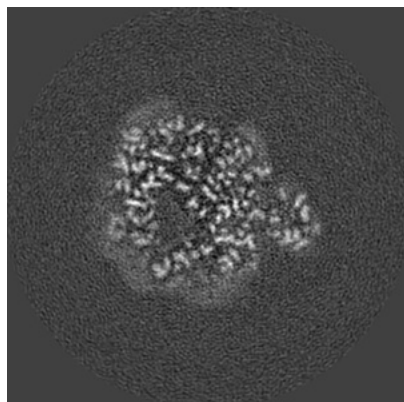


Y Index: 120

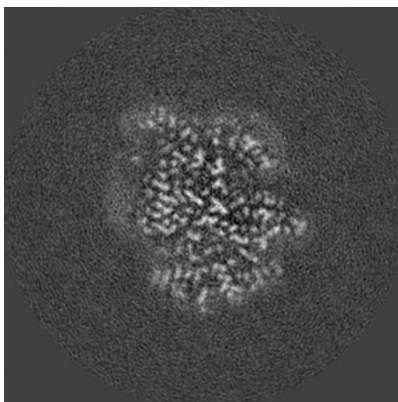


Z Index: 120

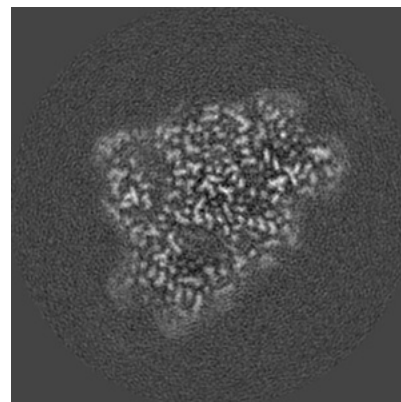
6.2.2 Raw map



X Index: 120



Y Index: 120

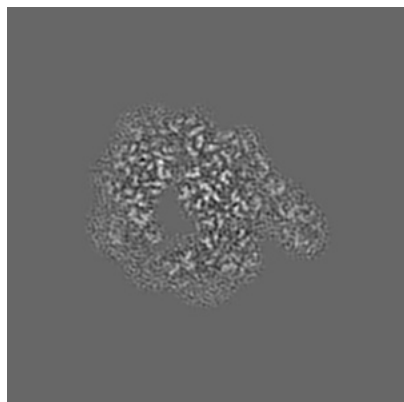


Z Index: 120

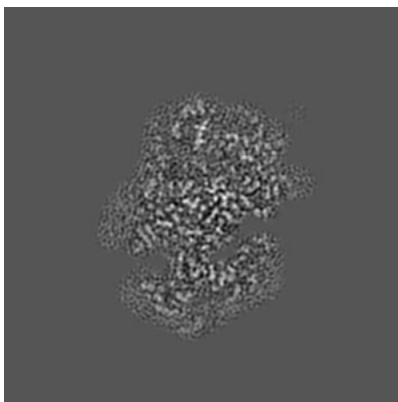
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

