



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 12:32 PM EDT

PDB ID : 2EIM / pdb_00002eim
Title : Zinc ion binding structure of bovine heart cytochrome C oxidase in the fully reduced state
Authors : Muramoto, K.; Hirata, K.; Shinzawa-Itoh, K.; Yoko-o, S.; Yamashita, E.; Aoyama, H.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2007-03-13
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

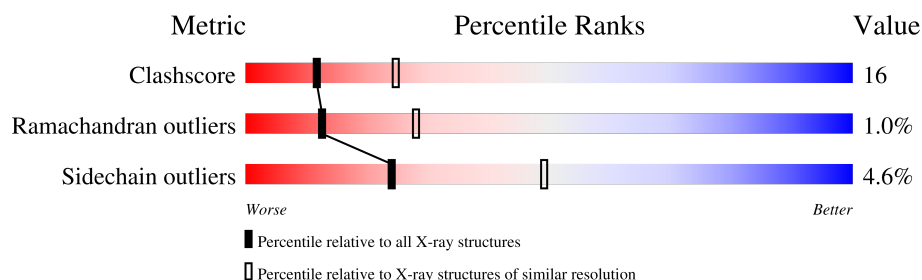
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)

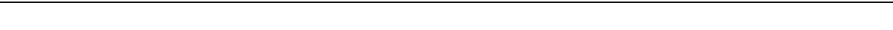
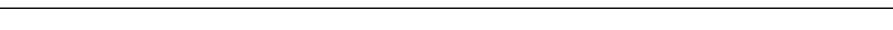
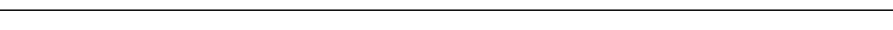
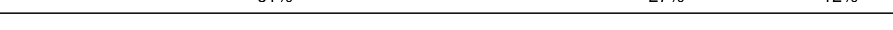
The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	514	
1	N	514	
2	B	227	
2	O	227	
3	C	261	
3	P	261	
4	D	147	
4	Q	147	

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Mol	Chain	Length	Quality of chain
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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
20	CHD	C	271	X	-	-	-
20	CHD	J	60	X	-	-	-
20	CHD	W	1060	X	-	-	-
20	CHD	W	1271	X	-	-	-
22	TGL	L	522	-	-	X	-
24	DMU	C	272	X	-	-	-
24	DMU	M	526	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	DMU	P	1272	X	-	-	-
24	DMU	Z	1526	X	-	-	-
26	CDL	G	269	-	-	X	-
26	CDL	T	1269	-	-	X	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 31961 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			
1	N	514	Total	C	N	O	S	0	0	0
			4027	2691	623	678	35			

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			
2	O	227	Total	C	N	O	S	0	0	0
			1824	1185	281	340	18			

- Molecule 3 is a protein called Cytochrome c oxidase subunit 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			
3	P	259	Total	C	N	O	S	0	0	0
			2110	1412	336	350	12			

- Molecule 4 is a protein called Cytochrome c oxidase subunit 4 isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			
4	Q	144	Total	C	N	O	S	0	0	0
			1195	777	196	218	4			

- Molecule 5 is a protein called Cytochrome c oxidase polypeptide Va.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			
5	R	105	Total	C	N	O	S	0	0	0
			852	544	144	162	2			

- Molecule 6 is a protein called Cytochrome c oxidase polypeptide Vb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			
6	S	98	Total	C	N	O	S	0	0	0
			748	464	134	145	5			

- Molecule 7 is a protein called Cytochrome c oxidase polypeptide VIa-heart.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		
7	T	84	Total	C	N	O	P	S	0	0
			675	431	129	113	1	1		

- Molecule 8 is a protein called Cytochrome c oxidase subunit VIb isoform 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			
8	U	79	Total	C	N	O	S	0	0	0
			662	417	121	119	5			

- Molecule 9 is a protein called Cytochrome c oxidase polypeptide VIc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			
9	V	73	Total	C	N	O	S	0	0	0
			601	390	107	100	4			

- Molecule 10 is a protein called Cytochrome c oxidase polypeptide VIIa-heart.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	58	Total	C	N	O	S	0	0	0
			460	297	78	82	3			

- Molecule 11 is a protein called Cytochrome c oxidase polypeptide VIIb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			
11	X	49	Total	C	N	O	S	0	0	0
			384	250	65	67	2			

- Molecule 12 is a protein called Cytochrome c oxidase polypeptide VIIc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			
12	Y	46	Total	C	N	O	S	0	0	0
			380	254	64	60	2			

- Molecule 13 is a protein called Cytochrome c oxidase polypeptide VIII-heart.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
13	M	43	Total	C	N	O	0	0	0
			335	223	53	59			
13	Z	43	Total	C	N	O	0	0	0
			335	223	53	59			

- Molecule 14 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total	Cu	0	0
			1	1		
14	N	1	Total	Cu	0	0
			1	1		

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	1	Total	Mg	0	0
			1	1		
15	N	1	Total	Mg	0	0
			1	1		

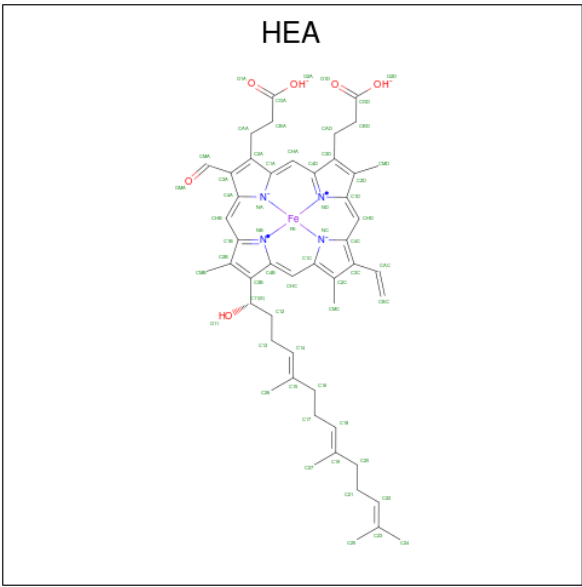
- Molecule 16 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Zn	0	0
			1	1		
17	C	1	Total	Zn	0	0
			1	1		
17	F	1	Total	Zn	0	0
			1	1		
17	N	1	Total	Zn	0	0
			1	1		
17	P	1	Total	Zn	0	0
			1	1		
17	S	1	Total	Zn	0	0
			1	1		

- Molecule 18 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



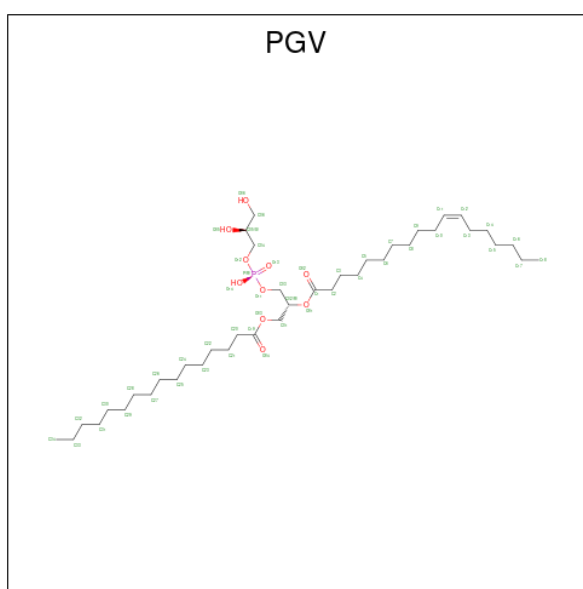
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	A	1	Total	C	Fe	N	O	
			60	49	1	4	6	
18	N	1	Total	C	Fe	N	O	
			60	49	1	4	6	
18	N	1	Total	C	Fe	N	O	
			60	49	1	4	6	

- Molecule 19 is (1R)-2-{{[[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: C₄₀H₇₇O₁₀P).



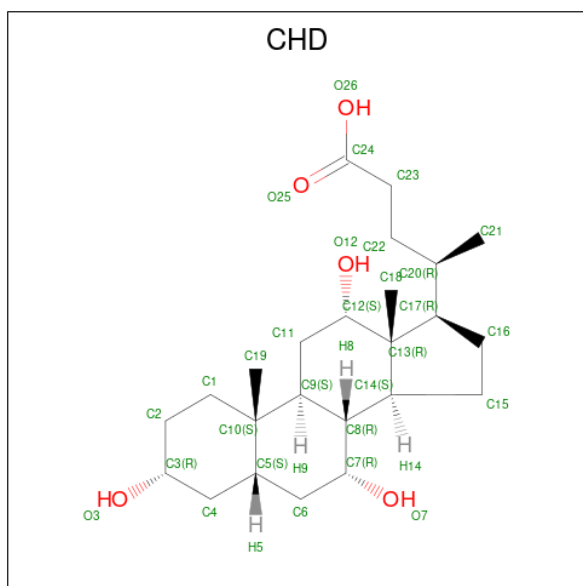
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P		
			51	40	10	1	0	0
19	C	1	Total	C	O	P		
			51	40	10	1	0	0
19	C	1	Total	C	O	P		
			51	40	10	1	0	0
19	C	1	Total	C	O	P		
			51	40	10	1	0	0
19	N	1	Total	C	O	P		
			51	40	10	1	0	0
19	P	1	Total	C	O	P		
			51	40	10	1	0	0
19	P	1	Total	C	O	P		
			51	40	10	1	0	0

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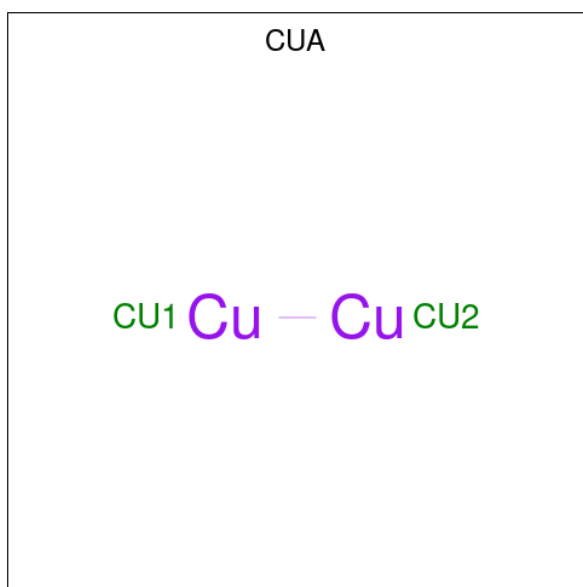
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	P	1	Total	C	O	P	0	0
			51	40	10	1		

- Molecule 20 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



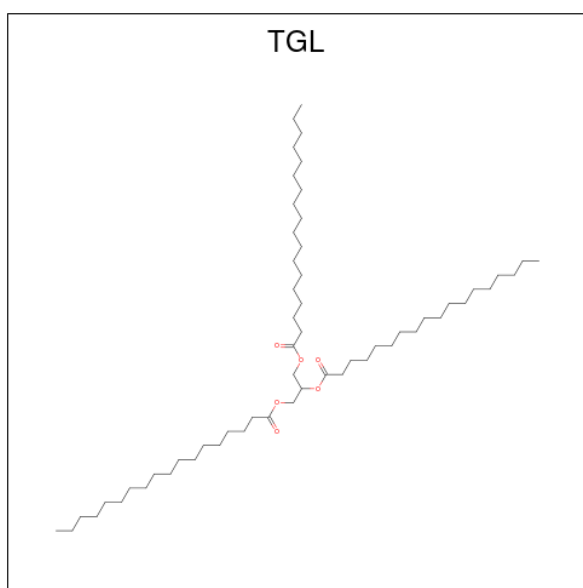
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O		0	0
			29	24	5			
20	B	1	Total	C	O		0	0
			29	24	5			
20	C	1	Total	C	O		0	0
			29	24	5			
20	J	1	Total	C	O		0	0
			29	24	5			
20	N	1	Total	C	O		0	0
			29	24	5			
20	P	1	Total	C	O		0	0
			29	24	5			
20	W	1	Total	C	O		0	0
			29	24	5			
20	W	1	Total	C	O		0	0
			29	24	5			

- Molecule 21 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	Cu		0	0
			2	2			
21	O	1	Total	Cu		0	0
			2	2			

- Molecule 22 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



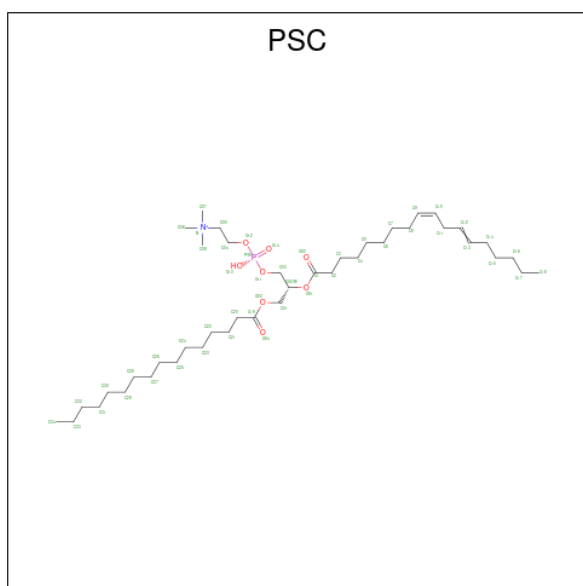
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			63	57	6		
22	D	1	Total	C	O	0	0
			63	57	6		

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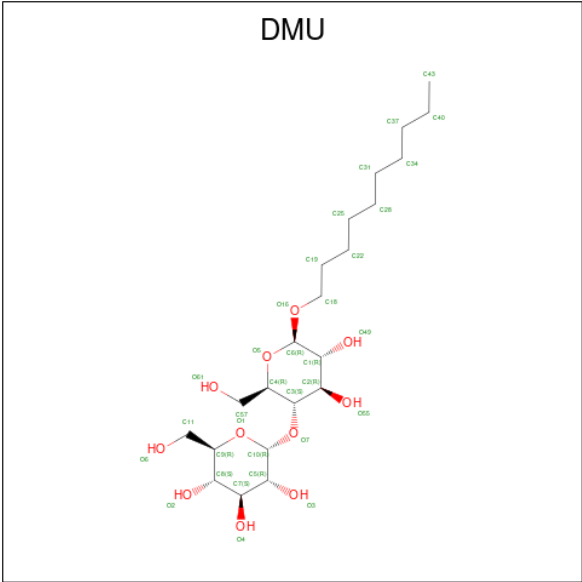
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	L	1	Total	C	O	0	0
			63	57	6		
22	N	1	Total	C	O	0	0
			63	57	6		
22	N	1	Total	C	O	0	0
			63	57	6		
22	O	1	Total	C	O	0	0
			63	57	6		

- Molecule 23 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: $C_{42}H_{81}NO_8P$).



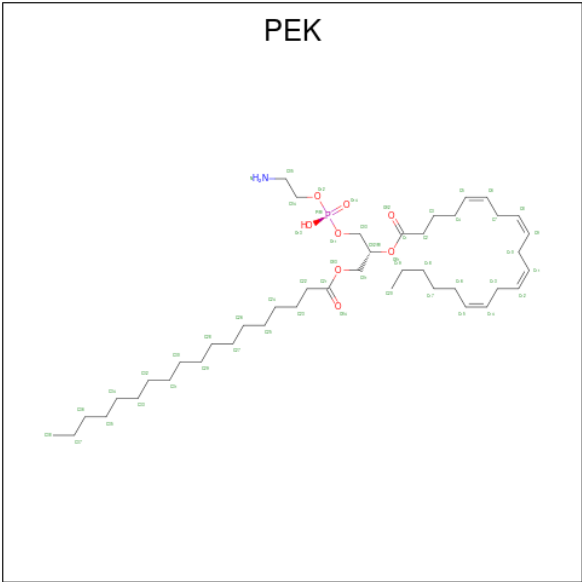
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
23	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 24 is DECYL-BETA-D-MALTOPYRANOSIDE (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).



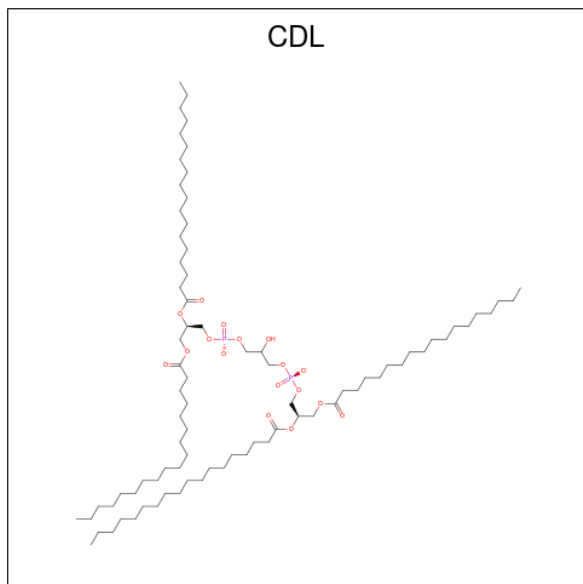
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			33	22	11		
24	M	1	Total	C	O	0	0
			33	22	11		
24	P	1	Total	C	O	0	0
			33	22	11		
24	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: C₄₃H₇₈NO₈P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
25	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	C	1	Total	C	O	P	0	0
			100	81	17	2		
26	G	1	Total	C	O	P	0	0
			100	81	17	2		
26	P	1	Total	C	O	P	0	0
			100	81	17	2		
26	T	1	Total	C	O	P	0	0
			100	81	17	2		

- Molecule 27 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	A	182	Total O 182 182	0	0
27	B	96	Total O 96 96	0	0
27	C	82	Total O 82 82	0	0
27	D	61	Total O 61 61	0	0
27	E	43	Total O 43 43	0	0
27	F	52	Total O 52 52	0	0
27	G	37	Total O 37 37	0	0
27	H	35	Total O 35 35	0	0
27	I	22	Total O 22 22	0	0
27	J	12	Total O 12 12	0	0
27	K	12	Total O 12 12	0	0
27	L	13	Total O 13 13	0	0
27	M	13	Total O 13 13	0	0
27	N	171	Total O 171 171	0	0
27	O	79	Total O 79 79	0	0
27	P	73	Total O 73 73	0	0
27	Q	42	Total O 42 42	0	0
27	R	30	Total O 30 30	0	0
27	S	42	Total O 42 42	0	0
27	T	30	Total O 30 30	0	0
27	U	30	Total O 30 30	0	0
27	V	19	Total O 19 19	0	0

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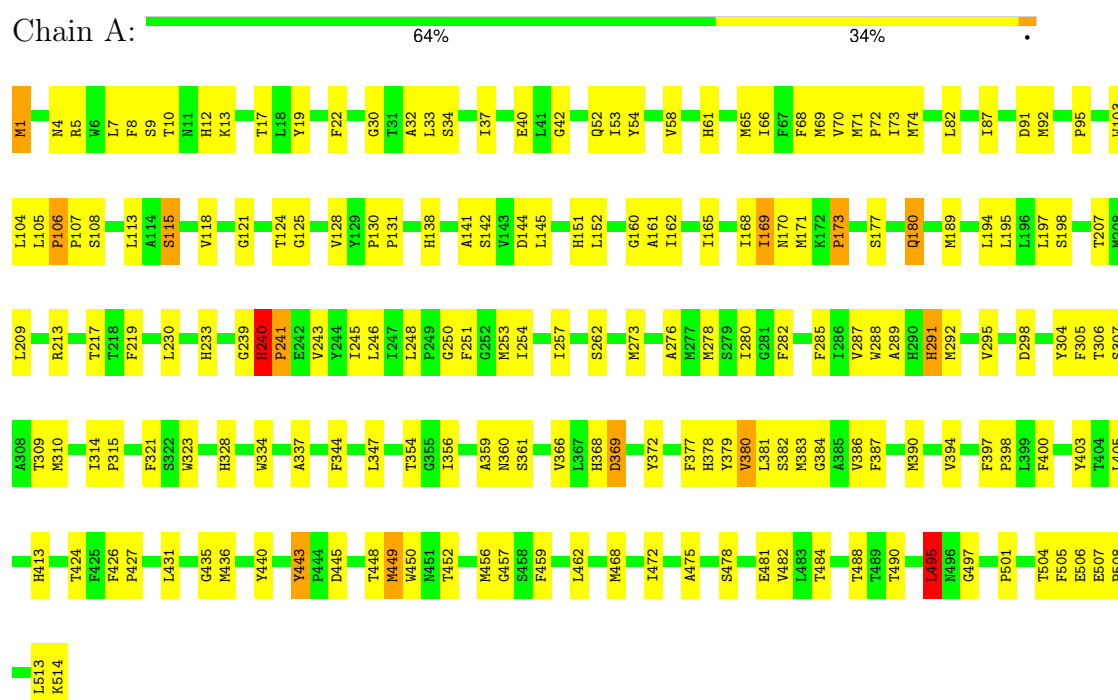
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	W	8	Total 8	O 8	0	0
27	X	18	Total 18	O 18	0	0
27	Y	14	Total 14	O 14	0	0
27	Z	11	Total 11	O 11	0	0

3 Residue-property plots

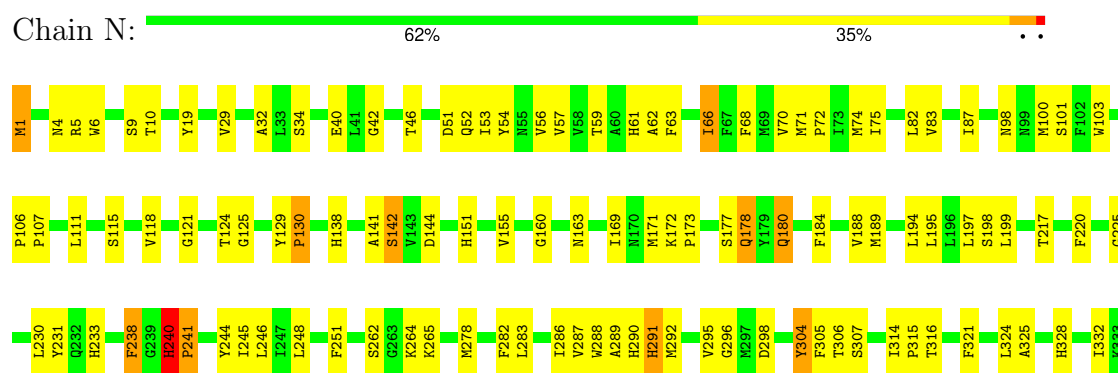
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

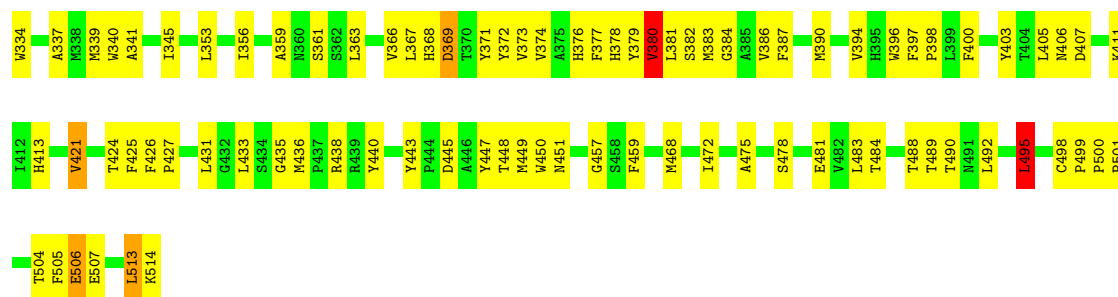
Note EDS was not executed.

• Molecule 1: Cytochrome c oxidase subunit 1

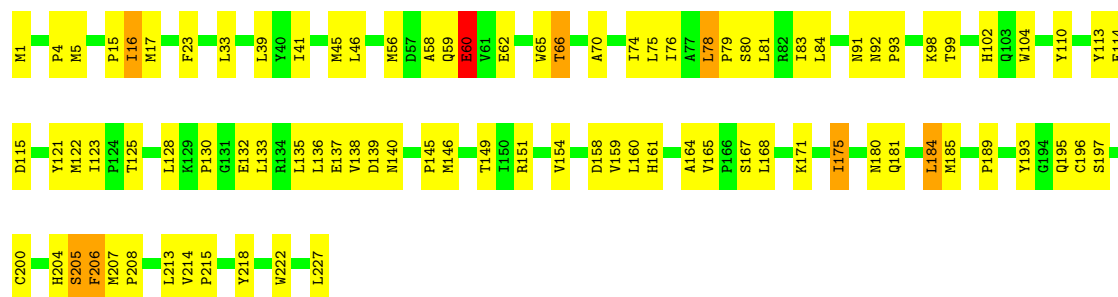


• Molecule 1: Cytochrome c oxidase subunit 1

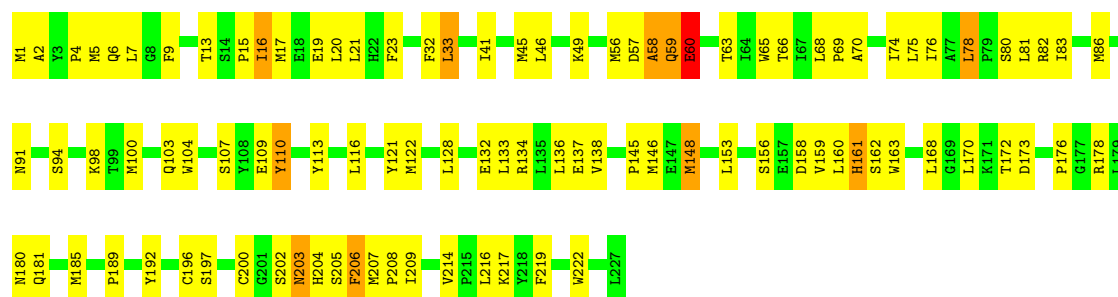




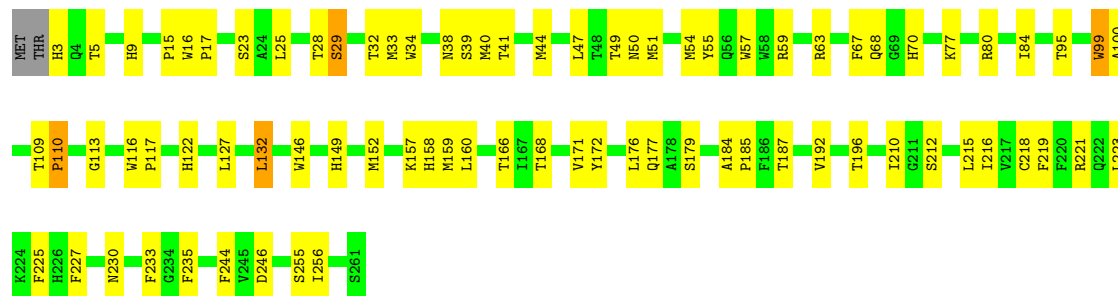
• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2

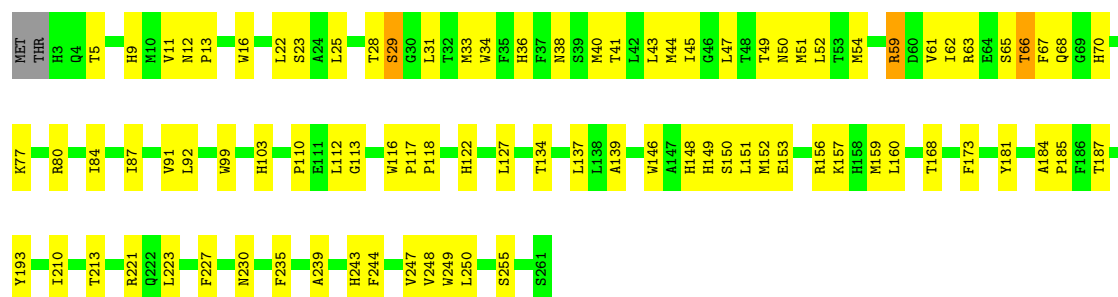


• Molecule 3: Cytochrome c oxidase subunit 3



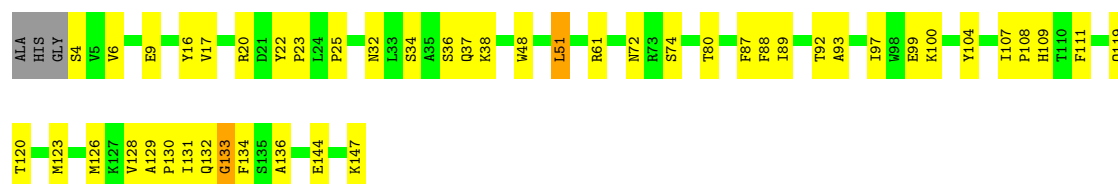
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:  66% 33% ..



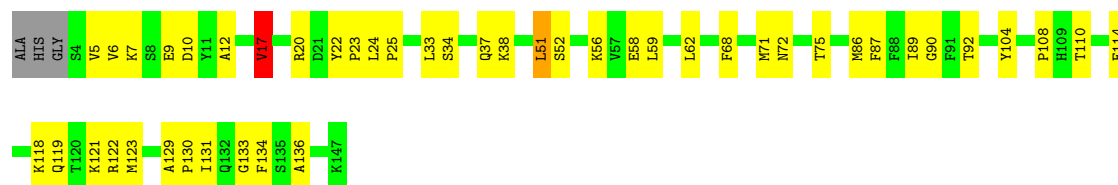
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D:  66% 31% ..



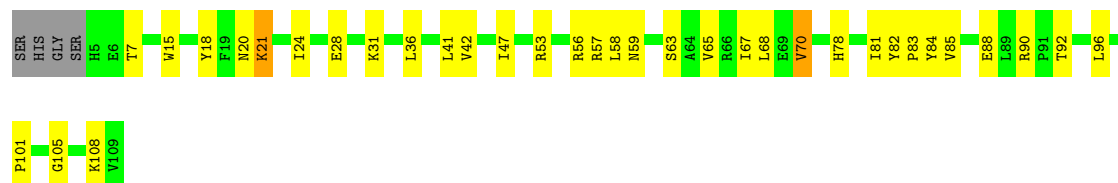
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q:  67% 30% ..



- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain E:  64% 30% ..



- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain R:  76% 20% .



- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F:  64% 31% ..



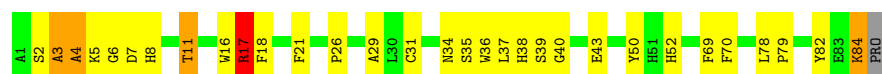
- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S:  73% 19% 6% ..



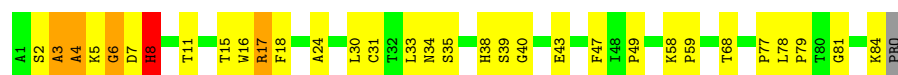
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G:  62% 31% 5% ..



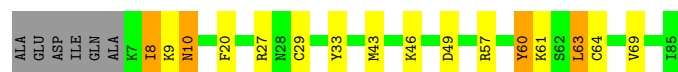
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T:  61% 32% 5% ..



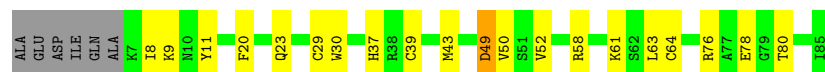
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain H:  74% 14% 5% 7%



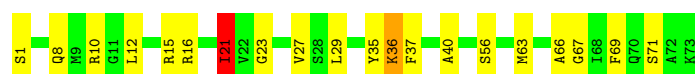
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain U:  69% 22% 7% ..



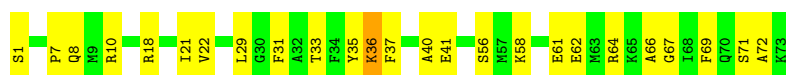
- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I:  73% 25% ..



- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V:  66% 33%



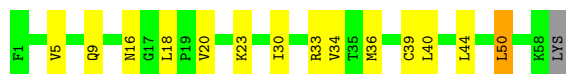
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain J:  78% 19%



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain W:  75% 22%



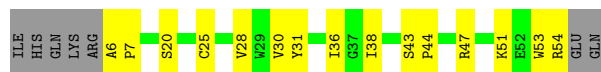
- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K:  66% 21% 12%



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X:  61% 27% 12%



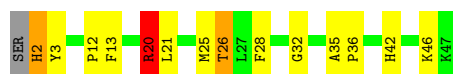
- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:  70% 26%



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

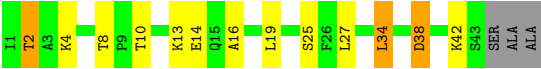
Chain Y:  68% 23%



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



● Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	183.91Å 206.72Å 178.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.204 , 0.256	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	31961	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, TGL, TPO, SAC, FME, DMU, CDL, PGV, MG, HEA, PEK, CU, CHD, PSC, CUA, ZN

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	0.87	3/4156 (0.1%)	1.21	30/5678 (0.5%)
1	N	0.78	0/4156	1.21	36/5678 (0.6%)
2	B	0.75	0/1860	1.14	11/2534 (0.4%)
2	O	0.72	0/1860	1.14	7/2534 (0.3%)
3	C	0.80	0/2197	1.07	8/3005 (0.3%)
3	P	0.73	0/2197	1.09	7/3005 (0.2%)
4	D	0.70	0/1229	1.08	4/1658 (0.2%)
4	Q	0.76	3/1229 (0.2%)	1.07	2/1658 (0.1%)
5	E	0.71	0/871	1.08	4/1182 (0.3%)
5	R	0.68	0/871	1.19	7/1182 (0.6%)
6	F	0.78	1/765 (0.1%)	1.20	5/1038 (0.5%)
6	S	0.75	1/765 (0.1%)	1.19	7/1038 (0.7%)
7	G	0.75	0/690	1.13	3/937 (0.3%)
7	T	0.74	0/690	1.11	3/937 (0.3%)
8	H	0.76	0/682	1.13	7/921 (0.8%)
8	U	0.69	0/682	1.16	4/921 (0.4%)
9	I	0.71	0/605	0.99	3/802 (0.4%)
9	V	0.65	0/605	0.96	2/802 (0.2%)
10	J	0.70	0/471	1.05	0/636
10	W	0.64	0/471	1.05	0/636
11	K	0.81	0/398	1.16	2/546 (0.4%)
11	X	0.66	0/398	1.13	0/546
12	L	0.77	0/393	1.12	4/526 (0.8%)
12	Y	0.75	1/393 (0.3%)	1.12	1/526 (0.2%)
13	M	0.71	0/345	1.08	2/470 (0.4%)
13	Z	0.64	0/345	1.15	1/470 (0.2%)
All	All	0.76	9/29324 (0.0%)	1.14	160/39866 (0.4%)

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
1	A	0	3
1	N	0	5
2	B	0	1
2	O	0	1
All	All	0	10

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	PRO	CA-C	7.45	1.59	1.52
4	Q	5	VAL	CA-CB	6.83	1.61	1.53
12	Y	2	HIS	CD2-NE2	6.37	1.44	1.37
6	F	6	VAL	CA-CB	5.82	1.61	1.54
1	A	295	VAL	CA-CB	5.68	1.61	1.54
1	A	106	PRO	CA-C	5.66	1.57	1.52
6	S	42	THR	CA-CB	5.41	1.60	1.53
4	Q	17	VAL	CA-CB	5.19	1.61	1.54
4	Q	6	VAL	CA-CB	5.08	1.61	1.54

All (160) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	PRO	N-CA-C	-10.01	98.48	110.70
1	N	130	PRO	N-CA-C	-9.52	99.09	110.70
1	A	82	LEU	N-CA-C	9.38	123.23	111.69
1	N	171	MET	N-CA-C	9.26	123.03	112.57
6	S	94	HIS	N-CA-C	8.64	129.20	110.80
5	R	42	VAL	N-CA-C	-8.56	97.95	108.05
1	A	445	ASP	N-CA-C	8.28	122.35	111.75
1	A	495	LEU	N-CA-C	8.28	121.23	111.71
6	F	94	HIS	N-CA-C	8.28	128.43	110.80
5	R	76	GLY	CA-C-N	8.16	127.80	119.56
5	R	76	GLY	C-N-CA	8.16	127.80	119.56
13	Z	27	LEU	N-CA-C	8.07	120.16	111.36
1	N	445	ASP	N-CA-C	8.04	122.03	111.75
1	A	288	TRP	N-CA-C	7.84	121.79	111.75
5	E	42	VAL	N-CA-C	-7.81	98.83	108.05
1	N	495	LEU	N-CA-C	7.77	120.64	111.71
1	N	288	TRP	N-CA-C	7.69	121.59	111.75
1	A	262	SER	N-CA-C	-7.61	103.99	113.28
1	N	425	PHE	N-CA-C	7.23	122.27	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	133	LEU	N-CA-C	7.16	119.76	108.67
1	N	83	VAL	N-CA-CB	7.16	115.31	110.52
2	B	66	THR	N-CA-C	-7.10	103.74	113.18
6	S	93	PRO	N-CA-C	7.06	127.02	112.47
6	F	93	PRO	N-CA-C	7.04	126.98	112.47
1	N	435	GLY	N-CA-C	7.00	125.68	115.32
4	D	22	TYR	CA-C-N	6.94	127.23	119.32
4	D	22	TYR	C-N-CA	6.94	127.23	119.32
2	B	76	ILE	N-CA-C	-6.93	106.28	111.90
1	A	74	MET	N-CA-C	6.92	118.71	111.03
1	N	506	GLU	N-CA-C	-6.90	103.76	111.28
13	M	27	LEU	N-CA-C	6.88	120.16	111.69
2	O	76	ILE	N-CA-C	-6.88	106.08	112.96
1	A	171	MET	N-CA-C	6.82	121.27	112.26
1	N	82	LEU	N-CA-C	6.80	121.90	112.45
1	N	262	SER	N-CA-C	-6.78	105.01	113.28
3	P	122	HIS	CA-C-N	6.78	126.80	119.89
3	P	122	HIS	C-N-CA	6.78	126.80	119.89
1	A	506	GLU	N-CA-C	-6.76	103.91	111.28
1	N	74	MET	N-CA-C	6.74	118.51	111.03
12	Y	20	ARG	N-CA-C	-6.70	103.91	111.07
2	O	206	PHE	N-CA-C	6.62	119.35	110.88
2	B	133	LEU	N-CA-C	6.61	118.92	108.67
1	A	435	GLY	N-CA-C	6.56	125.02	115.32
2	B	197	SER	N-CA-C	6.45	119.86	112.57
4	Q	22	TYR	CA-C-N	6.43	126.65	119.32
4	Q	22	TYR	C-N-CA	6.43	126.65	119.32
8	U	20	PHE	CA-C-N	6.41	127.56	120.45
8	U	20	PHE	C-N-CA	6.41	127.56	120.45
7	G	17	ARG	N-CA-C	-6.40	104.17	112.23
1	N	217	THR	N-CA-C	-6.38	101.08	110.52
8	U	49	ASP	N-CA-C	6.37	118.90	108.52
3	C	256	ILE	N-CA-C	6.37	117.00	110.82
3	P	255	SER	N-CA-C	6.35	118.08	111.03
3	C	113	GLY	N-CA-C	-6.35	106.13	115.72
3	P	113	GLY	N-CA-C	-6.31	106.43	115.64
3	C	99	TRP	N-CA-C	-6.30	104.11	110.97
1	N	10	THR	N-CA-C	-6.29	102.86	112.99
8	H	49	ASP	N-CA-C	6.27	118.75	108.52
12	L	11	ILE	CA-C-N	6.27	127.67	119.84
12	L	11	ILE	C-N-CA	6.27	127.67	119.84
1	A	217	THR	N-CA-C	-6.26	101.26	110.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	83	VAL	CB-CA-C	-6.25	107.76	113.70
11	K	6	ALA	CA-C-N	6.24	126.45	119.90
11	K	6	ALA	C-N-CA	6.24	126.45	119.90
1	N	70	VAL	N-CA-C	6.22	116.33	110.30
1	N	287	VAL	N-CA-C	6.20	119.15	113.20
1	N	372	TYR	N-CA-C	-6.16	104.65	111.36
1	A	198	SER	N-CA-C	6.11	118.85	111.40
1	A	169	ILE	CB-CA-C	-6.07	104.10	112.24
1	A	125	GLY	N-CA-C	-6.07	105.13	112.48
7	T	17	ARG	N-CA-C	-6.06	104.23	111.69
6	S	93	PRO	CA-C-N	6.05	133.10	121.54
6	S	93	PRO	C-N-CA	6.05	133.10	121.54
1	N	129	TYR	N-CA-C	6.02	117.39	109.93
3	C	255	SER	N-CA-C	6.01	117.70	111.03
1	N	287	VAL	CB-CA-C	-5.96	104.80	110.70
3	P	99	TRP	N-CA-C	-5.95	104.49	110.97
1	A	170	ASN	N-CA-C	5.90	120.75	113.50
2	B	161	HIS	N-CA-C	-5.89	100.18	108.96
1	N	66	ILE	N-CA-C	5.87	116.51	110.82
5	E	21	LYS	CA-C-N	5.82	125.29	119.24
5	E	21	LYS	C-N-CA	5.82	125.29	119.24
2	B	136	LEU	N-CA-C	5.81	120.38	113.12
1	A	207	THR	N-CA-C	-5.80	104.32	111.40
3	C	132	LEU	N-CA-C	-5.78	104.67	110.97
1	A	10	THR	N-CA-C	-5.73	103.76	112.99
8	U	64	CYS	N-CA-C	5.71	117.70	109.48
6	F	95	GLN	N-CA-C	5.70	122.94	110.80
3	C	59	ARG	N-CA-C	-5.66	104.75	111.03
8	H	63	LEU	N-CA-C	5.65	118.53	111.24
1	N	421	VAL	N-CA-C	5.64	116.42	110.72
8	H	20	PHE	CA-C-N	5.63	126.69	120.45
8	H	20	PHE	C-N-CA	5.63	126.69	120.45
12	L	20	ARG	N-CA-C	-5.62	105.23	111.36
7	T	8	HIS	N-CA-C	5.62	122.76	110.80
12	L	39	ILE	N-CA-C	-5.62	105.05	110.72
3	C	225	PHE	N-CA-C	5.56	119.65	112.86
1	N	198	SER	N-CA-C	5.55	118.17	111.40
7	T	6	GLY	N-CA-C	5.55	126.32	113.18
1	N	332	ILE	N-CA-C	5.53	116.14	108.84
9	I	69	PHE	N-CA-C	5.53	118.02	110.55
3	P	59	ARG	N-CA-C	-5.53	104.89	111.03
2	B	175	ILE	N-CA-C	5.51	113.89	107.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	GLN	N-CA-C	-5.49	105.38	111.36
1	A	449	MET	N-CA-C	5.49	117.69	111.11
1	A	372	TYR	N-CA-C	-5.48	104.95	111.69
1	N	291	HIS	N-CA-C	-5.48	106.18	112.92
1	A	168	ILE	N-CA-C	5.47	116.20	110.62
6	F	12	GLN	N-CA-C	5.46	120.96	113.97
1	N	125	GLY	N-CA-C	-5.45	104.88	112.18
1	A	197	LEU	N-CA-C	5.43	118.37	111.69
1	N	238	PHE	N-CA-C	-5.43	106.33	113.12
1	N	380	VAL	CB-CA-C	-5.43	104.86	111.87
5	R	21	LYS	CA-C-N	5.42	126.62	119.84
5	R	21	LYS	C-N-CA	5.42	126.62	119.84
1	A	103	TRP	N-CA-C	5.40	118.97	112.38
9	I	66	ALA	N-CA-C	-5.40	106.69	113.28
2	O	103	GLN	N-CA-C	-5.40	99.71	108.41
1	N	240	HIS	N-CA-CB	5.40	115.52	110.39
1	N	199	LEU	CA-C-N	5.39	125.46	119.32
1	N	199	LEU	C-N-CA	5.39	125.46	119.32
1	A	287	VAL	N-CA-C	5.37	118.36	113.20
7	G	6	GLY	N-CA-C	5.36	125.89	113.18
2	B	206	PHE	N-CA-C	5.35	117.73	110.88
2	O	161	HIS	N-CA-C	-5.35	101.36	108.74
9	V	69	PHE	N-CA-C	5.35	118.39	110.48
7	G	69	PHE	N-CA-C	5.34	117.79	111.33
3	C	9	HIS	N-CA-C	5.33	117.42	108.73
6	F	32	ASN	N-CA-C	5.32	118.53	111.30
1	N	448	THR	N-CA-C	5.30	116.74	111.07
1	N	407	ASP	N-CA-C	5.30	117.74	111.33
4	D	133	GLY	N-CA-C	5.29	125.72	113.18
9	V	66	ALA	N-CA-C	-5.28	106.89	113.38
4	D	89	ILE	N-CA-C	-5.28	104.37	111.44
1	A	240	HIS	N-CA-CB	5.26	115.39	110.39
1	N	396	TRP	N-CA-C	5.26	119.68	113.16
8	H	64	CYS	N-CA-C	5.21	116.99	109.48
2	O	136	LEU	N-CA-C	5.21	119.76	113.41
6	S	12	GLN	N-CA-C	5.20	120.63	113.97
1	A	380	VAL	CB-CA-C	-5.20	105.21	112.02
8	H	10	ASN	CA-C-N	5.19	128.21	120.95
8	H	10	ASN	C-N-CA	5.19	128.21	120.95
2	B	165	VAL	CA-C-N	5.18	124.63	119.24
2	B	165	VAL	C-N-CA	5.18	124.63	119.24
1	N	101	SER	N-CA-C	-5.18	105.63	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	193	TYR	N-CA-C	5.17	118.12	110.46
5	R	100	THR	CA-C-N	5.17	125.21	119.32
5	R	100	THR	C-N-CA	5.17	125.21	119.32
1	A	448	THR	N-CA-C	5.16	116.59	111.07
3	P	36	HIS	N-CA-C	5.15	120.95	114.31
1	A	291	HIS	N-CA-C	-5.12	106.72	113.17
1	N	449	MET	N-CA-C	5.10	117.23	111.11
1	A	124	THR	CB-CA-C	-5.09	100.80	109.65
6	S	29	ASP	CA-C-N	5.09	124.70	119.56
6	S	29	ASP	C-N-CA	5.09	124.70	119.56
1	A	70	VAL	N-CA-C	5.08	115.23	110.30
5	E	47	ILE	CB-CA-C	-5.08	105.39	112.04
2	O	58	ALA	N-CA-C	5.07	119.60	113.41
9	I	21	ILE	N-CA-C	-5.07	105.60	110.72
13	M	37	LEU	N-CA-C	5.03	116.76	111.28

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	TYR	Sidechain
1	A	240	HIS	Sidechain
1	A	443	TYR	Sidechain
2	B	218	TYR	Sidechain
1	N	19	TYR	Sidechain
1	N	240	HIS	Sidechain
1	N	244	TYR	Sidechain
1	N	304	TYR	Sidechain
1	N	379	TYR	Sidechain
2	O	192	TYR	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	143	0
1	N	4027	0	4001	155	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1824	0	1833	69	0
2	O	1824	0	1833	88	0
3	C	2110	0	2027	71	0
3	P	2110	0	2027	80	0
4	D	1195	0	1183	35	0
4	Q	1195	0	1183	39	0
5	E	852	0	845	25	0
5	R	852	0	845	12	0
6	F	748	0	728	25	0
6	S	748	0	728	18	0
7	G	675	0	644	36	0
7	T	675	0	644	41	0
8	H	662	0	623	10	0
8	U	662	0	623	17	0
9	I	601	0	613	14	0
9	V	601	0	613	16	0
10	J	460	0	459	12	0
10	W	460	0	459	11	0
11	K	384	0	366	8	0
11	X	384	0	366	9	0
12	L	380	0	380	22	0
12	Y	380	0	380	14	0
13	M	335	0	352	10	0
13	Z	335	0	352	11	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	F	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
17	S	1	0	0	0	0
18	A	120	0	108	5	0
18	N	120	0	108	9	0
19	A	51	0	76	7	0
19	C	153	0	228	13	0
19	N	51	0	76	10	0
19	P	153	0	228	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	A	29	0	39	1	0
20	B	29	0	39	1	0
20	C	29	0	39	2	0
20	J	29	0	37	5	0
20	N	29	0	39	2	0
20	P	29	0	39	2	0
20	W	58	0	76	5	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	63	0	110	6	0
22	D	63	0	110	5	0
22	L	63	0	110	28	0
22	N	126	0	220	23	0
22	O	63	0	110	8	0
23	B	52	0	80	19	0
23	O	52	0	80	18	0
24	C	33	0	36	3	0
24	M	33	0	38	1	0
24	P	33	0	37	4	0
24	Z	33	0	38	0	0
25	C	106	0	154	17	0
25	G	53	0	77	9	0
25	P	106	0	154	18	0
25	T	53	0	77	14	0
26	C	100	0	156	19	0
26	G	100	0	156	22	0
26	P	100	0	156	13	0
26	T	100	0	156	23	0
27	A	182	0	0	9	0
27	B	96	0	0	3	0
27	C	82	0	0	5	0
27	D	61	0	0	7	0
27	E	43	0	0	4	0
27	F	52	0	0	5	0
27	G	37	0	0	1	0
27	H	35	0	0	1	0
27	I	22	0	0	2	0
27	J	12	0	0	1	0
27	K	12	0	0	2	0
27	L	13	0	0	0	0
27	M	13	0	0	2	0
27	N	171	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	O	79	0	0	4	0
27	P	73	0	0	0	0
27	Q	42	0	0	1	0
27	R	30	0	0	2	0
27	S	42	0	0	0	0
27	T	30	0	0	3	0
27	U	30	0	0	0	0
27	V	19	0	0	3	0
27	W	8	0	0	0	0
27	X	18	0	0	1	0
27	Y	14	0	0	0	0
27	Z	11	0	0	2	0
All	All	31961	0	31295	988	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 16.

