



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:56 PM UTC

PDB ID : 2EIK / pdb_00002eik
Title : Cadmium 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 : 2.10 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)	:	2.49

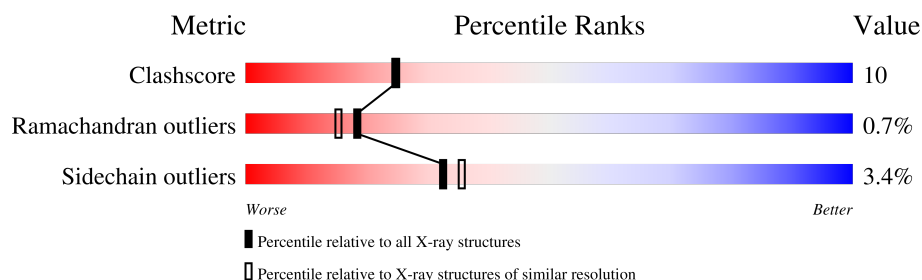
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	81% 18% .
1	N	514	77% 21% .
2	B	227	78% 19% ..
2	O	227	71% 26% .
3	C	261	82% 17% .
3	P	261	81% 17% ..
4	D	147	83% 15% .
4	Q	147	71% 26% ..

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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
19	TGL	L	522	-	-	X	-
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	-
23	CHD	P	1271	X	-	-	-
23	CHD	W	1060	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	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 32450 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		

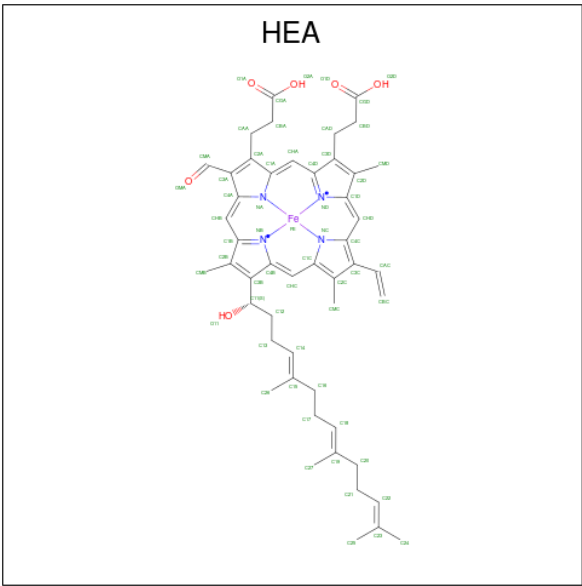
- Molecule 16 is SODIUM ION (CCD ID: NA) (formula: Na).

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 CADMIUM ION (CCD ID: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	1	Total	Cd	0	0
			1	1		
17	C	1	Total	Cd	0	0
			1	1		
17	E	1	Total	Cd	0	0
			1	1		
17	N	1	Total	Cd	0	0
			1	1		
17	P	2	Total	Cd	0	0
			2	2		

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



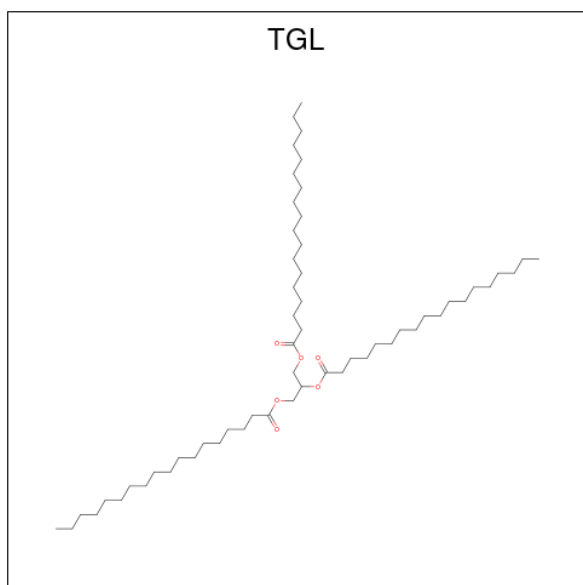
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
18	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