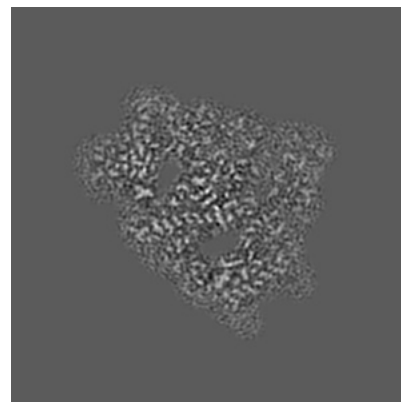
6.3.1 Primary map



X Index: 122

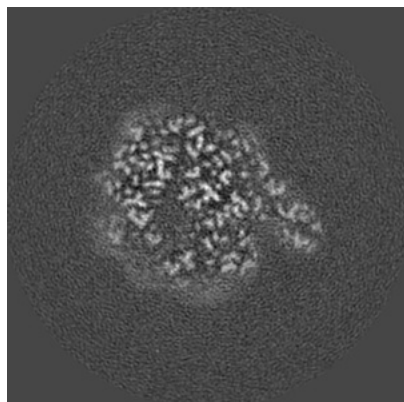


Y Index: 127

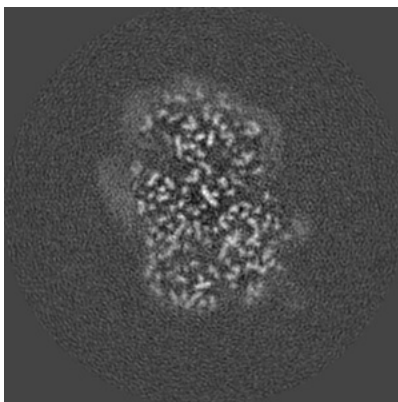


Z Index: 124

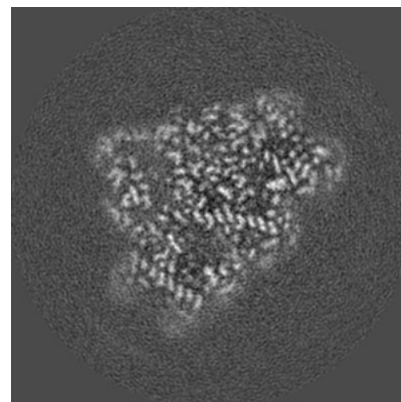
6.3.2 Raw map



X Index: 118



Y Index: 129

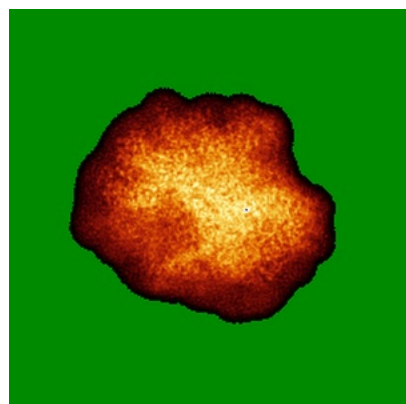


Z Index: 121

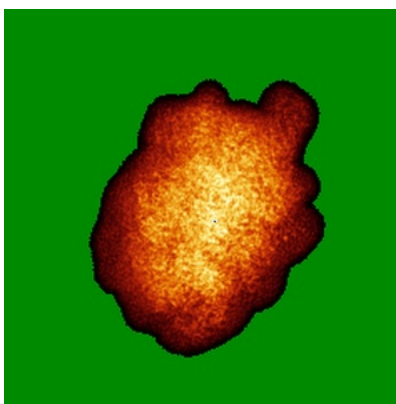
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