All (988) 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)
10:W:33:ARG:HG2	20:W:1060:CHD:H152	1.29	1.14
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.19	1.07
8:H:43:MET:HE1	8:U:43:MET:HE1	1.46	0.98
3:P:63:ARG:HE	26:P:1270:CDL:HA22	1.30	0.97
23:O:1230:PSC:H142	23:O:1230:PSC:H343	1.46	0.97
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.49	0.95
23:B:230:PSC:H343	23:B:230:PSC:H142	1.51	0.93
4:D:34:SER:H	4:D:37:GLN:HE21	1.04	0.93
7:G:84:LYS:H	7:G:84:LYS:HD2	1.33	0.93
7:T:84:LYS:HD2	7:T:84:LYS:H	1.34	0.92
7:G:31:CYS:SG	26:G:269:CDL:H532	2.10	0.92
3:P:50:ASN:ND2	3:P:54:MET:HE2	1.85	0.91
6:S:94:HIS:CD2	6:S:95:GLN:H	1.89	0.90
12:L:20:ARG:HH12	22:L:522:TGL:HC61	1.34	0.90
26:T:1269:CDL:H541	26:T:1269:CDL:H231	1.54	0.90
26:G:269:CDL:H541	26:G:269:CDL:H231	1.52	0.89
22:L:522:TGL:HC62	22:L:522:TGL:HC22	1.55	0.88
25:C:264:PEK:H161	25:C:264:PEK:H102	1.54	0.88
1:N:151:HIS:CD2	25:P:1264:PEK:H382	2.09	0.88
23:O:1230:PSC:H071	9:V:10:ARG:HE	1.39	0.88
7:G:5:LYS:HG3	25:G:1263:PEK:H383	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:33:ARG:HG2	20:J:60:CHD:H152	1.56	0.85
22:N:1522:TGL:HC62	22:N:1522:TGL:HC22	1.60	0.84
22:L:522:TGL:H242	22:L:522:TGL:H202	1.60	0.83
7:G:5:LYS:HB2	25:G:1263:PEK:H362	1.60	0.83
4:D:34:SER:H	4:D:37:GLN:NE2	1.77	0.82
1:N:151:HIS:HD2	25:P:1264:PEK:H382	1.44	0.82
1:N:472:ILE:HG21	22:N:1522:TGL:HA92	1.59	0.82
25:P:1264:PEK:H102	25:P:1264:PEK:H161	1.62	0.81
1:N:225:GLY:HA3	3:P:112:LEU:HD21	1.61	0.81
4:D:120:THR:HA	27:D:4164:HOH:O	1.78	0.81
7:G:5:LYS:HD3	1:N:278:MET:HB3	1.64	0.80
7:T:31:CYS:SG	26:T:1269:CDL:H532	2.21	0.80
22:N:1522:TGL:H242	22:N:1522:TGL:H202	1.63	0.79
12:L:13:PHE:HA	22:L:522:TGL:HC31	1.63	0.79
2:O:15:PRO:HD2	27:O:3142:HOH:O	1.83	0.79
2:O:41:ILE:HD13	23:O:1230:PSC:H342	1.63	0.79
26:G:269:CDL:H622	19:P:1268:PGV:H152	1.62	0.79
1:A:472:ILE:HG21	22:L:522:TGL:HA92	1.64	0.79
13:M:42:LYS:HE3	13:M:42:LYS:HA	1.64	0.79
23:O:1230:PSC:H21	23:O:1230:PSC:H222	1.64	0.78
3:C:80:ARG:NH1	25:T:263:PEK:H032	1.99	0.78
22:N:1522:TGL:HC31	12:Y:13:PHE:HA	1.64	0.78
12:L:24:MET:SD	22:L:522:TGL:H162	2.24	0.78
22:N:1522:TGL:H361	22:N:1522:TGL:HB91	1.66	0.78
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.32	0.78
23:B:230:PSC:H222	23:B:230:PSC:H21	1.66	0.77
3:C:80:ARG:HH11	25:T:263:PEK:H032	1.48	0.77
7:T:3:ALA:HB1	25:T:263:PEK:H382	1.65	0.77
22:B:521:TGL:H281	22:B:521:TGL:H102	1.67	0.76
3:C:160:LEU:HD13	20:C:271:CHD:H181	1.68	0.76
22:B:521:TGL:H102	22:B:521:TGL:C28	2.15	0.76
12:L:20:ARG:NH1	22:L:522:TGL:HC61	2.00	0.76
22:O:1521:TGL:C28	22:O:1521:TGL:H102	2.15	0.76
26:P:1270:CDL:H191	26:P:1270:CDL:H642	1.67	0.76
7:T:47:PHE:CD2	7:T:81:GLY:HA2	2.22	0.75
4:Q:130:PRO:HG2	4:Q:131:ILE:HD12	1.69	0.75
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.21	0.74
22:O:1521:TGL:H102	22:O:1521:TGL:H281	1.67	0.74
19:C:268:PGV:H152	26:T:1269:CDL:H622	1.70	0.74
26:C:270:CDL:H191	26:C:270:CDL:H642	1.67	0.74
6:F:51:SER:HB2	6:F:91:LEU:HD11	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:168:THR:HG22	25:C:265:PEK:H14	1.70	0.74
1:N:1:FME:HCN	1:N:4:ASN:H	1.53	0.73
27:A:4014:HOH:O	12:L:3:TYR:HB3	1.88	0.73
22:B:521:TGL:H241	22:B:521:TGL:H201	1.71	0.73
26:G:269:CDL:H541	26:G:269:CDL:C23	2.20	0.72
1:A:1:FME:HCN	1:A:4:ASN:H	1.54	0.72
3:P:168:THR:HG22	25:P:1265:PEK:H14	1.72	0.72
2:B:41:ILE:HD13	23:B:230:PSC:H342	1.71	0.71
3:P:168:THR:HG21	25:P:1265:PEK:H12	1.71	0.71
4:D:130:PRO:HG2	4:D:131:ILE:HD12	1.72	0.71
1:A:390:MET:HE2	1:A:413:HIS:CE1	2.25	0.71
7:T:38:HIS:NE2	26:T:1269:CDL:H111	2.05	0.70
1:A:278:MET:SD	7:T:5:LYS:HB3	2.31	0.70
2:O:146:MET:HE1	9:V:56:SER:HB2	1.72	0.70
22:O:1521:TGL:H241	22:O:1521:TGL:H201	1.73	0.70
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.74	0.70
1:A:160:GLY:HA3	27:A:2064:HOH:O	1.91	0.70
1:A:377:PHE:CD1	18:A:516:HEA:HAD1	2.27	0.69
1:A:390:MET:HE2	1:A:413:HIS:HE1	1.57	0.69
3:P:47:LEU:O	3:P:51:MET:HG2	1.92	0.69
12:L:20:ARG:HH22	22:L:522:TGL:HC61	1.55	0.69
1:A:87:ILE:O	1:A:173:PRO:HD3	1.91	0.69
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.75	0.69
7:G:5:LYS:HB3	1:N:278:MET:SD	2.33	0.69
1:A:484:THR:HB	13:M:2:THR:OG1	1.92	0.68
1:N:296:GLY:HA2	8:U:23:GLN:OE1	1.93	0.68
6:F:92:VAL:HG23	6:F:92:VAL:O	1.94	0.68
10:J:12:PHE:O	10:J:23:LYS:HE2	1.94	0.68
26:G:269:CDL:H522	26:G:269:CDL:H202	1.76	0.68
1:N:472:ILE:HG21	22:N:1522:TGL:CA9	2.22	0.68
3:P:34:TRP:CZ2	24:P:1272:DMU:H29	2.28	0.68
7:T:5:LYS:HG3	25:T:263:PEK:H383	1.76	0.68
5:E:68:LEU:HD12	5:E:101:PRO:HD3	1.76	0.68
3:C:210:ILE:HG23	19:C:267:PGV:H102	1.75	0.67
3:P:160:LEU:HD13	20:W:1271:CHD:H181	1.76	0.67
4:D:48:TRP:HA	4:D:51:LEU:HD22	1.77	0.67
4:D:16:TYR:CE1	4:D:25:PRO:HG2	2.29	0.67
1:N:177:SER:H	1:N:180:GLN:HE21	1.43	0.67
2:O:41:ILE:CD1	23:O:1230:PSC:H342	2.24	0.67
12:Y:20:ARG:HH11	12:Y:20:ARG:HB3	1.59	0.67
3:C:67:PHE:HE1	26:C:270:CDL:H1	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:371:TYR:CE2	1:N:436:MET:HE2	2.30	0.67
3:C:149:HIS:HA	3:C:152:MET:HE2	1.77	0.67
26:T:1269:CDL:H541	26:T:1269:CDL:C23	2.24	0.67
8:U:49:ASP:O	8:U:52:VAL:HG22	1.95	0.67
26:C:270:CDL:H431	27:J:4266:HOH:O	1.95	0.67
3:P:148:HIS:CE1	3:P:152:MET:SD	2.87	0.66
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.30	0.66
1:N:514:LYS:HE3	27:N:3395:HOH:O	1.94	0.66
12:Y:26:THR:HG23	13:Z:25:SER:HB2	1.77	0.66
7:T:47:PHE:CE2	7:T:81:GLY:HA2	2.31	0.66
1:A:219:PHE:HE2	3:C:196:THR:HG22	1.60	0.66
3:C:168:THR:CG2	25:C:265:PEK:H14	2.25	0.66
3:P:34:TRP:HZ2	24:P:1272:DMU:H29	1.61	0.66
1:A:278:MET:HE3	7:T:5:LYS:HD3	1.77	0.65
4:D:34:SER:N	4:D:37:GLN:HE21	1.87	0.65
1:A:1:FME:HE2	1:A:1:FME:HA	1.76	0.65
2:B:98:LYS:HD3	8:H:63:LEU:O	1.95	0.65
7:T:34:ASN:ND2	26:T:1269:CDL:H151	2.11	0.65
9:V:58:LYS:O	9:V:62:GLU:HG3	1.96	0.65
7:G:3:ALA:HB1	25:G:1263:PEK:H382	1.78	0.65
8:H:60:TYR:CD1	8:H:60:TYR:C	2.74	0.65
19:N:1524:PGV:H322	13:Z:19:LEU:HD23	1.79	0.65
2:O:160:LEU:HD23	2:O:176:PRO:HD2	1.78	0.65
3:P:67:PHE:HE1	26:P:1270:CDL:H1	1.61	0.65
3:P:80:ARG:O	3:P:84:ILE:HD12	1.96	0.65
3:C:54:MET:HE1	19:C:267:PGV:H141	1.77	0.65
1:A:32:ALA:HB3	12:L:36:PRO:HG2	1.78	0.65
1:A:73:ILE:HD11	18:A:515:HEA:H22	1.79	0.65
1:N:440:TYR:HE2	2:O:204:HIS:CE1	2.15	0.65
6:S:94:HIS:CD2	6:S:95:GLN:N	2.62	0.65
7:G:2:SER:OG	25:G:1263:PEK:H301	1.96	0.64
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.79	0.64
19:N:1524:PGV:H062	27:Z:3160:HOH:O	1.96	0.64
3:P:210:ILE:HG23	19:P:1267:PGV:H102	1.79	0.64
19:C:267:PGV:H182	26:C:270:CDL:H673	1.80	0.64
1:N:334:TRP:CZ3	22:N:1523:TGL:HA51	2.33	0.64
4:D:9:GLU:CD	4:D:9:GLU:H	2.05	0.64
22:L:522:TGL:H361	22:L:522:TGL:HB91	1.80	0.64
26:G:269:CDL:HB32	1:N:304:TYR:HD1	1.61	0.64
19:A:524:PGV:H062	27:M:2160:HOH:O	1.98	0.64
3:C:34:TRP:HZ2	24:C:272:DMU:H29	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.79	0.64
1:A:33:LEU:HD23	12:L:36:PRO:HB3	1.78	0.63
12:L:20:ARG:NH2	22:L:522:TGL:HC32	2.14	0.63
26:T:1269:CDL:H172	26:T:1269:CDL:H511	1.80	0.63
5:E:57:ARG:HG3	5:E:57:ARG:HH11	1.63	0.63
1:N:381:LEU:HD13	18:N:516:HEA:HBC2	1.81	0.63
3:C:50:ASN:ND2	3:C:54:MET:HE2	2.13	0.63
6:F:1:ALA:HB2	27:N:4346:HOH:O	1.99	0.63
5:R:87:GLN:HG2	5:R:88:GLU:N	2.13	0.63
2:B:184:LEU:HD23	2:B:185:MET:N	2.14	0.63
3:P:54:MET:HE1	19:P:1267:PGV:H141	1.81	0.63
1:N:376:HIS:O	1:N:380:VAL:HG22	1.98	0.63
22:O:1521:TGL:HC92	27:O:4117:HOH:O	1.99	0.63
4:Q:130:PRO:O	4:Q:136:ALA:HB2	1.99	0.62
1:N:341:ALA:O	1:N:345:ILE:HG13	2.00	0.62
23:O:1230:PSC:H142	23:O:1230:PSC:C34	2.27	0.62
12:L:20:ARG:NH2	22:L:522:TGL:HC61	2.14	0.62
23:O:1230:PSC:C07	9:V:10:ARG:HE	2.09	0.62
1:A:233:HIS:CE1	1:A:292:MET:HE1	2.34	0.62
1:A:436:MET:HE3	1:A:443:TYR:HB3	1.82	0.62
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.30	0.62
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.82	0.62
23:B:230:PSC:H072	9:I:10:ARG:HH21	1.65	0.62
7:G:37:LEU:HD21	26:G:269:CDL:H361	1.81	0.62
1:A:354:THR:HG21	27:A:2228:HOH:O	1.99	0.62
1:A:368:HIS:CD2	1:A:369:ASP:HB2	2.34	0.62
1:N:406:ASN:HD21	19:N:1524:PGV:C2	2.13	0.62
1:A:452:THR:O	1:A:456:MET:HG3	1.99	0.62
26:G:269:CDL:H511	26:G:269:CDL:H172	1.81	0.62
26:T:1269:CDL:H522	26:T:1269:CDL:H202	1.80	0.62
3:P:25:LEU:O	3:P:29:SER:HB2	2.01	0.61
1:N:321:PHE:CD2	23:O:1230:PSC:H341	2.36	0.61
1:A:472:ILE:HG21	22:L:522:TGL:CA9	2.30	0.61
1:N:87:ILE:O	1:N:173:PRO:HD3	2.00	0.61
6:F:85:CYS:SG	6:F:87:THR:HG23	2.41	0.61
1:N:324:LEU:HD13	2:O:41:ILE:HG22	1.82	0.61
6:S:22:LEU:O	6:S:25:ARG:HB3	2.00	0.61
1:A:306:THR:HG23	1:A:359:ALA:O	2.01	0.61
19:A:524:PGV:H311	13:M:16:ALA:HA	1.82	0.61
3:C:25:LEU:O	3:C:29:SER:HB2	2.01	0.61
19:N:1524:PGV:H311	13:Z:16:ALA:HA	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:50:ASN:HD22	3:P:54:MET:HE2	1.64	0.61
6:S:54:ASN:HD22	6:S:54:ASN:C	2.08	0.61
1:N:160:GLY:HA3	27:N:3064:HOH:O	2.00	0.61
12:L:20:ARG:HH22	22:L:522:TGL:HC32	1.65	0.61
2:O:163:TRP:NE1	2:O:209:ILE:HG12	2.15	0.61
2:B:99:THR:HG23	2:B:154:VAL:HG13	1.83	0.60
22:N:1523:TGL:H271	2:O:46:LEU:HD12	1.83	0.60
3:P:168:THR:CG2	25:P:1265:PEK:H14	2.31	0.60
2:O:68:LEU:CB	2:O:69:PRO:HD3	2.31	0.60
1:A:253:MET:O	1:A:257:ILE:HG13	2.01	0.60
7:G:84:LYS:H	7:G:84:LYS:CD	2.07	0.60
2:O:32:PHE:HE2	22:O:1521:TGL:HB91	1.66	0.60
12:Y:20:ARG:HB3	12:Y:20:ARG:NH1	2.15	0.60
3:C:47:LEU:O	3:C:51:MET:HG2	2.00	0.60
1:N:328:HIS:O	2:O:56:MET:HE1	2.01	0.60
24:P:1272:DMU:H25	25:P:1264:PEK:H341	1.84	0.60
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.37	0.60
6:F:8:THR:OG1	6:F:11:GLU:HG3	2.01	0.60
2:B:123:ILE:HG22	2:B:128:LEU:HD23	1.84	0.60
6:S:16:LEU:O	6:S:20:VAL:HG23	2.01	0.60
3:C:28:THR:HG22	19:C:266:PGV:H182	1.84	0.59
2:B:65:TRP:CZ3	23:B:230:PSC:H331	2.37	0.59
23:B:230:PSC:H032	27:E:2129:HOH:O	2.02	0.59
1:N:5:ARG:O	1:N:9:SER:HB2	2.01	0.59
1:N:367:LEU:HD21	1:N:433:LEU:HD23	1.84	0.59
2:O:116:LEU:HD21	2:O:222:TRP:CH2	2.37	0.59
1:A:151:HIS:CD2	25:C:264:PEK:H382	2.37	0.59
4:D:20:ARG:HG2	4:D:72:ASN:HD21	1.68	0.59
19:P:1267:PGV:H182	26:P:1270:CDL:H673	1.85	0.59
1:N:240:HIS:HB3	1:N:241:PRO:HD3	1.84	0.59
1:A:488:THR:HB	1:A:495:LEU:HD13	1.84	0.59
1:N:289:ALA:HB3	1:N:305:PHE:CD1	2.37	0.59
1:N:383:MET:HE2	1:N:421:VAL:HB	1.83	0.59
4:Q:20:ARG:HD2	4:Q:72:ASN:OD1	2.03	0.59
3:C:40:MET:O	3:C:44:MET:HG2	2.01	0.59
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.00	0.59
2:B:145:PRO:HA	2:B:214:VAL:O	2.03	0.58
3:C:122:HIS:HB3	27:C:4324:HOH:O	2.02	0.58
3:C:34:TRP:CZ2	24:C:272:DMU:H29	2.37	0.58
1:A:328:HIS:O	2:B:56:MET:HE1	2.02	0.58
8:H:46:LYS:HB2	8:U:52:VAL:HG12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:B:521:TGL:HC22	27:I:2383:HOH:O	2.02	0.58
10:W:16:ASN:ND2	10:W:18:LEU:HD12	2.19	0.58
2:B:15:PRO:HB2	27:B:4350:HOH:O	2.04	0.58
1:N:378:HIS:O	1:N:382:SER:HB2	2.02	0.58
3:P:250:LEU:HD22	26:T:1269:CDL:C67	2.34	0.58
1:A:508:PRO:HD2	3:C:5:THR:OG1	2.04	0.58
7:G:2:SER:O	25:G:1263:PEK:H322	2.04	0.58
1:A:33:LEU:CD2	12:L:36:PRO:HB3	2.34	0.58
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.67	0.58
2:B:122:MET:SD	2:B:206:PHE:HB3	2.43	0.58
6:F:51:SER:CB	6:F:91:LEU:HD11	2.34	0.58
1:A:361:SER:OG	2:B:84:LEU:HD13	2.04	0.58
1:N:177:SER:H	1:N:180:GLN:NE2	2.00	0.57
1:N:377:PHE:HA	1:N:380:VAL:CG2	2.34	0.57
3:P:40:MET:O	3:P:44:MET:HG2	2.03	0.57
7:G:17:ARG:HD2	27:N:2309:HOH:O	2.04	0.57
2:O:7:LEU:HD11	22:O:1521:TGL:H161	1.86	0.57
2:O:134:ARG:HD3	4:Q:110:THR:OG1	2.04	0.57
27:B:4027:HOH:O	25:P:1265:PEK:H292	2.03	0.57
1:N:71:MET:HE1	1:N:195:LEU:HD21	1.85	0.57
1:N:6:TRP:CD2	12:Y:12:PRO:HB3	2.39	0.57
3:P:41:THR:O	3:P:45:ILE:HG13	2.04	0.57
2:B:164:ALA:HB2	2:B:171:LYS:HG3	1.85	0.57
1:N:51:ASP:OD1	2:O:206:PHE:HE1	1.88	0.57
7:T:8:HIS:HE1	27:T:4411:HOH:O	1.86	0.57
19:C:267:PGV:H172	26:C:270:CDL:H662	1.86	0.57
9:I:36:LYS:HA	9:I:40:ALA:HB3	1.87	0.57
12:L:20:ARG:HH22	22:L:522:TGL:CC6	2.17	0.57
1:N:368:HIS:CD2	1:N:369:ASP:HB2	2.40	0.57
22:N:1522:TGL:H202	22:N:1522:TGL:C24	2.34	0.57
10:W:16:ASN:OD1	10:W:23:LYS:HE3	2.04	0.57
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.86	0.57
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.40	0.57
22:B:521:TGL:H222	22:B:521:TGL:HA82	1.87	0.56
2:O:146:MET:SD	2:O:189:PRO:HB3	2.45	0.56
11:K:24:PHE:O	11:K:28:VAL:HG12	2.04	0.56
22:D:523:TGL:HC61	27:D:4382:HOH:O	2.05	0.56
26:G:269:CDL:H231	26:G:269:CDL:C54	2.33	0.56
22:L:522:TGL:H202	22:L:522:TGL:C24	2.34	0.56
12:Y:21:LEU:O	12:Y:25:MET:HG3	2.05	0.56
1:A:177:SER:H	1:A:180:GLN:HE21	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:1521:TGL:HA82	22:O:1521:TGL:H222	1.87	0.56
1:A:42:GLY:HA3	4:D:104:TYR:OH	2.05	0.56
1:A:397:PHE:HB3	1:A:398:PRO:HD3	1.86	0.56
4:D:107:ILE:HD12	4:D:111:PHE:CD1	2.41	0.56
2:B:56:MET:HG2	23:B:230:PSC:H211	1.87	0.56
2:O:9:PHE:HB2	2:O:21:LEU:HD21	1.88	0.56
7:G:50:TYR:HB3	7:G:52:HIS:CE1	2.40	0.56
10:J:40:LEU:HD12	20:J:60:CHD:H183	1.87	0.56
1:N:406:ASN:HD21	19:N:1524:PGV:H22	1.70	0.56
2:B:135:LEU:HD22	2:B:206:PHE:CD2	2.41	0.55
25:C:265:PEK:H371	26:G:269:CDL:H261	1.88	0.55
12:L:20:ARG:HH12	22:L:522:TGL:CC6	2.14	0.55
2:B:74:ILE:O	2:B:78:LEU:HD22	2.06	0.55
1:N:481:GLU:HB2	13:Z:4:LYS:HE2	1.88	0.55
1:N:483:LEU:HD21	13:Z:4:LYS:HG2	1.88	0.55
3:P:244:PHE:O	3:P:248:VAL:HG23	2.07	0.55
6:S:40:SER:OG	6:S:42:THR:HG23	2.06	0.55
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.89	0.55
22:N:1523:TGL:HC21	22:N:1523:TGL:HG11	1.89	0.55
1:A:66:ILE:HG23	1:A:246:LEU:HD21	1.87	0.55
25:C:264:PEK:H102	25:C:264:PEK:C16	2.33	0.55
3:P:87:ILE:O	3:P:91:VAL:HG23	2.06	0.55
1:A:379:TYR:O	1:A:383:MET:HB2	2.07	0.55
2:B:214:VAL:HB	2:B:215:PRO:CD	2.36	0.55
1:A:306:THR:O	1:A:310:MET:HG3	2.07	0.55
5:E:24:ILE:O	5:E:58:LEU:HD21	2.05	0.55
1:N:431:LEU:HD21	1:N:450:TRP:HB2	1.88	0.55
6:S:94:HIS:CG	6:S:95:GLN:H	2.13	0.55
1:N:406:ASN:ND2	19:N:1524:PGV:H032	2.21	0.55
1:N:459:PHE:HB3	4:Q:92:THR:CG2	2.37	0.55
26:C:270:CDL:H642	26:C:270:CDL:C19	2.37	0.55
12:L:20:ARG:CZ	22:L:522:TGL:HC61	2.37	0.55
2:O:146:MET:CE	9:V:56:SER:HB2	2.37	0.55
6:S:13:ALA:O	6:S:18:ARG:HD2	2.07	0.55
1:A:405:LEU:HD23	1:A:475:ALA:HB2	1.89	0.54
6:F:18:ARG:HB3	27:F:4412:HOH:O	2.08	0.54
1:A:334:TRP:CZ3	22:D:523:TGL:HA51	2.42	0.54
4:D:130:PRO:O	4:D:136:ALA:HB2	2.06	0.54
1:A:69:MET:HE2	18:A:515:HEA:H18	1.89	0.54
23:B:230:PSC:H142	23:B:230:PSC:C34	2.31	0.54
3:C:146:TRP:CE2	7:G:17:ARG:HG3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:440:TYR:HE2	2:O:204:HIS:NE2	2.05	0.54
19:N:1524:PGV:H152	19:N:1524:PGV:H321	1.89	0.54
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.37	0.54
23:B:230:PSC:C07	9:I:10:ARG:HH21	2.20	0.54
1:A:161:ALA:O	1:A:165:ILE:HG13	2.07	0.54
12:L:25:MET:HG2	22:L:522:TGL:HA62	1.90	0.54
2:O:98:LYS:HE3	2:O:109:GLU:HB2	1.90	0.54
9:V:36:LYS:HA	9:V:40:ALA:HB3	1.88	0.54
1:A:243:VAL:HA	1:A:246:LEU:HD12	1.89	0.54
3:P:50:ASN:HD21	3:P:54:MET:HE2	1.71	0.54
5:E:57:ARG:HG3	5:E:57:ARG:NH1	2.23	0.54
1:A:115:SER:HA	1:A:145:LEU:HD12	1.89	0.54
6:F:63:GLU:HG3	27:F:4360:HOH:O	2.07	0.54
2:O:100:MET:HB2	2:O:107:SER:OG	2.08	0.54
1:A:282:PHE:HA	7:T:4:ALA:CB	2.38	0.54
3:C:50:ASN:HD21	3:C:54:MET:HE2	1.72	0.54
1:N:380:VAL:O	1:N:384:GLY:HA3	2.07	0.54
1:A:377:PHE:O	1:A:381:LEU:HB3	2.08	0.53
25:C:265:PEK:H231	7:G:21:PHE:CD2	2.43	0.53
3:P:187:THR:HG22	25:P:1264:PEK:H052	1.90	0.53
1:A:12:HIS:CD2	1:A:91:ASP:HA	2.43	0.53
1:A:34:SER:HB3	1:A:61:HIS:CE1	2.43	0.53
1:N:197:LEU:O	3:P:92:LEU:HD12	2.08	0.53
2:B:114:GLU:HG3	2:B:227:LEU:HD11	1.90	0.53
22:L:522:TGL:H231	22:L:522:TGL:H272	1.91	0.53
2:O:56:MET:HA	23:O:1230:PSC:H202	1.91	0.53
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.91	0.53
3:P:66:THR:HG23	19:P:1267:PGV:O05	2.09	0.53
1:A:472:ILE:HD13	22:L:522:TGL:HA91	1.91	0.53
1:N:169:ILE:HD11	1:N:189:MET:SD	2.48	0.53
1:N:289:ALA:HB3	1:N:305:PHE:CG	2.44	0.53
2:O:203:ASN:N	2:O:203:ASN:HD22	2.05	0.53
3:P:157:LYS:NZ	25:P:1265:PEK:H052	2.23	0.53
1:N:459:PHE:HB3	4:Q:92:THR:HG23	1.90	0.53
11:K:25:CYS:O	11:K:29:TRP:HD1	1.92	0.53
22:N:1522:TGL:HC21	22:N:1522:TGL:OA1	2.08	0.53
1:A:104:LEU:C	1:A:107:PRO:HD2	2.34	0.53
3:C:168:THR:HG21	25:C:265:PEK:H12	1.89	0.53
1:N:314:ILE:HB	1:N:315:PRO:CD	2.39	0.53
1:N:400:PHE:HB3	22:N:1522:TGL:H283	1.91	0.53
3:P:250:LEU:HD22	26:T:1269:CDL:H673	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:80:ARG:HH11	25:T:263:PEK:C03	2.18	0.53
5:E:53:ARG:NH2	5:E:92:THR:HG23	2.23	0.53
1:N:68:PHE:C	1:N:72:PRO:HG2	2.34	0.53
7:G:31:CYS:HG	26:G:269:CDL:H532	1.72	0.52
26:P:1270:CDL:H642	26:P:1270:CDL:C19	2.38	0.52
1:A:240:HIS:O	1:A:243:VAL:HG22	2.09	0.52
1:A:347:LEU:HD13	1:A:383:MET:SD	2.49	0.52
3:C:51:MET:SD	26:C:270:CDL:H622	2.49	0.52
2:O:74:ILE:O	2:O:78:LEU:HD22	2.10	0.52
2:O:122:MET:SD	2:O:206:PHE:HB3	2.49	0.52
4:Q:131:ILE:HD12	4:Q:131:ILE:N	2.25	0.52
1:A:165:ILE:O	1:A:169:ILE:HG12	2.08	0.52
4:Q:134:PHE:HE1	11:X:44:PRO:HD2	1.74	0.52
2:B:23:PHE:CZ	2:B:80:SER:HB2	2.44	0.52
3:C:68:GLN:HB2	3:C:70:HIS:HD2	1.74	0.52
1:N:339:MET:HE1	22:N:1523:TGL:HB31	1.89	0.52
1:A:440:TYR:CG	2:B:205:SER:HB3	2.45	0.52
7:G:79:PRO:HD2	27:G:2136:HOH:O	2.10	0.52
10:J:12:PHE:HD2	10:J:23:LYS:HG2	1.75	0.52
2:O:145:PRO:HB2	2:O:148:MET:HG3	1.90	0.52
10:W:16:ASN:CG	10:W:18:LEU:HD12	2.35	0.52
11:X:31:TYR:HB2	27:X:4091:HOH:O	2.08	0.52
1:N:52:GLN:O	1:N:56:VAL:HG23	2.10	0.52
5:R:12:ASP:CG	9:V:10:ARG:HH22	2.18	0.52
2:O:121:TYR:O	2:O:138:VAL:HA	2.09	0.52
1:A:33:LEU:HB3	1:A:61:HIS:HB2	1.91	0.52
4:D:144:GLU:HB2	27:D:4097:HOH:O	2.10	0.52
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.92	0.52
1:A:40:GLU:HG2	1:A:54:TYR:CD2	2.45	0.52
1:A:248:LEU:O	1:A:251:PHE:HB2	2.10	0.52
11:K:7:PRO:O	11:K:12:LYS:HE3	2.10	0.52
22:L:522:TGL:HC21	22:L:522:TGL:OA1	2.10	0.52
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.91	0.51
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.92	0.51
7:G:34:ASN:O	7:G:37:LEU:HB3	2.09	0.51
1:A:482:VAL:HG22	13:M:1:ILE:HD11	1.92	0.51
7:G:34:ASN:HD22	26:G:269:CDL:H151	1.76	0.51
2:O:4:PRO:HB2	11:X:43:SER:HA	1.91	0.51
2:O:163:TRP:CD1	2:O:209:ILE:HG12	2.46	0.51
25:C:265:PEK:H22	27:C:4087:HOH:O	2.09	0.51
4:D:80:THR:HA	11:K:17:VAL:HG11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:233:HIS:CE1	1:N:292:MET:HE1	2.45	0.51
19:P:1267:PGV:H172	26:P:1270:CDL:H662	1.91	0.51
3:C:51:MET:SD	26:C:270:CDL:C62	2.99	0.51
1:N:62:ALA:HB2	18:N:515:HEA:HBD1	1.93	0.51
3:P:28:THR:HG22	19:P:1266:PGV:H182	1.91	0.51
1:A:314:ILE:HB	1:A:315:PRO:CD	2.41	0.51
2:B:81:LEU:HD13	26:T:1269:CDL:H122	1.93	0.51
22:D:523:TGL:HC21	22:D:523:TGL:HG11	1.92	0.51
5:E:84:TYR:O	5:E:88:GLU:HG2	2.10	0.51
26:G:269:CDL:H182	1:N:307:SER:CB	2.39	0.51
2:B:123:ILE:CG2	2:B:128:LEU:HD23	2.40	0.51
2:B:146:MET:HE1	9:I:56:SER:HB2	1.93	0.51
2:B:200:CYS:SG	2:B:204:HIS:HA	2.50	0.51
4:Q:52:SER:O	4:Q:56:LYS:HG3	2.10	0.51
3:C:159:MET:SD	3:C:159:MET:C	2.94	0.51
2:O:222:TRP:HB2	9:V:71:SER:HB2	1.92	0.51
4:Q:118:LYS:HB3	11:X:53:TRP:HB3	1.93	0.51
1:A:1:FME:HA	1:A:1:FME:CE	2.41	0.51
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.91	0.51
3:P:62:ILE:HG23	3:P:221:ARG:HH21	1.74	0.51
1:A:309:THR:HG22	1:A:309:THR:O	2.10	0.51
1:A:459:PHE:O	1:A:462:LEU:HB3	2.11	0.51
1:N:151:HIS:O	1:N:155:VAL:HG23	2.11	0.51
1:N:411:LYS:HD3	22:N:1523:TGL:HB21	1.93	0.51
6:S:94:HIS:HD2	6:S:95:GLN:N	2.09	0.51
7:G:37:LEU:HD23	7:G:38:HIS:CE1	2.46	0.50
1:N:377:PHE:CD1	18:N:516:HEA:HAD1	2.46	0.50
1:A:398:PRO:HA	1:A:403:TYR:O	2.12	0.50
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.41	0.50
2:O:59:GLN:O	2:O:59:GLN:HG3	2.11	0.50
2:O:20:LEU:HD21	2:O:83:ILE:HG21	1.93	0.50
2:B:39:LEU:HD22	22:B:521:TGL:H141	1.92	0.50
6:F:47:ASN:HB2	6:F:89:TYR:CD1	2.46	0.50
1:N:115:SER:O	1:N:121:GLY:HA2	2.11	0.50
4:Q:129:ALA:HB1	4:Q:133:GLY:HA3	1.93	0.50
19:A:524:PGV:H152	19:A:524:PGV:H321	1.93	0.50
4:D:93:ALA:O	4:D:97:ILE:HG13	2.11	0.50
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.94	0.50
7:G:3:ALA:O	7:G:4:ALA:HB2	2.11	0.50
26:G:269:CDL:H182	1:N:307:SER:HB3	1.93	0.50
2:O:57:ASP:H	23:O:1230:PSC:H201	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:58:GLU:O	4:Q:62:LEU:HG	2.11	0.50
1:A:382:SER:O	1:A:386:VAL:HB	2.12	0.50
3:P:65:SER:HB2	19:P:1267:PGV:H041	1.94	0.50
5:R:8:ASP:HB3	9:V:10:ARG:CZ	2.41	0.50
1:A:240:HIS:HB3	1:A:241:PRO:HD3	1.93	0.50
2:B:4:PRO:HB2	11:K:43:SER:HA	1.94	0.50
3:C:157:LYS:NZ	25:C:265:PEK:H052	2.27	0.50
6:F:81:ARG:HG2	6:F:88:HIS:CD2	2.46	0.50
1:N:29:VAL:HG22	12:Y:32:GLY:O	2.12	0.50
4:Q:75:THR:HG22	27:Q:4352:HOH:O	2.11	0.50
1:A:37:ILE:HD11	1:A:58:VAL:HA	1.93	0.49
19:A:524:PGV:P	19:A:524:PGV:H061	2.52	0.49
1:N:298:ASP:HB3	27:N:3389:HOH:O	2.12	0.49
3:C:116:TRP:HA	3:C:117:PRO:C	2.37	0.49
3:C:212:SER:O	3:C:216:ILE:HG13	2.11	0.49
4:D:34:SER:O	4:D:38:LYS:HG3	2.12	0.49
7:G:18:PHE:HD2	7:G:18:PHE:O	1.95	0.49
1:N:440:TYR:CE2	2:O:204:HIS:NE2	2.80	0.49
4:Q:90:GLY:O	11:X:28:VAL:HG11	2.11	0.49
19:C:267:PGV:H12	19:C:267:PGV:H161	1.94	0.49
6:S:92:VAL:O	6:S:92:VAL:HG23	2.12	0.49
7:T:17:ARG:HD2	27:T:3309:HOH:O	2.11	0.49
1:N:390:MET:HE2	1:N:413:HIS:HE1	1.77	0.49
3:P:239:ALA:O	3:P:243:HIS:CD2	2.65	0.49
1:A:5:ARG:O	1:A:9:SER:HB2	2.12	0.49
1:A:131:PRO:HG3	27:A:4333:HOH:O	2.13	0.49
23:B:230:PSC:H212	23:B:230:PSC:O01	2.12	0.49
4:D:48:TRP:CH2	5:E:56:ARG:HA	2.47	0.49
4:Q:12:ALA:HA	6:S:73:TRP:CD1	2.48	0.49
1:A:304:TYR:HD1	26:T:1269:CDL:HB32	1.77	0.49
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.78	0.49
2:O:56:MET:HA	23:O:1230:PSC:C20	2.42	0.49
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.94	0.49
2:B:184:LEU:HD23	2:B:184:LEU:C	2.37	0.49
2:B:214:VAL:HB	2:B:215:PRO:HD2	1.95	0.49
25:G:1263:PEK:H9	3:P:244:PHE:HA	1.93	0.49
9:I:35:TYR:C	9:I:37:PHE:H	2.21	0.49
1:N:405:LEU:HD23	1:N:475:ALA:HB2	1.95	0.49
1:A:195:LEU:CD2	1:A:245:ILE:HD13	2.43	0.49
1:N:377:PHE:HA	1:N:380:VAL:HG23	1.93	0.49
9:V:67:GLY:HA2	27:V:3310:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:265:PEK:C38	26:G:269:CDL:H273	2.43	0.49
26:G:269:CDL:H322	26:G:269:CDL:HA62	1.93	0.49
9:I:23:GLY:O	9:I:27:VAL:HG23	2.13	0.49
1:N:381:LEU:CD1	18:N:516:HEA:HBC2	2.42	0.49
19:N:1524:PGV:H012	27:N:4191:HOH:O	2.11	0.49
3:P:193:TYR:C	3:P:193:TYR:CD2	2.90	0.49
7:T:78:LEU:HB3	7:T:79:PRO:HD2	1.94	0.49
3:P:50:ASN:O	3:P:54:MET:HG3	2.13	0.49
1:A:383:MET:O	1:A:387:PHE:HB2	2.12	0.48
8:H:43:MET:CE	8:U:43:MET:HE1	2.30	0.48
1:N:398:PRO:HA	1:N:403:TYR:O	2.12	0.48
2:O:172:THR:HG21	2:O:180:ASN:HB3	1.94	0.48
4:Q:33:LEU:HA	4:Q:37:GLN:NE2	2.28	0.48
1:N:507:GLU:HG3	3:P:5:THR:OG1	2.13	0.48
1:A:380:VAL:O	1:A:384:GLY:HA3	2.13	0.48
2:B:93:PRO:HA	2:B:149:THR:HG22	1.94	0.48
7:G:78:LEU:HB3	7:G:79:PRO:CD	2.42	0.48
1:N:115:SER:HB2	1:N:142:SER:O	2.13	0.48
3:P:59:ARG:HG3	26:P:1270:CDL:H512	1.94	0.48
26:T:1269:CDL:H322	26:T:1269:CDL:HA62	1.95	0.48
1:A:449:MET:SD	2:B:5:MET:HG2	2.53	0.48
10:J:31:LEU:HD12	10:J:31:LEU:HA	1.66	0.48
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.48	0.48
23:O:1230:PSC:O01	23:O:1230:PSC:H212	2.13	0.48
4:Q:129:ALA:HB3	4:Q:134:PHE:H	1.77	0.48
1:A:30:GLY:C	1:A:65:MET:HE2	2.38	0.48
2:B:135:LEU:HD22	2:B:206:PHE:HD2	1.77	0.48
1:N:337:ALA:HB2	1:N:394:VAL:HG23	1.96	0.48
2:O:2:ALA:HA	2:O:6:GLN:OE1	2.13	0.48
2:B:151:ARG:CD	2:B:181:GLN:HE21	2.26	0.48
2:O:156:SER:HB3	2:O:176:PRO:HD3	1.96	0.48
3:P:16:TRP:HA	3:P:16:TRP:CE3	2.49	0.48
3:P:151:LEU:HB2	3:P:159:MET:HG3	1.95	0.48
4:Q:33:LEU:HB2	4:Q:38:LYS:HG2	1.94	0.48
1:A:115:SER:HB2	1:A:142:SER:O	2.14	0.48
2:B:41:ILE:CD1	23:B:230:PSC:H342	2.41	0.48
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.01	0.48
6:F:95:GLN:HG3	27:F:4316:HOH:O	2.13	0.48
19:P:1267:PGV:H161	19:P:1267:PGV:H12	1.94	0.48
7:T:3:ALA:O	7:T:4:ALA:HB2	2.14	0.48
1:A:497:GLY:HA3	27:A:2398:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:MET:HE1	1:A:323:TRP:NE1	2.29	0.48
3:C:50:ASN:HD22	3:C:51:MET:HE2	1.79	0.48
3:C:57:TRP:CZ2	19:C:266:PGV:H21	2.49	0.48
4:D:129:ALA:HB1	4:D:133:GLY:HA3	1.96	0.48
1:N:380:VAL:HG23	1:N:381:LEU:H	1.78	0.48
1:N:492:LEU:O	1:N:492:LEU:HD12	2.14	0.48
22:N:1522:TGL:H272	22:N:1522:TGL:H231	1.95	0.48
2:O:122:MET:HE2	27:O:4368:HOH:O	2.13	0.48
3:P:157:LYS:HZ2	25:P:1265:PEK:H052	1.78	0.48
1:A:501:PRO:HG2	1:A:504:THR:HG22	1.94	0.47
26:G:269:CDL:H761	1:N:282:PHE:HZ	1.78	0.47
1:N:103:TRP:O	1:N:106:PRO:HD2	2.14	0.47
1:N:316:THR:HG21	18:N:516:HEA:H14	1.95	0.47
25:P:1264:PEK:H102	25:P:1264:PEK:C16	2.38	0.47
1:A:61:HIS:CE1	18:A:515:HEA:NB	2.82	0.47
1:A:310:MET:HE2	1:A:356:ILE:HG23	1.95	0.47
1:A:400:PHE:HB3	22:L:522:TGL:H283	1.96	0.47
2:B:45:MET:HE2	2:B:45:MET:HA	1.97	0.47
22:L:522:TGL:HC62	22:L:522:TGL:CC2	2.30	0.47
1:N:130:PRO:HD2	1:N:231:TYR:CD1	2.49	0.47
1:N:184:PHE:O	1:N:188:VAL:HG23	2.15	0.47
1:N:306:THR:HG23	1:N:359:ALA:O	2.14	0.47
26:T:1269:CDL:H231	26:T:1269:CDL:C54	2.36	0.47
7:G:78:LEU:HB3	7:G:79:PRO:HD2	1.97	0.47
2:O:68:LEU:HB3	2:O:69:PRO:HD3	1.97	0.47
1:A:282:PHE:HZ	26:T:1269:CDL:H761	1.80	0.47
1:A:449:MET:HB3	27:A:4144:HOH:O	2.13	0.47
6:F:92:VAL:O	6:F:92:VAL:CG2	2.63	0.47
3:P:43:LEU:O	3:P:47:LEU:HG	2.13	0.47
3:P:61:VAL:HG22	19:P:1266:PGV:H061	1.96	0.47
4:Q:131:ILE:HD12	4:Q:131:ILE:H	1.79	0.47
2:B:114:GLU:HB3	2:B:227:LEU:HD21	1.96	0.47
24:P:1272:DMU:H30	24:P:1272:DMU:O1	2.15	0.47
1:A:33:LEU:HD12	1:A:61:HIS:HA	1.97	0.47
19:C:267:PGV:H182	26:C:270:CDL:C67	2.43	0.47
7:G:4:ALA:CB	1:N:282:PHE:HA	2.45	0.47
1:N:390:MET:HE2	1:N:413:HIS:CE1	2.49	0.47
1:N:468:MET:HG2	1:N:468:MET:O	2.09	0.47
5:R:37:VAL:HG11	5:R:70:VAL:HG21	1.96	0.47
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.97	0.47
6:F:49:VAL:O	6:F:91:LEU:HD12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:2:SER:O	25:T:263:PEK:H322	2.14	0.47
7:T:6:GLY:O	25:T:263:PEK:H311	2.15	0.47
1:A:195:LEU:HG	1:A:245:ILE:HD13	1.97	0.47
4:D:109:HIS:HD2	27:D:2159:HOH:O	1.97	0.47
13:M:4:LYS:HE3	27:M:4199:HOH:O	2.15	0.47
1:N:124:THR:HB	27:N:4378:HOH:O	2.14	0.47
9:V:64:ARG:HG3	9:V:72:ALA:O	2.15	0.47
4:D:88:PHE:HZ	13:M:19:LEU:HD21	1.80	0.47
1:N:151:HIS:HD2	25:P:1264:PEK:C38	2.22	0.47
2:O:20:LEU:CD2	2:O:83:ILE:HG21	2.45	0.47
25:P:1265:PEK:H041	6:S:1:ALA:N	2.30	0.47
7:T:2:SER:OG	25:T:263:PEK:H301	2.14	0.47
1:A:177:SER:H	1:A:180:GLN:NE2	2.12	0.46
4:D:129:ALA:HB3	4:D:134:PHE:H	1.79	0.46
1:N:230:LEU:HD13	3:P:103:HIS:CG	2.50	0.46
22:O:1521:TGL:HC22	27:V:3383:HOH:O	2.15	0.46
23:O:1230:PSC:H032	27:R:3129:HOH:O	2.15	0.46
3:P:9:HIS:CE1	3:P:11:VAL:HG22	2.50	0.46
1:A:17:THR:OG1	22:L:522:TGL:H281	2.15	0.46
2:B:17:MET:HE2	27:B:4017:HOH:O	2.16	0.46
2:B:79:PRO:O	2:B:83:ILE:HG13	2.14	0.46
2:O:110:TYR:N	2:O:110:TYR:CD2	2.83	0.46
3:P:221:ARG:NH1	3:P:227:PHE:HE1	2.13	0.46
1:N:304:TYR:HD2	1:N:305:PHE:CD2	2.33	0.46
1:N:436:MET:HE1	1:N:451:ASN:OD1	2.15	0.46
1:A:426:PHE:N	1:A:427:PRO:CD	2.79	0.46
3:C:109:THR:HB	3:C:110:PRO:HD2	1.98	0.46
3:C:244:PHE:HA	25:T:263:PEK:H9	1.98	0.46
1:N:59:THR:HG22	1:N:63:PHE:CE2	2.50	0.46
9:V:35:TYR:C	9:V:37:PHE:H	2.23	0.46
10:W:30:ILE:O	10:W:34:VAL:HG23	2.15	0.46
1:A:71:MET:HE1	1:A:195:LEU:HD21	1.97	0.46
1:A:194:LEU:CB	1:A:245:ILE:HD11	2.46	0.46
1:N:472:ILE:HD13	22:N:1522:TGL:HA91	1.97	0.46
26:T:1269:CDL:H571	26:T:1269:CDL:H601	1.45	0.46
1:A:115:SER:O	1:A:121:GLY:HA2	2.15	0.46
1:N:488:THR:HB	1:N:495:LEU:HD13	1.96	0.46
9:V:18:ARG:HG2	9:V:18:ARG:HH11	1.80	0.46
22:D:523:TGL:HG31	27:D:4040:HOH:O	2.16	0.46
5:E:105:GLY:O	5:E:108:LYS:HG2	2.16	0.46
3:P:51:MET:HB3	26:P:1270:CDL:H622	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:139:ALA:CB	7:T:24:ALA:HB1	2.45	0.46
1:N:398:PRO:HG3	27:N:4079:HOH:O	2.15	0.46
7:T:38:HIS:CD2	26:T:1269:CDL:HA21	2.50	0.46
20:W:1060:CHD:H212	20:W:1060:CHD:H161	1.76	0.46
1:A:344:PHE:CD1	1:A:344:PHE:C	2.93	0.46
4:D:23:PRO:HB3	5:E:70:VAL:HG21	1.97	0.46
4:D:131:ILE:HG22	4:D:132:GLN:HG3	1.98	0.46
3:P:213:THR:HG23	26:P:1270:CDL:H762	1.97	0.46
1:A:239:GLY:O	1:A:243:VAL:HG13	2.16	0.45
2:B:139:ASP:OD2	2:B:140:ASN:N	2.49	0.45
23:B:230:PSC:H212	23:B:230:PSC:C02	2.47	0.45
19:N:1524:PGV:P	19:N:1524:PGV:H061	2.56	0.45
1:A:514:LYS:HE2	27:F:2339:HOH:O	2.16	0.45
2:B:168:LEU:HD13	2:B:184:LEU:HG	1.98	0.45
5:E:65:VAL:HG13	5:E:101:PRO:HG3	1.98	0.45
1:N:325:ALA:HA	23:O:1230:PSC:H291	1.98	0.45
3:P:187:THR:CB	7:T:68:THR:HG21	2.46	0.45
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.16	0.45
3:C:184:ALA:HA	3:C:185:PRO:HD2	1.88	0.45
26:C:270:CDL:H672	26:C:270:CDL:H641	1.80	0.45
1:N:295:VAL:HG12	2:O:173:ASP:OD2	2.16	0.45
1:N:513:LEU:HD22	1:N:513:LEU:HA	1.80	0.45
2:O:65:TRP:CZ3	23:O:1230:PSC:H331	2.51	0.45
2:O:170:LEU:HD23	27:O:4107:HOH:O	2.15	0.45
2:O:200:CYS:SG	2:O:204:HIS:HA	2.56	0.45
25:P:1264:PEK:H71	25:P:1264:PEK:H32	1.97	0.45
4:Q:23:PRO:HD2	5:R:34:ASN:OD1	2.17	0.45
1:A:230:LEU:HD21	3:C:100:ALA:HA	1.98	0.45
1:A:481:GLU:O	13:M:3:ALA:HB1	2.17	0.45
3:C:55:TYR:CD1	26:C:270:CDL:H532	2.52	0.45
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.82	0.45
2:O:113:TYR:HE1	8:U:11:TYR:O	2.00	0.45
2:O:145:PRO:HA	2:O:214:VAL:O	2.16	0.45
3:P:68:GLN:HE21	3:P:70:HIS:CD2	2.34	0.45
3:P:134:THR:OG1	3:P:249:TRP:NE1	2.41	0.45
7:T:8:HIS:ND1	25:T:263:PEK:H312	2.32	0.45
10:W:5:VAL:O	10:W:9:GLN:HG3	2.16	0.45
1:A:321:PHE:CD2	23:B:230:PSC:H341	2.51	0.45
3:C:246:ASP:HB2	27:C:4141:HOH:O	2.15	0.45
3:P:12:ASN:O	3:P:13:PRO:C	2.59	0.45
4:Q:56:LYS:NZ	5:R:97:GLY:O	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16:TRP:CE3	3:C:16:TRP:HA	2.51	0.45
1:N:100:MET:HE1	19:P:1266:PGV:H81	1.98	0.45
2:O:98:LYS:HD3	8:U:63:LEU:O	2.17	0.45
25:P:1265:PEK:H371	26:T:1269:CDL:H261	1.98	0.45
4:Q:114:GLU:HG3	11:X:51:LYS:HZ2	1.82	0.45
20:W:1271:CHD:H112	20:W:1271:CHD:H12A	1.61	0.45
1:A:194:LEU:HD12	1:A:245:ILE:HG13	1.99	0.45
3:C:171:VAL:HA	27:C:4409:HOH:O	2.16	0.45
5:E:56:ARG:HG2	5:E:96:LEU:HD22	1.99	0.45
26:G:269:CDL:H122	2:O:81:LEU:HD13	1.99	0.45
2:O:172:THR:CG2	2:O:180:ASN:HB3	2.46	0.45
7:T:47:PHE:CD2	7:T:77:PRO:HB2	2.52	0.45
1:A:276:ALA:O	1:A:280:ILE:HG13	2.17	0.45
2:O:58:ALA:O	2:O:60:GLU:N	2.48	0.45
3:P:213:THR:HG21	19:P:1267:PGV:H11	1.98	0.45
4:Q:24:LEU:HD12	5:R:33:MET:HB2	1.99	0.45
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.99	0.45
6:S:77:GLY:O	6:S:90:LYS:NZ	2.36	0.45
1:A:306:THR:HG23	1:A:360:ASN:HA	1.99	0.45
2:B:146:MET:SD	2:B:189:PRO:HB3	2.57	0.45
3:C:158:HIS:NE2	25:C:265:PEK:H051	2.32	0.45
3:C:166:THR:HG22	3:C:215:LEU:HD13	1.99	0.45
3:P:116:TRP:HA	3:P:117:PRO:C	2.40	0.45
12:Y:42:HIS:NE2	12:Y:46:LYS:HD2	2.32	0.45
2:B:74:ILE:HD11	26:T:1269:CDL:H452	1.98	0.45
7:G:34:ASN:ND2	26:G:269:CDL:H151	2.31	0.45
9:I:15:ARG:HD3	9:I:16:ARG:N	2.32	0.45
3:P:243:HIS:O	3:P:247:VAL:HG23	2.16	0.45
9:V:37:PHE:HA	9:V:41:GLU:HB2	1.99	0.45
2:B:62:GLU:HA	2:B:65:TRP:CD1	2.52	0.44
3:C:63:ARG:NH1	10:J:20:VAL:O	2.49	0.44
3:C:187:THR:HG22	25:C:264:PEK:H052	1.99	0.44
5:E:78:HIS:CD2	9:I:12:LEU:HD13	2.53	0.44
6:F:64:GLU:O	6:F:65:ASP:HB2	2.17	0.44
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.16	0.44
1:N:489:THR:HA	6:S:71:TRP:O	2.18	0.44
4:Q:119:GLN:O	4:Q:123:MET:HG3	2.17	0.44
1:A:321:PHE:HB3	2:B:65:TRP:CZ3	2.52	0.44
1:A:505:PHE:HB3	27:A:2194:HOH:O	2.18	0.44
3:C:51:MET:HB3	26:C:270:CDL:H622	1.98	0.44
1:N:220:PHE:CE1	1:N:231:TYR:HB2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:N:1523:TGL:H311	4:Q:89:ILE:HD13	2.00	0.44
7:T:2:SER:O	7:T:3:ALA:HB3	2.18	0.44
7:T:79:PRO:HD2	27:T:3136:HOH:O	2.17	0.44
1:A:377:PHE:CE2	1:A:378:HIS:CE1	3.04	0.44
2:B:58:ALA:O	2:B:60:GLU:N	2.49	0.44
2:B:160:LEU:O	2:B:200:CYS:HB3	2.15	0.44
23:B:230:PSC:H251	23:B:230:PSC:H221	1.71	0.44
8:H:46:LYS:CB	8:U:52:VAL:HG12	2.48	0.44
3:P:184:ALA:HA	3:P:185:PRO:HD2	1.85	0.44
11:X:36:ILE:HG13	11:X:38:ILE:HG13	1.99	0.44
2:B:70:ALA:O	2:B:74:ILE:HG13	2.18	0.44
4:D:99:GLU:HB3	27:D:4113:HOH:O	2.17	0.44
5:E:63:SER:O	5:E:67:ILE:HG13	2.18	0.44
6:F:13:ALA:O	6:F:18:ARG:HD2	2.17	0.44
11:K:15:ASN:HB2	27:K:2386:HOH:O	2.16	0.44
12:L:25:MET:HE3	22:L:522:TGL:HA62	2.00	0.44
1:N:106:PRO:HB2	1:N:107:PRO:HD3	2.00	0.44
3:P:187:THR:HB	7:T:68:THR:HG21	2.00	0.44
25:P:1265:PEK:C38	26:T:1269:CDL:H273	2.47	0.44
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.17	0.44
20:A:525:CHD:H112	20:A:525:CHD:H12A	1.78	0.44
2:B:78:LEU:HD12	2:B:78:LEU:HA	1.83	0.44
1:N:66:ILE:O	1:N:71:MET:HG3	2.17	0.44
3:P:156:ARG:HH22	3:P:223:LEU:HA	1.81	0.44
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.53	0.44
20:B:1086:CHD:H212	20:B:1086:CHD:H12	1.99	0.44
1:N:383:MET:O	1:N:387:PHE:HB2	2.18	0.44
2:O:203:ASN:N	2:O:203:ASN:ND2	2.66	0.44
10:W:36:MET:HB3	20:W:1060:CHD:H181	1.99	0.44
2:B:213:LEU:N	2:B:213:LEU:CD2	2.81	0.44
3:C:68:GLN:HB3	27:C:2153:HOH:O	2.18	0.44
4:D:107:ILE:HB	4:D:108:PRO:HD2	1.98	0.44
6:F:95:GLN:NE2	27:F:4185:HOH:O	2.49	0.44
27:N:3090:HOH:O	3:P:13:PRO:HG3	2.17	0.44
1:A:53:ILE:CD1	12:L:44:LEU:HD23	2.48	0.44
1:A:145:LEU:HD21	3:C:32:THR:HG21	2.00	0.44
1:A:307:SER:CB	26:T:1269:CDL:H182	2.48	0.44
3:C:63:ARG:O	3:C:68:GLN:HG3	2.17	0.44
3:C:221:ARG:NH1	3:C:227:PHE:CE1	2.86	0.44
5:E:28:GLU:HG2	27:E:4385:HOH:O	2.17	0.44
26:G:269:CDL:HB32	1:N:304:TYR:CD1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:40:GLU:OE1	1:N:46:THR:HA	2.18	0.44
1:N:68:PHE:HA	1:N:72:PRO:HG2	2.00	0.44
1:N:68:PHE:O	1:N:72:PRO:HG2	2.18	0.44
2:O:216:LEU:O	2:O:219:PHE:HB3	2.18	0.44
7:T:5:LYS:HD2	25:T:263:PEK:H371	2.00	0.44
1:A:92:MET:O	1:A:95:PRO:HD3	2.18	0.44
3:C:233:PHE:N	19:C:267:PGV:O14	2.47	0.44
4:D:23:PRO:HB3	5:E:70:VAL:CG2	2.48	0.44
1:N:34:SER:HB3	1:N:61:HIS:CE1	2.53	0.44
1:N:506:GLU:HB2	27:N:4072:HOH:O	2.18	0.44
2:O:41:ILE:O	2:O:45:MET:HG2	2.17	0.44
7:T:78:LEU:HB3	7:T:79:PRO:CD	2.48	0.44
2:B:65:TRP:HZ3	23:B:230:PSC:H331	1.81	0.43
23:B:230:PSC:H12	23:B:230:PSC:H322	2.01	0.43
8:H:27:ARG:NH1	27:H:2303:HOH:O	2.48	0.43
1:N:382:SER:O	1:N:386:VAL:HB	2.18	0.43
2:O:5:MET:HE2	2:O:5:MET:HB3	1.83	0.43
8:U:43:MET:HE2	8:U:52:VAL:HG21	1.99	0.43
4:D:126:MET:HG3	4:D:128:VAL:HG23	1.99	0.43
6:F:21:MET:HE2	6:F:21:MET:HB3	1.90	0.43
6:F:54:ASN:OD1	6:F:76:LYS:HD2	2.17	0.43
1:N:356:ILE:HD13	1:N:356:ILE:HA	1.83	0.43
1:N:363:LEU:HD23	1:N:363:LEU:HA	1.88	0.43
1:N:366:VAL:HG12	27:N:3400:HOH:O	2.18	0.43
2:O:132:GLU:HA	4:Q:122:ARG:NH1	2.34	0.43
4:Q:51:LEU:HD21	4:Q:59:LEU:HD11	1.99	0.43
7:T:49:PRO:HD2	8:U:80:THR:HG22	2.00	0.43
10:W:50:LEU:O	10:W:50:LEU:HD22	2.19	0.43
26:C:270:CDL:H202	26:C:270:CDL:H171	1.79	0.43
20:N:1604:CHD:H212	20:N:1604:CHD:H12	2.00	0.43
3:P:63:ARG:NH1	10:W:20:VAL:O	2.52	0.43
2:B:151:ARG:NE	2:B:181:GLN:NE2	2.66	0.43
3:C:218:CYS:SG	3:C:235:PHE:HA	2.59	0.43
10:J:36:MET:HG2	20:J:60:CHD:H222	1.99	0.43
4:Q:129:ALA:CB	4:Q:134:PHE:H	2.31	0.43
1:A:68:PHE:HA	1:A:72:PRO:HG2	1.99	0.43
2:B:102:HIS:O	2:B:104:TRP:HA	2.19	0.43
2:B:175:ILE:HD12	2:B:180:ASN:HD21	1.82	0.43
3:C:16:TRP:HA	3:C:16:TRP:HE3	1.83	0.43
4:D:119:GLN:O	4:D:123:MET:HG3	2.18	0.43
5:E:20:ASN:O	5:E:21:LYS:C	2.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:321:PHE:CZ	23:O:1230:PSC:H171	2.54	0.43
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.99	0.43
23:O:1230:PSC:H212	23:O:1230:PSC:C02	2.48	0.43
4:Q:34:SER:N	4:Q:37:GLN:HE21	2.08	0.43
1:A:141:ALA:O	1:A:144:ASP:N	2.51	0.43
11:K:41:ASN:ND2	27:K:2283:HOH:O	2.48	0.43
1:N:498:CYS:HA	1:N:499:PRO:HA	1.85	0.43
3:P:16:TRP:HA	3:P:16:TRP:HE3	1.82	0.43
3:P:149:HIS:O	3:P:153:GLU:HG3	2.18	0.43
8:U:39:CYS:O	8:U:43:MET:HG2	2.18	0.43
19:A:524:PGV:H152	19:A:524:PGV:H301	2.01	0.43
1:N:53:ILE:O	1:N:57:VAL:HG23	2.19	0.43
1:N:377:PHE:CE2	1:N:378:HIS:CE1	3.06	0.43
1:N:443:TYR:HB2	1:N:447:TYR:HD2	1.83	0.43
1:A:108:SER:HB2	1:A:152:LEU:HB2	2.01	0.43
1:N:369:ASP:C	1:N:438:ARG:HG3	2.44	0.43
2:O:160:LEU:O	2:O:200:CYS:HB3	2.19	0.43
2:O:161:HIS:CE1	2:O:200:CYS:HB2	2.54	0.43
3:P:139:ALA:HB1	7:T:24:ALA:HB1	2.00	0.43
7:T:3:ALA:CB	25:T:263:PEK:H382	2.43	0.43
20:P:1525:CHD:H12A	20:P:1525:CHD:H112	1.82	0.43
4:Q:68:PHE:HA	4:Q:71:MET:HE3	2.01	0.43
6:S:54:ASN:ND2	6:S:55:LYS:HG2	2.34	0.43
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.19	0.43
1:A:7:LEU:C	1:A:8:PHE:HD1	2.27	0.43
25:C:264:PEK:H041	7:G:70:PHE:HB2	2.01	0.43
5:E:84:TYR:HE1	27:E:4265:HOH:O	2.01	0.43
22:N:1522:TGL:HB62	12:Y:28:PHE:CZ	2.53	0.43
7:T:30:LEU:HD23	7:T:30:LEU:HA	1.87	0.43
8:U:78:GLU:O	8:U:78:GLU:HG2	2.19	0.43
1:A:413:HIS:NE2	1:A:468:MET:HB2	2.34	0.42
1:A:507:GLU:HA	3:C:5:THR:OG1	2.19	0.42
10:J:45:TYR:O	10:J:48:TYR:HB3	2.19	0.42
1:N:505:PHE:HB3	27:N:3194:HOH:O	2.19	0.42
3:P:173:PHE:C	3:P:173:PHE:CD2	2.97	0.42
8:U:37:HIS:CD2	8:U:76:ARG:CZ	3.02	0.42
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.01	0.42
1:A:307:SER:HB3	26:T:1269:CDL:H182	2.00	0.42
2:B:121:TYR:O	2:B:138:VAL:HA	2.19	0.42
7:G:26:PRO:O	7:G:29:ALA:HB3	2.19	0.42
25:G:1263:PEK:H132	3:P:247:VAL:CG1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:34:SER:HB2	18:N:515:HEA:C2B	2.49	0.42
1:N:501:PRO:HG2	1:N:504:THR:HG22	2.01	0.42
2:O:9:PHE:HB2	2:O:21:LEU:CD2	2.48	0.42
8:U:58:ARG:HD2	8:U:58:ARG:HA	1.73	0.42
6:F:6:VAL:HA	6:F:7:PRO:HD2	1.92	0.42
8:H:57:ARG:O	8:H:61:LYS:HB2	2.19	0.42
7:T:58:LYS:HA	7:T:59:PRO:HD2	1.92	0.42
1:A:106:PRO:N	1:A:107:PRO:CD	2.83	0.42
4:D:61:ARG:HD3	4:D:61:ARG:HA	1.83	0.42
4:D:100:LYS:HE2	11:K:37:GLY:O	2.19	0.42
12:L:46:LYS:O	12:L:47:LYS:HB2	2.19	0.42
1:N:40:GLU:HG2	1:N:54:TYR:CD2	2.54	0.42
1:N:106:PRO:N	1:N:107:PRO:CD	2.83	0.42
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.54	0.42
3:C:132:LEU:HD13	7:G:31:CYS:C	2.44	0.42
5:E:41:LEU:C	5:E:41:LEU:HD12	2.44	0.42
6:S:35:ALA:HA	6:S:36:PRO:HD2	1.94	0.42
23:B:230:PSC:H042	27:E:2401:HOH:O	2.20	0.42
8:H:9:LYS:HB3	8:H:10:ASN:H	1.61	0.42
4:Q:17:VAL:O	4:Q:25:PRO:HG3	2.19	0.42
13:Z:38:ASP:HB2	27:Z:4321:HOH:O	2.20	0.42
1:A:289:ALA:HB3	1:A:305:PHE:CG	2.55	0.42
1:A:478:SER:HA	13:M:8:THR:O	2.19	0.42
3:C:158:HIS:CE1	25:C:265:PEK:H051	2.55	0.42
6:F:48:LEU:O	6:F:50:PRO:HD3	2.19	0.42
1:N:111:LEU:HA	1:N:111:LEU:HD23	1.78	0.42
1:N:424:THR:OG1	1:N:457:GLY:C	2.63	0.42
4:Q:68:PHE:HA	4:Q:71:MET:HG2	2.02	0.42
4:D:87:PHE:CD2	4:D:87:PHE:C	2.98	0.42
5:E:81:ILE:O	5:E:85:VAL:HG23	2.20	0.42
7:G:5:LYS:CB	25:G:1263:PEK:H362	2.40	0.42
1:N:353:LEU:O	1:N:356:ILE:HB	2.20	0.42
2:O:20:LEU:HD23	2:O:83:ILE:HD13	2.02	0.42
2:O:68:LEU:CB	2:O:69:PRO:CD	2.98	0.42
3:P:31:LEU:HA	3:P:31:LEU:HD23	1.69	0.42
26:P:1270:CDL:H171	26:P:1270:CDL:H202	1.79	0.42
5:R:81:ILE:HG12	9:V:7:PRO:HG2	2.01	0.42
6:S:95:GLN:O	6:S:96:LEU:HB3	2.18	0.42
2:B:41:ILE:O	2:B:45:MET:HG2	2.19	0.42
3:C:216:ILE:O	3:C:219:PHE:HB3	2.20	0.42
3:C:223:LEU:HD23	3:C:223:LEU:HA	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:172:LYS:NZ	1:N:178:GLN:HE22	2.18	0.42
1:N:194:LEU:HD12	1:N:245:ILE:HG13	2.01	0.42
2:O:13:THR:HB	2:O:168:LEU:HD23	2.01	0.42
2:O:128:LEU:HD11	2:O:134:ARG:HA	2.02	0.42
3:P:156:ARG:HG3	3:P:156:ARG:HH11	1.84	0.42
10:W:40:LEU:O	10:W:44:LEU:HG	2.19	0.42
1:A:8:PHE:CE2	3:C:15:PRO:HB3	2.55	0.42
2:B:56:MET:HA	23:B:230:PSC:H202	2.02	0.42
3:C:63:ARG:HE	26:C:270:CDL:CA2	2.09	0.42
5:E:15:TRP:O	5:E:18:TYR:HB3	2.19	0.42
5:E:56:ARG:NH2	5:E:59:ASN:OD1	2.48	0.42
1:N:426:PHE:N	1:N:427:PRO:CD	2.82	0.42
22:N:1523:TGL:HG11	22:N:1523:TGL:CC2	2.50	0.42
8:U:9:LYS:HB2	8:U:9:LYS:HE2	1.85	0.42
13:Z:34:LEU:HD12	13:Z:34:LEU:HA	1.89	0.42
1:A:250:GLY:O	1:A:254:ILE:HG12	2.20	0.41
1:A:440:TYR:OH	2:B:195:GLN:HB3	2.20	0.41
1:A:459:PHE:HB3	4:D:92:THR:CG2	2.50	0.41
19:A:524:PGV:H202	19:A:524:PGV:H011	1.94	0.41
3:C:99:TRP:CE2	19:C:268:PGV:H232	2.55	0.41
5:E:15:TRP:CD2	5:E:36:LEU:HD13	2.55	0.41
5:E:31:LYS:HE3	6:F:83:PRO:O	2.19	0.41
1:N:246:LEU:HD13	1:N:381:LEU:HD21	2.02	0.41
1:N:472:ILE:CG2	22:N:1522:TGL:HA92	2.42	0.41
2:O:162:SER:HB3	2:O:197:SER:C	2.45	0.41
1:A:13:LYS:NZ	27:A:2081:HOH:O	2.53	0.41
12:L:24:MET:SD	22:L:522:TGL:C16	3.04	0.41
1:N:53:ILE:HG12	27:N:3076:HOH:O	2.18	0.41
1:N:283:LEU:HD23	1:N:286:ILE:HD11	2.02	0.41
1:N:468:MET:O	1:N:472:ILE:HG13	2.20	0.41
1:A:240:HIS:O	1:A:241:PRO:C	2.63	0.41
2:B:125:THR:HA	2:B:128:LEU:HG	2.02	0.41
23:B:230:PSC:C07	9:I:10:ARG:HE	2.33	0.41
7:G:2:SER:HB3	1:N:197:LEU:HD11	2.01	0.41
8:H:33:TYR:HE1	8:H:69:VAL:HG13	1.85	0.41
13:M:42:LYS:HA	13:M:42:LYS:CE	2.36	0.41
1:N:440:TYR:CZ	2:O:205:SER:HA	2.55	0.41
2:O:33:LEU:HD12	2:O:33:LEU:HA	1.87	0.41
2:O:110:TYR:N	2:O:110:TYR:HD2	2.19	0.41
5:R:53:ARG:HD2	27:R:4076:HOH:O	2.20	0.41
9:V:31:PHE:HA	27:V:4259:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:HD13	1:A:61:HIS:N	2.35	0.41
4:D:17:VAL:HA	27:D:4085:HOH:O	2.21	0.41
4:D:32:ASN:HD22	4:D:32:ASN:HA	1.70	0.41
22:N:1523:TGL:H271	2:O:46:LEU:CD1	2.49	0.41
6:S:54:ASN:C	6:S:54:ASN:ND2	2.76	0.41
8:U:50:VAL:O	8:U:50:VAL:HG12	2.20	0.41
1:A:113:LEU:CD1	22:L:522:TGL:H292	2.50	0.41
24:C:272:DMU:H25	25:C:264:PEK:H341	2.03	0.41
5:E:57:ARG:HH11	5:E:57:ARG:CG	2.33	0.41
6:F:59:GLY:HA2	6:F:70:ILE:O	2.20	0.41
1:N:381:LEU:HD13	18:N:516:HEA:CBC	2.49	0.41
2:O:59:GLN:O	2:O:59:GLN:CG	2.68	0.41
2:O:98:LYS:HE3	2:O:98:LYS:HB2	1.90	0.41
2:O:153:LEU:HD23	2:O:181:GLN:HA	2.02	0.41
3:P:22:LEU:HD23	3:P:22:LEU:HA	1.89	0.41
3:P:146:TRP:CE2	7:T:17:ARG:HG3	2.56	0.41
1:A:424:THR:OG1	1:A:457:GLY:C	2.63	0.41
3:C:3:HIS:HE1	6:F:31:TYR:OH	2.04	0.41
3:C:23:SER:HB2	3:C:49:THR:OG1	2.21	0.41
3:P:137:LEU:HA	3:P:137:LEU:HD23	1.81	0.41
26:P:1270:CDL:H561	26:P:1270:CDL:H532	1.80	0.41
1:A:33:LEU:HD23	1:A:33:LEU:HA	1.78	0.41
1:A:209:LEU:O	1:A:213:ARG:HG3	2.21	0.41
1:A:334:TRP:CZ2	2:B:46:LEU:HB3	2.56	0.41
2:B:146:MET:CE	9:I:56:SER:HB2	2.50	0.41
3:C:41:THR:HG21	10:J:45:TYR:CE2	2.56	0.41
3:C:172:TYR:O	3:C:176:LEU:HG	2.21	0.41
7:G:38:HIS:NE2	26:G:269:CDL:H111	2.36	0.41
26:G:269:CDL:H571	26:G:269:CDL:H601	1.51	0.41
20:N:1604:CHD:H112	20:N:1604:CHD:H12A	1.90	0.41
19:N:1524:PGV:H12	4:Q:87:PHE:CD2	2.55	0.41
2:O:82:ARG:NH1	2:O:86:MET:HE1	2.36	0.41
2:O:158:ASP:O	2:O:176:PRO:HG3	2.21	0.41
3:P:134:THR:HG22	26:T:1269:CDL:H591	2.02	0.41
1:A:337:ALA:HB2	1:A:394:VAL:CG2	2.51	0.41
20:J:60:CHD:H161	20:J:60:CHD:H212	1.71	0.41
1:N:42:GLY:HA3	4:Q:104:TYR:OH	2.20	0.41
1:N:248:LEU:O	1:N:251:PHE:HB2	2.20	0.41
1:N:340:TRP:HZ2	1:N:413:HIS:ND1	2.18	0.41
3:P:181:TYR:O	25:P:1264:PEK:C04	2.69	0.41
19:P:1267:PGV:H182	26:P:1270:CDL:C67	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:61:PHE:O	5:R:64:ALA:HB3	2.20	0.41
11:X:6:ALA:HA	11:X:7:PRO:HD2	1.92	0.41
1:A:22:PHE:CZ	1:A:105:LEU:HB3	2.55	0.41
1:A:53:ILE:HD12	12:L:44:LEU:HD23	2.03	0.41
1:A:219:PHE:CE2	3:C:196:THR:HG22	2.48	0.41
2:B:78:LEU:CB	2:B:79:PRO:CD	2.98	0.41
25:G:1263:PEK:H102	3:P:247:VAL:HG11	2.02	0.41
1:N:98:ASN:HB2	1:N:163:ASN:HD21	1.84	0.41
1:N:374:VAL:HA	1:N:377:PHE:CE1	2.56	0.41
1:N:483:LEU:HB2	13:Z:2:THR:OG1	2.20	0.41
1:N:500:PRO:HB3	27:N:3186:HOH:O	2.19	0.41
2:O:16:ILE:HG22	2:O:17:MET:N	2.35	0.41
2:O:185:MET:SD	2:O:185:MET:C	3.04	0.41
5:R:36:LEU:O	5:R:39:TYR:HD2	2.04	0.41
7:T:15:THR:O	7:T:18:PHE:HB3	2.21	0.41
12:Y:2:HIS:HB3	12:Y:3:TYR:H	1.66	0.41
1:A:289:ALA:C	1:A:291:HIS:H	2.28	0.41
1:A:501:PRO:HG2	1:A:504:THR:CG2	2.50	0.41
2:B:151:ARG:NE	2:B:181:GLN:HE21	2.18	0.41
2:B:213:LEU:N	2:B:213:LEU:HD22	2.36	0.41
2:B:222:TRP:HB2	9:I:71:SER:HB2	2.02	0.41
7:G:2:SER:O	7:G:3:ALA:HB3	2.21	0.41
1:N:400:PHE:HB3	22:N:1522:TGL:C28	2.51	0.41
3:P:49:THR:HB	10:W:39:CYS:SG	2.61	0.41
20:P:1525:CHD:H111	20:P:1525:CHD:H182	1.74	0.41
4:Q:86:MET:O	11:X:25:CYS:HB2	2.21	0.41
26:C:270:CDL:H242	26:C:270:CDL:H661	2.03	0.40
10:J:50:LEU:O	10:J:50:LEU:HD22	2.21	0.40
2:O:19:GLU:OE2	2:O:19:GLU:HA	2.21	0.40
26:P:1270:CDL:H641	26:P:1270:CDL:H672	1.77	0.40
7:T:47:PHE:CE2	7:T:77:PRO:HB2	2.56	0.40
1:A:298:ASP:HB3	27:A:2389:HOH:O	2.21	0.40
19:A:524:PGV:O14	19:A:524:PGV:H02	2.21	0.40
2:B:16:ILE:HD13	2:B:16:ILE:HA	1.90	0.40
2:B:189:PRO:O	9:I:63:MET:HE1	2.21	0.40
3:C:50:ASN:OD1	19:C:266:PGV:H91	2.21	0.40
25:C:265:PEK:H041	6:F:1:ALA:N	2.36	0.40
2:O:202:SER:HB2	2:O:203:ASN:HD22	1.86	0.40
23:O:1230:PSC:H251	23:O:1230:PSC:H221	1.70	0.40
7:T:18:PHE:HD2	7:T:18:PHE:O	2.03	0.40
3:C:84:ILE:HG12	25:T:263:PEK:H32	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:C:267:PGV:H181	26:C:270:CDL:H812	2.04	0.40
26:C:270:CDL:H632	26:C:270:CDL:H602	1.78	0.40
26:C:270:CDL:PA1	26:C:270:CDL:HB22	2.61	0.40
20:C:271:CHD:H12A	20:C:271:CHD:H112	1.60	0.40
9:I:21:ILE:HD13	9:I:21:ILE:HA	1.94	0.40
12:L:20:ARG:HH22	22:L:522:TGL:CC3	2.32	0.40
13:M:32:TRP:N	24:M:526:DMU:H1	2.36	0.40
1:N:141:ALA:O	1:N:144:ASP:N	2.54	0.40
22:N:1522:TGL:HB62	12:Y:28:PHE:HZ	1.86	0.40
3:P:49:THR:HA	3:P:52:LEU:HD12	2.04	0.40
1:A:34:SER:HB2	18:A:515:HEA:C2B	2.51	0.40
1:A:459:PHE:HB3	4:D:92:THR:HG23	2.02	0.40
10:J:36:MET:HB3	20:J:60:CHD:H181	2.03	0.40
1:N:61:HIS:CE1	18:N:515:HEA:NB	2.87	0.40
1:N:296:GLY:O	2:O:178:ARG:NH2	2.53	0.40
1:N:478:SER:HA	13:Z:8:THR:O	2.21	0.40
3:P:112:LEU:HD13	3:P:118:PRO:HG3	2.03	0.40
3:P:146:TRP:HB2	7:T:16:TRP:HB3	2.03	0.40
3:P:148:HIS:CD2	3:P:235:PHE:HE2	2.40	0.40
22:D:523:TGL:H212	22:D:523:TGL:H242	1.86	0.40
9:I:67:GLY:HA2	27:I:2310:HOH:O	2.22	0.40
10:J:11:LEU:O	10:J:11:LEU:HD12	2.21	0.40
1:N:373:VAL:HG13	18:N:516:HEA:HBA1	2.04	0.40
2:O:70:ALA:O	2:O:74:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	512/514 (100%)	488 (95%)	24 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	512/514 (100%)	484 (94%)	27 (5%)	1 (0%)	43	66
2	B	225/227 (99%)	210 (93%)	10 (4%)	5 (2%)	5	10
2	O	225/227 (99%)	206 (92%)	16 (7%)	3 (1%)	9	21
3	C	257/261 (98%)	249 (97%)	7 (3%)	1 (0%)	30	51
3	P	257/261 (98%)	249 (97%)	7 (3%)	1 (0%)	30	51
4	D	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
5	E	103/109 (94%)	97 (94%)	6 (6%)	0	100	100
5	R	103/109 (94%)	94 (91%)	9 (9%)	0	100	100
6	F	96/98 (98%)	85 (88%)	8 (8%)	3 (3%)	3	5
6	S	96/98 (98%)	85 (88%)	7 (7%)	4 (4%)	2	3
7	G	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	0	0
7	T	81/85 (95%)	65 (80%)	10 (12%)	6 (7%)	1	1
8	H	77/85 (91%)	69 (90%)	7 (9%)	1 (1%)	9	21
8	U	77/85 (91%)	69 (90%)	7 (9%)	1 (1%)	9	21
9	I	71/73 (97%)	66 (93%)	4 (6%)	1 (1%)	9	19
9	V	71/73 (97%)	66 (93%)	4 (6%)	1 (1%)	9	19
10	J	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	6	14
10	W	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
11	K	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
13	Z	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
All	All	3504/3614 (97%)	3279 (94%)	189 (5%)	36 (1%)	12	28