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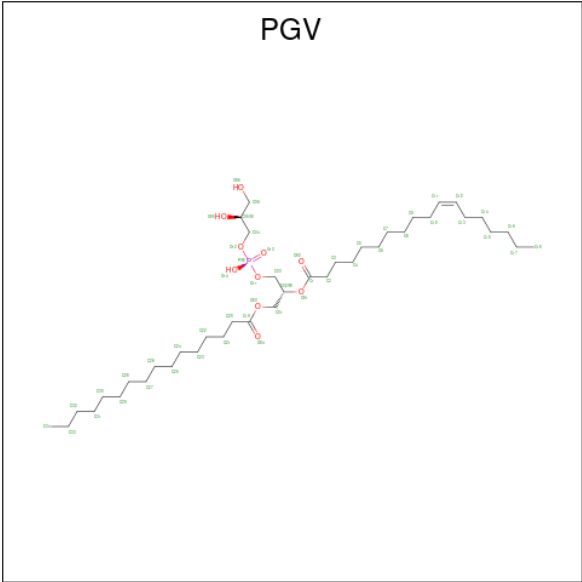
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	N	1	Total	C	Fe	N	O	
			60	49	1	4	6	
18	N	1	Total	C	Fe	N	O	
			60	49	1	4	6	

- Molecule 19 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: $C_{57}H_{110}O_6$).



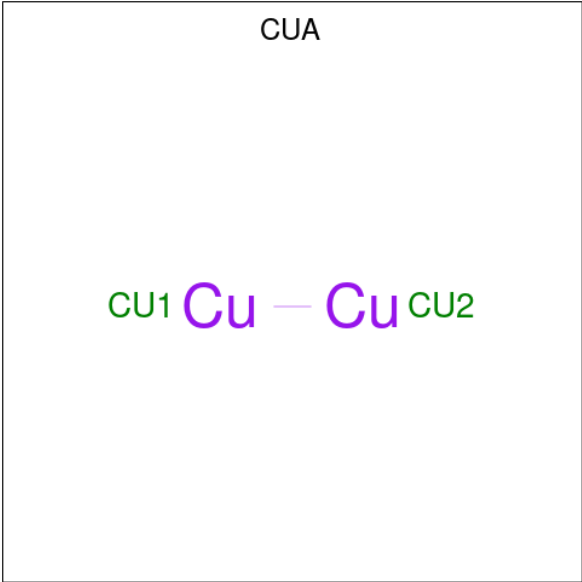
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O		
			63	57	6		
19	A	1	Total	C	O		
			63	57	6		
19	L	1	Total	C	O		
			63	57	6		
19	N	1	Total	C	O		
			63	57	6		
19	Q	1	Total	C	O		
			63	57	6		
19	Y	1	Total	C	O		
			63	57	6		

- Molecule 20 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (CCD ID: PGV) (formula: $C_{40}H_{77}O_{10}P$).



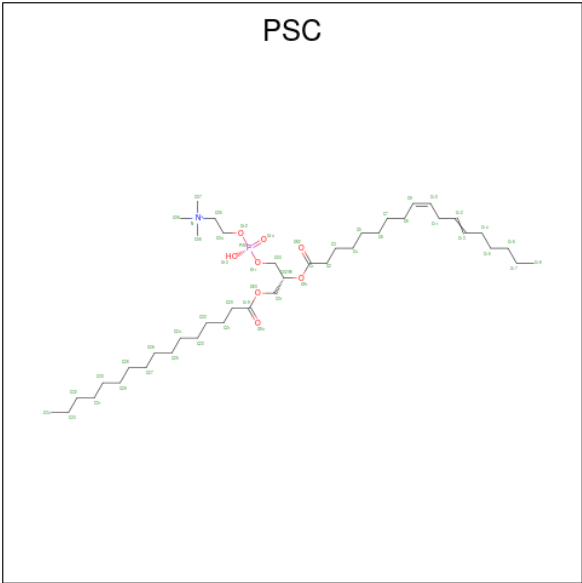
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0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