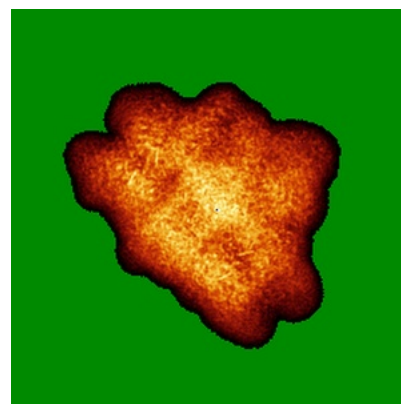
6.4.1 Primary map



X

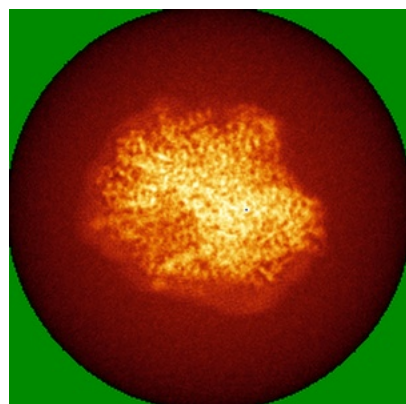


Y

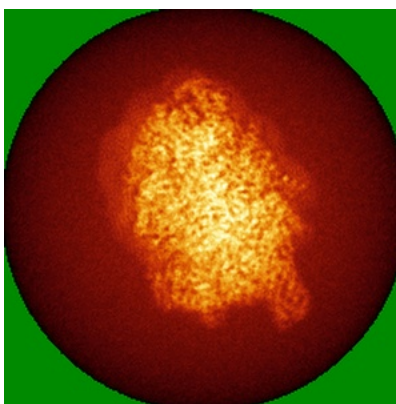


Z

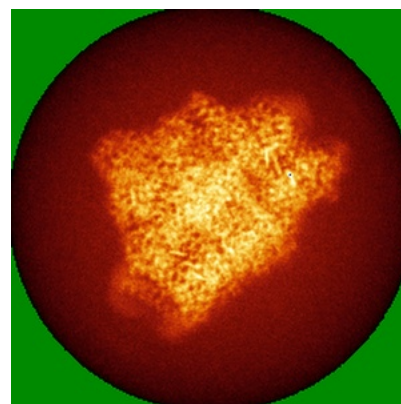
6.4.2 Raw map



X



Y

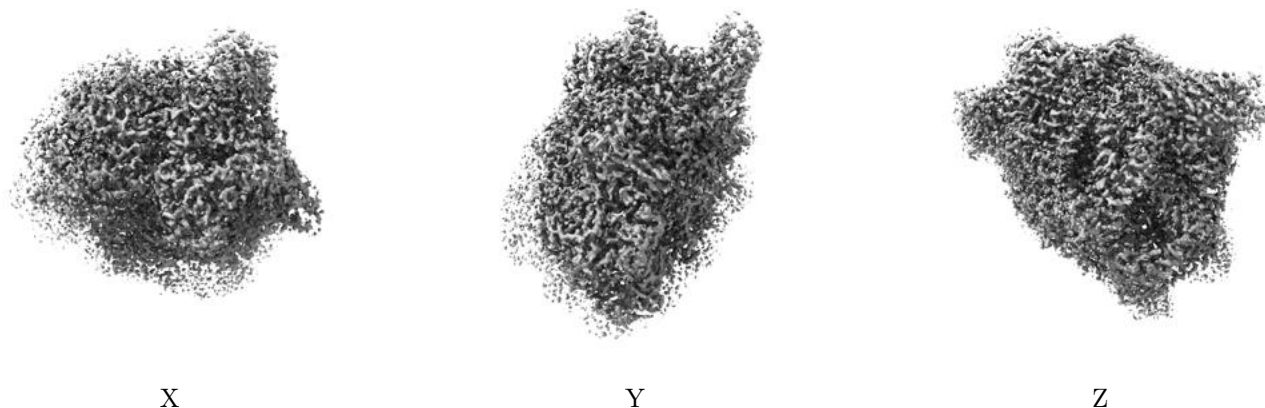


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

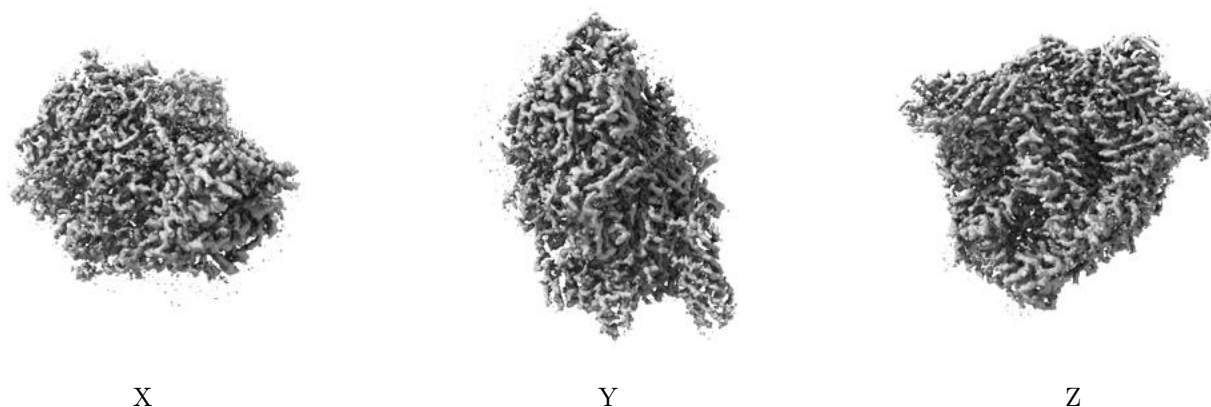
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0316. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

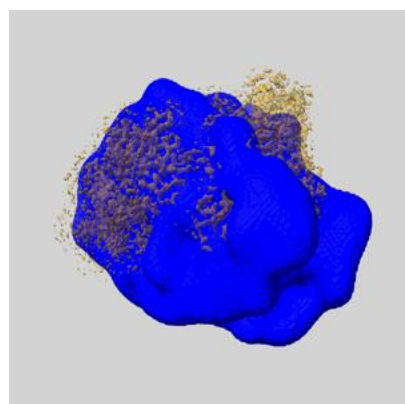
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

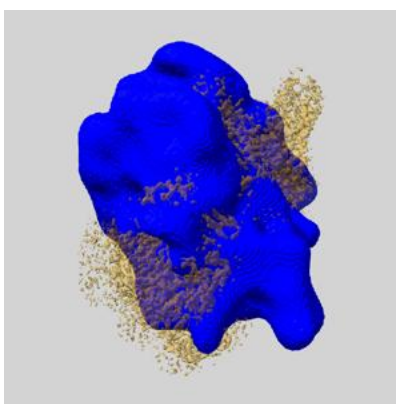
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

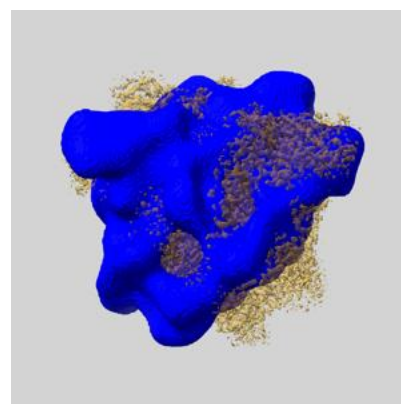
6.6.1 emd_31062_msk_1.map [i](#)