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	94	HIS
7	G	4	ALA
7	G	7	ASP

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Mol	Chain	Res	Type
7	G	39	SER
6	S	94	HIS
6	S	95	GLN
7	T	4	ALA
7	T	7	ASP
7	T	39	SER
2	B	59	GLN
6	F	95	GLN
7	G	3	ALA
7	G	8	HIS
7	G	40	GLY
8	H	8	ILE
10	J	15	ASP
2	O	59	GLN
7	T	3	ALA
7	T	8	HIS
7	T	40	GLY
2	B	60	GLU
2	O	60	GLU
3	P	38	ASN
8	U	8	ILE
7	G	82	TYR
9	V	36	LYS
3	C	38	ASN
9	I	36	LYS
1	N	142	SER
6	S	96	LEU
2	B	158	ASP
6	S	93	PRO
2	B	159	VAL
2	O	159	VAL
2	B	92	ASN
6	F	93	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	412 (97%)	14 (3%)	33	61
1	N	426/426 (100%)	412 (97%)	14 (3%)	33	61
2	B	210/210 (100%)	196 (93%)	14 (7%)	15	33
2	O	210/210 (100%)	197 (94%)	13 (6%)	16	36
3	C	224/226 (99%)	213 (95%)	11 (5%)	22	47
3	P	224/226 (99%)	216 (96%)	8 (4%)	31	58
4	D	128/129 (99%)	122 (95%)	6 (5%)	23	48
4	Q	128/129 (99%)	123 (96%)	5 (4%)	28	55
5	E	92/95 (97%)	89 (97%)	3 (3%)	33	61
5	R	92/95 (97%)	91 (99%)	1 (1%)	65	84
6	F	81/81 (100%)	78 (96%)	3 (4%)	30	57
6	S	81/81 (100%)	76 (94%)	5 (6%)	16	36
7	G	67/68 (98%)	62 (92%)	5 (8%)	12	28
7	T	67/68 (98%)	64 (96%)	3 (4%)	24	50
8	H	71/75 (95%)	68 (96%)	3 (4%)	26	52
8	U	71/75 (95%)	69 (97%)	2 (3%)	38	66
9	I	57/57 (100%)	54 (95%)	3 (5%)	20	43
9	V	57/57 (100%)	51 (90%)	6 (10%)	6	14
10	J	49/50 (98%)	48 (98%)	1 (2%)	48	74
10	W	49/50 (98%)	48 (98%)	1 (2%)	48	74
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	39/46 (85%)	35 (90%)	4 (10%)	7	15
12	L	39/40 (98%)	37 (95%)	2 (5%)	21	45
12	Y	39/40 (98%)	37 (95%)	2 (5%)	21	45
13	M	37/38 (97%)	30 (81%)	7 (19%)	1	2
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4	7
All	All	3040/3082 (99%)	2899 (95%)	141 (5%)	24	49

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	115	SER
1	A	118	VAL
1	A	128	VAL

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Mol	Chain	Res	Type
1	A	138	HIS
1	A	162	ILE
1	A	173	PRO
1	A	180	GLN
1	A	189	MET
1	A	241	PRO
1	A	366	VAL
1	A	369	ASP
1	A	490	THR
1	A	495	LEU
1	A	513	LEU
2	B	16	ILE
2	B	33	LEU
2	B	60	GLU
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	110	TYR
2	B	113	TYR
2	B	115	ASP
2	B	130	PRO
2	B	167	SER
2	B	184	LEU
2	B	205	SER
3	C	17	PRO
3	C	29	SER
3	C	33	MET
3	C	39	SER
3	C	77	LYS
3	C	95	THR
3	C	110	PRO
3	C	127	LEU
3	C	179	SER
3	C	192	VAL
3	C	230	ASN
4	D	4	SER
4	D	6	VAL
4	D	36	SER
4	D	51	LEU
4	D	74	SER
4	D	147	LYS

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Mol	Chain	Res	Type
5	E	7	THR
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
6	F	53	THR
6	F	95	GLN
7	G	17	ARG
7	G	35	SER
7	G	36	TRP
7	G	43	GLU
7	G	84	LYS
8	H	8	ILE
8	H	29	CYS
8	H	60	TYR
9	I	8	GLN
9	I	21	ILE
9	I	29	LEU
10	J	50	LEU
12	L	2	HIS
12	L	26	THR
13	M	4	LYS
13	M	5	PRO
13	M	13	LYS
13	M	34	LEU
13	M	37	LEU
13	M	38	ASP
13	M	42	LYS
1	N	75	ILE
1	N	118	VAL
1	N	138	HIS
1	N	178	GLN
1	N	180	GLN
1	N	238	PHE
1	N	241	PRO
1	N	264	LYS
1	N	361	SER
1	N	369	ASP
1	N	380	VAL
1	N	484	THR
1	N	495	LEU
1	N	513	LEU
2	O	16	ILE

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Mol	Chain	Res	Type
2	O	33	LEU
2	O	60	GLU
2	O	63	THR
2	O	66	THR
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	110	TYR
2	O	148	MET
2	O	203	ASN
2	O	217	LYS
3	P	23	SER
3	P	29	SER
3	P	33	MET
3	P	66	THR
3	P	77	LYS
3	P	127	LEU
3	P	150	SER
3	P	230	ASN
4	Q	9	GLU
4	Q	17	VAL
4	Q	51	LEU
4	Q	108	PRO
4	Q	121	LYS
5	R	86	ILE
6	S	12	GLN
6	S	48	LEU
6	S	53	THR
6	S	54	ASN
6	S	94	HIS
7	T	33	LEU
7	T	35	SER
7	T	43	GLU
8	U	29	CYS
8	U	61	LYS
9	V	8	GLN
9	V	21	ILE
9	V	22	VAL
9	V	29	LEU
9	V	33	THR
9	V	61	GLU

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Mol	Chain	Res	Type
10	W	50	LEU
11	X	20	SER
11	X	30	VAL
11	X	47	ARG
11	X	54	ARG
12	Y	20	ARG
12	Y	26	THR
13	Z	2	THR
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	HIS
1	A	178	GLN
1	A	180	GLN
1	A	360	ASN
1	A	413	HIS
2	B	10	GLN
2	B	91	ASN
2	B	102	HIS
2	B	181	GLN
3	C	3	HIS
3	C	9	HIS
3	C	50	ASN
3	C	68	GLN
3	C	70	HIS
3	C	76	GLN
3	C	230	ASN
3	C	243	HIS
4	D	32	ASN
4	D	37	GLN
4	D	109	HIS
5	E	78	HIS
5	E	94	ASN
7	G	34	ASN
8	H	31	GLN
11	K	35	GLN
1	N	52	GLN

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Mol	Chain	Res	Type
1	N	178	GLN
1	N	180	GLN
1	N	232	GLN
1	N	406	ASN
1	N	491	ASN
1	N	512	ASN
2	O	10	GLN
2	O	52	HIS
2	O	203	ASN
3	P	3	HIS
3	P	12	ASN
3	P	50	ASN
3	P	68	GLN
3	P	122	HIS
3	P	161	GLN
3	P	243	HIS
4	Q	37	GLN
4	Q	101	HIS
5	R	78	HIS
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
6	S	95	GLN
7	T	41	HIS
7	T	66	ASN
8	U	31	GLN
10	W	57	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 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$
7	TPO	G	11	7	8,10,11	1.74	2 (25%)	10,14,16	1.03	0
1	FME	A	1	1	8,9,10	0.79	0	8,9,11	1.11	1 (12%)
2	FME	O	1	2	8,9,10	0.73	0	8,9,11	2.09	2 (25%)
7	TPO	T	11	7	8,10,11	1.43	1 (12%)	10,14,16	1.12	1 (10%)
2	FME	B	1	2	8,9,10	0.89	0	8,9,11	1.57	2 (25%)
9	SAC	I	1	9	7,8,9	2.49	2 (28%)	7,9,11	1.54	2 (28%)
1	FME	N	1	1	8,9,10	0.89	0	8,9,11	1.19	1 (12%)
9	SAC	V	1	9	7,8,9	2.80	2 (28%)	7,9,11	1.92	3 (42%)

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
7	TPO	G	11	7	-	4/9/11/13	-
1	FME	A	1	1	-	3/7/9/11	-
2	FME	O	1	2	-	2/7/9/11	-
7	TPO	T	11	7	-	3/9/11/13	-
2	FME	B	1	2	-	2/7/9/11	-
9	SAC	I	1	9	-	3/7/8/10	-
1	FME	N	1	1	-	3/7/9/11	-
9	SAC	V	1	9	-	3/7/8/10	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	OAC-C1A	5.51	1.35	1.23
9	I	1	SAC	OAC-C1A	5.26	1.35	1.23
9	V	1	SAC	CA-N	4.22	1.52	1.46
9	I	1	SAC	CA-N	3.59	1.51	1.46
7	G	11	TPO	CB-CA	3.22	1.60	1.53
7	T	11	TPO	P-O1P	2.58	1.58	1.50
7	G	11	TPO	P-O1P	2.16	1.57	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	FME	C-CA-N	4.54	118.27	109.50
2	O	1	FME	CA-N-CN	-3.50	117.45	122.82
9	V	1	SAC	C2A-C1A-N	3.03	121.15	116.12
2	B	1	FME	CA-N-CN	-2.80	118.51	122.82
2	B	1	FME	C-CA-N	2.71	114.72	109.50
9	I	1	SAC	C-CA-N	-2.65	104.38	109.50
9	V	1	SAC	OAC-C1A-C2A	-2.52	117.57	122.05
9	V	1	SAC	C-CA-N	-2.51	104.65	109.50
1	N	1	FME	CA-N-CN	-2.51	118.97	122.82
7	T	11	TPO	O3P-P-OG1	2.12	114.11	105.85
1	A	1	FME	CA-N-CN	-2.12	119.57	122.82
9	I	1	SAC	C2A-C1A-N	2.00	119.44	116.12