- Molecule 21 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



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 (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



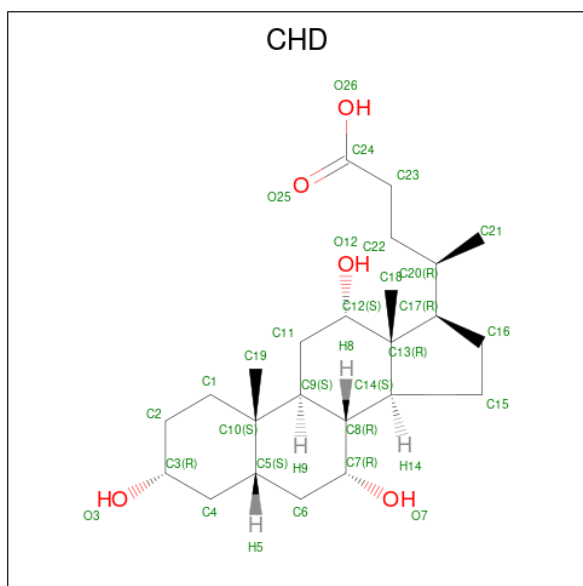
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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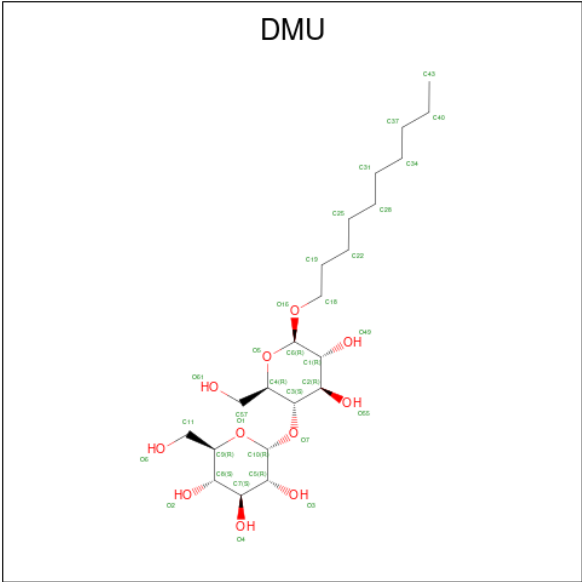
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 23 is CHOLIC ACID (CCD ID: CHD) (formula: $C_{24}H_{40}O_5$).



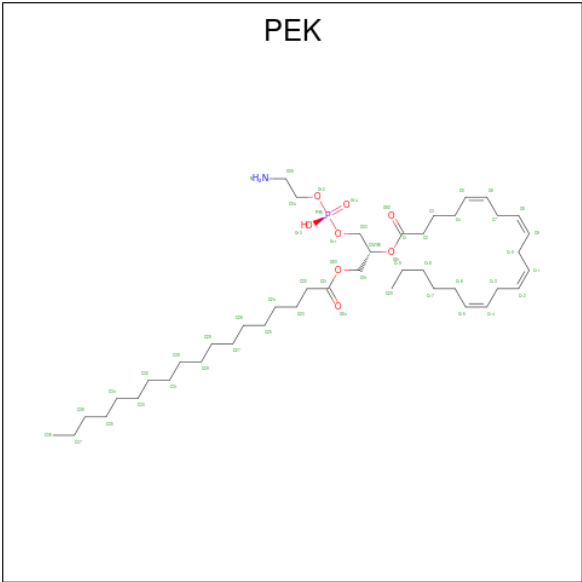
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		
23	J	1	Total	C	O	0	0
			29	24	5		
23	O	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	W	1	Total	C	O	0	0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