X



Y

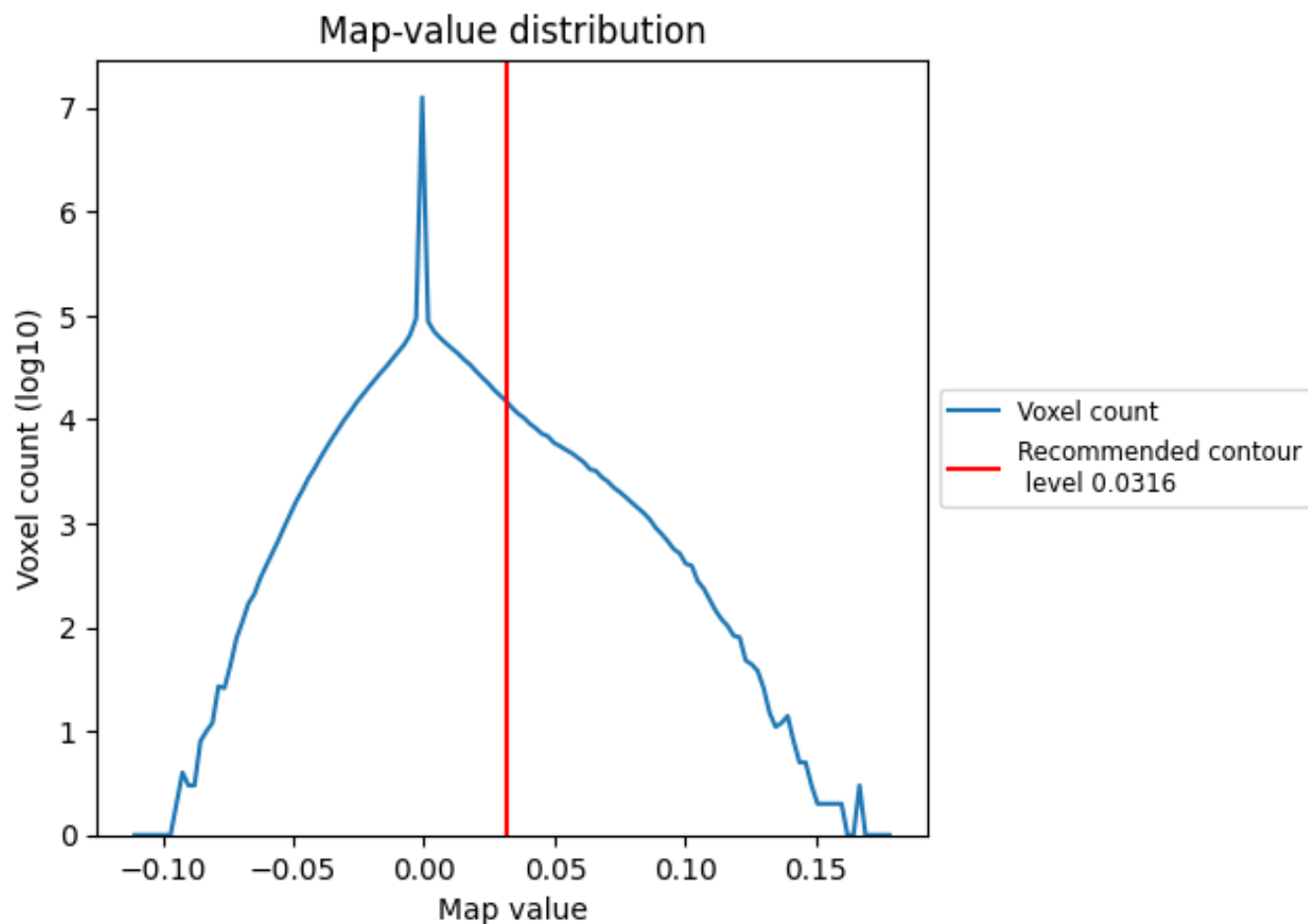


Z

7 Map analysis [i](#)

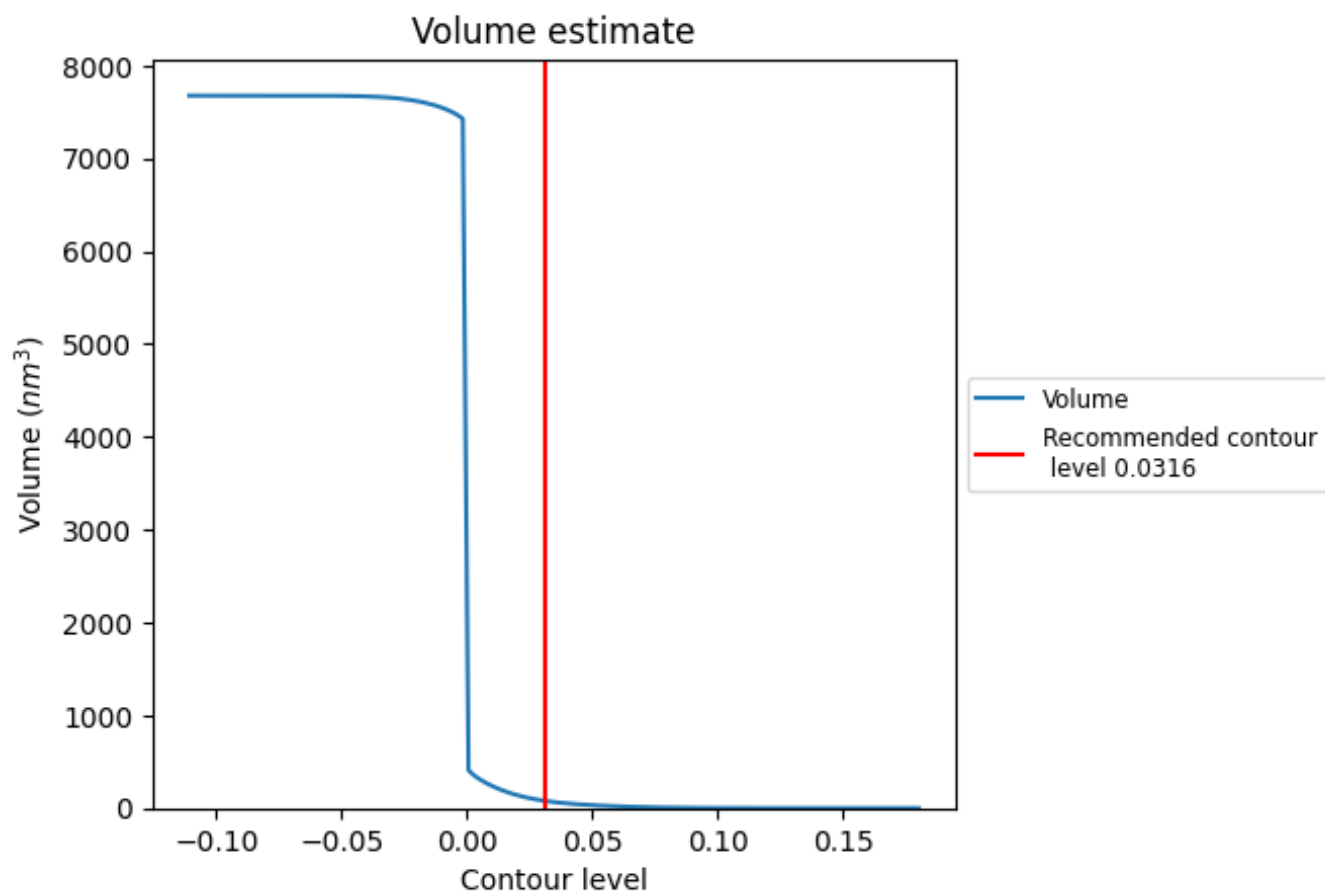
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