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
9	I	1	SAC	CB-CA-N-C1A
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
2	O	1	FME	O1-CN-N-CA
2	O	1	FME	CB-CA-N-CN
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	CB-CA-N-C1A
1	A	1	FME	C-CA-CB-CG
2	B	1	FME	CB-CA-N-CN
7	G	11	TPO	CB-OG1-P-O2P

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	1	0
1	A	1	FME	3	0
1	N	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 12 are monoatomic - leaving 44 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$
19	PGV	C	268	-	50,50,50	1.50	7 (14%)	53,56,56	0.92	2 (3%)
22	TGL	N	1523	-	62,62,62	0.99	3 (4%)	65,65,65	1.26	7 (10%)
20	CHD	P	1525	-	32,32,32	1.05	2 (6%)	51,51,51	2.57	23 (45%)
21	CUA	B	228	2	0,1,1	-	-	-	-	-
25	PEK	C	264	-	52,52,52	1.49	6 (11%)	55,57,57	1.24	3 (5%)
20	CHD	B	1086	-	32,32,32	0.87	0	51,51,51	2.47	20 (39%)
18	HEA	N	515	1	67,67,67	1.49	12 (17%)	81,103,103	1.67	16 (19%)
19	PGV	N	1524	-	50,50,50	1.25	5 (10%)	53,56,56	0.90	1 (1%)
19	PGV	C	266	-	50,50,50	1.18	5 (10%)	53,56,56	0.96	3 (5%)
26	CDL	G	269	-	99,99,99	1.28	11 (11%)	105,111,111	1.00	8 (7%)
22	TGL	D	523	-	62,62,62	1.05	3 (4%)	65,65,65	1.31	9 (13%)
19	PGV	A	524	-	50,50,50	1.29	6 (12%)	53,56,56	0.83	1 (1%)
19	PGV	P	1267	-	50,50,50	0.98	3 (6%)	53,56,56	1.03	4 (7%)
22	TGL	L	522	-	62,62,62	1.38	5 (8%)	65,65,65	1.69	12 (18%)
22	TGL	N	1522	-	62,62,62	1.52	6 (9%)	65,65,65	1.65	10 (15%)
18	HEA	N	516	1	67,67,67	1.43	8 (11%)	81,103,103	1.42	11 (13%)
24	DMU	C	272	-	34,34,34	2.64	16 (47%)	45,45,45	4.06	18 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	DMU	M	526	-	34,34,34	3.39	8 (23%)	45,45,45	3.97	21 (46%)
25	PEK	P	1265	-	52,52,52	1.81	11 (21%)	55,57,57	1.19	6 (10%)
26	CDL	T	1269	-	99,99,99	1.28	11 (11%)	105,111,111	1.00	7 (6%)
18	HEA	A	515	1	67,67,67	1.71	9 (13%)	81,103,103	1.48	14 (17%)
20	CHD	W	1060	-	32,32,32	2.08	8 (25%)	51,51,51	3.99	28 (54%)
18	HEA	A	516	1	67,67,67	1.48	9 (13%)	81,103,103	1.31	10 (12%)
25	PEK	C	265	-	52,52,52	1.79	12 (23%)	55,57,57	1.21	7 (12%)
25	PEK	P	1264	-	52,52,52	1.68	9 (17%)	55,57,57	1.37	7 (12%)
26	CDL	P	1270	-	99,99,99	1.24	9 (9%)	105,111,111	1.11	6 (5%)
21	CUA	O	228	2	0,1,1	-	-	-	-	-
24	DMU	P	1272	-	34,34,34	2.70	15 (44%)	45,45,45	4.02	17 (37%)
19	PGV	P	1266	-	50,50,50	1.37	6 (12%)	53,56,56	1.06	4 (7%)
19	PGV	P	1268	-	50,50,50	1.47	5 (10%)	53,56,56	0.89	1 (1%)
20	CHD	J	60	-	32,32,32	1.93	10 (31%)	51,51,51	3.93	28 (54%)
20	CHD	A	525	-	32,32,32	1.01	2 (6%)	51,51,51	2.46	18 (35%)
22	TGL	B	521	-	62,62,62	1.11	3 (4%)	65,65,65	1.48	9 (13%)
20	CHD	W	1271	-	32,32,32	1.33	4 (12%)	51,51,51	3.53	25 (49%)
22	TGL	O	1521	-	62,62,62	1.14	5 (8%)	65,65,65	1.49	9 (13%)
23	PSC	O	1230	-	51,51,51	1.54	8 (15%)	57,59,59	1.00	2 (3%)
20	CHD	N	1604	-	32,32,32	1.00	2 (6%)	51,51,51	2.42	17 (33%)
24	DMU	Z	1526	-	34,34,34	3.28	8 (23%)	45,45,45	3.98	20 (44%)
25	PEK	T	263	-	52,52,52	2.14	12 (23%)	55,57,57	1.34	4 (7%)
23	PSC	B	230	-	51,51,51	1.43	6 (11%)	57,59,59	1.01	2 (3%)
20	CHD	C	271	-	32,32,32	1.39	3 (9%)	51,51,51	3.61	24 (47%)
25	PEK	G	1263	-	52,52,52	2.11	11 (21%)	55,57,57	1.31	4 (7%)
26	CDL	C	270	-	99,99,99	1.10	8 (8%)	105,111,111	1.10	9 (8%)
19	PGV	C	267	-	50,50,50	1.06	3 (6%)	53,56,56	1.06	5 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	PGV	C	268	-	-	34/55/55/55	-
22	TGL	N	1523	-	-	15/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CHD	P	1525	-	-	2/9/74/74	0/4/4/4
25	PEK	C	264	-	-	23/56/56/56	-
20	CHD	B	1086	-	-	2/9/74/74	0/4/4/4
18	HEA	N	515	1	-	9/36/76/76	-
19	PGV	N	1524	-	-	34/55/55/55	-
19	PGV	C	266	-	-	16/55/55/55	-
26	CDL	G	269	-	-	60/110/110/110	-
22	TGL	D	523	-	-	15/65/65/65	-
19	PGV	A	524	-	-	34/55/55/55	-
19	PGV	P	1267	-	-	17/55/55/55	-
22	TGL	L	522	-	-	19/65/65/65	-
22	TGL	N	1522	-	-	18/65/65/65	-
18	HEA	N	516	1	-	5/36/76/76	-
24	DMU	C	272	-	6/6/10/10	10/19/59/59	0/2/2/2
24	DMU	M	526	-	5/5/10/10	8/19/59/59	0/2/2/2
25	PEK	P	1265	-	-	20/56/56/56	-
26	CDL	T	1269	-	-	60/110/110/110	-
18	HEA	A	515	1	-	9/36/76/76	-
20	CHD	W	1060	-	5/5/12/12	8/9/74/74	0/4/4/4
18	HEA	A	516	1	-	6/36/76/76	-
25	PEK	C	265	-	-	20/56/56/56	-
25	PEK	P	1264	-	-	24/56/56/56	-
26	CDL	P	1270	-	-	68/110/110/110	-
24	DMU	P	1272	-	6/6/10/10	11/19/59/59	0/2/2/2
19	PGV	P	1266	-	-	15/55/55/55	-
19	PGV	P	1268	-	-	35/55/55/55	-
20	CHD	J	60	-	5/5/12/12	8/9/74/74	0/4/4/4
20	CHD	A	525	-	-	2/9/74/74	0/4/4/4
22	TGL	B	521	-	-	14/65/65/65	-
20	CHD	W	1271	-	5/5/12/12	8/9/74/74	0/4/4/4
22	TGL	O	1521	-	-	14/65/65/65	-
24	DMU	Z	1526	-	5/5/10/10	8/19/59/59	0/2/2/2
20	CHD	N	1604	-	-	3/9/74/74	0/4/4/4
23	PSC	O	1230	-	-	36/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	PEK	T	263	-	-	30/56/56/56	-
23	PSC	B	230	-	-	36/55/55/55	-
20	CHD	C	271	-	5/5/12/12	8/9/74/74	0/4/4/4
25	PEK	G	1263	-	-	29/56/56/56	-
26	CDL	C	270	-	-	67/110/110/110	-
19	PGV	C	267	-	-	17/55/55/55	-

All (295) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	526	DMU	O7-C3	-8.77	1.21	1.43
24	M	526	DMU	O16-C6	-8.16	1.26	1.40
24	Z	1526	DMU	O7-C3	-7.95	1.23	1.43
24	Z	1526	DMU	O16-C6	-7.65	1.27	1.40
24	Z	1526	DMU	O1-C9	-7.48	1.26	1.44
24	M	526	DMU	O1-C9	-7.46	1.26	1.44
24	Z	1526	DMU	O16-C18	-6.84	1.24	1.43
18	A	515	HEA	C11-C3B	-6.75	1.43	1.51
24	M	526	DMU	O7-C10	-6.66	1.23	1.41
18	A	516	HEA	FE-NC	6.62	2.17	1.95
24	M	526	DMU	O5-C4	-6.57	1.28	1.44
24	M	526	DMU	O16-C18	-6.36	1.25	1.43
22	N	1522	TGL	OG1-CA1	6.35	1.51	1.33
24	Z	1526	DMU	O7-C10	-6.30	1.24	1.41
20	W	1060	CHD	C13-C17	6.21	1.65	1.55
24	Z	1526	DMU	O5-C4	-6.20	1.29	1.44
24	P	1272	DMU	O16-C18	-6.13	1.26	1.43
25	T	263	PEK	O03-C21	5.99	1.50	1.33
20	J	60	CHD	C13-C17	5.89	1.65	1.55
24	C	272	DMU	O16-C18	-5.87	1.27	1.43
24	M	526	DMU	O1-C10	-5.61	1.27	1.41
23	O	1230	PSC	C2-C1	5.55	1.66	1.50
19	P	1266	PGV	O03-C19	5.52	1.49	1.33
25	G	1263	PEK	O03-C21	5.42	1.49	1.33
18	N	516	HEA	FE-NC	5.41	2.13	1.95
18	N	515	HEA	C11-C3B	-5.41	1.44	1.51
24	P	1272	DMU	O16-C6	-5.38	1.31	1.40
25	T	263	PEK	C12-C11	5.23	1.61	1.31
24	Z	1526	DMU	O1-C10	-5.21	1.28	1.41
18	A	515	HEA	C1D-ND	-5.12	1.31	1.40
19	C	268	PGV	C12-C11	5.04	1.60	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	272	DMU	O16-C6	-5.02	1.31	1.40
25	G	1263	PEK	C01-C02	5.02	1.66	1.50
25	G	1263	PEK	C12-C11	4.98	1.60	1.31
25	T	263	PEK	C01-C02	4.97	1.66	1.50
25	C	264	PEK	C15-C14	4.96	1.59	1.31
24	C	272	DMU	O1-C9	-4.93	1.32	1.44
22	L	522	TGL	OG2-CB1	4.87	1.48	1.34
23	O	1230	PSC	C10-C9	4.85	1.59	1.31
19	P	1268	PGV	C12-C11	4.84	1.59	1.31
22	N	1522	TGL	OG2-CB1	4.84	1.47	1.34
25	G	1263	PEK	C9-C8	4.82	1.59	1.31
24	C	272	DMU	O7-C3	-4.81	1.31	1.43
24	P	1272	DMU	O7-C3	-4.75	1.31	1.43
23	B	230	PSC	C10-C9	4.72	1.58	1.31
25	T	263	PEK	C6-C5	4.72	1.58	1.31
25	C	264	PEK	C12-C11	4.71	1.58	1.31
25	G	1263	PEK	C6-C5	4.71	1.58	1.31
25	C	264	PEK	C6-C5	4.70	1.58	1.31
18	N	515	HEA	CHD-C1D	-4.69	1.29	1.38
22	L	522	TGL	OG1-CA1	4.69	1.47	1.33
25	P	1265	PEK	C12-C11	4.69	1.58	1.31
25	T	263	PEK	C9-C8	4.69	1.58	1.31
25	P	1264	PEK	C6-C5	4.68	1.58	1.31
24	C	272	DMU	O5-C4	-4.68	1.32	1.44
25	P	1265	PEK	C9-C8	4.61	1.57	1.31
24	P	1272	DMU	O1-C9	-4.59	1.33	1.44
25	P	1264	PEK	C12-C11	4.57	1.57	1.31
25	C	265	PEK	C12-C11	4.56	1.57	1.31
25	C	265	PEK	C15-C14	4.53	1.57	1.31
25	C	265	PEK	C9-C8	4.51	1.57	1.31
24	P	1272	DMU	C6-C1	4.47	1.65	1.52
19	N	1524	PGV	C12-C11	4.47	1.57	1.31
25	T	263	PEK	C15-C14	4.46	1.57	1.31
25	P	1264	PEK	C15-C14	4.46	1.57	1.31
24	Z	1526	DMU	O5-C6	-4.45	1.30	1.41
25	P	1264	PEK	C9-C8	4.44	1.56	1.31
19	C	266	PGV	O03-C19	4.44	1.46	1.33
25	P	1265	PEK	C15-C14	4.43	1.56	1.31
26	G	269	CDL	OA6-CA5	4.42	1.46	1.34
25	G	1263	PEK	C15-C14	4.42	1.56	1.31
24	M	526	DMU	O5-C6	-4.41	1.30	1.41
24	P	1272	DMU	C8-C7	4.39	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	1263	PEK	C03-C02	4.34	1.64	1.50
19	A	524	PGV	C12-C11	4.29	1.56	1.31
18	A	515	HEA	C4B-C3B	-4.28	1.37	1.44
25	T	263	PEK	C03-C02	4.27	1.64	1.50
25	C	264	PEK	C9-C8	4.26	1.55	1.31
26	T	1269	CDL	OA6-CA5	4.24	1.46	1.34
18	N	516	HEA	FE-NB	-4.18	1.82	1.94
19	A	524	PGV	O03-C19	4.18	1.45	1.33
25	P	1265	PEK	C6-C5	4.16	1.55	1.31
18	A	515	HEA	CHD-C1D	-4.13	1.30	1.38
19	P	1268	PGV	O01-C1	4.13	1.45	1.34
19	P	1266	PGV	C12-C11	4.04	1.54	1.31
22	D	523	TGL	OG2-CB1	4.02	1.45	1.34
24	P	1272	DMU	C3-C4	4.01	1.63	1.52
25	C	265	PEK	C6-C5	3.97	1.54	1.31
19	C	266	PGV	C12-C11	3.96	1.54	1.31
24	C	272	DMU	C6-C1	3.92	1.64	1.52
26	G	269	CDL	C11-CA5	3.89	1.62	1.50
23	B	230	PSC	C13-C12	3.87	1.53	1.31
22	B	521	TGL	OG2-CB1	3.81	1.45	1.34
19	C	268	PGV	O01-C1	3.79	1.45	1.34
23	O	1230	PSC	C13-C12	3.74	1.52	1.31
18	A	516	HEA	FE-NB	-3.73	1.83	1.94
26	T	1269	CDL	CB6-CB4	3.65	1.62	1.50
20	W	1060	CHD	C20-C17	3.65	1.60	1.54
26	P	1270	CDL	PA1-OA5	3.61	1.73	1.59
19	C	268	PGV	C04-C05	3.57	1.63	1.51
24	P	1272	DMU	O5-C4	-3.56	1.35	1.44
18	A	515	HEA	CMA-C3A	-3.55	1.37	1.45
19	P	1268	PGV	C04-C05	3.54	1.62	1.51
18	N	515	HEA	C1D-ND	-3.52	1.34	1.40
24	C	272	DMU	C3-C4	3.49	1.62	1.52
26	T	1269	CDL	C11-CA5	3.48	1.60	1.50
20	C	271	CHD	C13-C14	3.48	1.61	1.55
25	G	1263	PEK	P-O11	3.47	1.73	1.59
20	W	1060	CHD	C10-C5	3.47	1.60	1.55
26	P	1270	CDL	OA8-CA7	3.46	1.43	1.33
20	J	60	CHD	C10-C5	3.45	1.60	1.55
22	O	1521	TGL	CB2-CB1	3.43	1.60	1.50
19	P	1266	PGV	C01-C02	3.42	1.61	1.50
26	P	1270	CDL	C31-CA7	3.42	1.60	1.50
23	B	230	PSC	C2-C1	3.40	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	W	1060	CHD	C8-C7	3.36	1.59	1.53
19	C	267	PGV	O01-C1	3.35	1.43	1.34
22	O	1521	TGL	OG2-CB1	3.33	1.43	1.34
26	G	269	CDL	CB6-CB4	3.33	1.61	1.50
24	P	1272	DMU	O7-C10	-3.33	1.32	1.41
24	C	272	DMU	O1-C10	-3.33	1.33	1.41
24	C	272	DMU	O7-C10	-3.32	1.32	1.41
22	L	522	TGL	CG1-CG2	3.32	1.61	1.50
20	W	1271	CHD	C13-C17	3.30	1.61	1.55
25	C	265	PEK	O03-C21	3.29	1.43	1.33
26	P	1270	CDL	C71-CB7	3.28	1.60	1.50
19	P	1267	PGV	C12-C11	3.28	1.50	1.31
25	T	263	PEK	P-O11	3.27	1.72	1.59
25	P	1265	PEK	O03-C21	3.27	1.42	1.33
25	P	1264	PEK	O03-C21	3.26	1.42	1.33
20	C	271	CHD	C13-C12	3.22	1.59	1.54
18	A	516	HEA	FE-ND	3.21	2.04	1.94
26	P	1270	CDL	CA3-CA4	3.20	1.60	1.50
26	T	1269	CDL	CB2-C1	3.18	1.61	1.51
26	C	270	CDL	C71-CB7	3.18	1.59	1.50
19	C	267	PGV	C12-C11	3.17	1.49	1.31
20	C	271	CHD	C13-C17	3.17	1.60	1.55
22	N	1522	TGL	CG1-CG2	3.16	1.60	1.50
26	P	1270	CDL	CA6-CA4	3.10	1.60	1.50
23	B	230	PSC	O01-C1	3.09	1.43	1.34
25	C	265	PEK	C03-C02	3.08	1.60	1.50
22	N	1523	TGL	OG2-CB1	3.07	1.43	1.34
25	P	1264	PEK	O01-C1	3.05	1.42	1.34
22	L	522	TGL	CG3-CG2	3.05	1.60	1.50
20	J	60	CHD	C8-C9	3.04	1.59	1.53
20	J	60	CHD	C8-C7	3.04	1.59	1.53
19	C	267	PGV	O03-C19	3.04	1.42	1.33
26	C	270	CDL	CA6-CA4	3.03	1.60	1.50
20	W	1060	CHD	C13-C12	3.03	1.59	1.54
22	N	1522	TGL	CA2-CA1	3.03	1.59	1.50
26	G	269	CDL	PB2-OB2	3.02	1.71	1.59
19	C	266	PGV	C03-C02	2.99	1.60	1.50
26	T	1269	CDL	PB2-OB2	2.98	1.71	1.59
26	G	269	CDL	CB2-C1	2.98	1.61	1.51
19	C	268	PGV	P-O12	2.97	1.71	1.59
24	P	1272	DMU	C10-C5	2.96	1.61	1.52
20	W	1271	CHD	C13-C12	2.95	1.59	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	P	1272	DMU	C7-C5	2.94	1.60	1.52
20	W	1060	CHD	C10-C9	2.93	1.61	1.56
19	P	1268	PGV	P-O12	2.93	1.70	1.59
25	P	1265	PEK	C03-C02	2.93	1.60	1.50
24	C	272	DMU	C7-C5	2.92	1.59	1.52
25	P	1265	PEK	P-O11	2.92	1.70	1.59
25	C	265	PEK	P-O11	2.92	1.70	1.59
24	C	272	DMU	O5-C6	-2.92	1.34	1.41
26	T	1269	CDL	CB3-CB4	2.90	1.59	1.50
26	G	269	CDL	CB3-CB4	2.88	1.59	1.50
22	N	1522	TGL	CG3-CG2	2.86	1.59	1.50
22	B	521	TGL	CG3-CG2	2.86	1.59	1.50
26	G	269	CDL	OB6-CB5	2.85	1.42	1.34
25	P	1265	PEK	C01-C02	2.84	1.59	1.50
22	O	1521	TGL	CG3-CG2	2.84	1.59	1.50
18	N	516	HEA	CMA-C3A	-2.83	1.39	1.45
24	P	1272	DMU	C8-C9	2.82	1.59	1.53
22	B	521	TGL	CB2-CB1	2.81	1.58	1.50
20	W	1271	CHD	C13-C14	2.79	1.60	1.55
20	W	1060	CHD	C8-C14	2.77	1.59	1.53
19	N	1524	PGV	C03-C02	2.76	1.59	1.50
25	G	1263	PEK	P-O12	2.76	1.70	1.59
25	G	1263	PEK	O03-C01	2.75	1.51	1.45
24	C	272	DMU	C8-C7	2.74	1.59	1.52
18	N	515	HEA	C1C-C2C	2.73	1.49	1.43
25	P	1265	PEK	C22-C21	2.72	1.58	1.50
26	P	1270	CDL	OB6-CB5	2.72	1.42	1.34
20	W	1060	CHD	C8-C9	2.72	1.59	1.53
25	P	1264	PEK	C2-C1	2.71	1.58	1.50
20	J	60	CHD	C13-C12	2.70	1.58	1.54
25	T	263	PEK	O03-C01	2.69	1.51	1.45
23	O	1230	PSC	P-O12	2.69	1.69	1.59
24	C	272	DMU	C8-C9	2.68	1.58	1.53
19	N	1524	PGV	O03-C19	2.66	1.41	1.33
18	A	515	HEA	C4D-C3D	-2.65	1.40	1.45
25	P	1265	PEK	O01-C1	2.65	1.41	1.34
22	D	523	TGL	CB2-CB1	2.65	1.58	1.50
26	C	270	CDL	C31-CA7	2.65	1.58	1.50
25	C	265	PEK	C01-C02	2.65	1.59	1.50
26	P	1270	CDL	C11-CA5	2.65	1.58	1.50
18	A	516	HEA	CAC-C3C	2.65	1.54	1.47
19	P	1266	PGV	C20-C19	2.64	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	P	1272	DMU	O5-C6	-2.64	1.35	1.41
25	T	263	PEK	C22-C21	2.63	1.58	1.50
19	P	1267	PGV	O03-C19	2.61	1.41	1.33
18	A	515	HEA	C1A-C2A	-2.60	1.40	1.45
19	P	1266	PGV	O01-C1	2.60	1.41	1.34
22	N	1522	TGL	CB2-CB1	2.57	1.58	1.50
18	N	515	HEA	CMA-C3A	-2.57	1.39	1.45
26	C	270	CDL	CA3-CA4	2.56	1.58	1.50
26	P	1270	CDL	PB2-OB2	2.55	1.69	1.59
19	C	266	PGV	O01-C1	2.54	1.41	1.34
26	C	270	CDL	OA8-CA7	2.53	1.40	1.33
19	P	1267	PGV	C01-C02	2.52	1.58	1.50
18	A	516	HEA	CMA-C3A	-2.52	1.39	1.45
24	C	272	DMU	C10-C5	2.51	1.59	1.52
19	C	268	PGV	C06-C05	2.51	1.61	1.51
25	P	1265	PEK	P-O12	2.51	1.69	1.59
26	G	269	CDL	CA6-CA4	2.50	1.58	1.50
24	P	1272	DMU	C2-C1	2.48	1.58	1.52
19	P	1266	PGV	C03-C02	2.47	1.58	1.50
26	T	1269	CDL	C31-CA7	2.47	1.57	1.50
20	J	60	CHD	C8-C14	2.47	1.58	1.53
18	A	516	HEA	C16-C15	2.47	1.56	1.51
18	N	516	HEA	C17-C18	2.47	1.57	1.50
26	T	1269	CDL	C71-CB7	2.46	1.57	1.50
20	N	1604	CHD	C13-C12	-2.44	1.50	1.54
25	C	265	PEK	O01-C1	2.44	1.41	1.34
18	N	516	HEA	FE-ND	2.43	2.02	1.94
26	C	270	CDL	PA1-OA5	2.42	1.68	1.59
18	A	515	HEA	C26-C15	2.41	1.56	1.50
25	C	265	PEK	C22-C21	2.40	1.57	1.50
24	P	1272	DMU	O1-C10	-2.39	1.35	1.41
20	P	1525	CHD	C13-C14	2.39	1.59	1.55
22	O	1521	TGL	OG3-CC1	2.37	1.40	1.33
26	C	270	CDL	PB2-OB2	2.37	1.68	1.59
20	J	60	CHD	C1-C10	2.37	1.58	1.54
25	G	1263	PEK	C22-C21	2.35	1.57	1.50
19	A	524	PGV	C03-C02	2.35	1.58	1.50
25	C	265	PEK	P-O12	2.35	1.68	1.59
20	J	60	CHD	C20-C17	2.34	1.58	1.54
19	N	1524	PGV	O01-C1	2.34	1.40	1.34
18	N	515	HEA	C4B-C3B	-2.32	1.40	1.44
20	J	60	CHD	C10-C9	2.31	1.60	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	T	1269	CDL	OB6-CB5	2.31	1.40	1.34
22	L	522	TGL	CB2-CB1	2.31	1.57	1.50
19	A	524	PGV	C20-C19	2.30	1.57	1.50
23	O	1230	PSC	C3-C2	2.29	1.60	1.52
26	T	1269	CDL	CA6-CA4	2.29	1.58	1.50
22	N	1523	TGL	OG3-CC1	2.29	1.40	1.33
23	B	230	PSC	P-O12	2.27	1.68	1.59
25	T	263	PEK	C2-C1	2.27	1.57	1.50
18	N	516	HEA	CHB-C1B	-2.27	1.34	1.39
19	C	266	PGV	C20-C19	2.26	1.57	1.50
18	N	515	HEA	CMC-C2C	2.26	1.55	1.50
25	T	263	PEK	P-O12	2.26	1.68	1.59
19	N	1524	PGV	C20-C19	2.25	1.57	1.50
25	C	264	PEK	O03-C01	-2.25	1.40	1.45
22	D	523	TGL	OG3-CC1	2.20	1.39	1.33
26	T	1269	CDL	C51-CB5	2.20	1.57	1.50
19	C	268	PGV	P-O11	2.20	1.68	1.59
24	C	272	DMU	C2-C3	2.20	1.58	1.52
19	A	524	PGV	C06-C05	2.19	1.60	1.51
18	N	515	HEA	C1C-NC	2.19	1.43	1.39
18	N	515	HEA	FE-NC	-2.18	1.88	1.95
24	C	272	DMU	C2-C1	2.18	1.58	1.52
23	B	230	PSC	P-O11	2.18	1.67	1.59
18	N	516	HEA	CHB-C4A	-2.17	1.34	1.38
20	W	1271	CHD	C1-C10	2.16	1.57	1.54
18	A	516	HEA	C20-C19	2.16	1.55	1.51
19	P	1268	PGV	C06-C05	2.14	1.59	1.51
18	A	516	HEA	C17-C18	2.14	1.57	1.50
18	N	516	HEA	CMB-C2B	2.14	1.55	1.50
18	N	515	HEA	CHC-C4B	-2.13	1.34	1.38
20	N	1604	CHD	C19-C10	-2.13	1.50	1.54
20	A	525	CHD	C10-C9	-2.13	1.52	1.56
18	A	515	HEA	C3A-C4A	-2.12	1.42	1.46
22	O	1521	TGL	CA2-CA1	2.12	1.56	1.50
26	C	270	CDL	C11-CA5	2.12	1.56	1.50
26	G	269	CDL	C71-CB7	2.10	1.56	1.50
20	P	1525	CHD	C8-C9	2.09	1.57	1.53
23	O	1230	PSC	C01-C02	2.09	1.57	1.50
25	P	1264	PEK	C22-C21	2.09	1.56	1.50
19	C	268	PGV	C20-C19	2.08	1.56	1.50
18	N	515	HEA	FE-ND	-2.08	1.88	1.94
22	N	1523	TGL	CG3-CG2	2.08	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	524	PGV	C04-C05	2.06	1.58	1.51
25	C	264	PEK	C4-C5	2.05	1.61	1.50
20	J	60	CHD	C13-C14	2.05	1.58	1.55
25	C	265	PEK	C29-C28	2.05	1.62	1.51
18	N	515	HEA	CHC-C1C	-2.04	1.34	1.39
26	G	269	CDL	PA1-OA5	2.04	1.67	1.59
18	A	516	HEA	C18-C19	2.03	1.37	1.33
23	O	1230	PSC	O01-C1	2.02	1.40	1.34
23	O	1230	PSC	C05-C04	2.02	1.57	1.51
26	G	269	CDL	PB2-OB5	2.01	1.67	1.59
25	P	1264	PEK	P-O11	2.01	1.67	1.59
20	A	525	CHD	C10-C5	2.00	1.58	1.55