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



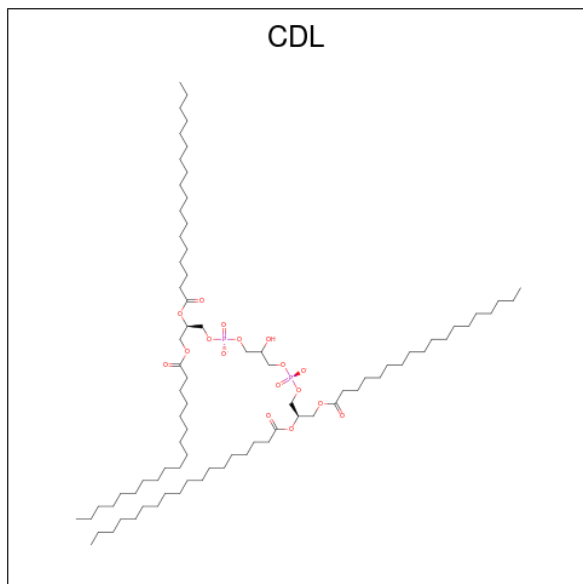
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			33	22	11		
24	M	1	Total	C	O	0	0
			33	22	11		
24	P	1	Total	C	O	0	0
			33	22	11		
24	Z	1	Total	C	O	0	0
			33	22	11		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	F	1	Total 1	Zn 1	0	0
27	S	1	Total 1	Zn 1	0	0

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	223	Total 223	O 223	0	0
28	B	146	Total 146	O 146	0	0
28	C	102	Total 102	O 102	0	0
28	D	98	Total 98	O 98	0	0
28	E	60	Total 60	O 60	0	0
28	F	85	Total 85	O 85	0	0
28	G	41	Total 41	O 41	0	0
28	H	49	Total 49	O 49	0	0
28	I	44	Total 44	O 44	0	0
28	J	26	Total 26	O 26	0	0
28	K	25	Total 25	O 25	0	0
28	L	23	Total 23	O 23	0	0
28	M	22	Total 22	O 22	0	0
28	N	213	Total 213	O 213	0	0
28	O	116	Total 116	O 116	0	0
28	P	103	Total 103	O 103	0	0
28	Q	52	Total 52	O 52	0	0
28	R	41	Total 41	O 41	0	0

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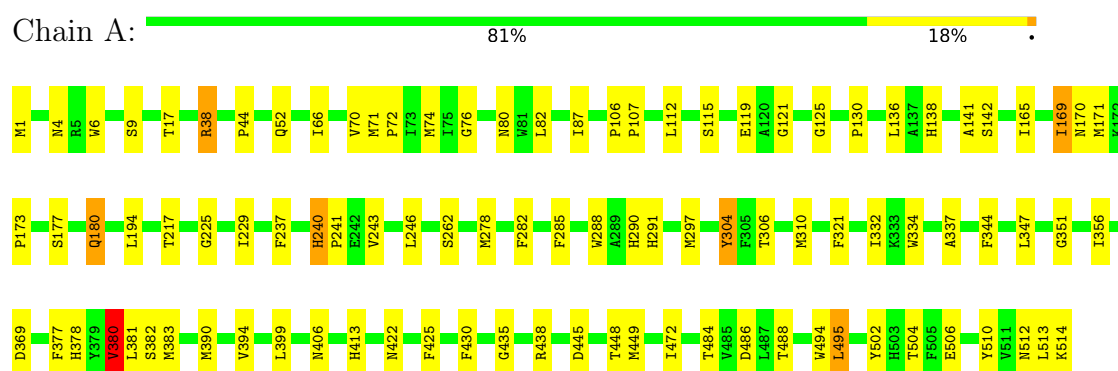
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	S	69	Total 69	O 69	0	0
28	T	47	Total 47	O 47	0	0
28	U	43	Total 43	O 43	0	0
28	V	25	Total 25	O 25	0	0
28	W	15	Total 15	O 15	0	0
28	X	17	Total 17	O 17	0	0
28	Y	15	Total 15	O 15	0	0
28	Z	14	Total 14	O 14	0	0