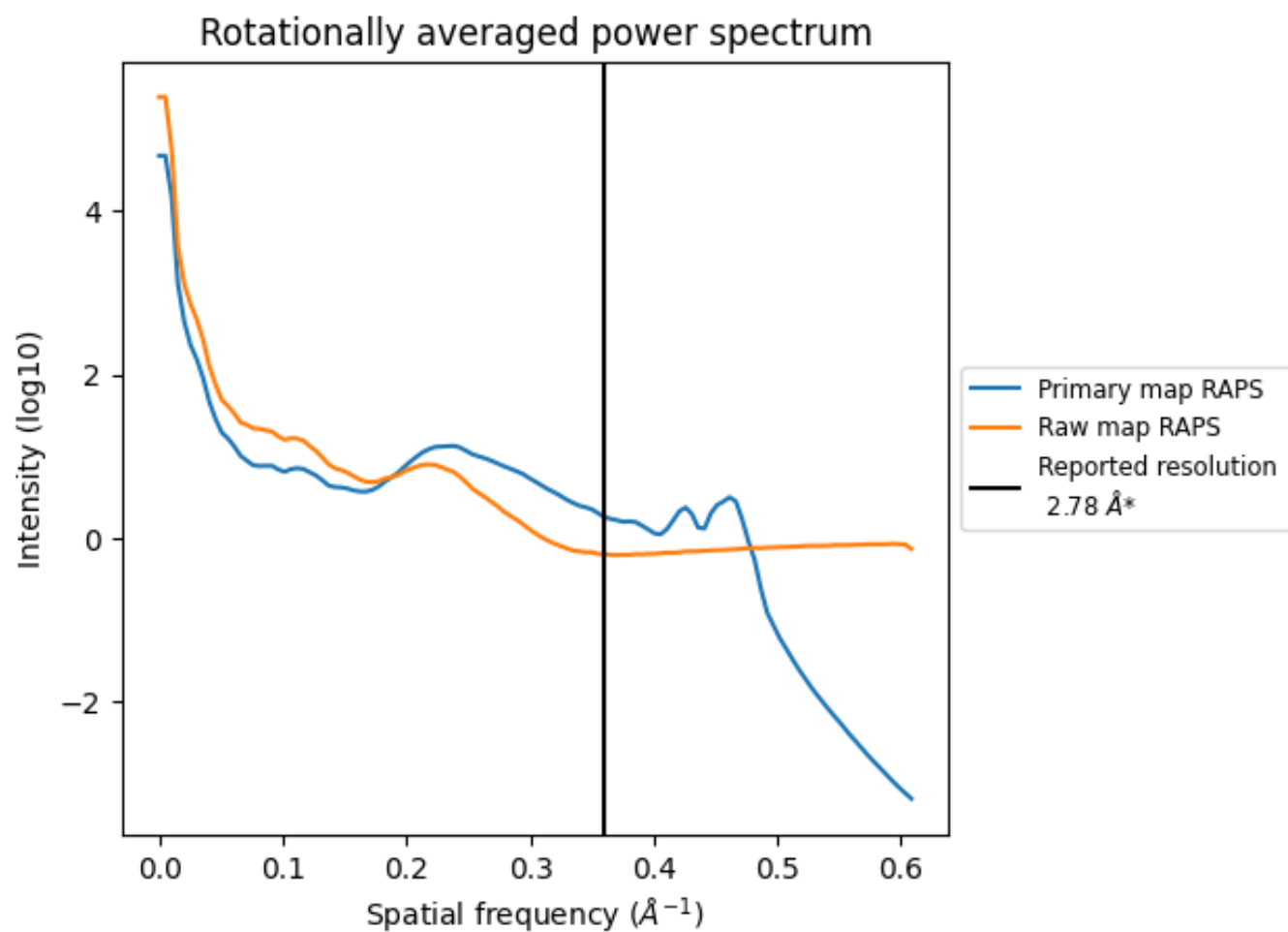
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 77 nm³; this corresponds to an approximate mass of 69 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