All (452) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	1272	DMU	O16-C6-C1	12.21	126.82	108.27
24	C	272	DMU	O16-C6-C1	11.04	125.04	108.27
24	M	526	DMU	C1-C2-C3	9.92	132.19	109.68
24	Z	1526	DMU	C1-C2-C3	9.81	131.95	109.68
20	B	1086	CHD	C18-C13-C12	-9.71	99.33	109.06
20	C	271	CHD	C10-C9-C8	9.30	122.21	111.84
20	W	1060	CHD	C10-C9-C8	8.96	121.82	111.84
24	C	272	DMU	C1-C2-C3	8.92	129.92	109.68
20	J	60	CHD	C10-C9-C8	8.78	121.63	111.84
20	W	1271	CHD	C10-C9-C8	8.77	121.62	111.84
24	C	272	DMU	O1-C9-C11	8.74	128.09	106.44
20	W	1271	CHD	C19-C10-C9	-8.71	99.47	111.18
20	C	271	CHD	C17-C13-C14	8.56	108.70	100.11
20	C	271	CHD	C19-C10-C9	-8.45	99.82	111.18
20	N	1604	CHD	C18-C13-C12	-8.32	100.73	109.06
20	W	1060	CHD	O12-C12-C13	8.17	124.83	111.02
24	P	1272	DMU	O5-C4-C3	8.09	126.44	109.72
24	P	1272	DMU	O1-C9-C11	8.04	126.37	106.44
20	W	1271	CHD	C17-C13-C14	8.03	108.17	100.11
24	P	1272	DMU	C1-C2-C3	7.99	127.81	109.68
24	M	526	DMU	O1-C9-C11	7.97	126.19	106.44
24	Z	1526	DMU	O1-C9-C11	7.89	125.98	106.44
20	W	1271	CHD	C17-C13-C12	-7.84	110.61	117.67
24	Z	1526	DMU	C7-C8-C9	7.80	124.37	110.23
20	W	1060	CHD	C6-C5-C10	7.77	120.93	112.66
24	P	1272	DMU	O7-C3-C4	7.72	129.74	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	60	CHD	O12-C12-C13	7.69	124.01	111.02
24	C	272	DMU	C6-O5-C4	7.58	128.52	113.72
24	M	526	DMU	C10-C5-C7	7.48	125.75	110.01
24	C	272	DMU	O5-C4-C3	7.45	125.13	109.72
20	J	60	CHD	C6-C5-C10	7.44	120.57	112.66
24	Z	1526	DMU	O5-C4-C3	7.40	125.03	109.72
20	W	1060	CHD	C13-C17-C20	7.39	128.43	119.48
20	C	271	CHD	C17-C13-C12	-7.38	111.02	117.67
20	W	1060	CHD	C17-C13-C14	7.33	107.47	100.11
20	J	60	CHD	C17-C13-C14	7.29	107.42	100.11
24	C	272	DMU	O7-C3-C4	7.24	128.48	109.48
24	M	526	DMU	C7-C8-C9	7.21	123.30	110.23
24	Z	1526	DMU	C10-C5-C7	7.20	125.16	110.01
20	J	60	CHD	C11-C12-C13	7.15	118.54	111.26
24	M	526	DMU	C6-O5-C4	7.13	127.65	113.72
24	M	526	DMU	O5-C4-C3	7.11	124.43	109.72
20	J	60	CHD	C13-C17-C20	7.10	128.09	119.48
20	W	1060	CHD	C11-C9-C10	7.00	120.81	113.70
20	W	1060	CHD	C4-C3-C2	6.98	119.14	110.62
24	M	526	DMU	O5-C4-C57	6.94	123.65	106.44
24	Z	1526	DMU	C6-O5-C4	6.92	127.24	113.72
20	W	1271	CHD	C14-C13-C12	6.89	113.71	107.42
20	C	271	CHD	C14-C13-C12	6.80	113.63	107.42
24	Z	1526	DMU	O5-C4-C57	6.80	123.28	106.44
20	J	60	CHD	C5-C6-C7	6.61	122.25	114.40
20	W	1060	CHD	C11-C12-C13	6.47	117.85	111.26
24	M	526	DMU	O1-C9-C8	6.44	121.30	109.70
24	Z	1526	DMU	O1-C9-C8	6.36	121.16	109.70
20	P	1525	CHD	C10-C9-C8	6.32	118.88	111.84
20	A	525	CHD	C10-C9-C8	6.31	118.87	111.84
20	P	1525	CHD	C11-C12-C13	-6.25	104.91	111.26
20	J	60	CHD	C11-C9-C10	6.24	120.03	113.70
20	W	1060	CHD	C18-C13-C14	-6.18	101.52	111.20
20	J	60	CHD	C4-C3-C2	6.17	118.14	110.62
20	W	1060	CHD	C5-C6-C7	6.12	121.68	114.40
24	P	1272	DMU	O1-C9-C8	6.10	120.68	109.70
24	P	1272	DMU	C6-O5-C4	5.97	125.39	113.72
24	P	1272	DMU	O5-C6-C1	5.95	122.59	110.37
24	C	272	DMU	C18-O16-C6	5.91	123.78	113.68
20	C	271	CHD	C1-C10-C5	5.88	116.19	107.75
24	M	526	DMU	O5-C6-C1	5.85	122.39	110.37
24	C	272	DMU	O7-C3-C2	5.84	122.08	107.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Z	1526	DMU	C8-C7-C5	-5.83	100.59	110.83
20	C	271	CHD	C9-C8-C7	5.80	119.16	111.86
24	P	1272	DMU	C18-O16-C6	5.80	123.58	113.68
20	W	1271	CHD	C9-C8-C7	5.79	119.15	111.86
20	C	271	CHD	C4-C3-C2	5.78	117.67	110.62
22	B	521	TGL	CG2-OG2-CB1	5.78	131.63	117.80
20	W	1271	CHD	C4-C3-C2	5.78	117.66	110.62
24	C	272	DMU	C8-C7-C5	5.61	120.67	110.83
22	O	1521	TGL	CG2-OG2-CB1	5.56	131.10	117.80
24	P	1272	DMU	O7-C3-C2	5.47	121.13	107.23
20	W	1060	CHD	C14-C8-C9	5.46	117.38	109.75
24	P	1272	DMU	C8-C7-C5	5.46	120.41	110.83
24	C	272	DMU	O5-C4-C57	5.45	119.96	106.44
24	Z	1526	DMU	O5-C6-C1	5.45	121.58	110.37
24	M	526	DMU	C8-C7-C5	-5.45	101.26	110.83
24	C	272	DMU	O7-C10-C5	5.44	121.47	108.09
24	P	1272	DMU	O5-C4-C57	5.37	119.74	106.44
24	C	272	DMU	O5-C6-C1	5.31	121.28	110.37
20	J	60	CHD	C18-C13-C14	-5.31	102.89	111.20
20	W	1271	CHD	C15-C14-C8	-5.27	111.13	118.36
20	B	1086	CHD	C1-C10-C5	5.22	115.24	107.75
24	Z	1526	DMU	O5-C6-O16	5.20	122.33	110.04
20	W	1060	CHD	C15-C14-C8	-5.17	111.26	118.36
20	W	1271	CHD	C1-C10-C5	5.14	115.12	107.75
20	C	271	CHD	C15-C14-C8	-5.13	111.33	118.36
20	N	1604	CHD	C10-C9-C8	5.12	117.55	111.84
22	N	1522	TGL	C12-C11-C10	-5.11	88.52	114.37
24	M	526	DMU	O5-C6-O16	5.09	122.08	110.04
20	J	60	CHD	C14-C8-C9	5.07	116.83	109.75
20	J	60	CHD	C15-C14-C8	-5.05	111.43	118.36
20	W	1060	CHD	C19-C10-C1	-5.03	100.31	108.31
24	C	272	DMU	O1-C9-C8	4.97	118.66	109.70
24	Z	1526	DMU	O16-C6-C1	4.96	115.81	108.27
20	C	271	CHD	C18-C13-C12	-4.96	104.09	109.06
20	A	525	CHD	C13-C17-C20	4.96	125.49	119.48
20	A	525	CHD	C4-C3-C2	4.95	116.66	110.62
20	J	60	CHD	C19-C10-C1	-4.94	100.45	108.31
24	M	526	DMU	O7-C3-C2	4.93	119.76	107.23
22	L	522	TGL	C12-C11-C10	-4.90	89.60	114.37
20	J	60	CHD	C13-C14-C8	4.90	120.92	114.72
20	P	1525	CHD	C5-C6-C7	4.88	120.21	114.40
24	P	1272	DMU	O7-C10-C5	4.88	120.09	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Z	1526	DMU	O7-C3-C2	4.85	119.57	107.23
18	A	515	HEA	C26-C15-C16	4.84	123.64	115.23
25	T	263	PEK	O03-C01-C02	4.83	122.31	108.40
20	N	1604	CHD	C1-C10-C5	4.81	114.66	107.75
20	A	525	CHD	C5-C6-C7	4.81	120.12	114.40
25	G	1263	PEK	O03-C01-C02	4.75	122.09	108.40
20	P	1525	CHD	C1-C10-C5	4.74	114.55	107.75
18	N	515	HEA	C26-C15-C16	4.71	123.41	115.23
20	C	271	CHD	C4-C5-C10	4.69	117.65	112.66
20	W	1060	CHD	C1-C10-C5	4.65	114.42	107.75
20	W	1060	CHD	C13-C14-C8	4.64	120.59	114.72
24	M	526	DMU	O16-C6-C1	4.62	115.30	108.27
20	J	60	CHD	C2-C1-C10	4.61	120.52	112.74
20	J	60	CHD	C9-C8-C7	4.59	117.64	111.86
20	A	525	CHD	C11-C12-C13	-4.59	106.59	111.26
20	W	1060	CHD	C2-C1-C10	4.57	120.45	112.74
24	Z	1526	DMU	O7-C3-C4	4.55	121.41	109.48
20	P	1525	CHD	C13-C17-C20	4.53	124.97	119.48
24	C	272	DMU	C10-O1-C9	4.52	122.54	113.72
22	N	1522	TGL	CB9-CB8-CB7	-4.48	91.70	114.37
18	A	516	HEA	C12-C11-C3B	4.47	119.11	112.12
20	N	1604	CHD	C17-C13-C12	4.45	121.67	117.67
20	W	1060	CHD	C9-C8-C7	4.42	117.42	111.86
20	W	1271	CHD	C4-C5-C10	4.41	117.36	112.66
18	N	516	HEA	C12-C11-C3B	4.37	118.95	112.12
25	T	263	PEK	C02-O01-C1	4.26	127.99	117.80
26	C	270	CDL	PA1-OA5-CA3	4.24	145.67	121.35
20	J	60	CHD	C1-C10-C5	4.24	113.83	107.75
24	Z	1526	DMU	O7-C10-O1	4.24	121.85	110.69
20	C	271	CHD	C19-C10-C1	-4.22	101.60	108.31
20	C	271	CHD	C6-C5-C10	4.19	117.12	112.66
19	P	1266	PGV	O01-C1-C2	-4.19	102.42	111.48
26	P	1270	CDL	PA1-OA5-CA3	4.19	145.33	121.35
22	L	522	TGL	CB9-CB8-CB7	-4.18	93.26	114.37
25	T	263	PEK	P-O11-C03	4.17	145.24	121.35
24	M	526	DMU	O7-C3-C4	4.16	120.39	109.48
20	A	525	CHD	C1-C10-C5	4.16	113.72	107.75
20	J	60	CHD	C18-C13-C12	-4.13	104.92	109.06
24	Z	1526	DMU	C18-O16-C6	4.11	120.69	113.68
22	L	522	TGL	C11-C10-CB9	4.09	135.06	114.37
20	C	271	CHD	C9-C11-C12	4.09	119.65	114.29
24	P	1272	DMU	O1-C10-C5	4.03	118.66	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	W	1060	CHD	C14-C8-C7	4.03	117.20	111.85
19	C	266	PGV	O01-C1-C2	-4.01	102.80	111.48
20	P	1525	CHD	C15-C14-C8	-4.01	112.85	118.36
20	N	1604	CHD	C15-C14-C13	-4.01	99.65	103.54
22	O	1521	TGL	CG1-OG1-CA1	-4.00	102.48	117.12
18	N	515	HEA	C12-C13-C14	-3.99	101.67	112.16
24	C	272	DMU	O7-C10-O1	3.95	121.08	110.69
22	N	1522	TGL	C15-CC9-CC8	3.95	134.31	114.37
25	G	1263	PEK	P-O11-C03	3.94	143.95	121.35
20	W	1271	CHD	O12-C12-C13	3.90	117.61	111.02
20	P	1525	CHD	C6-C5-C10	3.89	116.80	112.66
20	P	1525	CHD	C4-C3-C2	3.88	115.36	110.62
22	L	522	TGL	C15-CC9-CC8	3.87	133.93	114.37
23	B	230	PSC	C01-O03-C19	-3.86	103.01	117.12
24	M	526	DMU	C18-O16-C6	3.84	120.24	113.68
22	L	522	TGL	C16-C15-CC9	3.83	133.75	114.37
20	N	1604	CHD	C16-C17-C13	-3.82	99.84	103.54
20	P	1525	CHD	C9-C8-C7	3.81	116.66	111.86
22	N	1522	TGL	C16-C15-CC9	3.77	133.44	114.37
22	N	1522	TGL	C11-C10-CB9	3.77	133.41	114.37
18	N	516	HEA	C3C-C4C-NC	3.75	112.96	109.80
25	P	1264	PEK	O03-C21-C22	-3.75	100.40	111.83
20	A	525	CHD	C15-C14-C8	-3.74	113.23	118.36
25	G	1263	PEK	C02-O01-C1	3.74	126.74	117.80
20	B	1086	CHD	C10-C9-C8	3.72	115.99	111.84
20	W	1271	CHD	C18-C13-C12	-3.72	105.34	109.06
20	J	60	CHD	C1-C2-C3	3.71	115.40	110.48
20	N	1604	CHD	C15-C14-C8	-3.70	113.28	118.36
26	C	270	CDL	CB6-OB8-CB7	-3.69	103.62	117.12
19	C	267	PGV	O01-C1-C2	-3.68	103.52	111.48
23	O	1230	PSC	C01-O03-C19	-3.66	103.74	117.12
20	B	1086	CHD	C6-C5-C10	3.65	116.54	112.66
20	J	60	CHD	C14-C8-C7	3.59	116.61	111.85
20	P	1525	CHD	C18-C13-C14	3.59	116.82	111.20
22	B	521	TGL	CG1-OG1-CA1	-3.58	104.05	117.12
24	P	1272	DMU	O7-C10-O1	3.57	120.10	110.69
26	P	1270	CDL	CB6-OB8-CB7	-3.57	104.06	117.12
20	A	525	CHD	C5-C4-C3	3.57	118.09	112.71
18	N	515	HEA	C1C-CHC-C4B	-3.56	117.88	126.25
26	P	1270	CDL	OB6-CB5-C51	-3.56	103.78	111.48
20	J	60	CHD	C5-C4-C3	3.55	118.06	112.71
20	W	1271	CHD	C5-C4-C3	3.55	118.06	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	1086	CHD	C15-C14-C8	-3.55	113.49	118.36
24	M	526	DMU	C10-O7-C3	3.55	126.38	117.98
20	B	1086	CHD	C16-C17-C13	-3.54	100.11	103.54
19	P	1267	PGV	O01-C1-C2	-3.50	103.90	111.48
20	C	271	CHD	O12-C12-C13	3.50	116.94	111.02
25	P	1264	PEK	C3-C2-C1	-3.49	100.92	113.69
20	W	1271	CHD	C9-C11-C12	3.48	118.85	114.29
18	N	515	HEA	C17-C18-C19	-3.47	119.68	127.62
24	P	1272	DMU	C10-O1-C9	3.47	120.49	113.72
22	N	1522	TGL	C13-C12-C11	3.46	131.84	114.37
25	C	265	PEK	C11-C10-C9	3.45	129.03	112.02
20	B	1086	CHD	C17-C13-C12	3.45	120.77	117.67
20	B	1086	CHD	C1-C2-C3	3.42	115.02	110.48
22	B	521	TGL	CG3-CG2-CG1	3.42	119.77	111.78
22	O	1521	TGL	CG3-CG2-CG1	3.42	119.76	111.78
20	N	1604	CHD	C1-C2-C3	3.42	115.00	110.48
25	P	1265	PEK	C11-C10-C9	3.41	128.83	112.02
24	M	526	DMU	O7-C10-O1	3.39	119.61	110.69
20	A	525	CHD	C18-C13-C14	3.37	116.48	111.20
18	A	515	HEA	C25-C23-C24	3.36	122.31	114.59
20	P	1525	CHD	C4-C5-C10	3.35	116.22	112.66
20	W	1060	CHD	C1-C2-C3	3.34	114.91	110.48
18	N	516	HEA	C27-C19-C20	3.34	121.02	115.23
20	N	1604	CHD	C5-C4-C3	3.32	117.72	112.71
22	D	523	TGL	CG2-OG2-CB1	3.31	125.72	117.80
24	Z	1526	DMU	C2-C3-C4	-3.31	103.59	110.93
25	C	264	PEK	C3-C2-C1	-3.29	101.66	113.69
20	P	1525	CHD	C14-C13-C12	-3.28	104.42	107.42
20	A	525	CHD	C6-C5-C10	3.28	116.15	112.66
20	W	1271	CHD	C6-C5-C10	3.27	116.14	112.66
18	N	515	HEA	CHC-C4B-NB	3.27	128.41	124.37
18	A	516	HEA	C26-C15-C16	3.26	120.89	115.23
20	W	1271	CHD	C18-C13-C14	-3.26	106.09	111.20
20	P	1525	CHD	C1-C2-C3	3.26	114.80	110.48
25	C	265	PEK	P-O11-C03	3.26	140.03	121.35
24	M	526	DMU	C10-O1-C9	3.26	120.08	113.72
20	W	1060	CHD	C18-C13-C12	-3.25	105.80	109.06
20	A	525	CHD	C4-C5-C10	3.24	116.10	112.66
20	W	1271	CHD	C19-C10-C1	-3.23	103.17	108.31
26	P	1270	CDL	OB6-CB5-OB7	3.23	131.26	123.70
20	P	1525	CHD	C5-C4-C3	3.23	117.58	112.71
18	N	516	HEA	C3D-C4D-ND	3.23	113.47	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	515	HEA	C12-C13-C14	-3.22	103.69	112.16
20	W	1271	CHD	C2-C1-C10	3.21	118.16	112.74
20	B	1086	CHD	C14-C13-C12	3.21	110.35	107.42
25	P	1265	PEK	P-O11-C03	3.20	139.67	121.35
22	L	522	TGL	C13-C12-C11	3.17	130.40	114.37
18	A	516	HEA	C2B-C1B-NB	3.16	113.56	109.90
20	W	1271	CHD	C5-C6-C7	3.15	118.15	114.40
20	W	1060	CHD	C9-C11-C12	3.15	118.41	114.29
26	C	270	CDL	OB6-CB5-C51	-3.13	104.70	111.48
22	D	523	TGL	CG1-OG1-CA1	-3.13	105.67	117.12
20	A	525	CHD	C9-C8-C7	3.13	115.79	111.86
24	M	526	DMU	C2-C3-C4	-3.12	104.01	110.93
22	N	1523	TGL	CG1-OG1-CA1	-3.12	105.73	117.12
20	W	1060	CHD	C16-C15-C14	3.11	111.24	105.14
19	P	1266	PGV	O03-C01-C02	3.10	117.33	108.40
20	W	1060	CHD	C5-C4-C3	3.10	117.38	112.71
20	A	525	CHD	C14-C13-C12	-3.08	104.60	107.42
25	P	1264	PEK	C23-C22-C21	-3.06	102.47	113.69
20	C	271	CHD	C11-C12-C13	3.05	114.36	111.26
20	C	271	CHD	C1-C2-C3	3.04	114.51	110.48
24	M	526	DMU	O7-C10-C5	3.04	115.58	108.09
18	A	515	HEA	C3C-C2C-C1C	-3.04	103.59	107.17
20	C	271	CHD	C5-C4-C3	3.02	117.27	112.71
26	G	269	CDL	C22-C21-C20	3.00	129.56	114.37
20	J	60	CHD	C1-C10-C9	2.99	115.99	111.34
20	J	60	CHD	C15-C16-C17	2.99	110.99	105.14
20	C	271	CHD	C5-C6-C7	2.98	117.94	114.40
22	D	523	TGL	CB3-CB2-CB1	2.98	124.61	113.69
26	T	1269	CDL	C23-C22-C21	2.96	129.35	114.37
22	N	1523	TGL	OG2-CG2-CG3	2.96	118.97	108.34
18	N	515	HEA	CHA-C4D-C3D	-2.96	120.46	124.77
22	N	1523	TGL	CG2-OG2-CB1	2.96	124.87	117.80
26	T	1269	CDL	C22-C21-C20	2.96	129.31	114.37
20	N	1604	CHD	C17-C13-C14	2.95	103.08	100.11
20	J	60	CHD	O7-C7-C6	2.95	117.18	109.86
20	P	1525	CHD	C17-C13-C12	2.94	120.32	117.67
20	A	525	CHD	C18-C13-C17	-2.93	106.61	111.20
24	C	272	DMU	O1-C10-C5	2.93	116.39	110.37
20	C	271	CHD	C15-C16-C17	2.91	110.85	105.14
24	C	272	DMU	C10-O7-C3	2.91	124.87	117.98
20	A	525	CHD	C17-C13-C12	2.91	120.28	117.67
24	Z	1526	DMU	O1-C10-C5	2.89	116.30	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	1264	PEK	O03-C21-O04	2.87	130.81	123.63
24	Z	1526	DMU	C10-O7-C3	2.87	124.78	117.98
22	L	522	TGL	CC4-CC3-CC2	2.87	123.67	113.13
20	J	60	CHD	C16-C15-C14	2.86	110.74	105.14
22	L	522	TGL	OG1-CG1-CG2	2.84	116.58	108.40
20	B	1086	CHD	C9-C8-C7	2.84	115.43	111.86
20	W	1060	CHD	C15-C16-C17	2.84	110.69	105.14
25	C	264	PEK	O03-C21-C22	-2.83	103.21	111.83
18	N	515	HEA	C3C-C2C-C1C	-2.83	103.84	107.17
20	B	1086	CHD	C15-C14-C13	-2.83	100.80	103.54
20	J	60	CHD	C9-C11-C12	2.82	117.98	114.29
26	C	270	CDL	OB6-CB5-OB7	2.80	130.25	123.70
19	C	267	PGV	O01-C1-O02	2.80	130.25	123.70
18	N	515	HEA	C25-C23-C24	2.79	121.01	114.59
20	W	1271	CHD	C1-C10-C9	2.79	115.67	111.34
20	N	1604	CHD	C6-C5-C10	2.78	115.62	112.66
25	C	265	PEK	P-O12-C04	2.76	134.41	121.26
20	B	1086	CHD	C5-C6-C7	2.76	117.68	114.40
20	C	271	CHD	C18-C13-C14	-2.76	106.88	111.20
18	A	515	HEA	CHA-C4D-C3D	-2.75	120.76	124.77
26	G	269	CDL	C23-C22-C21	2.75	128.27	114.37
20	W	1271	CHD	C11-C12-C13	2.75	114.06	111.26
22	D	523	TGL	CG3-OG3-CC1	2.74	127.14	117.12
20	B	1086	CHD	C5-C4-C3	2.74	116.84	112.71
20	N	1604	CHD	C4-C3-C2	2.73	113.95	110.62
20	C	271	CHD	C16-C15-C14	2.72	110.47	105.14
20	B	1086	CHD	C9-C11-C12	2.72	117.86	114.29
20	N	1604	CHD	C5-C6-C7	2.72	117.64	114.40
22	D	523	TGL	OG2-CG2-CG3	2.72	118.09	108.34
26	T	1269	CDL	OB8-CB7-C71	-2.71	103.57	111.83
20	W	1271	CHD	C16-C15-C14	2.71	110.44	105.14
25	P	1265	PEK	P-O12-C04	2.71	134.15	121.26
20	W	1271	CHD	C15-C16-C17	2.68	110.39	105.14
20	W	1271	CHD	C1-C2-C3	2.68	114.03	110.48
18	A	515	HEA	CHC-C4B-NB	2.67	127.67	124.37
22	B	521	TGL	CG3-OG3-CC1	2.67	126.87	117.12
22	D	523	TGL	OG1-CG1-CG2	2.66	116.07	108.40
20	W	1060	CHD	O7-C7-C6	2.65	116.45	109.86
25	P	1265	PEK	C24-C23-C22	2.65	122.86	113.13
22	O	1521	TGL	CG3-OG3-CC1	2.64	126.77	117.12
20	J	60	CHD	C17-C13-C12	2.63	120.03	117.67
22	B	521	TGL	CA8-CA7-CA6	-2.62	101.13	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	1604	CHD	C19-C10-C1	-2.62	104.15	108.31
20	C	271	CHD	C2-C1-C10	2.61	117.15	112.74
18	N	516	HEA	C26-C15-C16	2.61	119.76	115.23
20	B	1086	CHD	O7-C7-C6	-2.61	103.37	109.86
18	N	515	HEA	C27-C19-C20	2.60	119.75	115.23
26	T	1269	CDL	OB8-CB6-CB4	2.59	115.86	108.40
20	N	1604	CHD	C18-C13-C14	2.58	115.25	111.20
20	W	1060	CHD	C6-C5-C4	2.57	114.17	111.23
20	C	271	CHD	C1-C10-C9	2.57	115.33	111.34
20	A	525	CHD	C2-C1-C10	2.56	117.06	112.74
25	C	265	PEK	C24-C23-C22	2.56	122.53	113.13
26	G	269	CDL	OB8-CB7-C71	-2.56	104.04	111.83
18	A	516	HEA	CHC-C4B-NB	2.56	127.53	124.37
18	A	515	HEA	C17-C18-C19	-2.55	121.78	127.62
22	N	1522	TGL	C20-CA9-CA8	2.55	127.25	114.37
22	N	1522	TGL	CC4-CC3-CC2	2.55	122.49	113.13
20	B	1086	CHD	O12-C12-C13	-2.54	106.73	111.02
20	B	1086	CHD	C4-C3-C2	2.54	113.72	110.62
18	N	515	HEA	C12-C11-C3B	-2.53	108.17	112.12
22	O	1521	TGL	CA8-CA7-CA6	-2.52	101.61	114.37
25	C	264	PEK	O03-C21-O04	2.51	129.91	123.63
22	N	1523	TGL	CG3-OG3-CC1	2.50	126.26	117.12
18	N	515	HEA	C16-C15-C14	-2.49	115.57	121.17
19	N	1524	PGV	O01-C02-C03	2.48	117.24	108.34
22	N	1523	TGL	CB3-CB2-CB1	2.48	122.77	113.69
22	L	522	TGL	CG2-OG2-CB1	2.48	123.72	117.80
18	A	515	HEA	C12-C11-C3B	-2.46	108.27	112.12
18	N	515	HEA	C2D-C1D-ND	2.46	112.67	109.84
22	L	522	TGL	C20-CA9-CA8	2.46	126.82	114.37
20	N	1604	CHD	O12-C12-C13	-2.46	106.86	111.02
26	G	269	CDL	OB8-CB6-CB4	2.46	115.48	108.40
22	N	1522	TGL	OG1-CG1-CG2	2.46	115.48	108.40
26	P	1270	CDL	OA8-CA6-CA4	2.45	115.47	108.40
20	J	60	CHD	C6-C5-C4	2.45	114.02	111.23
18	N	515	HEA	C3C-C4C-NC	2.45	111.86	109.80
25	C	265	PEK	C23-C22-C21	-2.44	104.76	113.69
25	G	1263	PEK	P-O12-C04	2.44	132.87	121.26
19	P	1266	PGV	C02-O01-C1	-2.43	111.97	117.80
19	P	1267	PGV	O03-C19-O04	2.43	129.71	123.63
26	C	270	CDL	C52-C51-CB5	-2.42	104.82	113.69
25	C	265	PEK	C03-C02-C01	2.42	117.42	111.78
18	A	516	HEA	C26-C15-C14	-2.41	117.44	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	272	DMU	C2-C3-C4	-2.41	105.59	110.93
20	P	1525	CHD	C19-C10-C9	-2.39	107.96	111.18
22	L	522	TGL	CC3-CC2-CC1	2.39	122.46	113.69
18	N	516	HEA	C2B-C1B-NB	2.39	112.67	109.90
24	M	526	DMU	O1-C10-C5	2.39	115.28	110.37
18	A	515	HEA	C16-C15-C14	-2.38	115.82	121.17
18	A	515	HEA	CHA-C4D-ND	2.37	126.98	124.42
18	N	516	HEA	C4C-C3C-C2C	-2.37	104.36	107.30
18	A	516	HEA	C27-C19-C20	2.37	119.33	115.23
18	A	516	HEA	C3D-C4D-ND	2.36	112.63	110.35
19	C	266	PGV	O03-C01-C02	2.35	115.17	108.40
22	O	1521	TGL	CB7-CB6-CB5	-2.35	102.50	114.37
20	A	525	CHD	C1-C2-C3	2.34	113.58	110.48
26	C	270	CDL	OA8-CA6-CA4	2.32	115.09	108.40
25	T	263	PEK	P-O12-C04	2.32	132.29	121.26
26	G	269	CDL	C19-C18-C17	2.30	126.00	114.37
26	T	1269	CDL	C20-C19-C18	2.29	125.95	114.37
20	A	525	CHD	C15-C14-C13	-2.29	101.32	103.54
22	N	1523	TGL	OG1-CG1-CG2	2.29	115.00	108.40
18	A	516	HEA	CHB-C4A-NA	-2.28	121.97	124.45
19	P	1268	PGV	O03-C01-C02	2.28	114.97	108.40
25	P	1264	PEK	C24-C23-C22	-2.28	104.75	113.13
20	B	1086	CHD	C14-C8-C9	-2.27	106.58	109.75
18	N	515	HEA	C3D-C4D-ND	2.27	112.54	110.35
18	A	516	HEA	CHB-C1B-C2B	-2.26	121.45	125.03
19	A	524	PGV	O01-C02-C03	2.26	116.45	108.34
24	Z	1526	DMU	O7-C10-C5	2.26	113.64	108.09
26	T	1269	CDL	C19-C18-C17	2.26	125.77	114.37
20	B	1086	CHD	C19-C10-C1	-2.25	104.72	108.31
18	A	515	HEA	C27-C19-C20	2.25	119.13	115.23
20	P	1525	CHD	C16-C17-C13	-2.24	101.37	103.54
23	B	230	PSC	P-O12-C04	2.23	131.90	121.26
18	A	516	HEA	O11-C11-C3B	2.23	115.34	111.26
25	P	1265	PEK	C23-C22-C21	-2.22	105.56	113.69
18	N	516	HEA	CHB-C4A-NA	-2.22	122.04	124.45
20	N	1604	CHD	C9-C11-C12	2.22	117.20	114.29
20	P	1525	CHD	C18-C13-C17	-2.21	107.74	111.20
18	A	515	HEA	C1A-CHA-C4D	-2.21	121.33	126.02
22	B	521	TGL	C10-CB9-CB8	2.19	125.46	114.37
20	B	1086	CHD	C18-C13-C14	2.19	114.64	111.20
20	P	1525	CHD	C15-C14-C13	-2.19	101.42	103.54
22	L	522	TGL	CC7-CC6-CC5	2.18	125.40	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G	269	CDL	C20-C19-C18	2.18	125.38	114.37
22	D	523	TGL	CC3-CC2-CC1	-2.17	105.72	113.69
22	N	1523	TGL	OG2-CG2-CG1	2.17	116.12	108.34
22	O	1521	TGL	C10-CB9-CB8	2.17	125.32	114.37
25	P	1265	PEK	C03-C02-C01	2.16	116.82	111.78
20	W	1060	CHD	C1-C10-C9	2.15	114.68	111.34
20	P	1525	CHD	O3-C3-C4	2.14	114.11	109.84
22	B	521	TGL	C33-C19-C18	2.14	125.19	114.37
19	P	1267	PGV	O01-C1-O02	2.13	128.70	123.70
22	O	1521	TGL	OG3-CC1-CC2	-2.13	105.33	111.83
18	N	516	HEA	CHC-C4B-NB	2.13	127.00	124.37
25	P	1264	PEK	C02-O01-C1	-2.12	112.71	117.80
18	A	515	HEA	C1C-CHC-C4B	-2.11	121.28	126.25
18	N	515	HEA	CHC-C4B-C3B	-2.11	120.47	125.80
19	C	267	PGV	C9-C10-C11	-2.11	100.77	112.60
20	P	1525	CHD	C19-C10-C1	-2.09	104.98	108.31
22	B	521	TGL	CB7-CB6-CB5	-2.09	103.82	114.37
19	C	267	PGV	C3-C2-C1	-2.09	106.05	113.69
24	P	1272	DMU	O55-C2-C1	2.09	115.29	110.38
26	T	1269	CDL	C83-C82-C81	2.08	124.86	114.37
26	C	270	CDL	C79-C78-C77	2.07	124.86	114.37
20	P	1525	CHD	C11-C9-C10	2.07	115.80	113.70
19	P	1266	PGV	O01-C1-O02	2.07	128.54	123.70
23	O	1230	PSC	P-O12-C04	2.07	131.10	121.26
26	C	270	CDL	C80-C79-C78	2.06	124.79	114.37
26	C	270	CDL	CB6-CB4-CB3	-2.06	106.98	111.78
19	P	1267	PGV	C3-C2-C1	-2.06	106.16	113.69
26	G	269	CDL	C83-C82-C81	2.05	124.75	114.37
22	D	523	TGL	C10-CB9-CB8	2.05	124.74	114.37
22	D	523	TGL	CB8-CB7-CB6	2.05	124.71	114.37
19	C	266	PGV	O01-C1-O02	2.04	128.49	123.70
26	G	269	CDL	O1-C1-CB2	2.04	116.75	109.70
18	N	516	HEA	C1D-ND-C4D	-2.04	102.79	105.21
19	C	267	PGV	O03-C19-O04	2.04	128.73	123.63
19	C	268	PGV	C04-C05-C06	2.04	118.63	111.77
18	N	515	HEA	C27-C19-C18	-2.03	118.42	123.63
25	C	265	PEK	O03-C01-C02	2.03	114.23	108.40
18	A	515	HEA	C27-C19-C18	-2.02	118.43	123.63
25	P	1264	PEK	C25-C24-C23	-2.02	104.15	114.37
18	N	516	HEA	CAA-C2A-C1A	2.01	128.95	124.85
20	W	1060	CHD	C18-C13-C17	2.01	114.35	111.20
22	O	1521	TGL	C19-C18-C17	2.01	124.52	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	P	1525	CHD	O3-C3-C2	2.01	115.41	110.17
19	C	268	PGV	O03-C01-C02	2.01	114.18	108.40
20	W	1271	CHD	C14-C8-C7	2.00	114.51	111.85
26	P	1270	CDL	C80-C79-C78	2.00	124.49	114.37
22	B	521	TGL	OG1-CG1-CG2	2.00	114.17	108.40
22	N	1522	TGL	CC3-CC2-CC1	2.00	121.03	113.69

All (42) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	C	271	CHD	C8
20	C	271	CHD	C9
20	C	271	CHD	C3
20	C	271	CHD	C12
20	C	271	CHD	C14
20	J	60	CHD	C8
20	J	60	CHD	C9
20	J	60	CHD	C12
20	J	60	CHD	C14
20	J	60	CHD	C17
20	W	1271	CHD	C8
20	W	1271	CHD	C9
20	W	1271	CHD	C3
20	W	1271	CHD	C12
20	W	1271	CHD	C14
20	W	1060	CHD	C8
20	W	1060	CHD	C9
20	W	1060	CHD	C12
20	W	1060	CHD	C14
20	W	1060	CHD	C17
24	C	272	DMU	C10
24	C	272	DMU	C9
24	C	272	DMU	C5
24	C	272	DMU	C2
24	C	272	DMU	C6
24	C	272	DMU	C4
24	M	526	DMU	C9
24	M	526	DMU	C5
24	M	526	DMU	C2
24	M	526	DMU	C6
24	M	526	DMU	C4
24	P	1272	DMU	C10

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Mol	Chain	Res	Type	Atom
24	P	1272	DMU	C9
24	P	1272	DMU	C5
24	P	1272	DMU	C2
24	P	1272	DMU	C6
24	P	1272	DMU	C4
24	Z	1526	DMU	C9
24	Z	1526	DMU	C5
24	Z	1526	DMU	C2
24	Z	1526	DMU	C6
24	Z	1526	DMU	C4

All (877) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	515	HEA	C2A-C3A-CMA-OMA
18	A	515	HEA	C4A-C3A-CMA-OMA
18	N	515	HEA	C2A-C3A-CMA-OMA
19	A	524	PGV	C04-O12-P-O11
19	A	524	PGV	C04-O12-P-O13
19	A	524	PGV	C04-O12-P-O14
19	A	524	PGV	C02-C03-O11-P
19	A	524	PGV	C05-C04-O12-P
19	A	524	PGV	C04-C05-C06-O06
19	A	524	PGV	O02-C1-O01-C02
19	A	524	PGV	C2-C1-O01-C02
19	A	524	PGV	C20-C19-O03-C01
19	C	266	PGV	C04-O12-P-O13
19	C	268	PGV	C04-O12-P-O11
19	C	268	PGV	C04-O12-P-O13
19	C	268	PGV	C04-O12-P-O14
19	C	268	PGV	O05-C05-C06-O06
19	N	1524	PGV	C04-O12-P-O11
19	N	1524	PGV	C04-O12-P-O13
19	N	1524	PGV	C04-O12-P-O14
19	N	1524	PGV	C02-C03-O11-P
19	N	1524	PGV	C05-C04-O12-P
19	N	1524	PGV	C04-C05-C06-O06
19	N	1524	PGV	O02-C1-O01-C02
19	N	1524	PGV	C2-C1-O01-C02
19	N	1524	PGV	C20-C19-O03-C01
19	P	1268	PGV	C04-O12-P-O11
19	P	1268	PGV	C04-O12-P-O13

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Mol	Chain	Res	Type	Atoms
19	P	1268	PGV	C04-O12-P-O14
19	P	1268	PGV	O05-C05-C06-O06
20	J	60	CHD	C16-C17-C20-C21
20	J	60	CHD	C16-C17-C20-C22
20	W	1060	CHD	C16-C17-C20-C21
20	W	1060	CHD	C16-C17-C20-C22
22	O	1521	TGL	CB2-CB1-OG2-CG2
23	B	230	PSC	C03-O11-P-O14
23	B	230	PSC	C04-O12-P-O14
23	O	1230	PSC	C03-O11-P-O14
23	O	1230	PSC	C04-O12-P-O14
24	M	526	DMU	O5-C6-O16-C18
24	Z	1526	DMU	O5-C6-O16-C18
25	C	265	PEK	C03-O11-P-O13
25	C	265	PEK	C04-O12-P-O11
25	C	265	PEK	C04-O12-P-O13
25	C	265	PEK	C04-O12-P-O14
25	G	1263	PEK	C03-O11-P-O12
25	G	1263	PEK	C03-O11-P-O13
25	G	1263	PEK	C03-O11-P-O14
25	G	1263	PEK	O12-C04-C05-N
25	P	1265	PEK	C03-O11-P-O13
25	P	1265	PEK	C04-O12-P-O11
25	P	1265	PEK	C04-O12-P-O13
25	P	1265	PEK	C04-O12-P-O14
25	T	263	PEK	C03-O11-P-O12
25	T	263	PEK	C03-O11-P-O14
25	T	263	PEK	O12-C04-C05-N
26	C	270	CDL	CA2-C1-CB2-OB2
26	C	270	CDL	CA2-OA2-PA1-OA3
26	C	270	CDL	CA2-OA2-PA1-OA4
26	C	270	CDL	CA2-OA2-PA1-OA5
26	C	270	CDL	CA4-CA3-OA5-PA1
26	C	270	CDL	C11-CA5-OA6-CA4
26	C	270	CDL	CB2-OB2-PB2-OB3
26	C	270	CDL	CB2-OB2-PB2-OB4
26	G	269	CDL	CB2-C1-CA2-OA2
26	G	269	CDL	CA2-OA2-PA1-OA3
26	G	269	CDL	C1-CB2-OB2-PB2
26	G	269	CDL	CB3-OB5-PB2-OB2
26	G	269	CDL	CB3-OB5-PB2-OB3
26	G	269	CDL	CB3-OB5-PB2-OB4

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Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	CA2-C1-CB2-OB2
26	P	1270	CDL	CA2-OA2-PA1-OA3
26	P	1270	CDL	CA2-OA2-PA1-OA4
26	P	1270	CDL	CA2-OA2-PA1-OA5
26	P	1270	CDL	CA4-CA3-OA5-PA1
26	P	1270	CDL	C11-CA5-OA6-CA4
26	P	1270	CDL	CB2-OB2-PB2-OB3
26	P	1270	CDL	CB2-OB2-PB2-OB4
26	T	1269	CDL	CB2-C1-CA2-OA2
26	T	1269	CDL	CA2-OA2-PA1-OA3
26	T	1269	CDL	C1-CB2-OB2-PB2
26	T	1269	CDL	CB3-OB5-PB2-OB2
26	T	1269	CDL	CB3-OB5-PB2-OB3
26	T	1269	CDL	CB3-OB5-PB2-OB4
19	A	524	PGV	O04-C19-O03-C01
19	N	1524	PGV	O04-C19-O03-C01
22	D	523	TGL	OC1-CC1-OG3-CG3
22	N	1523	TGL	OC1-CC1-OG3-CG3
22	B	521	TGL	OB1-CB1-OG2-CG2
22	O	1521	TGL	OB1-CB1-OG2-CG2
23	B	230	PSC	O02-C1-O01-C02
23	O	1230	PSC	O02-C1-O01-C02
22	B	521	TGL	CB2-CB1-OG2-CG2
18	A	515	HEA	C26-C15-C16-C17
18	N	515	HEA	C26-C15-C16-C17
18	A	515	HEA	C14-C15-C16-C17
18	N	515	HEA	C14-C15-C16-C17
22	O	1521	TGL	OA1-CA1-OG1-CG1
22	B	521	TGL	CA2-CA1-OG1-CG1
26	G	269	CDL	C31-CA7-OA8-CA6
26	T	1269	CDL	C31-CA7-OA8-CA6
22	O	1521	TGL	C16-C15-CC9-CC8
22	B	521	TGL	OA1-CA1-OG1-CG1
26	G	269	CDL	OA9-CA7-OA8-CA6
26	T	1269	CDL	OA9-CA7-OA8-CA6
26	C	270	CDL	OA7-CA5-OA6-CA4
26	P	1270	CDL	OA7-CA5-OA6-CA4
26	C	270	CDL	C80-C81-C82-C83
26	T	1269	CDL	C57-C58-C59-C60
26	C	270	CDL	C40-C41-C42-C43
26	C	270	CDL	C60-C61-C62-C63
26	G	269	CDL	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
26	G	269	CDL	C57-C58-C59-C60
26	P	1270	CDL	C80-C81-C82-C83
22	N	1522	TGL	C21-C20-CA9-CA8
26	C	270	CDL	C20-C21-C22-C23
26	C	270	CDL	C57-C58-C59-C60
26	C	270	CDL	C77-C78-C79-C80
26	G	269	CDL	C20-C21-C22-C23
26	G	269	CDL	C37-C38-C39-C40
26	G	269	CDL	C77-C78-C79-C80
26	P	1270	CDL	C40-C41-C42-C43
26	P	1270	CDL	C57-C58-C59-C60
26	P	1270	CDL	C60-C61-C62-C63
26	T	1269	CDL	C17-C18-C19-C20
26	T	1269	CDL	C20-C21-C22-C23
26	T	1269	CDL	C37-C38-C39-C40
26	T	1269	CDL	C40-C41-C42-C43
26	T	1269	CDL	C60-C61-C62-C63
26	T	1269	CDL	C77-C78-C79-C80
19	A	524	PGV	O12-C04-C05-O05
26	G	269	CDL	O1-C1-CA2-OA2
26	T	1269	CDL	O1-C1-CA2-OA2
22	D	523	TGL	CC2-CC1-OG3-CG3
22	N	1523	TGL	CC2-CC1-OG3-CG3
22	O	1521	TGL	CA2-CA1-OG1-CG1
23	B	230	PSC	C2-C1-O01-C02
23	O	1230	PSC	C2-C1-O01-C02
22	L	522	TGL	OA1-CA1-OG1-CG1
24	C	272	DMU	O6-C11-C9-O1
22	D	523	TGL	C21-C20-CA9-CA8
22	L	522	TGL	C21-C20-CA9-CA8
26	G	269	CDL	C17-C18-C19-C20
26	P	1270	CDL	C77-C78-C79-C80
22	B	521	TGL	C16-C15-CC9-CC8
26	P	1270	CDL	C20-C21-C22-C23
23	B	230	PSC	C20-C19-O03-C01
23	O	1230	PSC	C20-C19-O03-C01
26	P	1270	CDL	C17-C18-C19-C20
24	M	526	DMU	O6-C11-C9-C8
26	C	270	CDL	C17-C18-C19-C20
26	C	270	CDL	C37-C38-C39-C40
26	G	269	CDL	C60-C61-C62-C63
26	G	269	CDL	C80-C81-C82-C83

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Mol	Chain	Res	Type	Atoms
24	P	1272	DMU	O6-C11-C9-O1
22	D	523	TGL	C11-C10-CB9-CB8
22	N	1523	TGL	C21-C20-CA9-CA8
26	P	1270	CDL	C37-C38-C39-C40
22	N	1522	TGL	OA1-CA1-OG1-CG1
23	B	230	PSC	O04-C19-O03-C01
22	N	1523	TGL	C11-C10-CB9-CB8
26	T	1269	CDL	C80-C81-C82-C83
24	Z	1526	DMU	O6-C11-C9-C8
22	L	522	TGL	C16-C15-CC9-CC8
24	M	526	DMU	O5-C4-C57-O61
22	D	523	TGL	C16-C15-CC9-CC8
22	N	1522	TGL	C16-C15-CC9-CC8
22	O	1521	TGL	C21-C20-CA9-CA8
20	J	60	CHD	C17-C20-C22-C23
20	W	1060	CHD	C17-C20-C22-C23
22	B	521	TGL	C21-C20-CA9-CA8
22	N	1523	TGL	C16-C15-CC9-CC8
22	O	1521	TGL	C11-C10-CB9-CB8
22	B	521	TGL	C11-C10-CB9-CB8
22	N	1522	TGL	C11-C10-CB9-CB8
20	J	60	CHD	C21-C20-C22-C23
23	O	1230	PSC	O04-C19-O03-C01
19	A	524	PGV	O12-C04-C05-C06
19	N	1524	PGV	O12-C04-C05-C06
22	D	523	TGL	CA2-CA1-OG1-CG1
22	L	522	TGL	CA2-CA1-OG1-CG1
22	N	1522	TGL	CA2-CA1-OG1-CG1
22	N	1523	TGL	CA2-CA1-OG1-CG1
22	L	522	TGL	C11-C10-CB9-CB8
24	P	1272	DMU	C3-C4-C57-O61
20	W	1060	CHD	C21-C20-C22-C23
26	C	270	CDL	O1-C1-CB2-OB2
26	G	269	CDL	O1-C1-CB2-OB2
26	P	1270	CDL	O1-C1-CB2-OB2
26	T	1269	CDL	O1-C1-CB2-OB2
24	C	272	DMU	C3-C4-C57-O61
24	Z	1526	DMU	O5-C4-C57-O61
26	T	1269	CDL	C11-CA5-OA6-CA4
26	G	269	CDL	OB6-CB4-CB6-OB8
26	T	1269	CDL	OB6-CB4-CB6-OB8
19	A	524	PGV	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
19	N	1524	PGV	C19-C20-C21-C22
19	N	1524	PGV	O05-C05-C06-O06
22	N	1523	TGL	OA1-CA1-OG1-CG1
20	J	60	CHD	C13-C17-C20-C22
20	W	1060	CHD	C13-C17-C20-C22
25	G	1263	PEK	C1-C2-C3-C4
25	T	263	PEK	C1-C2-C3-C4
22	L	522	TGL	CC3-CC4-CC5-CC6
23	B	230	PSC	C20-C21-C22-C23
25	G	1263	PEK	C28-C29-C30-C31
25	T	263	PEK	C28-C29-C30-C31
19	C	268	PGV	O12-C04-C05-O05
19	N	1524	PGV	O12-C04-C05-O05
19	P	1268	PGV	O12-C04-C05-O05
20	C	271	CHD	C13-C17-C20-C22
23	O	1230	PSC	C20-C21-C22-C23
22	D	523	TGL	OA1-CA1-OG1-CG1
23	B	230	PSC	C1-C2-C3-C4
19	C	268	PGV	C2-C1-O01-C02
26	G	269	CDL	C11-CA5-OA6-CA4
22	O	1521	TGL	OC1-CC1-OG3-CG3
22	B	521	TGL	OC1-CC1-OG3-CG3
26	C	270	CDL	CB7-C71-C72-C73
26	G	269	CDL	OA7-CA5-OA6-CA4
26	T	1269	CDL	OA7-CA5-OA6-CA4
19	C	268	PGV	O12-C04-C05-C06
19	P	1268	PGV	O12-C04-C05-C06
26	G	269	CDL	CA2-C1-CB2-OB2
26	T	1269	CDL	CA2-C1-CB2-OB2
22	N	1522	TGL	CC3-CC4-CC5-CC6
20	W	1060	CHD	C13-C17-C20-C21
23	B	230	PSC	C22-C23-C24-C25
20	W	1271	CHD	C13-C17-C20-C22
26	G	269	CDL	CA5-C11-C12-C13
19	P	1268	PGV	C2-C1-O01-C02
19	C	268	PGV	O02-C1-O01-C02
19	P	1268	PGV	O02-C1-O01-C02
20	J	60	CHD	C13-C17-C20-C21
24	C	272	DMU	C1-C6-O16-C18
23	O	1230	PSC	C22-C23-C24-C25
23	O	1230	PSC	C1-C2-C3-C4
24	P	1272	DMU	O5-C4-C57-O61

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Mol	Chain	Res	Type	Atoms
19	C	268	PGV	C04-C05-C06-O06
19	P	1268	PGV	C04-C05-C06-O06
24	P	1272	DMU	O5-C6-O16-C18
25	G	1263	PEK	O03-C01-C02-O01
24	Z	1526	DMU	O16-C18-C19-C22
22	B	521	TGL	CB6-CB7-CB8-CB9
24	M	526	DMU	C25-C28-C31-C34
20	C	271	CHD	C17-C20-C22-C23
19	A	524	PGV	C4-C5-C6-C7
19	C	266	PGV	C6-C7-C8-C9
19	C	267	PGV	C7-C8-C9-C10
19	C	268	PGV	C22-C23-C24-C25
19	P	1266	PGV	C29-C30-C31-C32
19	P	1267	PGV	C7-C8-C9-C10
23	O	1230	PSC	C2-C3-C4-C5
26	P	1270	CDL	C51-C52-C53-C54
26	T	1269	CDL	C73-C74-C75-C76
19	N	1524	PGV	C4-C5-C6-C7
23	B	230	PSC	C2-C3-C4-C5
26	P	1270	CDL	C55-C56-C57-C58
19	C	267	PGV	C22-C23-C24-C25
19	C	268	PGV	C13-C14-C15-C16
19	P	1266	PGV	C6-C7-C8-C9
19	P	1267	PGV	C22-C23-C24-C25
19	P	1268	PGV	C13-C14-C15-C16
19	P	1268	PGV	C22-C23-C24-C25
25	C	265	PEK	C25-C26-C27-C28
26	G	269	CDL	C72-C73-C74-C75
26	T	1269	CDL	C58-C59-C60-C61
19	A	524	PGV	O05-C05-C06-O06
25	P	1265	PEK	C25-C26-C27-C28
26	C	270	CDL	C16-C17-C18-C19
26	C	270	CDL	C55-C56-C57-C58
26	T	1269	CDL	CA5-C11-C12-C13
24	Z	1526	DMU	C25-C28-C31-C34
26	P	1270	CDL	C16-C17-C18-C19
19	C	266	PGV	C29-C30-C31-C32
26	G	269	CDL	C58-C59-C60-C61
26	P	1270	CDL	C72-C73-C74-C75
26	T	1269	CDL	C72-C73-C74-C75
25	P	1265	PEK	C21-C22-C23-C24
26	P	1270	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
19	C	268	PGV	C24-C25-C26-C27
19	P	1268	PGV	C24-C25-C26-C27
26	C	270	CDL	C51-C52-C53-C54
26	P	1270	CDL	C13-C14-C15-C16
24	M	526	DMU	O16-C18-C19-C22
26	C	270	CDL	C13-C14-C15-C16
23	B	230	PSC	C29-C30-C31-C32
22	O	1521	TGL	CB6-CB7-CB8-CB9
20	W	1271	CHD	C17-C20-C22-C23
25	G	1263	PEK	C27-C28-C29-C30
25	T	263	PEK	C29-C30-C31-C32
26	C	270	CDL	CA5-C11-C12-C13
19	C	268	PGV	C3-C4-C5-C6
19	N	1524	PGV	C24-C25-C26-C27
22	L	522	TGL	CB4-CB5-CB6-CB7
23	O	1230	PSC	C29-C30-C31-C32
25	C	264	PEK	C23-C24-C25-C26
25	G	1263	PEK	C29-C30-C31-C32
25	T	263	PEK	C27-C28-C29-C30
26	G	269	CDL	C13-C14-C15-C16
26	T	1269	CDL	C13-C14-C15-C16
19	A	524	PGV	C24-C25-C26-C27
25	P	1264	PEK	C23-C24-C25-C26
26	C	270	CDL	C72-C73-C74-C75
26	G	269	CDL	C79-C80-C81-C82
26	T	1269	CDL	C79-C80-C81-C82
19	A	524	PGV	C5-C6-C7-C8
19	P	1268	PGV	C3-C4-C5-C6
25	G	1263	PEK	C25-C26-C27-C28
26	C	270	CDL	C74-C75-C76-C77
26	P	1270	CDL	CA5-C11-C12-C13
22	N	1522	TGL	CB4-CB5-CB6-CB7
25	T	263	PEK	C25-C26-C27-C28
26	C	270	CDL	C73-C74-C75-C76
26	G	269	CDL	C73-C74-C75-C76
23	O	1230	PSC	C13-C14-C15-C16
22	B	521	TGL	CC2-CC1-OG3-CG3
22	N	1522	TGL	CC2-CC1-OG3-CG3
22	N	1522	TGL	CC2-CC3-CC4-CC5
26	C	270	CDL	C59-C60-C61-C62
25	C	264	PEK	C1-C2-C3-C4
19	A	524	PGV	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
22	L	522	TGL	CC2-CC3-CC4-CC5
26	G	269	CDL	C56-C57-C58-C59
25	P	1265	PEK	C16-C17-C18-C19
19	P	1266	PGV	C23-C24-C25-C26
19	N	1524	PGV	C5-C6-C7-C8
19	N	1524	PGV	C28-C29-C30-C31
25	C	265	PEK	C21-C22-C23-C24
22	O	1521	TGL	CC2-CC1-OG3-CG3
25	C	264	PEK	C22-C21-O03-C01
22	B	521	TGL	C12-C13-C14-C29
24	P	1272	DMU	C25-C28-C31-C34
26	T	1269	CDL	C56-C57-C58-C59
25	C	265	PEK	C16-C17-C18-C19
26	P	1270	CDL	C73-C74-C75-C76
24	P	1272	DMU	C1-C6-O16-C18
19	N	1524	PGV	C22-C23-C24-C25
25	C	265	PEK	C29-C30-C31-C32
25	P	1264	PEK	C1-C2-C3-C4
19	A	524	PGV	C22-C23-C24-C25
19	C	266	PGV	C23-C24-C25-C26
25	C	264	PEK	C31-C32-C33-C34
19	C	266	PGV	C5-C6-C7-C8
19	P	1268	PGV	C27-C28-C29-C30
24	C	272	DMU	C25-C28-C31-C34
25	P	1265	PEK	C29-C30-C31-C32
26	P	1270	CDL	C18-C19-C20-C21
26	P	1270	CDL	C74-C75-C76-C77
25	P	1264	PEK	C22-C21-O03-C01
26	P	1270	CDL	C51-CB5-OB6-CB4
24	Z	1526	DMU	C3-C4-C57-O61
26	T	1269	CDL	CB5-C51-C52-C53
26	P	1270	CDL	C59-C60-C61-C62
19	C	267	PGV	C11-C10-C9-C8
19	P	1267	PGV	C11-C10-C9-C8
23	B	230	PSC	C13-C14-C15-C16
26	C	270	CDL	C18-C19-C20-C21
19	P	1266	PGV	C5-C6-C7-C8
26	G	269	CDL	CB5-C51-C52-C53
19	C	268	PGV	C27-C28-C29-C30
24	M	526	DMU	C22-C25-C28-C31
25	G	1263	PEK	C16-C17-C18-C19
24	Z	1526	DMU	C22-C25-C28-C31