3 Residue-property plots

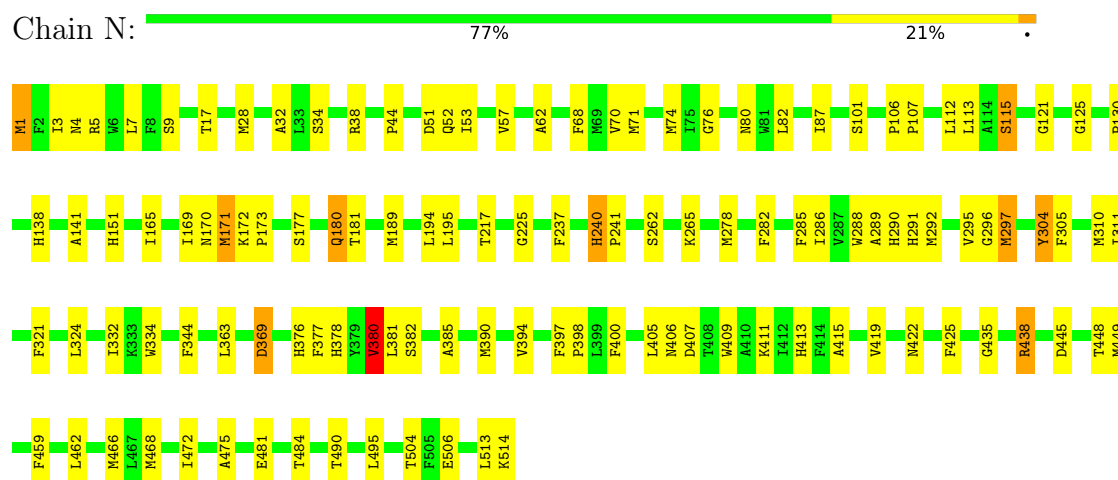
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

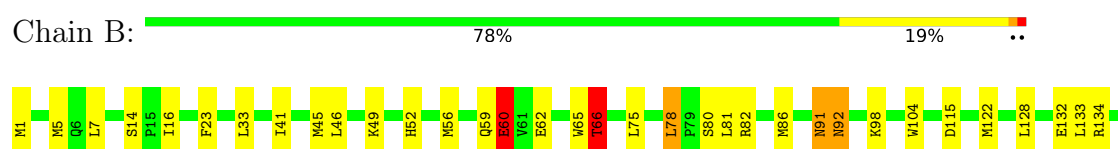
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 1: Cytochrome c oxidase subunit 1



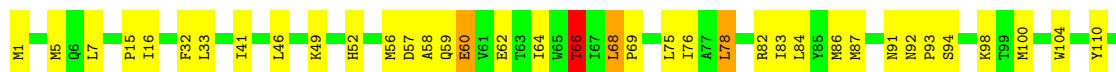
• Molecule 2: Cytochrome c oxidase subunit 2





• Molecule 2: Cytochrome c oxidase subunit 2

Chain O: 71% 26% .



• Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 82% 17% .



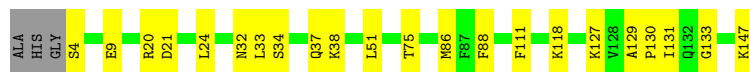
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 81% 17% ..



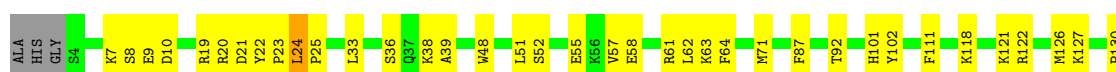
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D: 83% 15% .



• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q: 71% 26% ..



- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain E:  84% 12% .



- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain R:  64% 31% ..



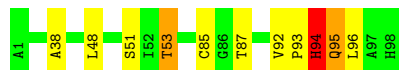
- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F:  83% 15% ..



- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S:  89% 8% ..



- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G:  74% 19% 6% .



- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T:  72% 21% 6% .



- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain H:  81% 9% .. 7%



- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain U:  75% 14% • 7%



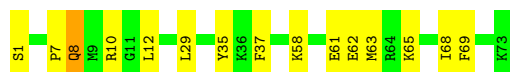
- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I:  85% 14% •



- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V:  79% 19% •



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain J:  85% 12% • •



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain W:  85% 12% • •



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K:  70% 18% 12%



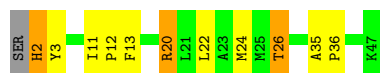
- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X:  73% 12% • 12%



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:  74% 17% 6% .



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y:  74% 21% . .



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M:  72% 20% . 7%



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain Z:  72% 22% 7%



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	183.32Å 206.53Å 178.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.199 , 0.228	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32450	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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: PGV, CUA, CDL, PEK, PSC, CU, ZN, NA, TGL, DMU, MG, CHD, FME, SAC, TPO, CD, HEA

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	0.68	1/4156 (0.0%)	1.08	28/5678 (0.5%)
1	N	0.61	0/4156	1.06	23/5678 (0.4%)
2	B	0.64	0/1860	1.04	5/2534 (0.2%)
2	O	0.63	0/1860	1.07	6/2534 (0.2%)
3	C	0.59	0/2197	0.95	6/3005 (0.2%)
3	P	0.56	0/2197	0.98	7/3005 (0.2%)
4	D	0.58	0/1229	1.00	5/1658 (0.3%)
4	Q	0.63	0/1229	1.03	4/1658 (0.2%)
5	E	0.64	0/871	1.04	2/1182 (0.2%)
5	R	0.64	0/871	1.11	5/1182 (0.4%)
6	F	0.62	0/765	1.15	3/1038 (0.3%)
6	S	0.64	0/765	1.13	4/1038 (0.4%)
7	G	0.60	0/690	1.02	1/937 (0.1%)
7	T	0.62	0/690	1.02	2/937 (0.2%)
8	H	0.60	0/682	1.04	4/921 (0.4%)
8	U	0.57	0/682	1.03	3/921 (0.3%)
9	I	0.55	0/605	0.92	2/802 (0.2%)
9	V	0.54	0/605	0.91	1/802 (0.1%)
10	J	0.57	0/471	0.93	1/636 (0.2%)
10	W	0.54	0/471	0.97	1/636 (0.2%)
11	K	0.66	0/398	1.15	3/546 (0.5%)
11	X	0.58	0/398	1.11	3/546 (0.5%)
12	L	0.66	0/393	0.96	1/526 (0.2%)
12	Y	0.61	0/393	1.00	1/526 (0.2%)
13	M	0.58	0/345	0.98	1/470 (0.2%)
13	Z	0.53	0/345	0.98	1/470 (0.2%)
All	All	0.61	1/29324 (0.0%)	1.04	123/39866 (0.3%)

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	2
1	N	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	PRO	CA-C	6.05	1.57	1.52