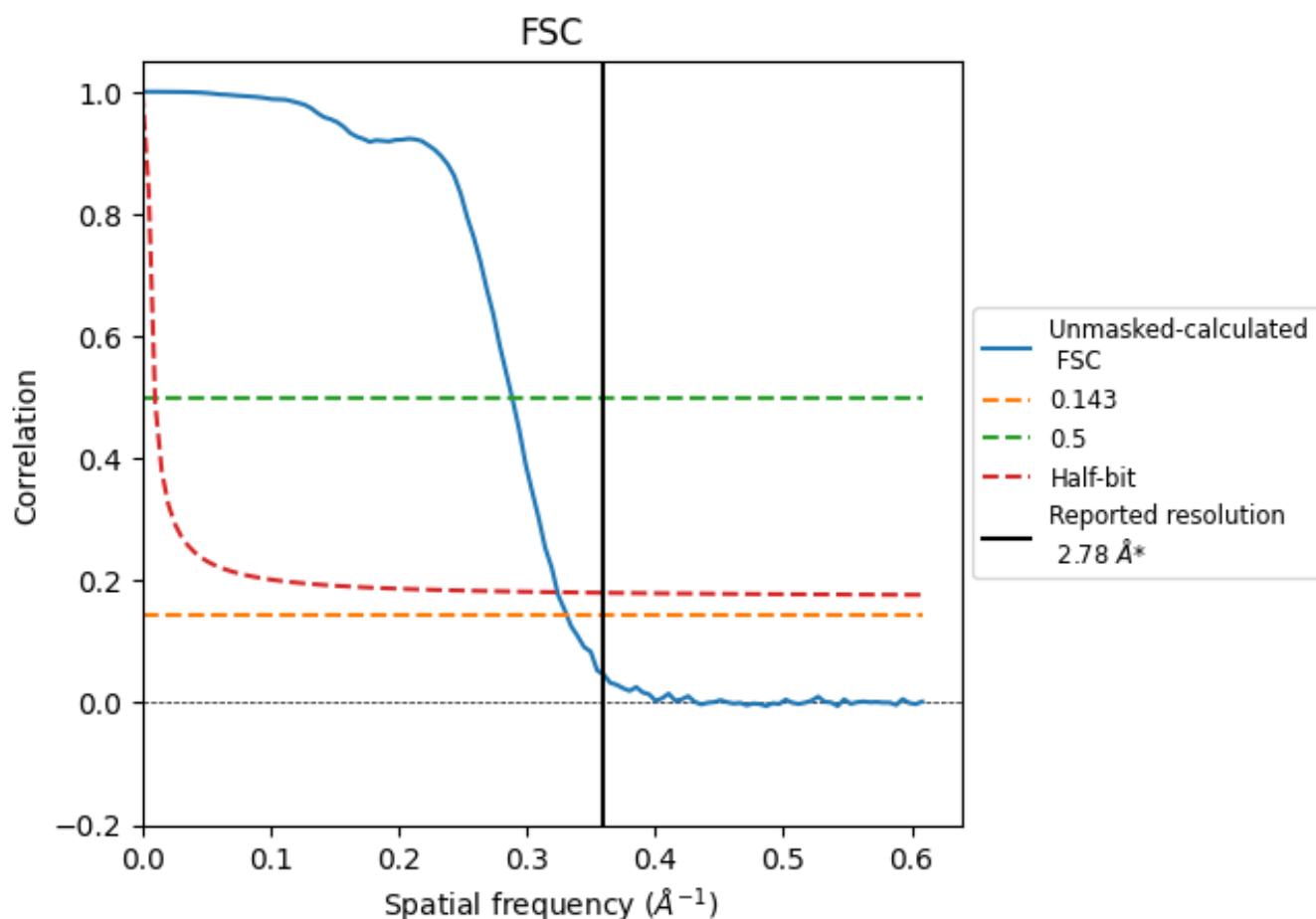


*Reported resolution corresponds to spatial frequency of 0.360 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.360 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