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Mol	Chain	Res	Type	Atoms
25	P	1265	PEK	C31-C32-C33-C34
25	C	265	PEK	C31-C32-C33-C34
26	T	1269	CDL	C43-C44-C45-C46
22	L	522	TGL	CC2-CC1-OG3-CG3
19	P	1268	PGV	C1-C2-C3-C4
20	C	271	CHD	C21-C20-C22-C23
25	P	1264	PEK	C31-C32-C33-C34
25	T	263	PEK	C16-C17-C18-C19
26	G	269	CDL	C43-C44-C45-C46
19	C	268	PGV	C1-C2-C3-C4
25	T	263	PEK	O03-C01-C02-O01
19	P	1267	PGV	C20-C21-C22-C23
26	C	270	CDL	C32-C33-C34-C35
26	G	269	CDL	C82-C83-C84-C85
26	P	1270	CDL	C75-C76-C77-C78
26	T	1269	CDL	C82-C83-C84-C85
19	C	267	PGV	C20-C21-C22-C23
19	P	1267	PGV	C13-C14-C15-C16
19	C	267	PGV	C13-C14-C15-C16
26	P	1270	CDL	C32-C33-C34-C35
26	C	270	CDL	C64-C65-C66-C67
19	P	1266	PGV	C7-C8-C9-C10
22	L	522	TGL	OB1-CB1-OG2-CG2
26	C	270	CDL	OB7-CB5-OB6-CB4
19	C	266	PGV	C4-C5-C6-C7
25	P	1264	PEK	C16-C17-C18-C19
26	P	1270	CDL	C36-C37-C38-C39
19	C	266	PGV	C7-C8-C9-C10
26	P	1270	CDL	C64-C65-C66-C67
25	C	264	PEK	C2-C1-O01-C02
19	P	1267	PGV	C23-C24-C25-C26
20	C	271	CHD	C16-C17-C20-C22
19	A	524	PGV	C12-C13-C14-C15
19	N	1524	PGV	C12-C13-C14-C15
19	P	1268	PGV	C12-C13-C14-C15
19	P	1268	PGV	C25-C26-C27-C28
25	T	263	PEK	C01-C02-C03-O11
26	C	270	CDL	OB5-CB3-CB4-CB6
22	N	1522	TGL	OB1-CB1-OG2-CG2
26	P	1270	CDL	OB7-CB5-OB6-CB4
19	C	268	PGV	C25-C26-C27-C28
25	G	1263	PEK	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
25	C	264	PEK	O04-C21-O03-C01
20	C	271	CHD	C13-C17-C20-C21
25	T	263	PEK	C34-C35-C36-C37
26	C	270	CDL	C75-C76-C77-C78
26	P	1270	CDL	C63-C64-C65-C66
26	C	270	CDL	C63-C64-C65-C66
20	W	1271	CHD	C16-C17-C20-C22
19	C	268	PGV	C30-C31-C32-C33
19	P	1268	PGV	C30-C31-C32-C33
25	C	264	PEK	C22-C23-C24-C25
26	C	270	CDL	C36-C37-C38-C39
25	G	1263	PEK	C34-C35-C36-C37
20	W	1271	CHD	C16-C17-C20-C21
23	B	230	PSC	O03-C01-C02-C03
23	O	1230	PSC	O03-C01-C02-C03
25	G	1263	PEK	O03-C01-C02-C03
25	P	1264	PEK	O03-C01-C02-C03
25	T	263	PEK	O03-C01-C02-C03
26	C	270	CDL	CB3-CB4-CB6-OB8
26	G	269	CDL	CB3-CB4-CB6-OB8
26	P	1270	CDL	CB3-CB4-CB6-OB8
26	T	1269	CDL	CB3-CB4-CB6-OB8
19	C	268	PGV	C11-C10-C9-C8
19	C	268	PGV	C12-C13-C14-C15
25	C	264	PEK	C16-C17-C18-C19
25	T	263	PEK	C26-C27-C28-C29
19	P	1266	PGV	C4-C5-C6-C7
20	C	271	CHD	C16-C17-C20-C21
26	C	270	CDL	C71-C72-C73-C74
26	P	1270	CDL	C71-C72-C73-C74
25	C	264	PEK	C25-C26-C27-C28
25	P	1264	PEK	C22-C23-C24-C25
19	C	267	PGV	C23-C24-C25-C26
20	W	1271	CHD	C13-C17-C20-C21
23	O	1230	PSC	C27-C28-C29-C30
26	G	269	CDL	C33-C34-C35-C36
26	T	1269	CDL	C33-C34-C35-C36
19	A	524	PGV	C03-C02-O01-C1
19	N	1524	PGV	C03-C02-O01-C1
26	T	1269	CDL	C53-C54-C55-C56
19	P	1268	PGV	C11-C10-C9-C8
23	B	230	PSC	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
26	G	269	CDL	C21-C22-C23-C24
26	G	269	CDL	C53-C54-C55-C56
19	P	1266	PGV	C19-C20-C21-C22
23	B	230	PSC	C23-C24-C25-C26
23	O	1230	PSC	C23-C24-C25-C26
26	C	270	CDL	OA5-CA3-CA4-OA6
26	P	1270	CDL	OA5-CA3-CA4-OA6
19	C	267	PGV	C15-C16-C17-C18
19	C	268	PGV	C28-C29-C30-C31
19	P	1268	PGV	C28-C29-C30-C31
26	P	1270	CDL	C42-C43-C44-C45
19	A	524	PGV	C26-C27-C28-C29
26	C	270	CDL	C11-C12-C13-C14
26	G	269	CDL	C71-C72-C73-C74
26	T	1269	CDL	C14-C15-C16-C17
26	T	1269	CDL	C21-C22-C23-C24
19	P	1267	PGV	C15-C16-C17-C18
26	T	1269	CDL	C71-C72-C73-C74
25	P	1264	PEK	C26-C27-C28-C29
26	P	1270	CDL	C11-C12-C13-C14
26	P	1270	CDL	C61-C62-C63-C64
20	W	1271	CHD	C21-C20-C22-C23
22	L	522	TGL	CC7-CC8-CC9-C15
22	N	1522	TGL	CC7-CC8-CC9-C15
26	C	270	CDL	C42-C43-C44-C45
19	C	268	PGV	C23-C24-C25-C26
26	G	269	CDL	C14-C15-C16-C17
26	C	270	CDL	C51-CB5-OB6-CB4
26	C	270	CDL	C44-C45-C46-C47
26	P	1270	CDL	C44-C45-C46-C47
26	C	270	CDL	C61-C62-C63-C64
25	P	1264	PEK	C25-C26-C27-C28
26	C	270	CDL	C84-C85-C86-C87
26	G	269	CDL	C41-C42-C43-C44
18	A	516	HEA	C4D-C3D-CAD-CBD
18	N	516	HEA	C4D-C3D-CAD-CBD
19	N	1524	PGV	C26-C27-C28-C29
25	G	1263	PEK	C30-C31-C32-C33
26	T	1269	CDL	C31-C32-C33-C34
19	C	268	PGV	C31-C32-C33-C34
26	P	1270	CDL	C84-C85-C86-C87
19	P	1268	PGV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	C38-C39-C40-C41
19	C	266	PGV	C30-C31-C32-C33
25	C	265	PEK	C32-C33-C34-C35
26	P	1270	CDL	OB5-CB3-CB4-CB6
25	P	1264	PEK	C35-C36-C37-C38
19	P	1268	PGV	C31-C32-C33-C34
19	C	268	PGV	C14-C15-C16-C17
19	P	1267	PGV	C24-C25-C26-C27
25	T	263	PEK	C30-C31-C32-C33
23	B	230	PSC	C24-C25-C26-C27
25	P	1264	PEK	O04-C21-O03-C01
19	P	1266	PGV	C30-C31-C32-C33
26	T	1269	CDL	C35-C36-C37-C38
24	M	526	DMU	C34-C37-C40-C43
24	Z	1526	DMU	C34-C37-C40-C43
26	G	269	CDL	C35-C36-C37-C38
19	P	1268	PGV	C14-C15-C16-C17
19	C	268	PGV	C20-C19-O03-C01
26	G	269	CDL	C31-C32-C33-C34
26	P	1270	CDL	C34-C35-C36-C37
19	P	1268	PGV	C4-C5-C6-C7
23	O	1230	PSC	C24-C25-C26-C27
26	C	270	CDL	C34-C35-C36-C37
22	O	1521	TGL	C12-C13-C14-C29
25	C	264	PEK	O03-C01-C02-C03
26	G	269	CDL	CA3-CA4-CA6-OA8
25	C	264	PEK	C26-C27-C28-C29
26	G	269	CDL	C44-C45-C46-C47
26	T	1269	CDL	C44-C45-C46-C47
25	P	1265	PEK	C32-C33-C34-C35
19	C	266	PGV	C19-C20-C21-C22
26	G	269	CDL	C15-C16-C17-C18
26	T	1269	CDL	C41-C42-C43-C44
25	C	264	PEK	C17-C18-C19-C20
26	C	270	CDL	C38-C39-C40-C41
19	C	267	PGV	C25-C26-C27-C28
26	C	270	CDL	OB5-CB3-CB4-OB6
26	P	1270	CDL	OB5-CB3-CB4-OB6
24	P	1272	DMU	C34-C37-C40-C43
19	C	267	PGV	C02-C03-O11-P
25	P	1264	PEK	C17-C18-C19-C20
23	B	230	PSC	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	C78-C79-C80-C81
26	T	1269	CDL	C15-C16-C17-C18
25	C	264	PEK	C5-C6-C7-C8
25	C	264	PEK	C9-C10-C11-C12
25	C	265	PEK	C11-C12-C13-C14
25	G	1263	PEK	C6-C7-C8-C9
25	P	1264	PEK	C5-C6-C7-C8
25	P	1264	PEK	C9-C10-C11-C12
25	P	1265	PEK	C11-C12-C13-C14
25	T	263	PEK	C6-C7-C8-C9
22	N	1522	TGL	CC5-CC6-CC7-CC8
23	O	1230	PSC	C3-C4-C5-C6
19	P	1267	PGV	C1-C2-C3-C4
19	C	268	PGV	C4-C5-C6-C7
26	C	270	CDL	C39-C40-C41-C42
25	C	264	PEK	C35-C36-C37-C38
19	P	1267	PGV	C25-C26-C27-C28
22	D	523	TGL	CA9-C20-C21-C22
25	C	264	PEK	C27-C28-C29-C30
26	P	1270	CDL	C39-C40-C41-C42
23	O	1230	PSC	C14-C15-C16-C17
25	C	264	PEK	C24-C25-C26-C27
26	C	270	CDL	C43-C44-C45-C46
19	C	268	PGV	C15-C16-C17-C18
23	B	230	PSC	C14-C15-C16-C17
24	C	272	DMU	C22-C25-C28-C31
25	C	264	PEK	C32-C33-C34-C35
19	P	1268	PGV	C26-C27-C28-C29
23	O	1230	PSC	C31-C32-C33-C34
19	P	1268	PGV	C15-C16-C17-C18
19	A	524	PGV	C7-C8-C9-C10
22	N	1523	TGL	CA9-C20-C21-C22
25	P	1264	PEK	C24-C25-C26-C27
25	G	1263	PEK	C01-C02-C03-O11
26	G	269	CDL	OA5-CA3-CA4-CA6
26	T	1269	CDL	OA5-CA3-CA4-CA6
24	C	272	DMU	O5-C4-C57-O61
22	N	1522	TGL	CB5-CB6-CB7-CB8
26	P	1270	CDL	C43-C44-C45-C46
19	C	267	PGV	C24-C25-C26-C27
23	B	230	PSC	C31-C32-C33-C34
19	C	268	PGV	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
19	C	268	PGV	C5-C6-C7-C8
19	P	1268	PGV	O04-C19-O03-C01
22	N	1522	TGL	OC1-CC1-OG3-CG3
19	C	267	PGV	C1-C2-C3-C4
25	G	1263	PEK	C15-C16-C17-C18
19	P	1267	PGV	C31-C32-C33-C34
25	G	1263	PEK	O04-C21-O03-C01
25	P	1264	PEK	C27-C28-C29-C30
24	P	1272	DMU	O6-C11-C9-C8
19	A	524	PGV	O03-C01-C02-C03
19	N	1524	PGV	O03-C01-C02-C03
26	T	1269	CDL	CA3-CA4-CA6-OA8
19	C	267	PGV	C31-C32-C33-C34
25	T	263	PEK	O04-C21-O03-C01
26	C	270	CDL	C78-C79-C80-C81
26	C	270	CDL	OB6-CB4-CB6-OB8
26	G	269	CDL	OA6-CA4-CA6-OA8
26	P	1270	CDL	OB6-CB4-CB6-OB8
26	T	1269	CDL	OA6-CA4-CA6-OA8
19	P	1268	PGV	C5-C6-C7-C8
19	P	1266	PGV	C26-C27-C28-C29
22	L	522	TGL	CC5-CC6-CC7-CC8
26	G	269	CDL	C19-C20-C21-C22
22	L	522	TGL	OC1-CC1-OG3-CG3
19	N	1524	PGV	C7-C8-C9-C10
26	T	1269	CDL	C19-C20-C21-C22
25	C	265	PEK	C35-C36-C37-C38
19	P	1268	PGV	C20-C19-O03-C01
22	L	522	TGL	CB5-CB6-CB7-CB8
22	B	521	TGL	CG2-CG3-OG3-CC1
26	C	270	CDL	OA5-CA3-CA4-CA6
19	C	268	PGV	C26-C27-C28-C29
25	G	1263	PEK	C32-C33-C34-C35
25	G	1263	PEK	C22-C21-O03-C01
25	T	263	PEK	C22-C21-O03-C01
23	B	230	PSC	C4-C5-C6-C7
22	O	1521	TGL	CG2-CG3-OG3-CC1
26	P	1270	CDL	C83-C84-C85-C86
24	M	526	DMU	C3-C4-C57-O61
26	C	270	CDL	C24-C25-C26-C27
25	G	1263	PEK	O01-C02-C03-O11
25	P	1265	PEK	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	C24-C25-C26-C27
18	N	515	HEA	C4A-C3A-CMA-OMA
19	A	524	PGV	O03-C01-C02-O01
19	N	1524	PGV	O03-C01-C02-O01
23	B	230	PSC	O03-C01-C02-O01
23	O	1230	PSC	O03-C01-C02-O01
25	C	264	PEK	O03-C01-C02-O01
25	P	1264	PEK	O03-C01-C02-O01
22	N	1522	TGL	CA5-CA6-CA7-CA8
26	T	1269	CDL	C64-C65-C66-C67
25	T	263	PEK	C32-C33-C34-C35
18	A	515	HEA	O11-C11-C3B-C2B
18	N	515	HEA	O11-C11-C3B-C2B
19	A	524	PGV	C03-O11-P-O13
19	N	1524	PGV	C03-O11-P-O13
19	P	1266	PGV	C04-O12-P-O13
23	B	230	PSC	C04-O12-P-O11
23	B	230	PSC	C04-O12-P-O13
23	B	230	PSC	C04-C05-N-C08
23	O	1230	PSC	C04-O12-P-O11
23	O	1230	PSC	C04-O12-P-O13
23	O	1230	PSC	C04-C05-N-C08
25	C	265	PEK	C03-O11-P-O12
25	C	265	PEK	C03-O11-P-O14
25	P	1264	PEK	O12-C04-C05-N
25	P	1265	PEK	C03-O11-P-O12
25	P	1265	PEK	C03-O11-P-O14
25	T	263	PEK	C03-O11-P-O13
26	C	270	CDL	CB2-OB2-PB2-OB5
26	P	1270	CDL	CB2-OB2-PB2-OB5
26	T	1269	CDL	CB7-C71-C72-C73
19	P	1267	PGV	C02-C03-O11-P
26	G	269	CDL	CB4-CB3-OB5-PB2
26	T	1269	CDL	CB4-CB3-OB5-PB2
19	A	524	PGV	C20-C21-C22-C23
19	N	1524	PGV	C20-C21-C22-C23
25	G	1263	PEK	C21-C22-C23-C24
25	T	263	PEK	C21-C22-C23-C24
25	P	1264	PEK	C32-C33-C34-C35
23	O	1230	PSC	C4-C5-C6-C7
19	A	524	PGV	C01-C02-C03-O11
19	N	1524	PGV	C01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
22	O	1521	TGL	C13-C14-C29-C30
26	G	269	CDL	CB7-C71-C72-C73
25	T	263	PEK	O01-C02-C03-O11
19	C	266	PGV	C26-C27-C28-C29
19	A	524	PGV	C11-C10-C9-C8
19	P	1266	PGV	C9-C10-C11-C12
25	C	265	PEK	C3-C4-C5-C6
25	P	1265	PEK	C3-C4-C5-C6
26	C	270	CDL	C23-C24-C25-C26
26	G	269	CDL	C24-C25-C26-C27
26	P	1270	CDL	C23-C24-C25-C26
24	C	272	DMU	O5-C6-O16-C18
19	A	524	PGV	C25-C26-C27-C28
23	B	230	PSC	C04-C05-N-C07
26	P	1270	CDL	C76-C77-C78-C79
25	G	1263	PEK	C02-C03-O11-P
26	G	269	CDL	C64-C65-C66-C67
26	T	1269	CDL	C24-C25-C26-C27
26	G	269	CDL	C12-C13-C14-C15
19	C	266	PGV	C25-C26-C27-C28
20	A	525	CHD	C22-C23-C24-O26
19	N	1524	PGV	C11-C10-C9-C8
26	C	270	CDL	C83-C84-C85-C86
22	L	522	TGL	CA5-CA6-CA7-CA8
19	P	1268	PGV	O03-C01-C02-O01
20	P	1525	CHD	C22-C23-C24-O26
25	P	1265	PEK	C30-C31-C32-C33
25	G	1263	PEK	C31-C32-C33-C34
23	B	230	PSC	C11-C12-C13-C14
19	C	266	PGV	C02-C01-O03-C19
19	A	524	PGV	C21-C22-C23-C24
25	T	263	PEK	C02-C03-O11-P
26	T	1269	CDL	C54-C55-C56-C57
26	G	269	CDL	C54-C55-C56-C57
25	T	263	PEK	C31-C32-C33-C34
26	T	1269	CDL	C12-C13-C14-C15
18	A	516	HEA	CAA-CBA-CGA-O2A
26	C	270	CDL	C52-C53-C54-C55
26	T	1269	CDL	C38-C39-C40-C41
19	P	1266	PGV	O03-C19-C20-C21
23	B	230	PSC	C03-C02-O01-C1
23	O	1230	PSC	C03-C02-O01-C1

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Mol	Chain	Res	Type	Atoms
18	N	515	HEA	CAD-CBD-CGD-O1D
20	B	1086	CHD	C22-C23-C24-O25
20	B	1086	CHD	C22-C23-C24-O26
20	N	1604	CHD	C22-C23-C24-O26
20	P	1525	CHD	C22-C23-C24-O25
20	W	1271	CHD	C22-C23-C24-O25
18	A	516	HEA	CAD-CBD-CGD-O2D
20	A	525	CHD	C22-C23-C24-O25
19	C	268	PGV	O01-C02-C03-O11
19	N	1524	PGV	C21-C22-C23-C24
25	C	265	PEK	C30-C31-C32-C33
20	C	271	CHD	C22-C23-C24-O25
20	C	271	CHD	C22-C23-C24-O26
19	C	266	PGV	C9-C10-C11-C12
26	C	270	CDL	C76-C77-C78-C79
18	A	515	HEA	CAD-CBD-CGD-O2D
18	N	516	HEA	CAD-CBD-CGD-O2D
20	N	1604	CHD	C22-C23-C24-O25
23	B	230	PSC	C01-C02-C03-O11
19	N	1524	PGV	C25-C26-C27-C28
18	A	516	HEA	CAD-CBD-CGD-O1D
18	N	516	HEA	CAA-CBA-CGA-O2A
20	W	1271	CHD	C22-C23-C24-O26
24	P	1272	DMU	C22-C25-C28-C31
19	C	268	PGV	O03-C01-C02-O01
26	G	269	CDL	C39-C40-C41-C42
23	B	230	PSC	C9-C10-C11-C12
23	O	1230	PSC	C9-C10-C11-C12
25	C	265	PEK	C12-C13-C14-C15
25	P	1265	PEK	C12-C13-C14-C15
25	C	265	PEK	C26-C27-C28-C29
26	G	269	CDL	C38-C39-C40-C41
24	C	272	DMU	C28-C31-C34-C37
23	O	1230	PSC	C04-C05-N-C07
26	C	270	CDL	C41-C42-C43-C44
26	G	269	CDL	C36-C37-C38-C39
18	N	516	HEA	CAA-CBA-CGA-O1A
18	N	516	HEA	CAD-CBD-CGD-O1D
25	P	1265	PEK	C17-C18-C19-C20
26	P	1270	CDL	C52-C53-C54-C55
22	N	1522	TGL	CB2-CB1-OG2-CG2
19	P	1266	PGV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
25	C	264	PEK	O02-C1-O01-C02
26	P	1270	CDL	C56-C57-C58-C59
25	C	265	PEK	C17-C18-C19-C20
18	A	515	HEA	CAD-CBD-CGD-O1D
26	C	270	CDL	C1-CA2-OA2-PA1
26	P	1270	CDL	C1-CA2-OA2-PA1
24	C	272	DMU	C34-C37-C40-C43
22	L	522	TGL	OG2-CB1-CB2-CB3
20	N	1604	CHD	C17-C20-C22-C23
18	A	516	HEA	CAA-CBA-CGA-O1A
25	T	263	PEK	C33-C34-C35-C36
18	N	515	HEA	CAD-CBD-CGD-O2D
19	C	266	PGV	O03-C19-C20-C21
26	T	1269	CDL	C39-C40-C41-C42
26	T	1269	CDL	C52-C53-C54-C55
26	C	270	CDL	C56-C57-C58-C59
19	C	267	PGV	C14-C15-C16-C17
22	N	1522	TGL	OG2-CB1-CB2-CB3
23	O	1230	PSC	C11-C12-C13-C14
25	T	263	PEK	C15-C16-C17-C18
26	G	269	CDL	C52-C53-C54-C55
26	T	1269	CDL	C36-C37-C38-C39
19	P	1268	PGV	C01-C02-C03-O11
26	P	1270	CDL	OA5-CA3-CA4-CA6
22	N	1523	TGL	OG2-CG2-CG3-OG3
19	C	267	PGV	C9-C10-C11-C12
19	C	268	PGV	C02-C03-O11-P
19	P	1268	PGV	C02-C03-O11-P
22	B	521	TGL	C13-C14-C29-C30
24	P	1272	DMU	C4-C3-O7-C10
19	C	267	PGV	C29-C30-C31-C32
19	A	524	PGV	C9-C10-C11-C12
19	P	1267	PGV	C9-C10-C11-C12
23	O	1230	PSC	C7-C8-C9-C10
26	P	1270	CDL	C41-C42-C43-C44
23	O	1230	PSC	C04-C05-N-C06
22	B	521	TGL	CG1-CG2-OG2-CB1
19	C	266	PGV	C11-C12-C13-C14
19	C	267	PGV	C11-C12-C13-C14
23	B	230	PSC	C7-C8-C9-C10
22	D	523	TGL	C21-C22-C23-C24
24	P	1272	DMU	C18-C19-C22-C25

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Mol	Chain	Res	Type	Atoms
19	N	1524	PGV	C9-C10-C11-C12
25	C	264	PEK	C3-C4-C5-C6
19	C	267	PGV	C05-C04-O12-P
19	P	1268	PGV	O01-C02-C03-O11
19	P	1267	PGV	C14-C15-C16-C17
25	P	1264	PEK	C3-C4-C5-C6
23	B	230	PSC	O03-C19-C20-C21
19	P	1266	PGV	C20-C21-C22-C23
22	N	1523	TGL	CC3-CC4-CC5-CC6
19	C	266	PGV	C20-C21-C22-C23
22	D	523	TGL	OG2-CG2-CG3-OG3
19	P	1267	PGV	C11-C12-C13-C14
19	P	1267	PGV	C29-C30-C31-C32
22	L	522	TGL	OG3-CC1-CC2-CC3
23	O	1230	PSC	O03-C19-C20-C21
19	C	268	PGV	C01-C02-C03-O11
23	O	1230	PSC	C01-C02-C03-O11
26	P	1270	CDL	C22-C23-C24-C25
26	T	1269	CDL	C55-C56-C57-C58
25	G	1263	PEK	C33-C34-C35-C36
22	L	522	TGL	CB2-CB1-OG2-CG2
19	P	1266	PGV	C11-C12-C13-C14
25	T	263	PEK	C3-C4-C5-C6
18	A	516	HEA	C3B-C11-C12-C13
25	P	1265	PEK	C26-C27-C28-C29
22	N	1522	TGL	OG3-CC1-CC2-CC3
25	P	1264	PEK	O01-C1-C2-C3
26	G	269	CDL	C11-C12-C13-C14
26	P	1270	CDL	C32-C31-CA7-OA8
25	G	1263	PEK	C3-C4-C5-C6
25	G	1263	PEK	C14-C15-C16-C17
25	T	263	PEK	C14-C15-C16-C17
22	N	1523	TGL	C21-C22-C23-C24
22	N	1523	TGL	OG2-CB1-CB2-CB3
25	C	264	PEK	O01-C1-C2-C3
26	C	270	CDL	C32-C31-CA7-OA8
25	P	1264	PEK	C2-C1-O01-C02
26	C	270	CDL	C22-C23-C24-C25
26	T	1269	CDL	C59-C60-C61-C62
19	C	268	PGV	C05-C04-O12-P
24	C	272	DMU	C4-C3-O7-C10
18	A	515	HEA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	C11-C12-C13-C14
26	P	1270	CDL	C12-C11-CA5-OA6
25	C	265	PEK	O03-C01-C02-O01
25	P	1265	PEK	C34-C35-C36-C37
18	N	515	HEA	CAA-CBA-CGA-O1A
22	D	523	TGL	OG2-CB1-CB2-CB3
26	C	270	CDL	C12-C11-CA5-OA6
23	B	230	PSC	C15-C16-C17-C18
26	G	269	CDL	C78-C79-C80-C81
25	G	1263	PEK	C24-C25-C26-C27
22	D	523	TGL	CG1-CG2-OG2-CB1
22	N	1523	TGL	CG1-CG2-OG2-CB1
22	O	1521	TGL	CG1-CG2-OG2-CB1
23	B	230	PSC	C04-C05-N-C06
26	P	1270	CDL	C52-C51-CB5-OB6
22	D	523	TGL	CC3-CC4-CC5-CC6
19	P	1268	PGV	C05-C04-O12-P
26	P	1270	CDL	C15-C16-C17-C18
23	O	1230	PSC	C15-C16-C17-C18
26	C	270	CDL	C32-C31-CA7-OA9
26	P	1270	CDL	C32-C31-CA7-OA9
20	J	60	CHD	C22-C23-C24-O26
26	G	269	CDL	C55-C56-C57-C58
25	P	1264	PEK	O02-C1-O01-C02
18	A	515	HEA	C27-C19-C20-C21
22	D	523	TGL	OB1-CB1-CB2-CB3
19	N	1524	PGV	O01-C1-C2-C3
20	W	1060	CHD	C22-C23-C24-O26
19	N	1524	PGV	O02-C1-C2-C3
22	D	523	TGL	OC1-CC1-CC2-CC3
23	B	230	PSC	O04-C19-C20-C21
19	A	524	PGV	O02-C1-C2-C3
23	O	1230	PSC	O04-C19-C20-C21
25	P	1264	PEK	O02-C1-C2-C3
23	B	230	PSC	O01-C1-C2-C3
23	O	1230	PSC	O01-C1-C2-C3
26	C	270	CDL	C52-C51-CB5-OB6
22	N	1523	TGL	OC1-CC1-CC2-CC3
23	B	230	PSC	O02-C1-C2-C3
25	C	264	PEK	O02-C1-C2-C3
19	P	1267	PGV	C05-C04-O12-P
22	N	1523	TGL	OB1-CB1-CB2-CB3

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Mol	Chain	Res	Type	Atoms
23	O	1230	PSC	O02-C1-C2-C3
25	T	263	PEK	C02-C01-O03-C21
19	P	1268	PGV	C7-C8-C9-C10
19	A	524	PGV	O01-C1-C2-C3
25	T	263	PEK	C24-C25-C26-C27
18	N	515	HEA	CAA-CBA-CGA-O2A
20	W	1060	CHD	C22-C23-C24-O25
22	L	522	TGL	OC1-CC1-CC2-CC3
20	J	60	CHD	C22-C23-C24-O25

There are no ring outliers.

41 monomers are involved in 310 short contacts:

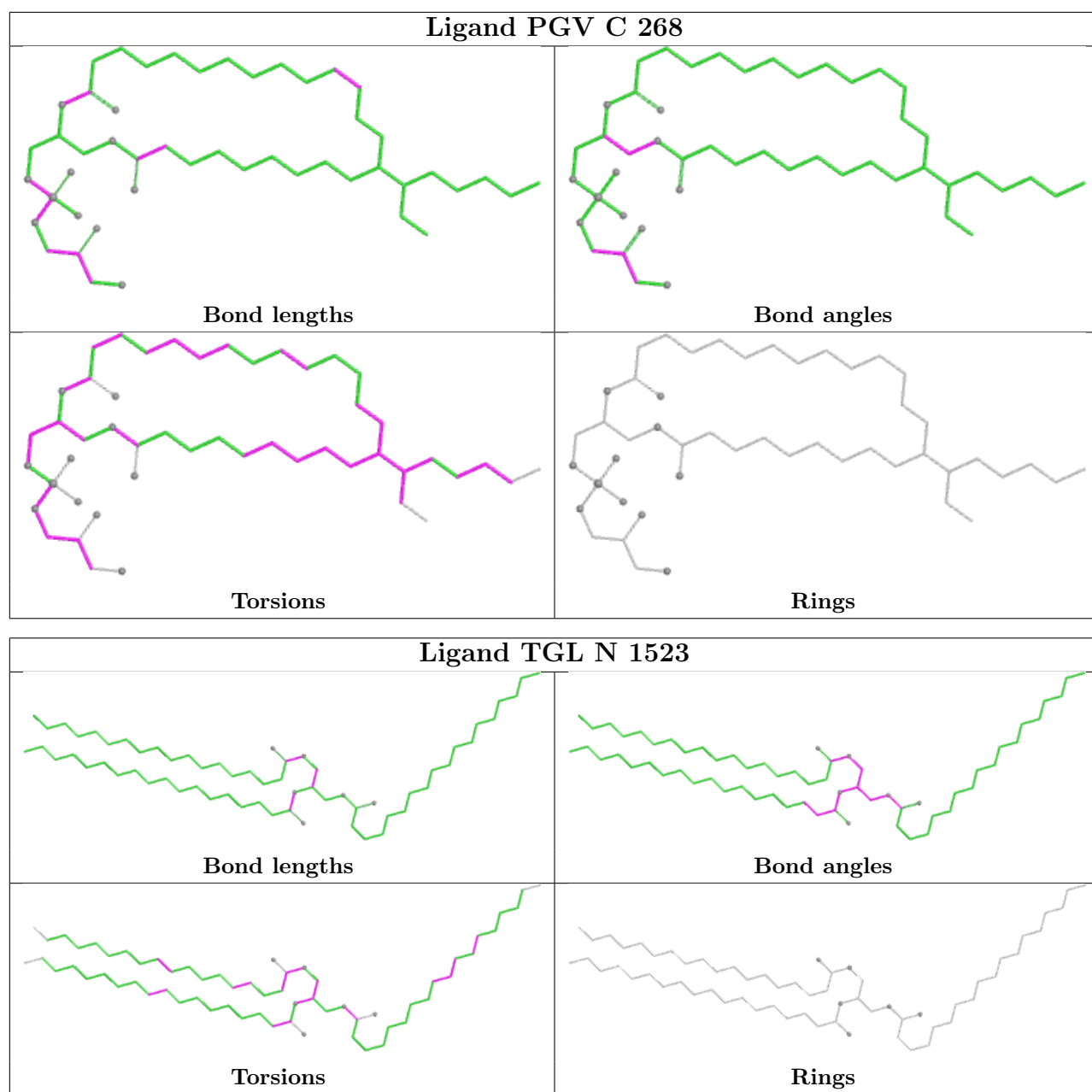
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	268	PGV	2	0
22	N	1523	TGL	8	0
20	P	1525	CHD	2	0
25	C	264	PEK	6	0
20	B	1086	CHD	1	0
18	N	515	HEA	3	0
19	N	1524	PGV	10	0
19	C	266	PGV	3	0
26	G	269	CDL	22	0
22	D	523	TGL	5	0
19	A	524	PGV	7	0
19	P	1267	PGV	9	0
22	L	522	TGL	28	0
22	N	1522	TGL	15	0
18	N	516	HEA	6	0
24	C	272	DMU	3	0
24	M	526	DMU	1	0
25	P	1265	PEK	9	0
26	T	1269	CDL	23	0
18	A	515	HEA	4	0
20	W	1060	CHD	3	0
18	A	516	HEA	1	0
25	C	265	PEK	11	0
25	P	1264	PEK	9	0
26	P	1270	CDL	13	0
24	P	1272	DMU	4	0
19	P	1266	PGV	3	0
19	P	1268	PGV	1	0

Continued on next page...

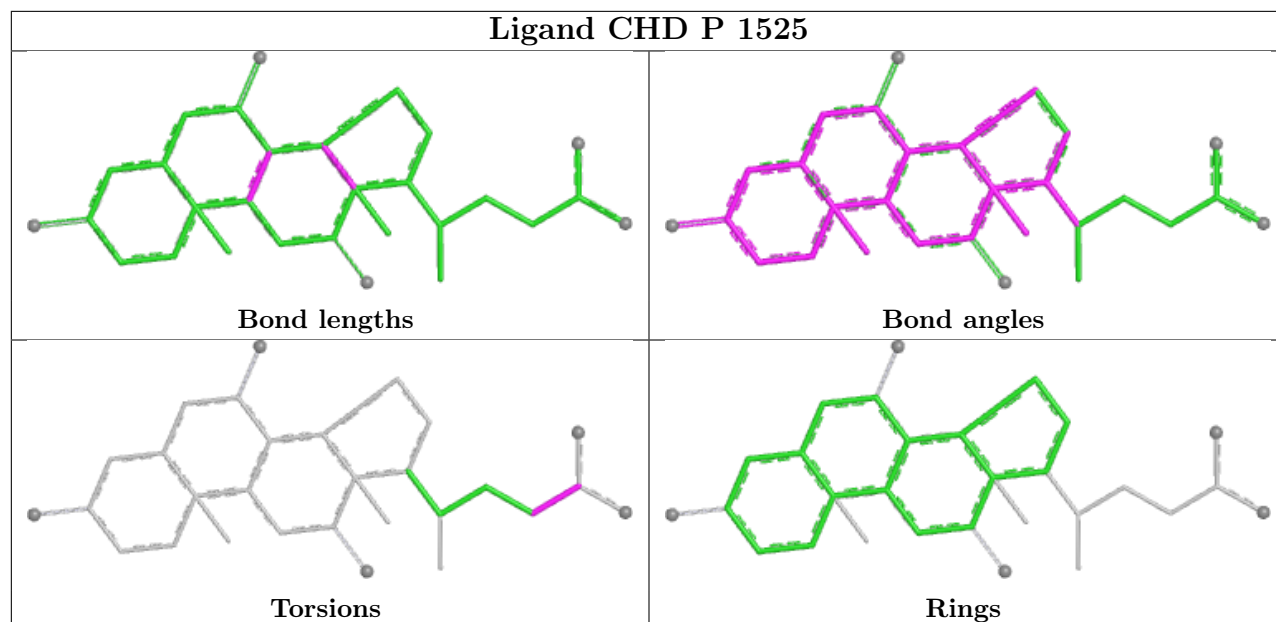
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	J	60	CHD	5	0
20	A	525	CHD	1	0
22	B	521	TGL	6	0
20	W	1271	CHD	2	0
22	O	1521	TGL	8	0
23	O	1230	PSC	18	0
20	N	1604	CHD	2	0
25	T	263	PEK	14	0
23	B	230	PSC	19	0
20	C	271	CHD	2	0
25	G	1263	PEK	9	0
26	C	270	CDL	19	0
19	C	267	PGV	8	0

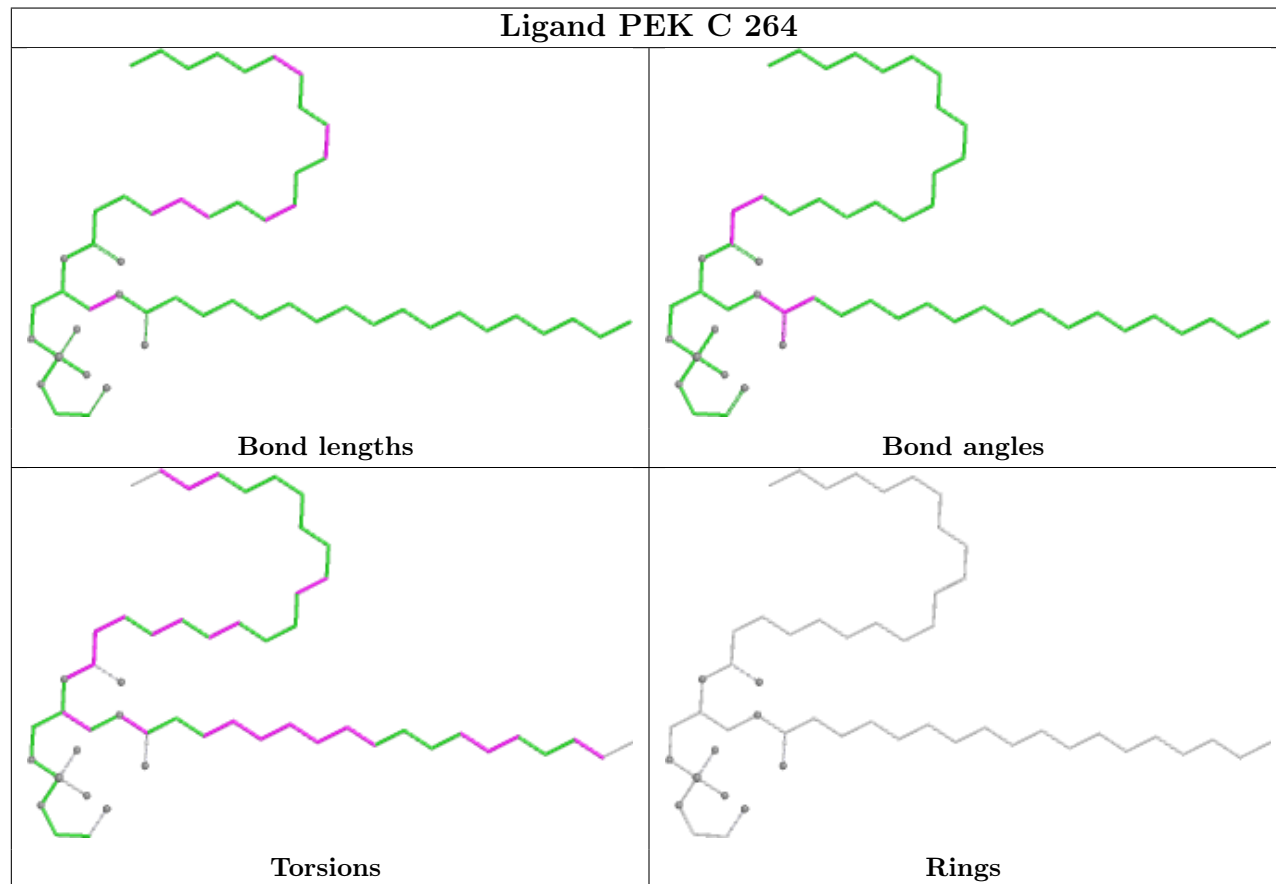
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

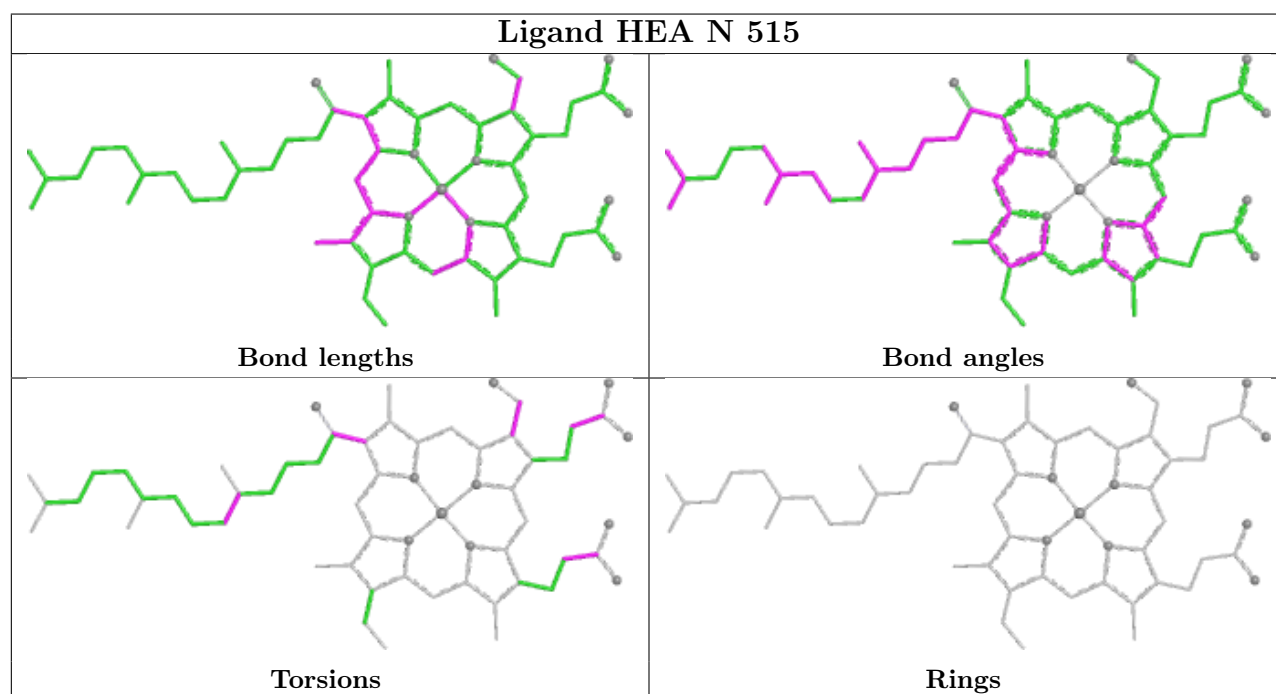
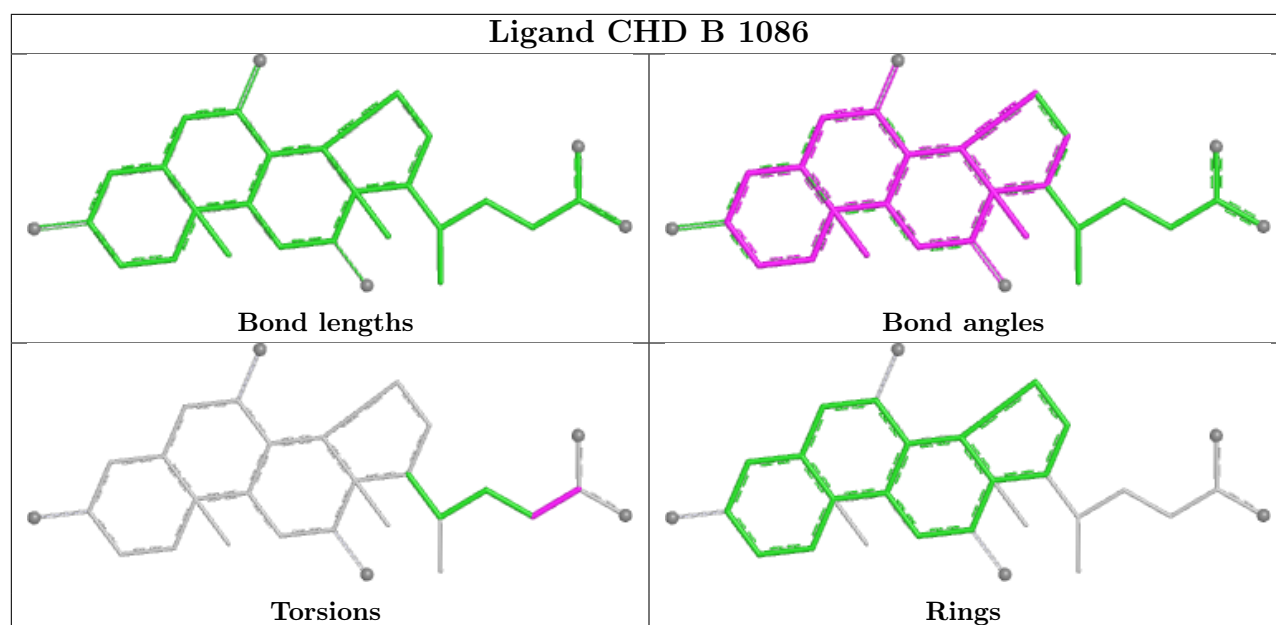


Ligand CHD P 1525

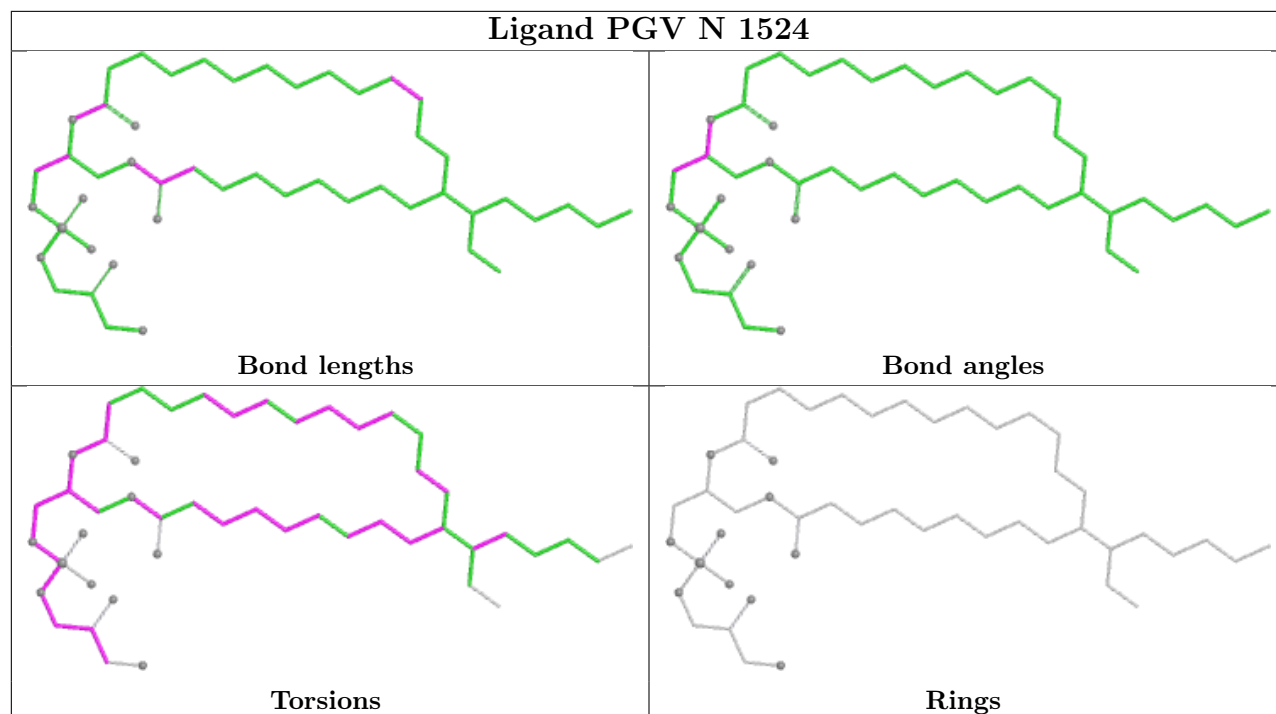


Ligand PEK C 264

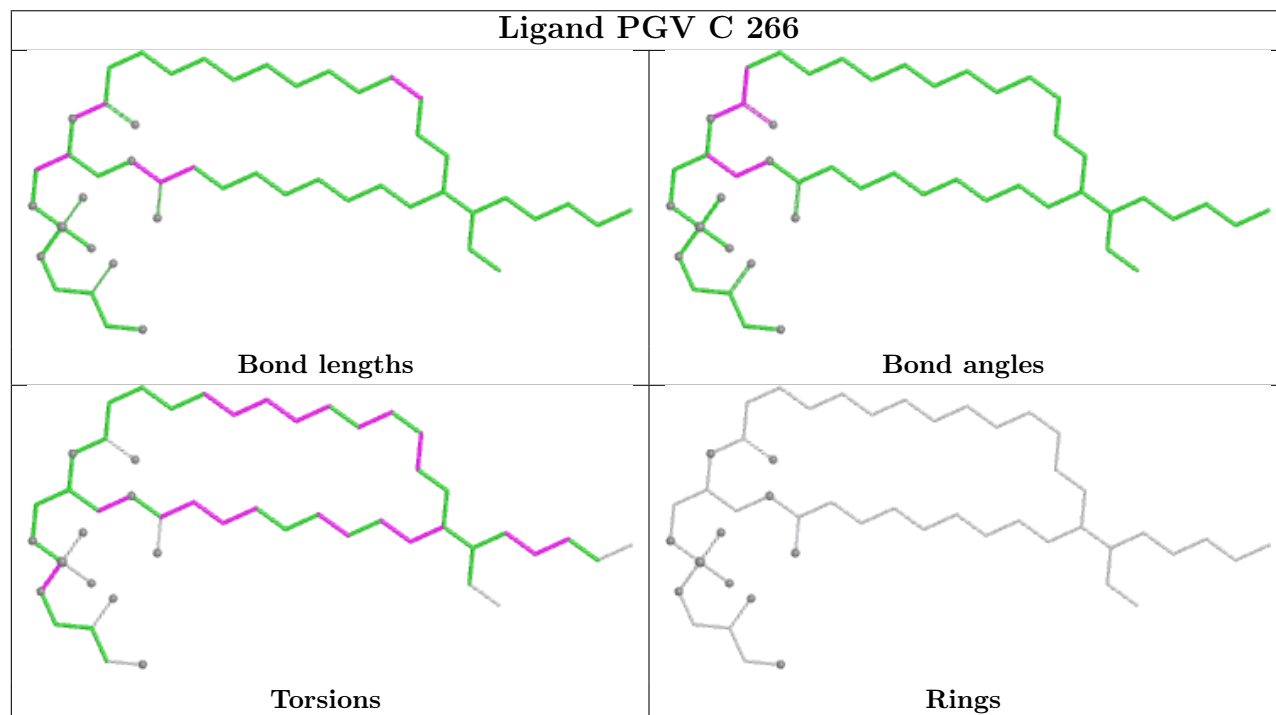


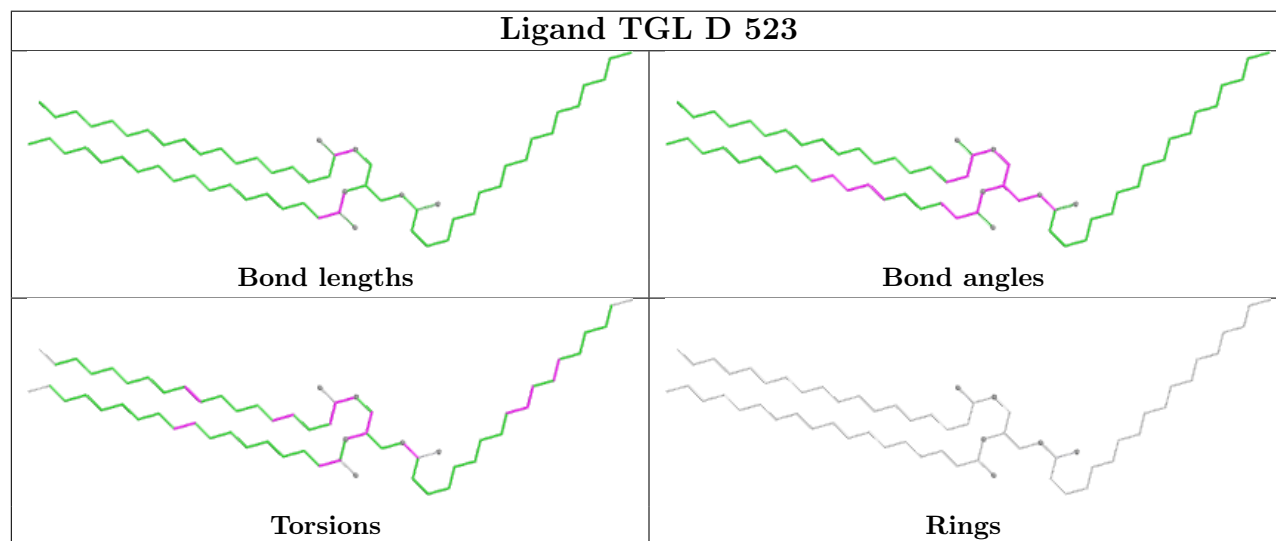
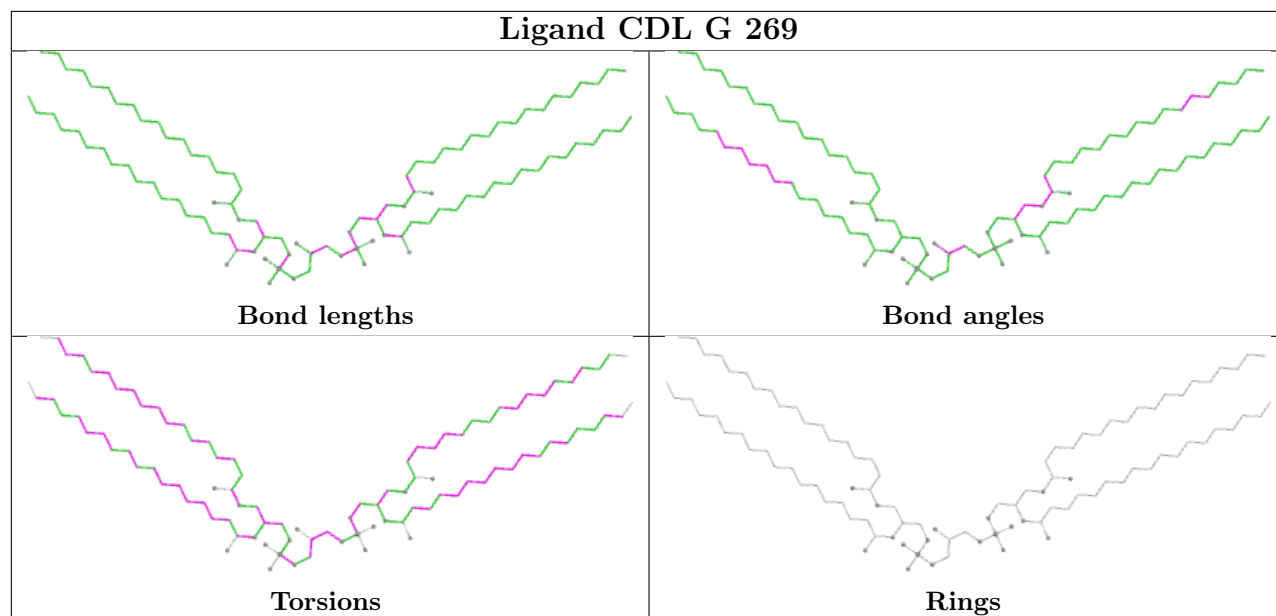