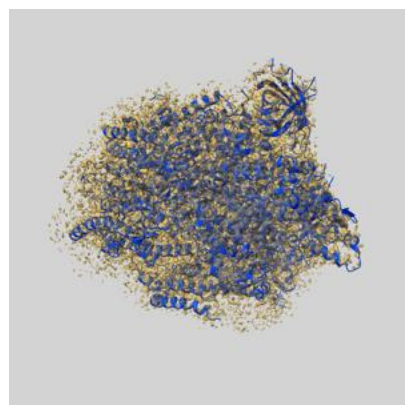
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.78	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.02	3.47	3.09

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

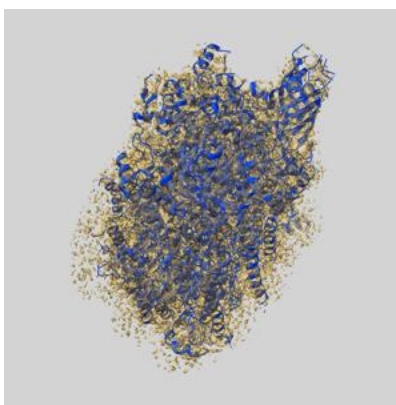
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31062 and PDB model 7EDA. Per-residue inclusion information can be found in section 3 on page 18.

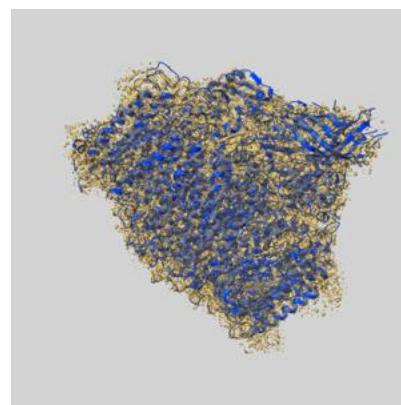
9.1 Map-model overlay [i](#)



X



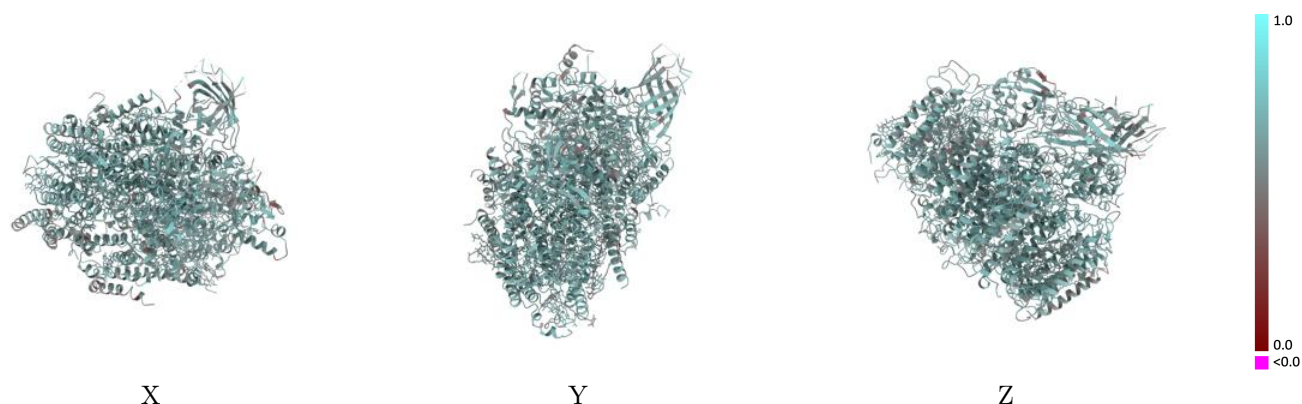
Y



Z

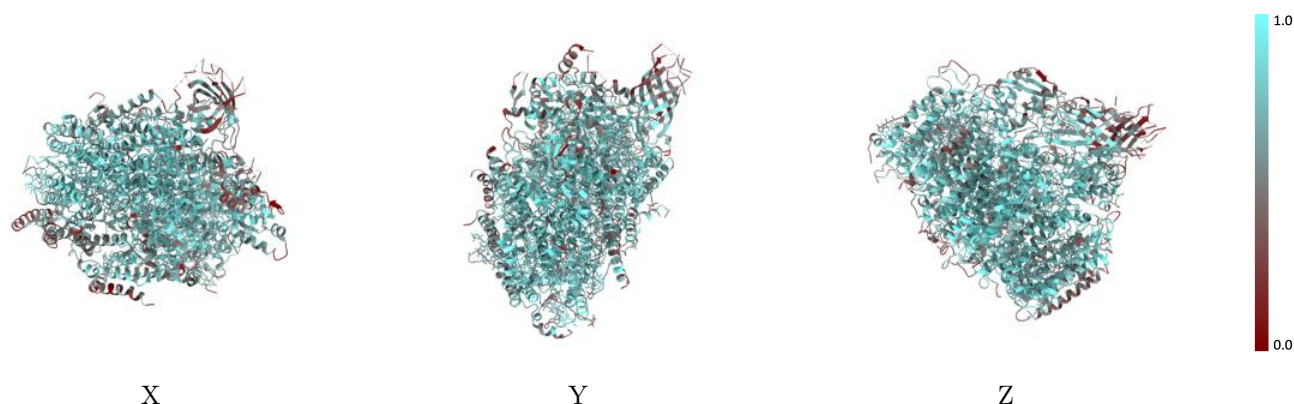
The images above show the 3D surface view of the map at the recommended contour level 0.0316 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