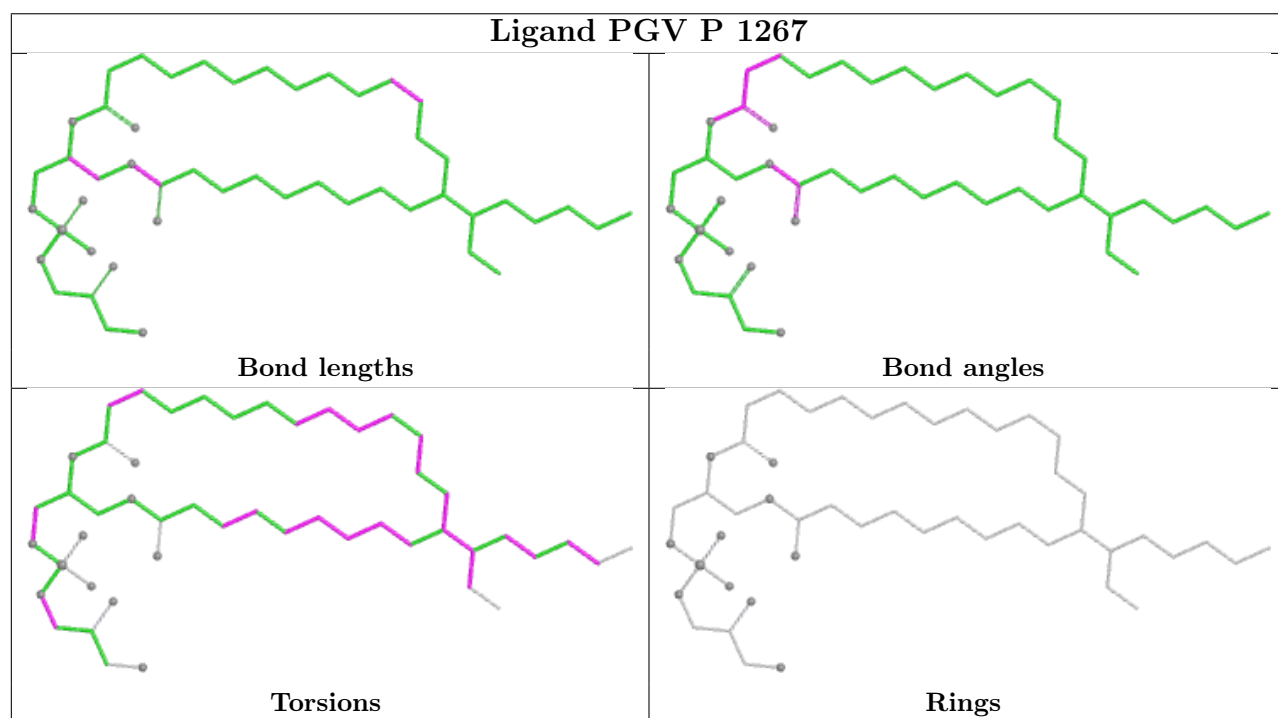
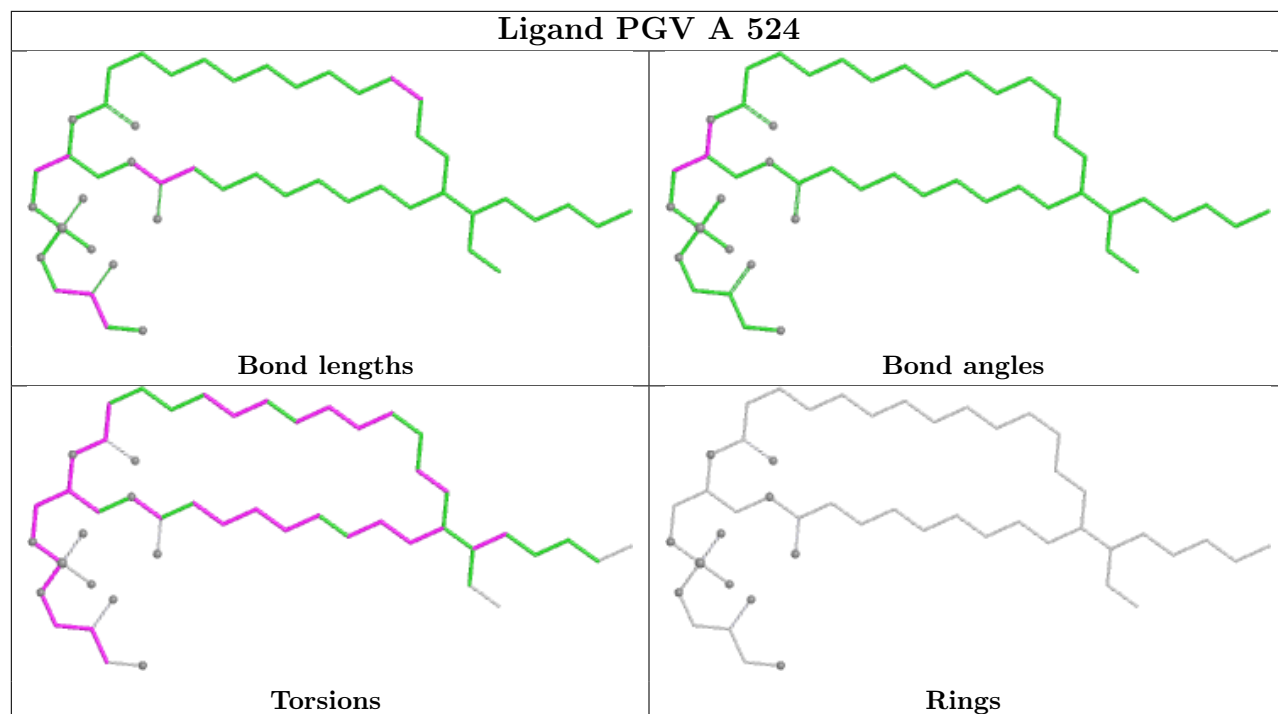
Ligand PGV N 1524

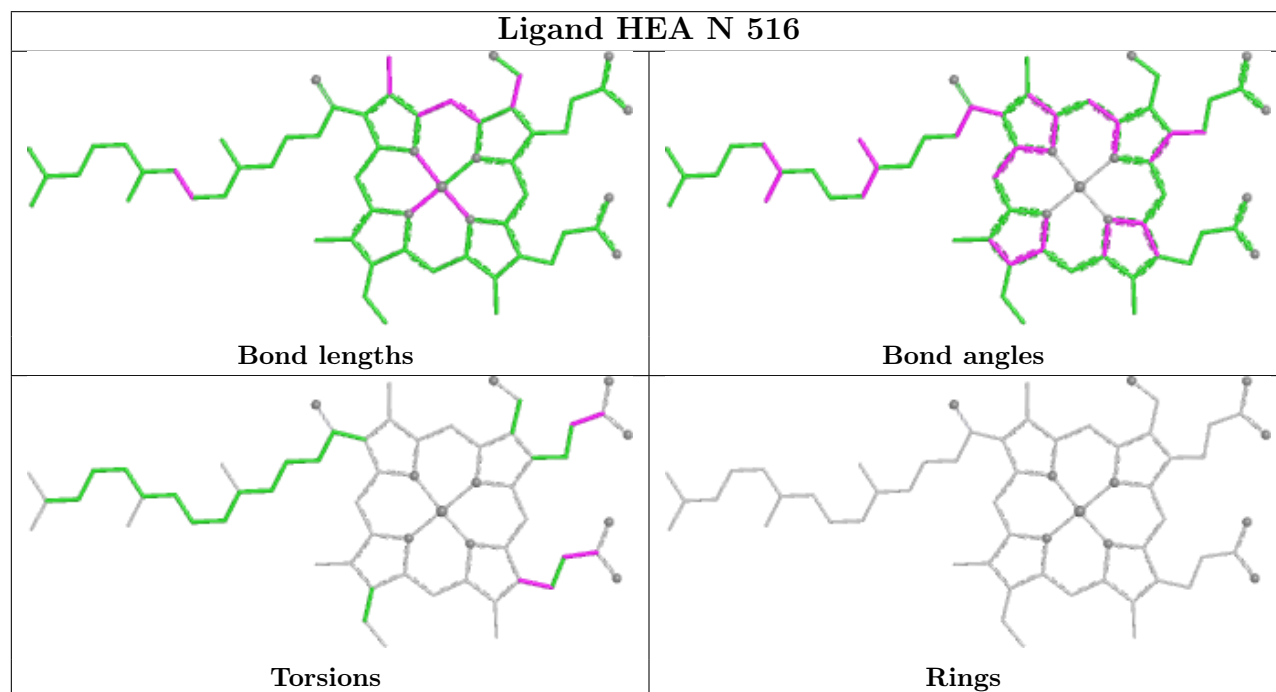
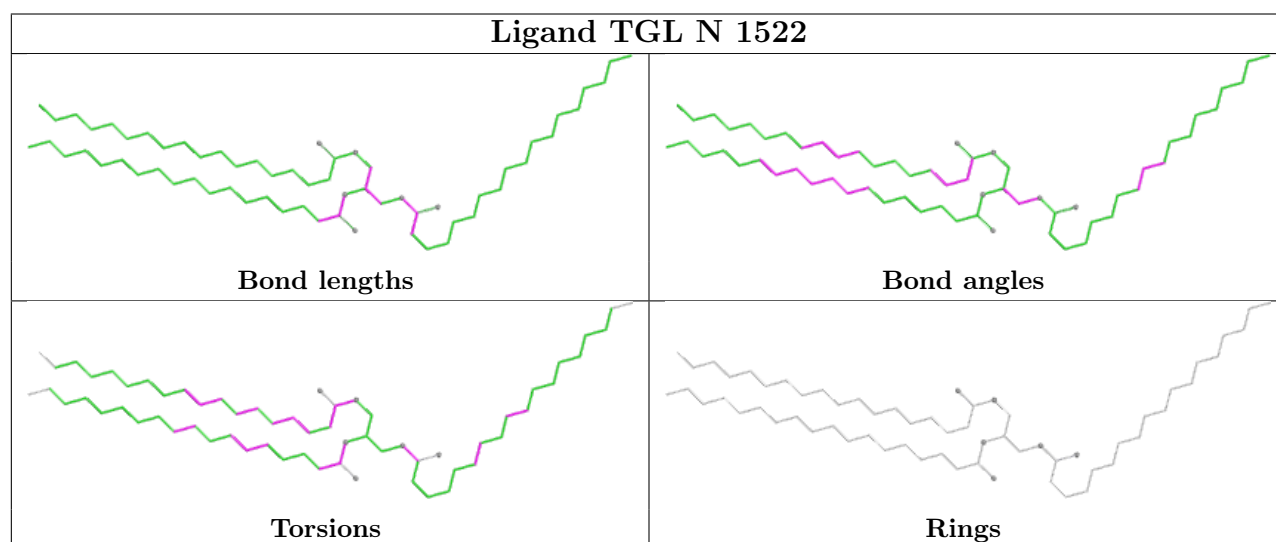
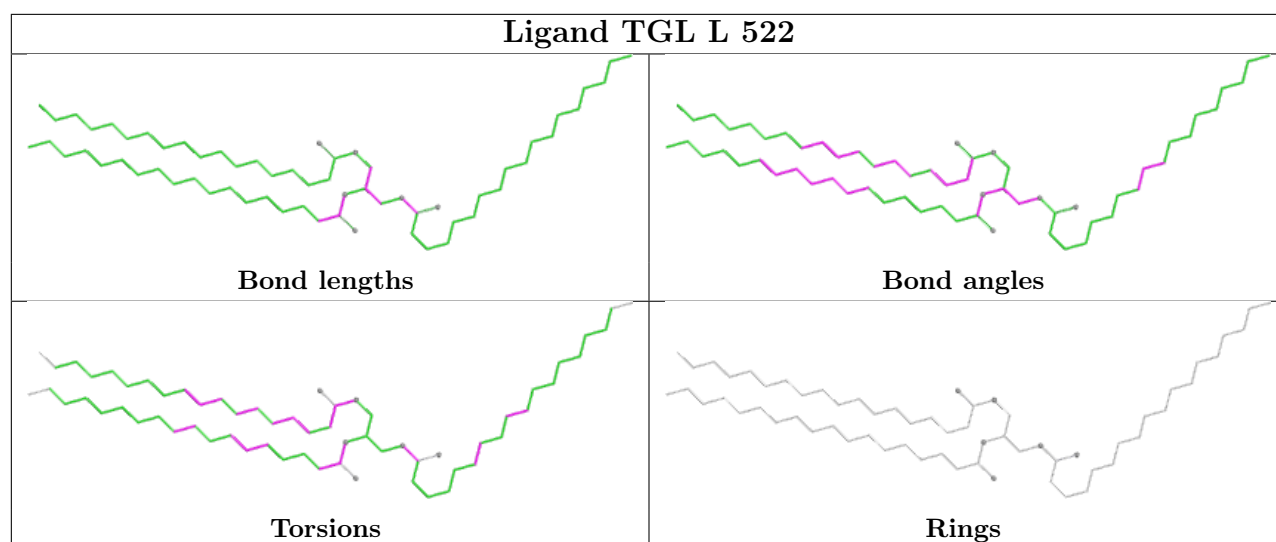


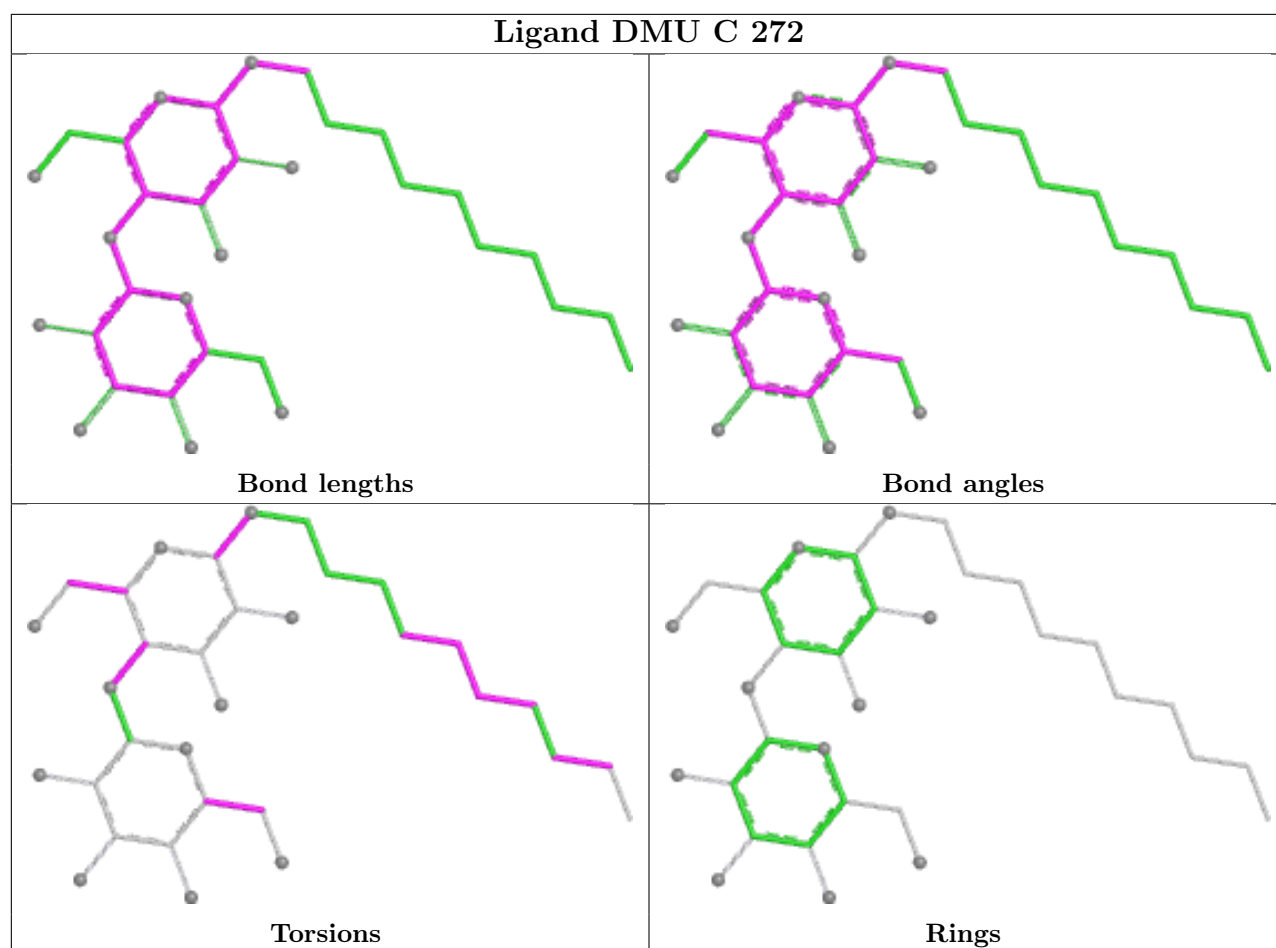
Ligand PGV C 266

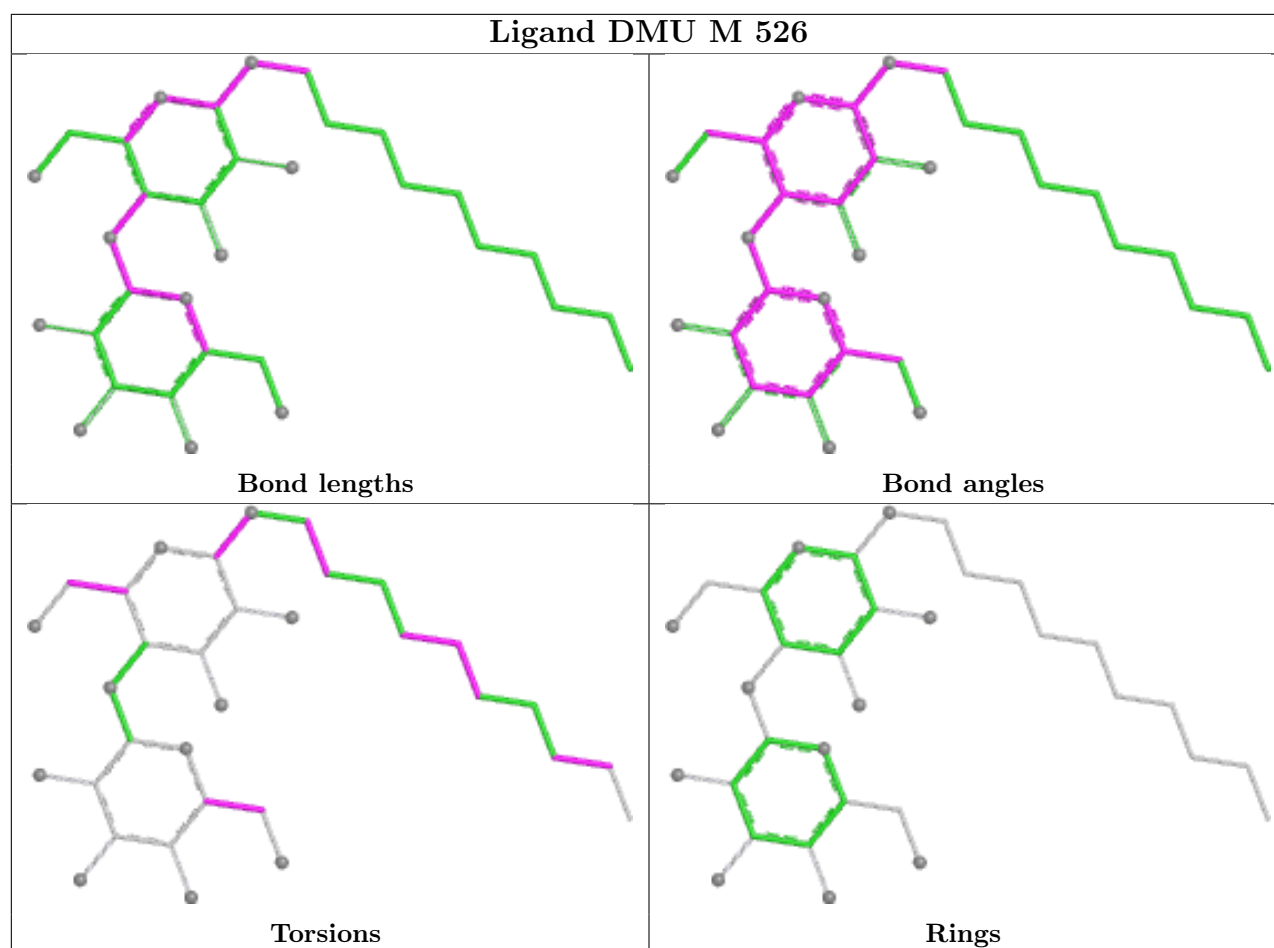


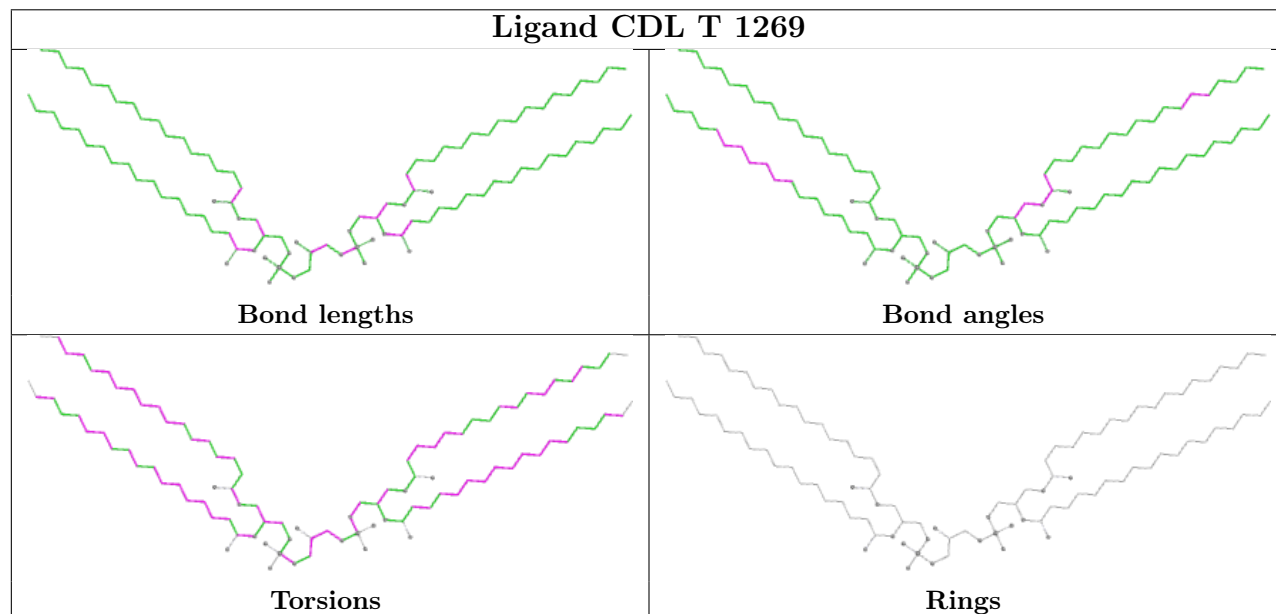
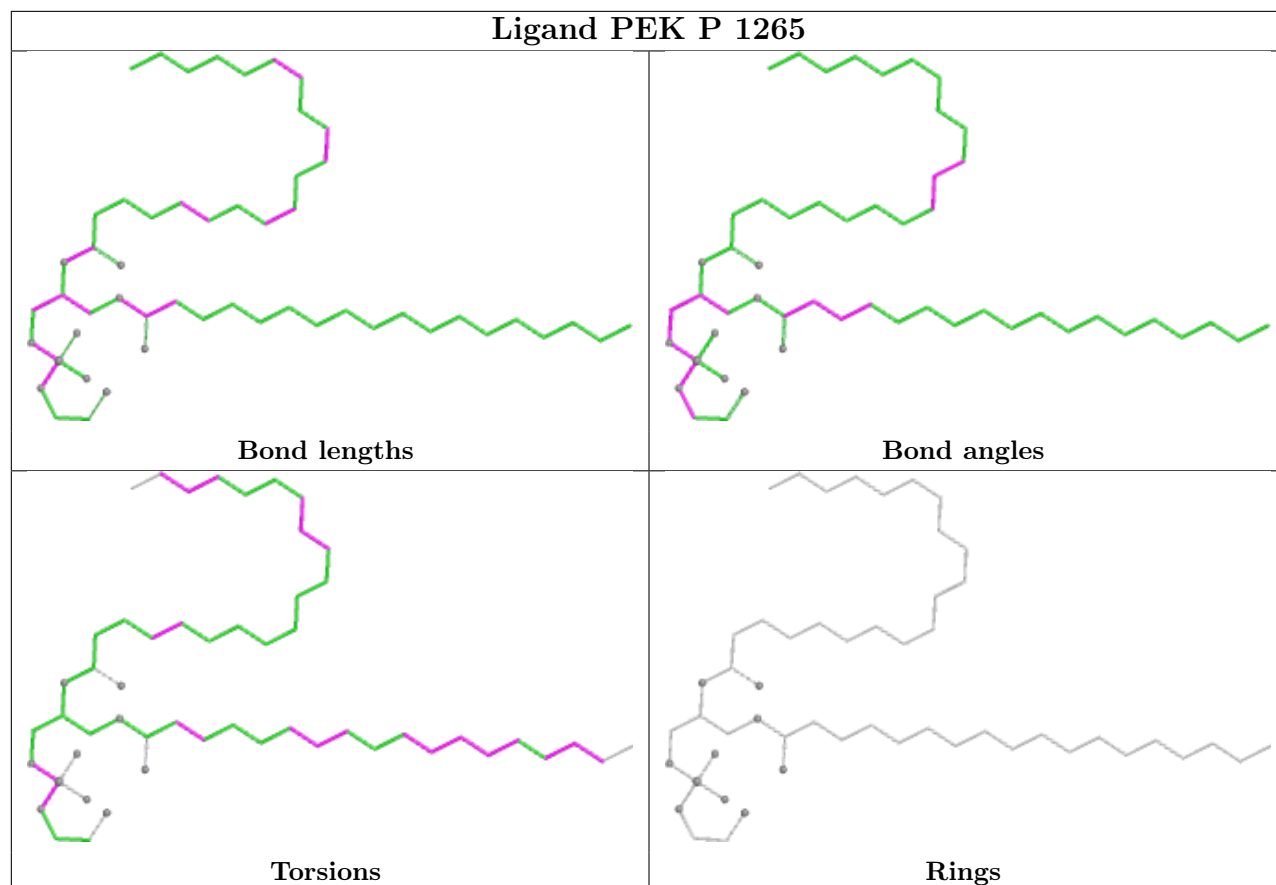


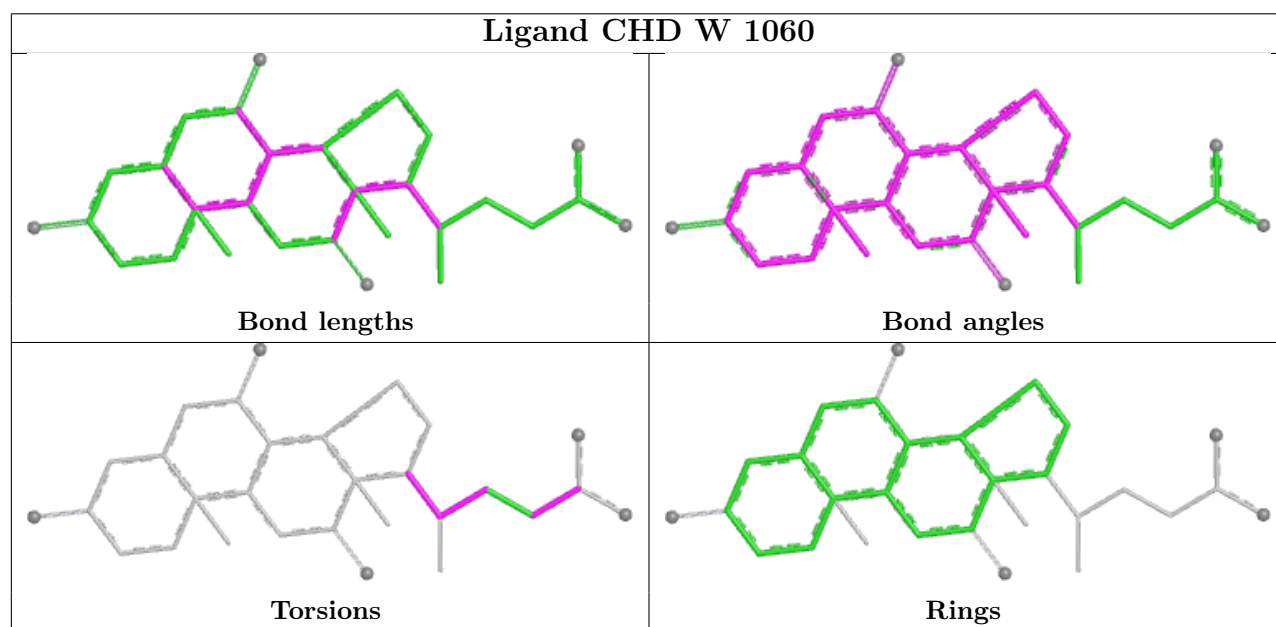
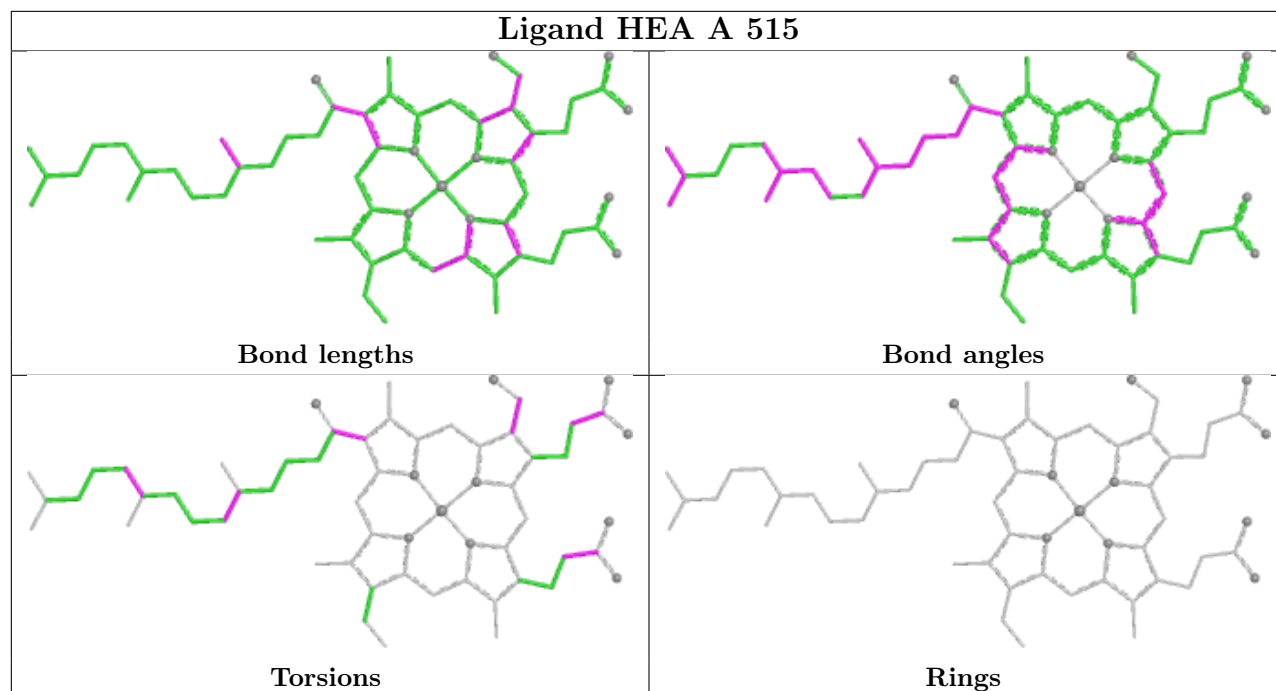


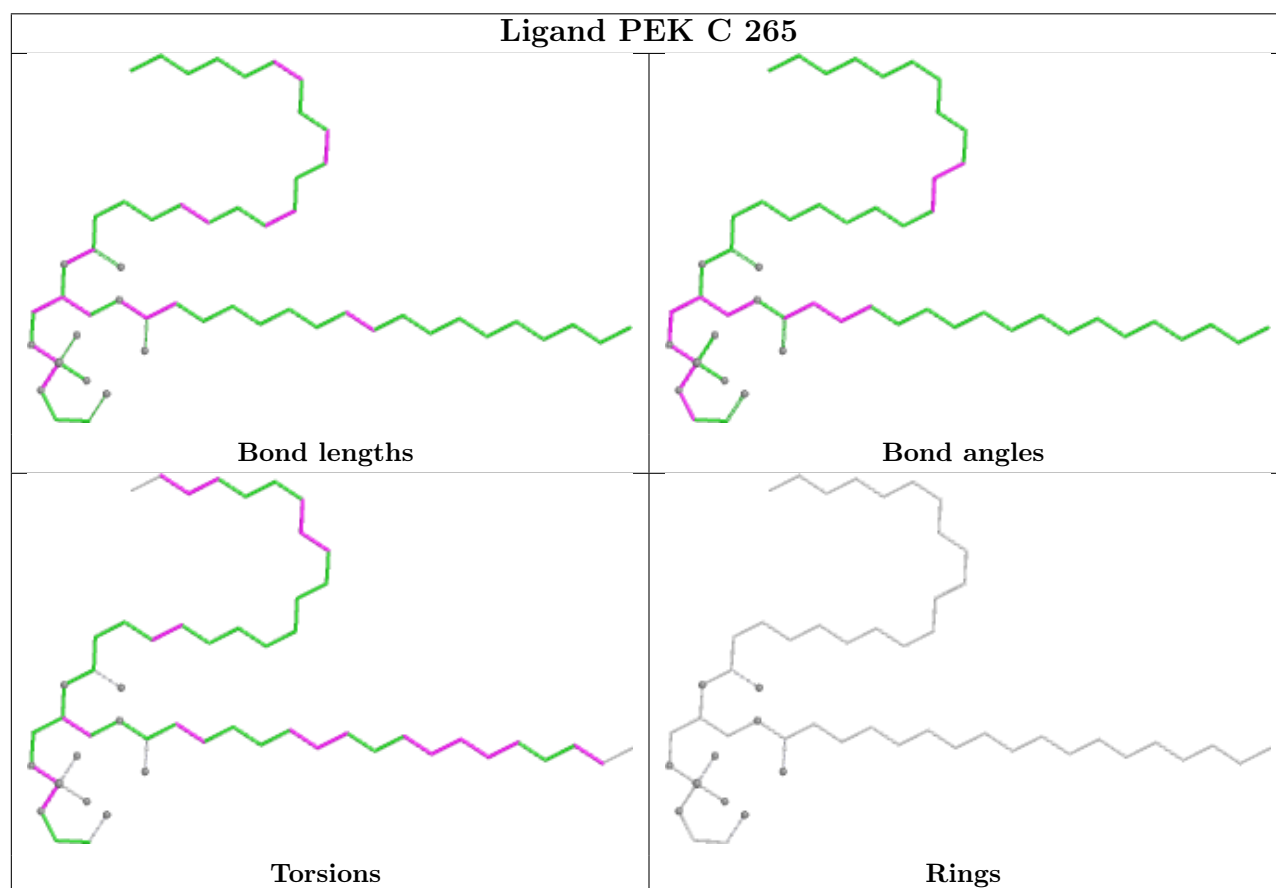
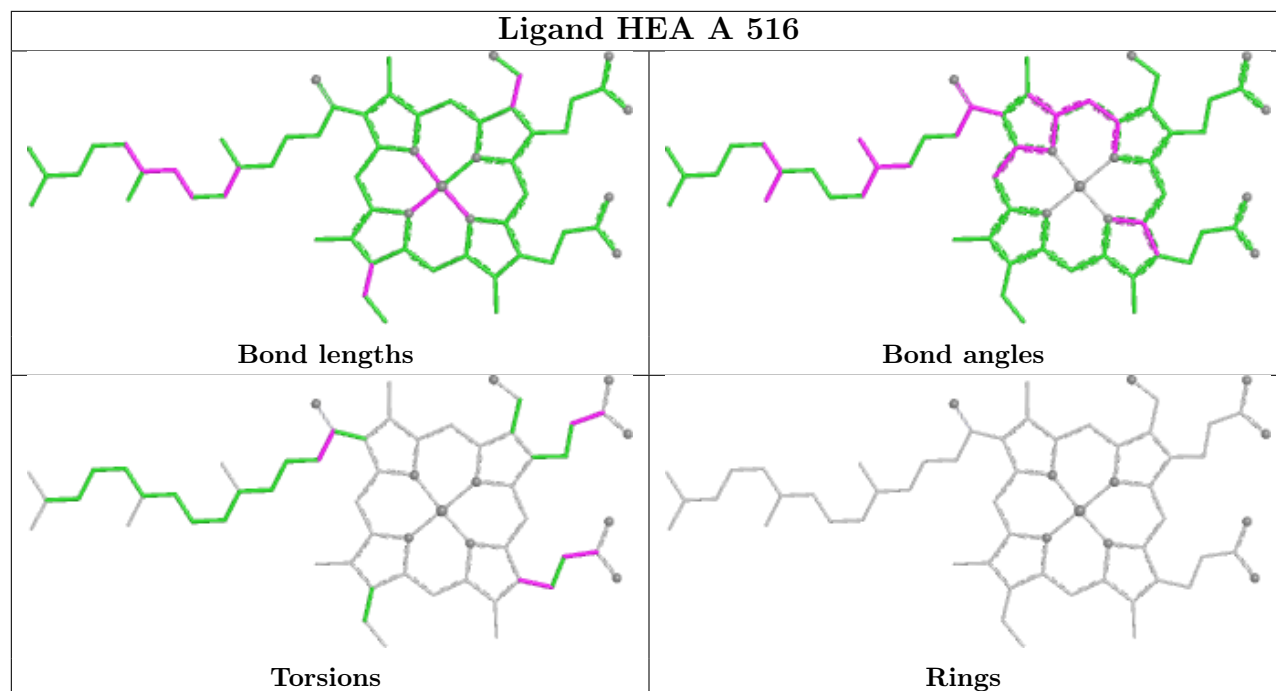


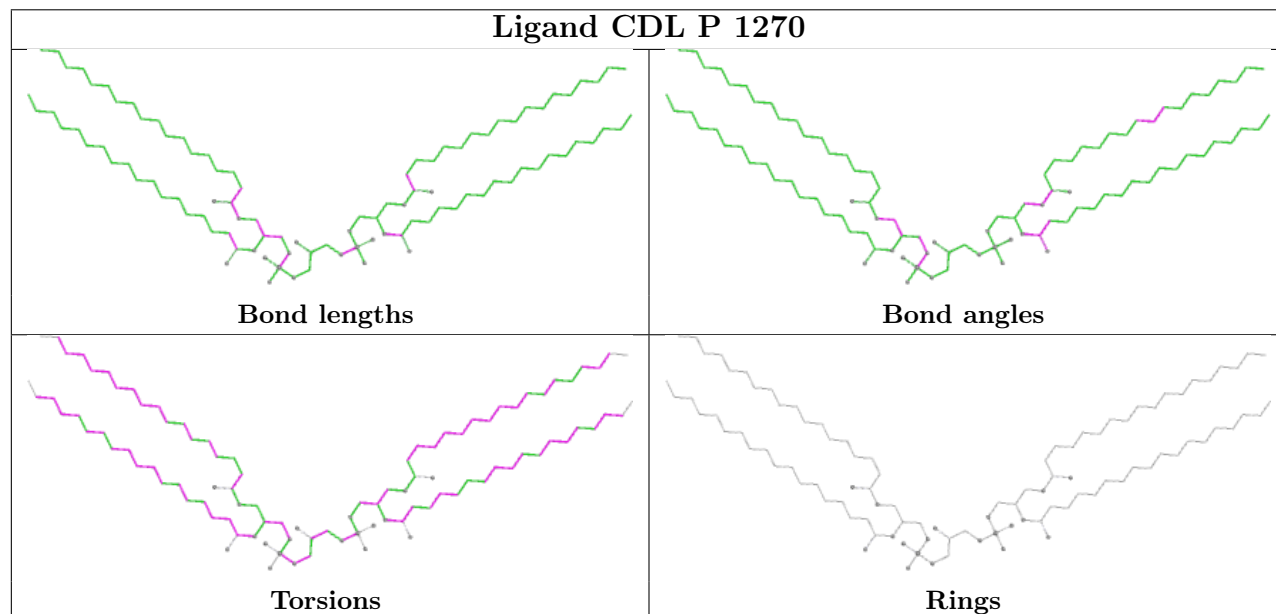
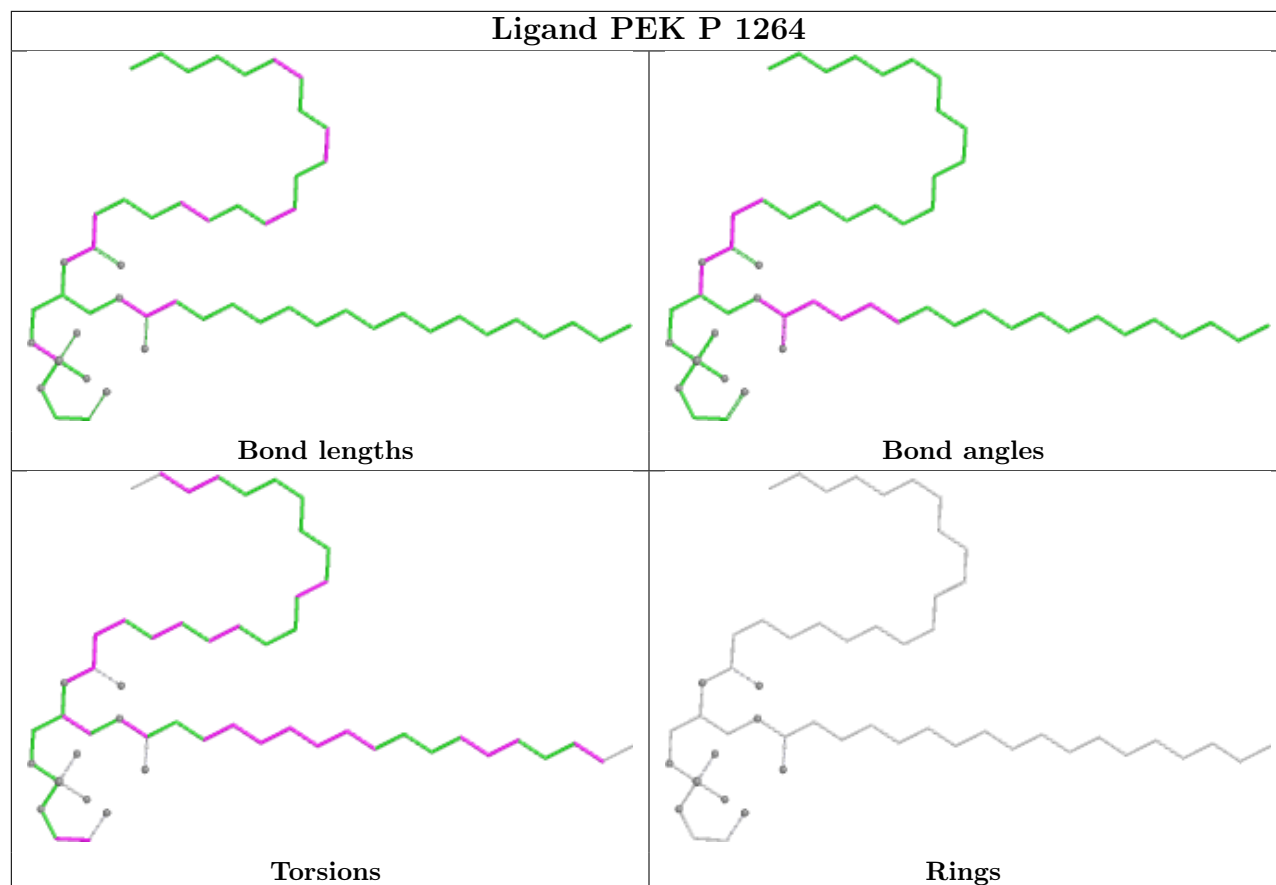