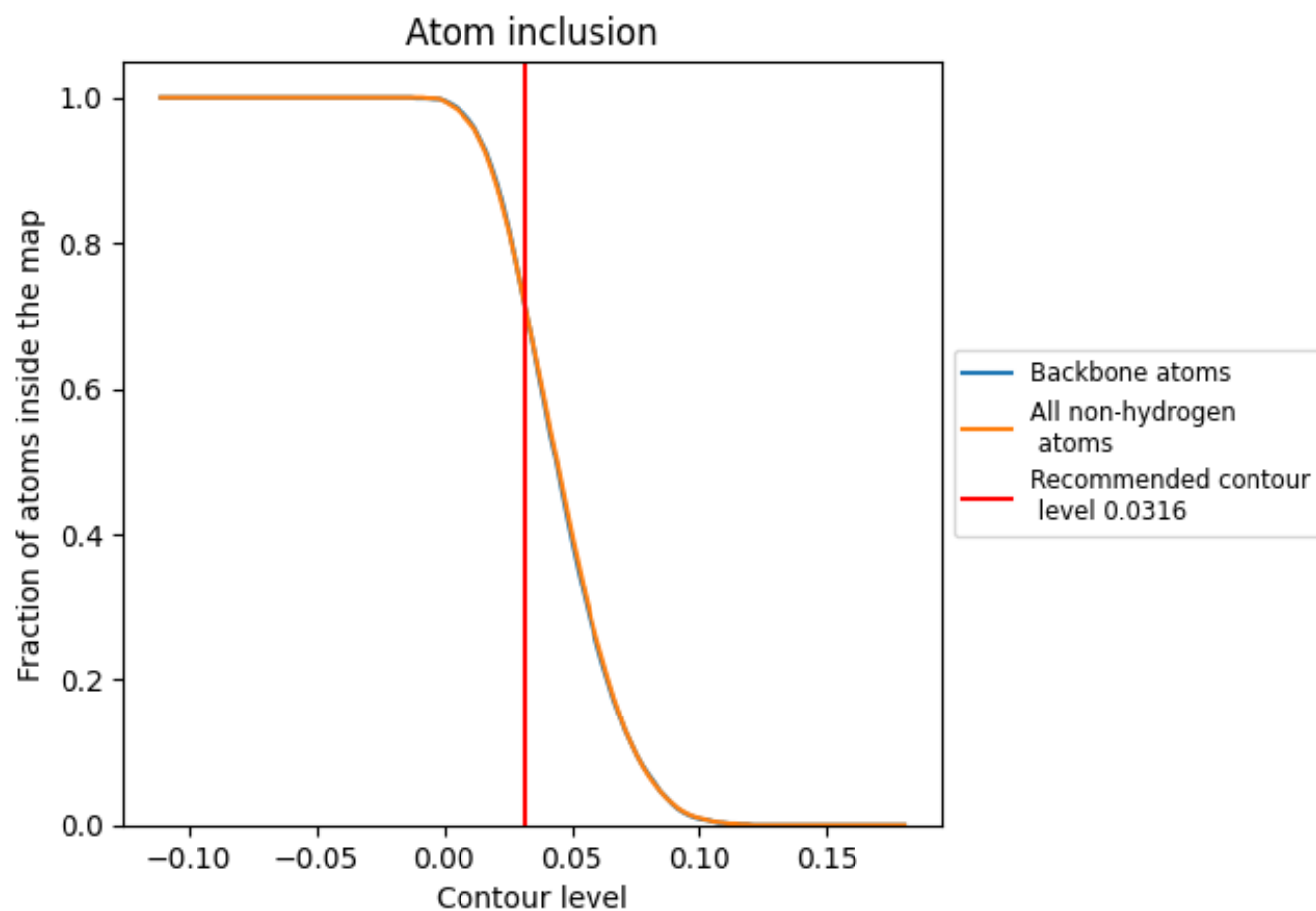
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0316).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0316) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7190	 0.6220
A	 0.8250	 0.6470
B	 0.7270	 0.6220
C	 0.7720	 0.6340
D	 0.8270	 0.6560
E	 0.6910	 0.6030
F	 0.7720	 0.6340
H	 0.6740	 0.6090
I	 0.6470	 0.6000
J	 0.6900	 0.6210
K	 0.6120	 0.5860
L	 0.7360	 0.6310
M	 0.5310	 0.5780
O	 0.5450	 0.5780
R	 0.3120	 0.5120
T	 0.5820	 0.5880
U	 0.5130	 0.5800
V	 0.6580	 0.6090
X	 0.5240	 0.5710
Y	 0.5000	 0.5650
Z	 0.4490	 0.5330