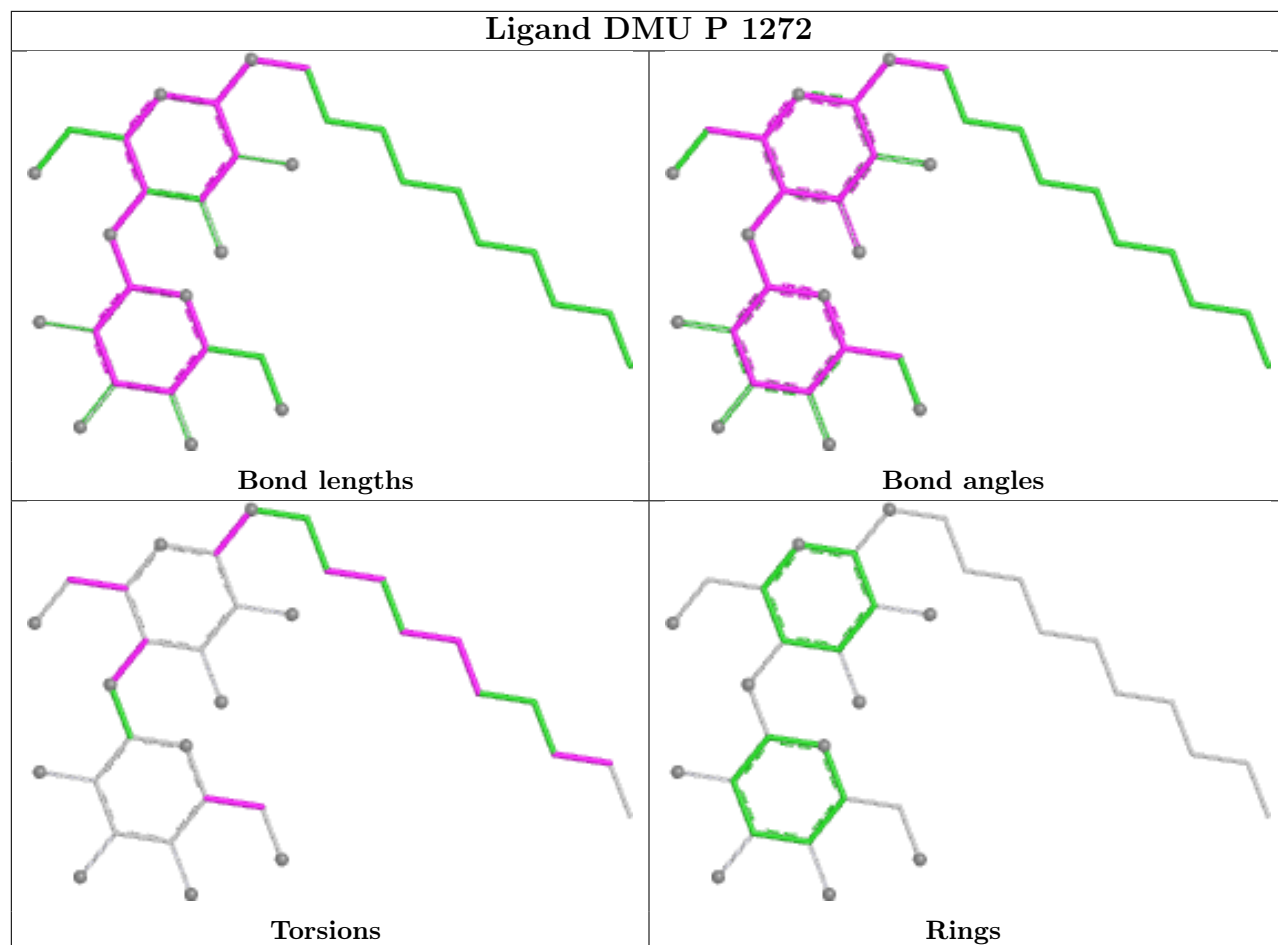




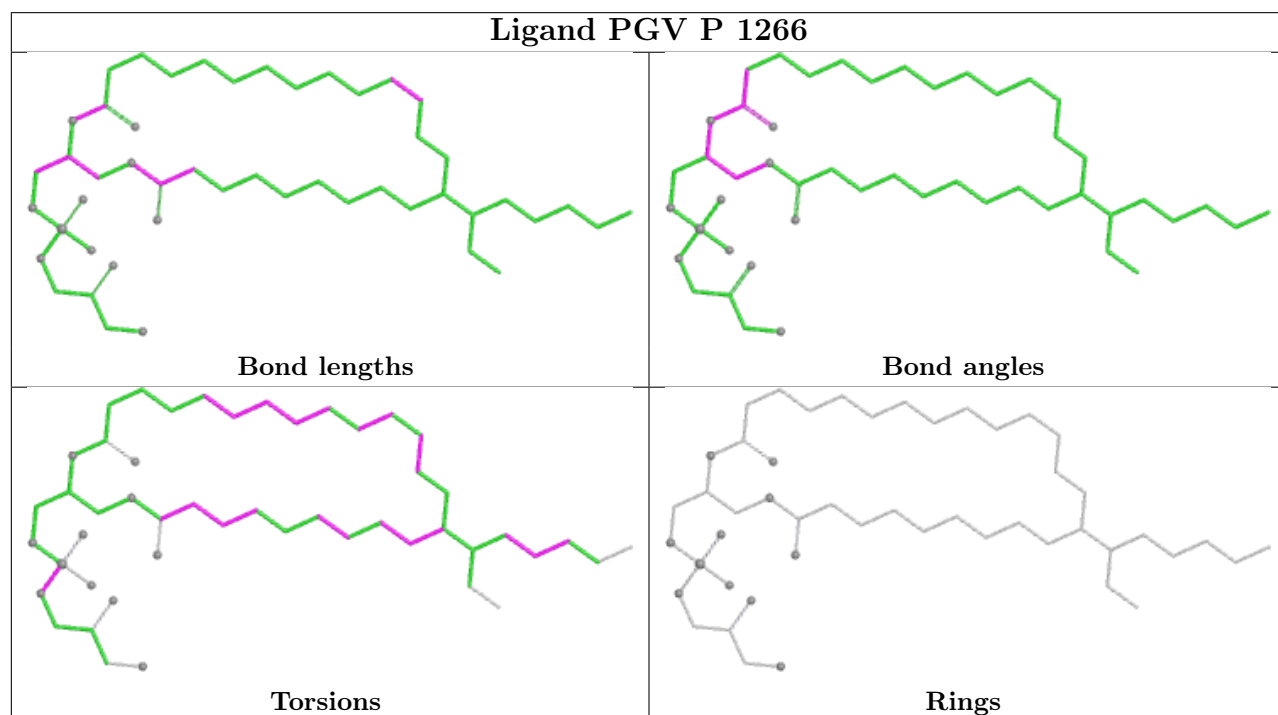


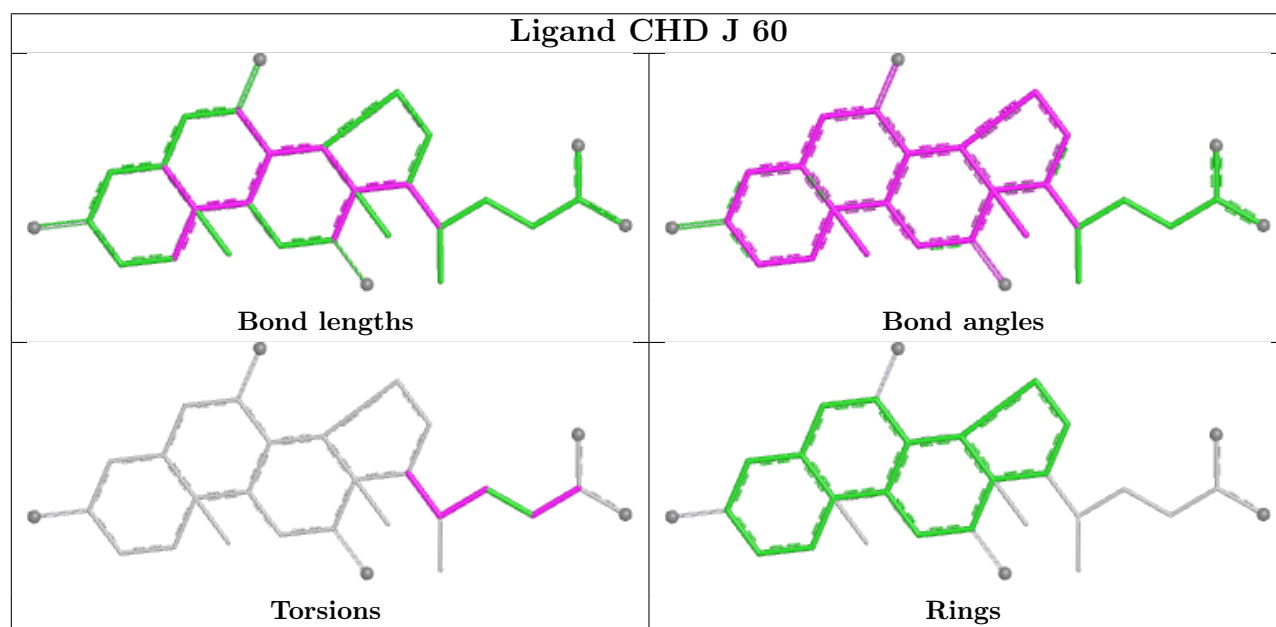
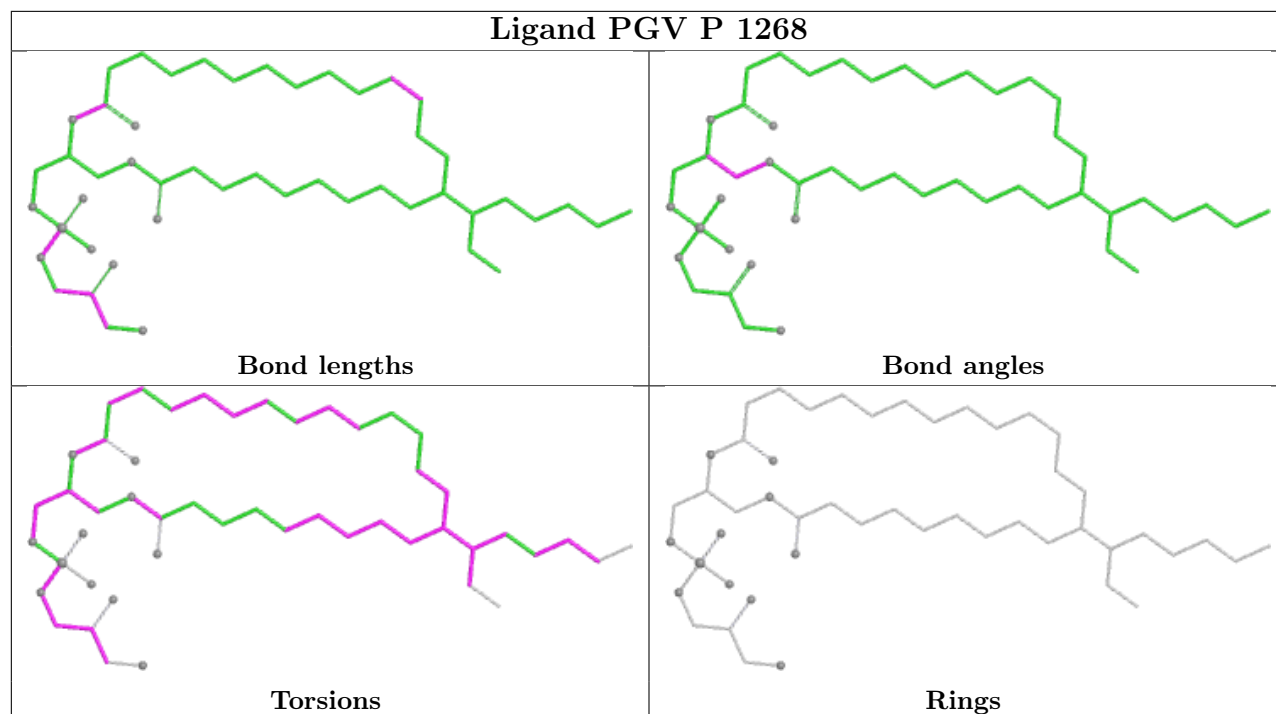


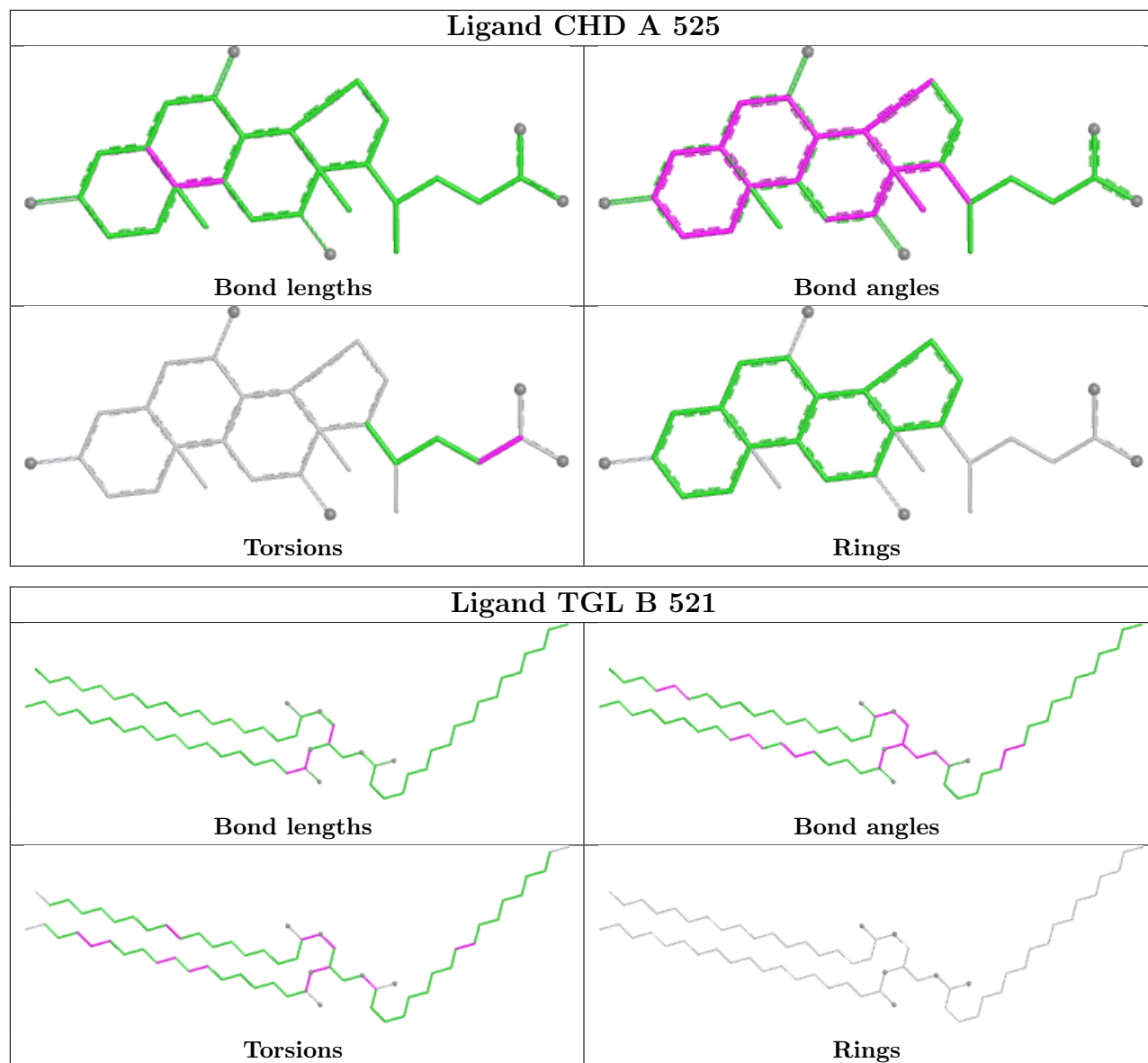
Ligand DMU P 1272



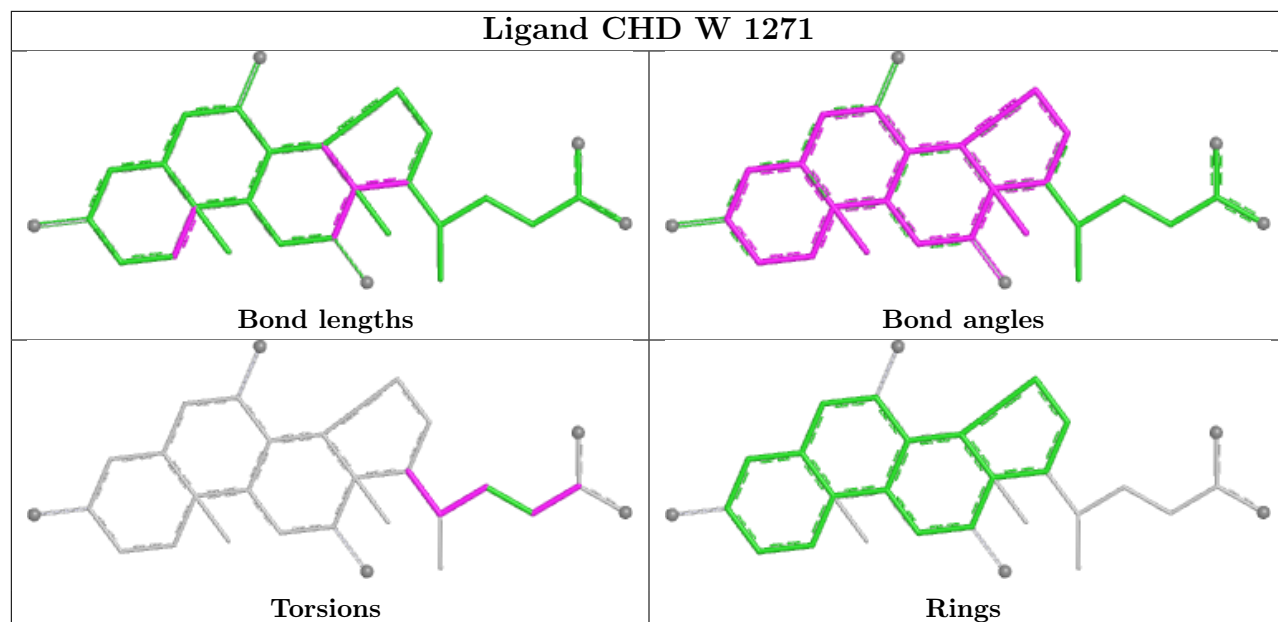
Ligand PGV P 1266



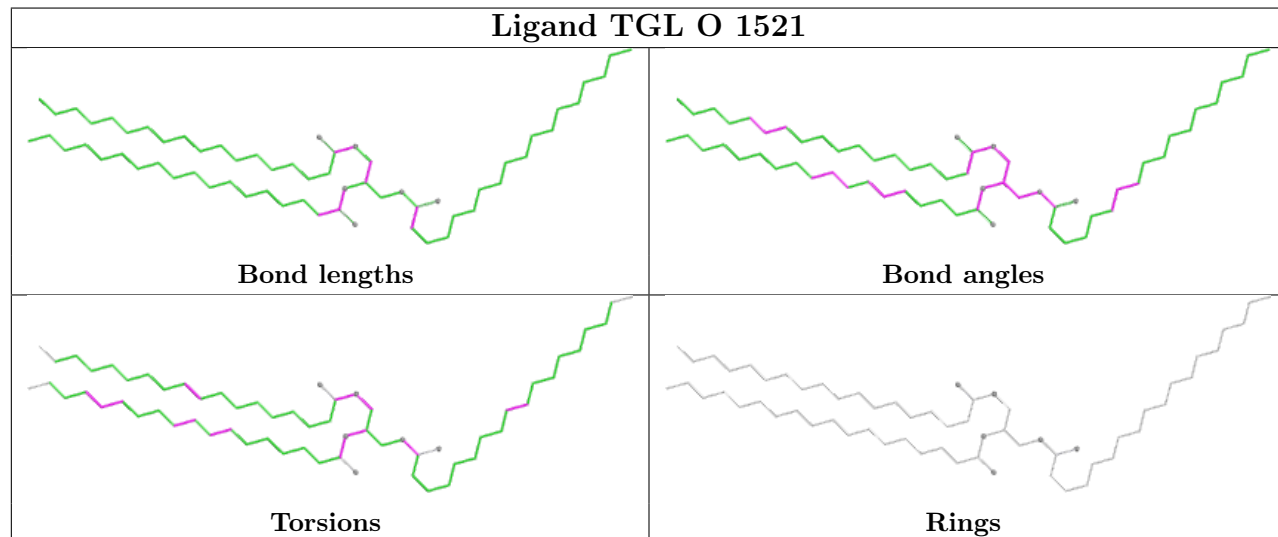


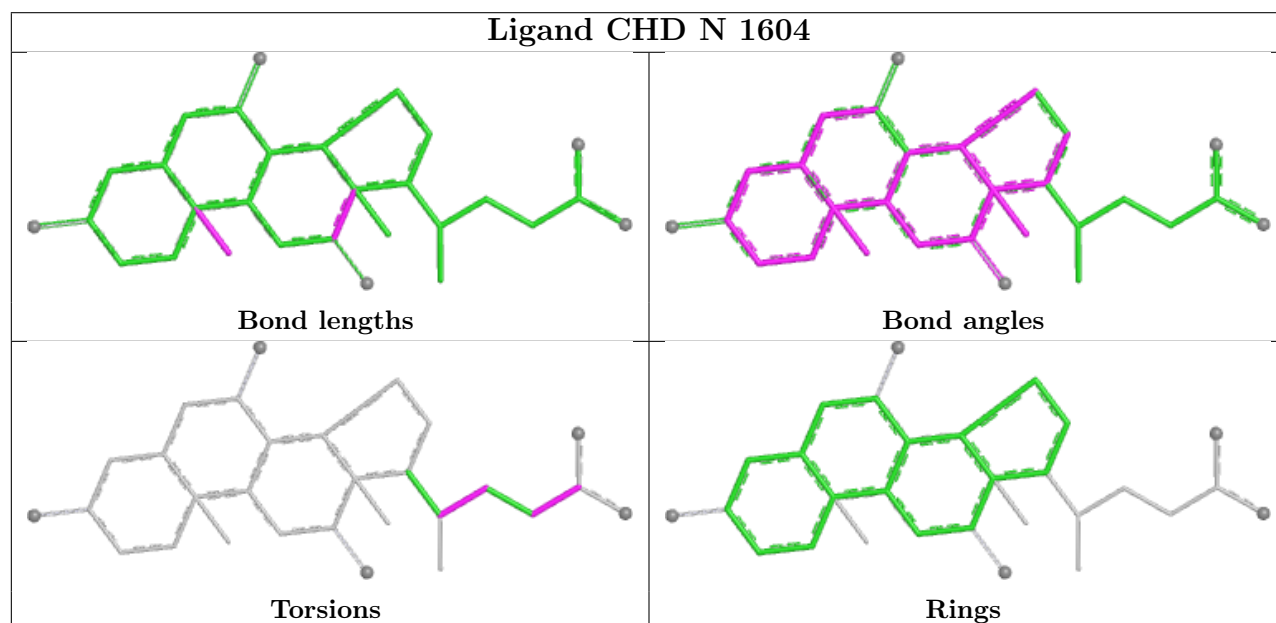
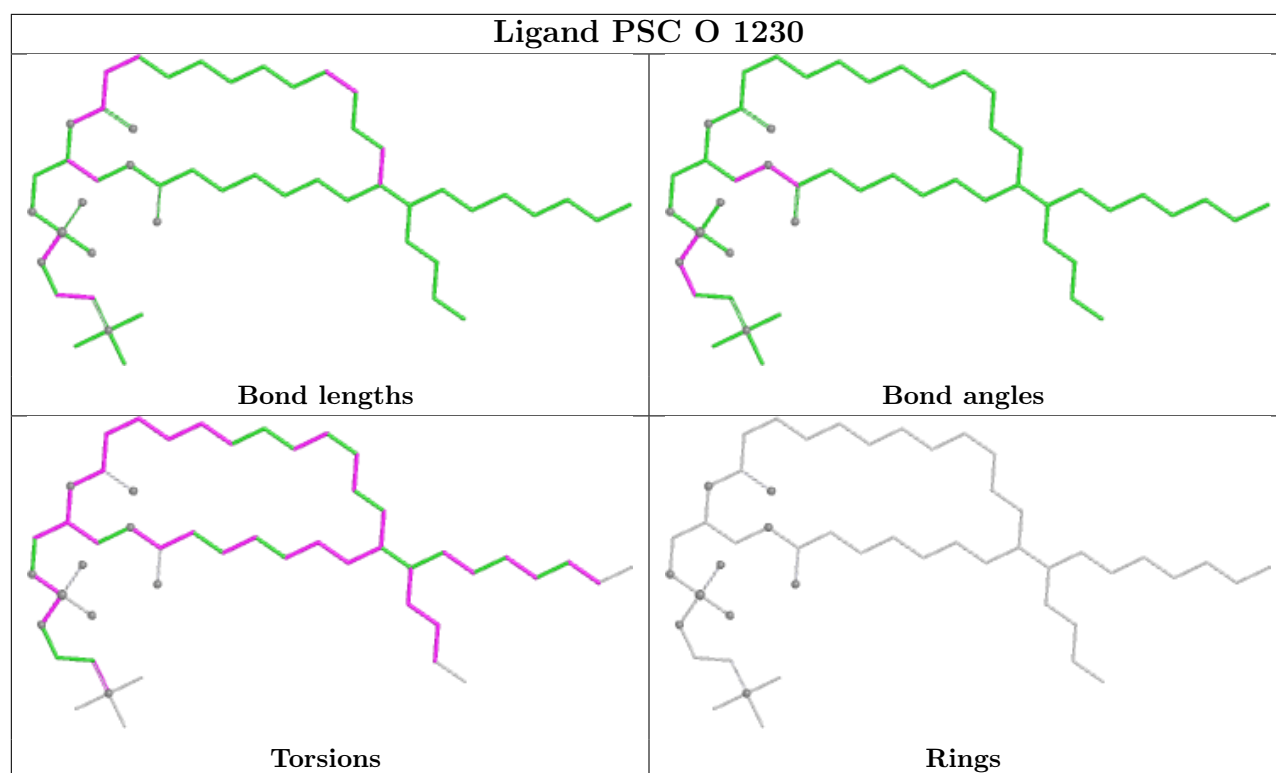


Ligand CHD W 1271

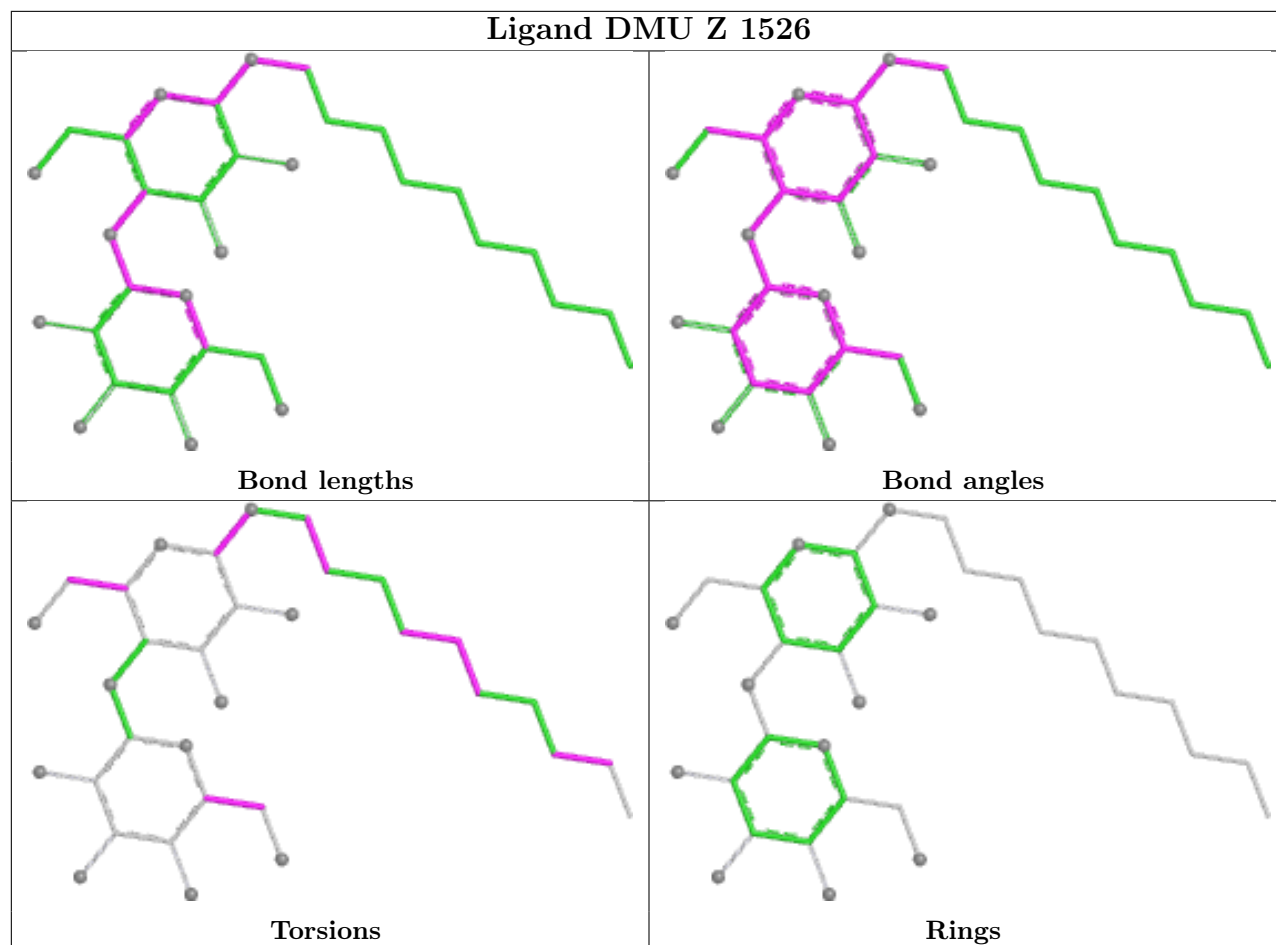


Ligand TGL O 1521

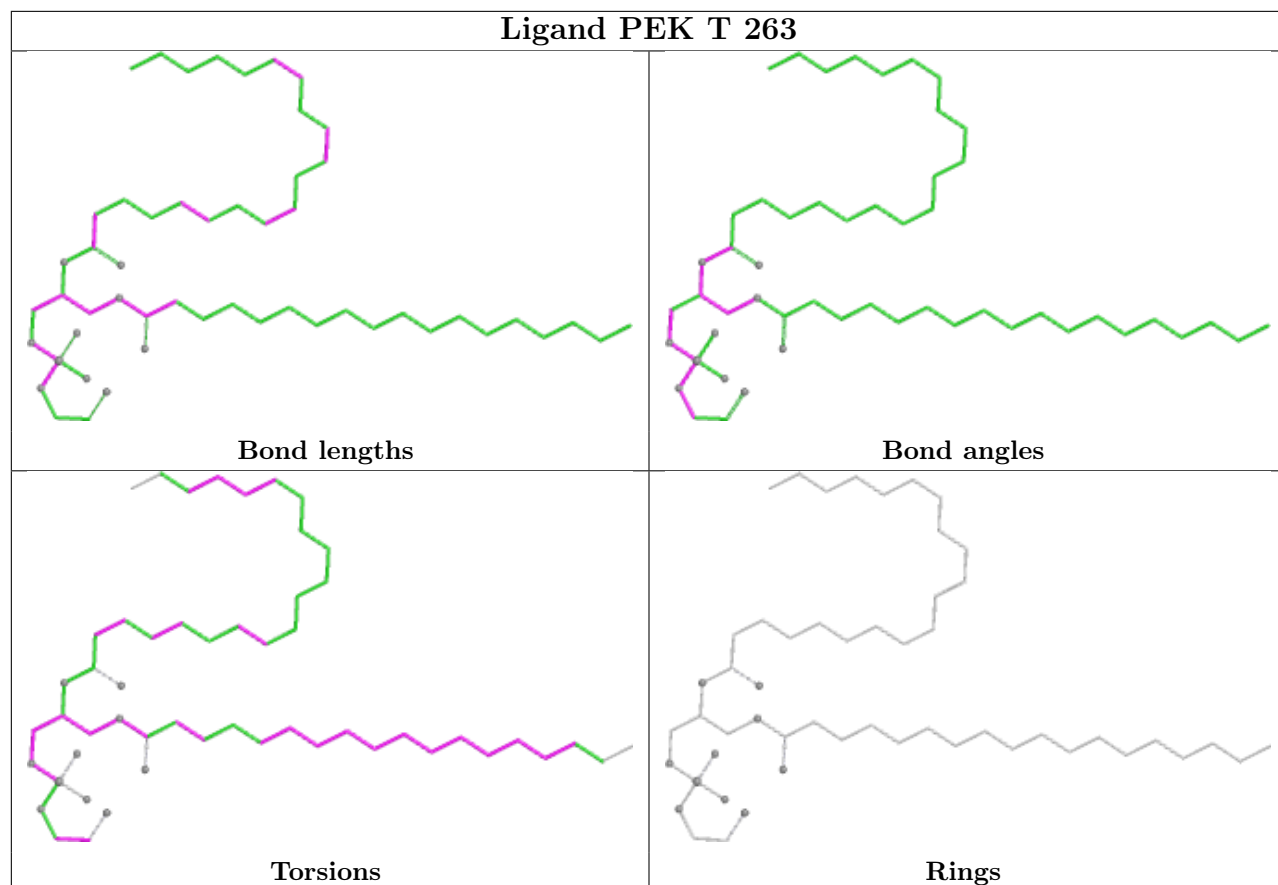




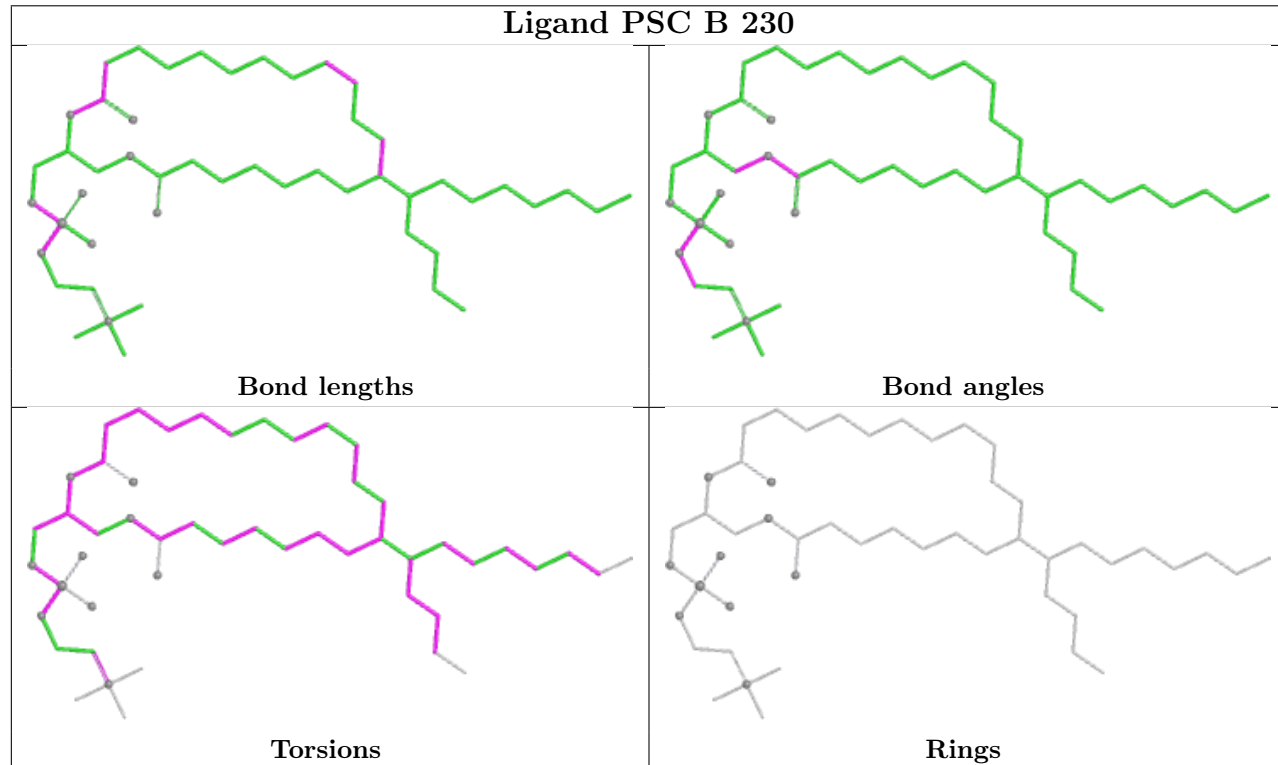
Ligand DMU Z 1526

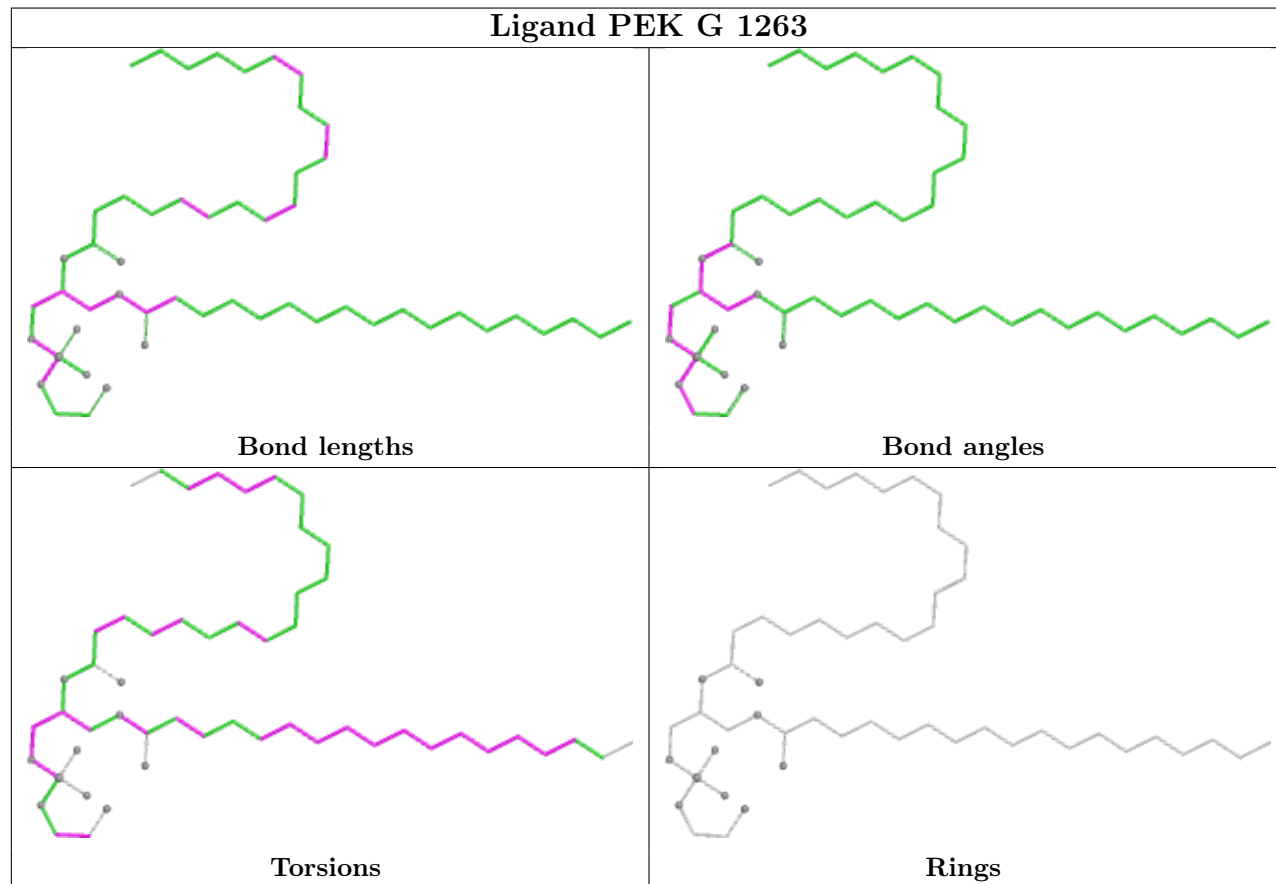
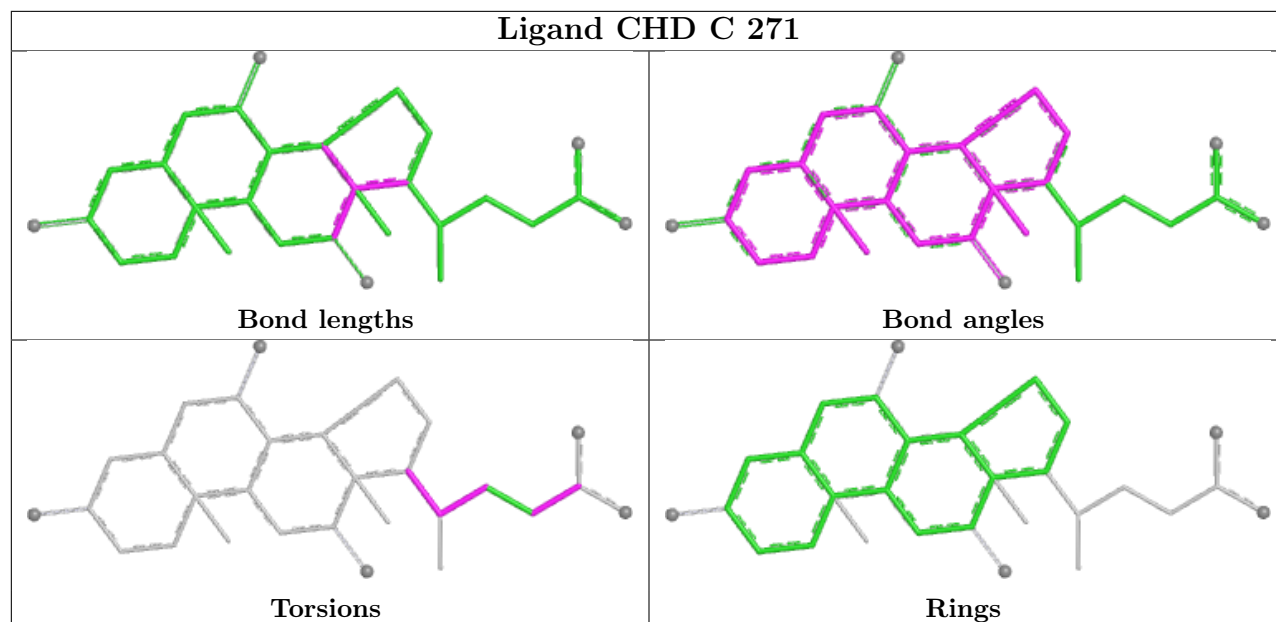


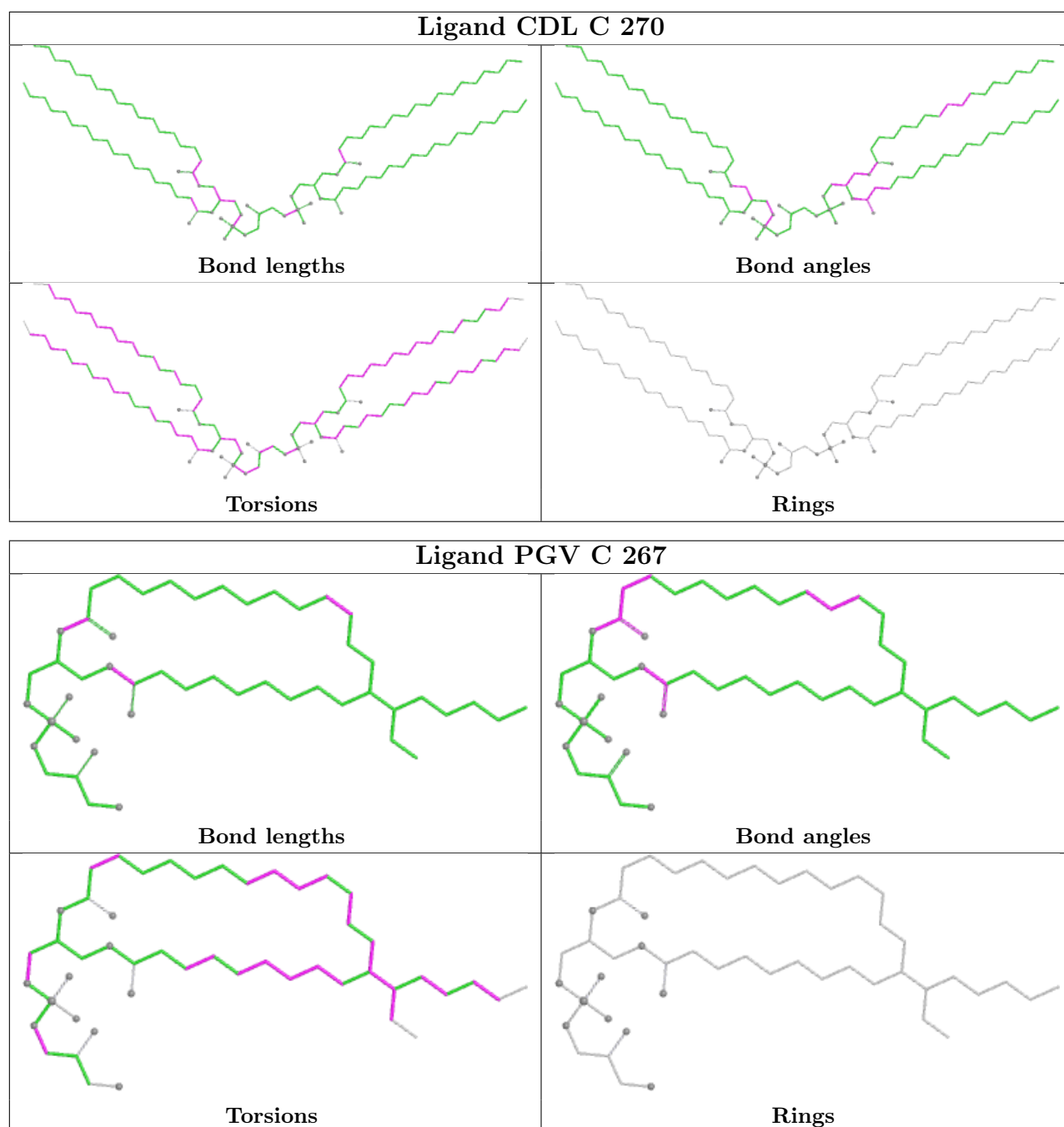
Ligand PEK T 263



Ligand PSC B 230







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.