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	133	GLY	N-CA-C	11.68	127.72	112.77
4	Q	133	GLY	N-CA-C	10.96	126.80	112.77
6	F	93	PRO	N-CA-C	10.49	126.33	111.33
6	S	93	PRO	N-CA-C	9.05	125.36	111.34
5	R	42	VAL	N-CA-C	-8.85	97.61	108.05
5	E	81	ILE	N-CA-C	8.47	119.04	110.23
6	S	94	HIS	N-CA-C	8.42	128.74	110.80
1	A	125	GLY	N-CA-C	-8.18	102.58	112.48
1	N	125	GLY	N-CA-C	-8.16	102.60	112.48
5	E	42	VAL	N-CA-C	-7.85	98.79	108.05
2	O	206	PHE	N-CA-C	7.80	119.80	110.44
6	F	94	HIS	N-CA-C	7.72	127.25	110.80
1	N	130	PRO	N-CA-C	-7.67	101.35	110.70
1	A	130	PRO	N-CA-C	-7.65	101.37	110.70
1	A	288	TRP	N-CA-C	7.58	120.50	111.33
12	Y	20	ARG	N-CA-C	-7.54	103.14	111.36
1	N	82	LEU	N-CA-C	7.47	120.87	111.69
1	A	82	LEU	N-CA-C	7.44	120.84	111.69
2	O	197	SER	N-CA-C	7.42	122.05	112.26
1	N	70	VAL	N-CA-C	7.41	117.53	110.42
1	N	288	TRP	N-CA-C	7.33	120.20	111.33
1	N	425	PHE	N-CA-C	7.33	122.52	113.50
1	N	332	ILE	N-CA-C	7.29	118.47	108.84
13	Z	27	LEU	N-CA-C	7.23	119.25	111.36
8	H	64	CYS	N-CA-C	7.18	118.69	109.65
11	K	36	ILE	N-CA-C	7.07	118.94	112.43
2	B	197	SER	N-CA-C	7.03	121.53	112.26
1	A	332	ILE	N-CA-C	7.00	118.38	108.93
8	U	64	CYS	N-CA-C	6.85	118.28	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	70	VAL	N-CA-C	6.85	116.94	110.30
1	N	171	MET	N-CA-C	6.84	121.29	112.26
8	H	54	GLU	N-CA-C	6.83	118.38	111.07
1	A	425	PHE	N-CA-C	6.82	121.73	113.41
11	X	36	ILE	N-CA-C	6.82	119.11	111.88
11	K	6	ALA	CA-C-N	6.68	127.73	119.98
11	K	6	ALA	C-N-CA	6.68	127.73	119.98
1	N	445	ASP	N-CA-C	6.63	119.35	111.33
1	A	170	ASN	N-CA-C	6.54	121.54	113.50
1	A	262	SER	N-CA-C	-6.50	104.98	113.17
1	A	52	GLN	N-CA-C	-6.44	104.34	111.36
12	L	20	ARG	N-CA-C	-6.43	104.35	111.36
1	A	448	THR	N-CA-C	6.38	117.90	111.07
1	A	169	ILE	CB-CA-C	-6.35	103.73	112.24
1	N	448	THR	N-CA-C	6.34	117.86	111.07
1	A	217	THR	N-CA-C	-6.26	102.45	110.53
1	N	262	SER	N-CA-C	-6.26	105.29	113.17
1	A	435	GLY	N-CA-C	6.23	124.74	115.64
1	A	171	MET	N-CA-C	6.19	120.14	112.59
1	A	380	VAL	CB-CA-C	-6.17	103.94	112.02
9	I	69	PHE	N-CA-C	6.09	119.49	110.48
1	N	435	GLY	N-CA-C	6.05	124.48	115.64
2	O	133	LEU	N-CA-C	6.05	118.50	109.25
1	A	142	SER	N-CA-C	6.02	118.37	111.02
6	S	93	PRO	CA-C-N	6.02	133.03	121.54
6	S	93	PRO	C-N-CA	6.02	133.03	121.54
13	M	27	LEU	N-CA-C	5.98	119.05	111.69
1	N	380	VAL	CB-CA-C	-5.93	104.25	112.02
3	C	256	ILE	N-CA-C	5.92	116.56	110.82
3	P	113	GLY	N-CA-C	-5.91	107.02	115.64
1	N	506	GLU	N-CA-C	-5.90	104.92	111.71
1	N	74	MET	N-CA-C	5.87	117.48	111.14
4	D	24	LEU	CA-C-N	5.84	126.17	119.92
4	D	24	LEU	C-N-CA	5.84	126.17	119.92
1	A	141	ALA	N-CA-C	5.83	119.65	112.54
9	V	69	PHE	N-CA-C	5.82	119.10	110.48
2	B	133	LEU	N-CA-C	5.82	118.15	109.25
1	A	438	ARG	N-CA-C	-5.79	103.06	110.53
3	C	9	HIS	N-CA-C	5.79	118.09	108.20
1	N	438	ARG	N-CA-C	-5.78	103.07	110.53
1	A	74	MET	N-CA-C	5.75	117.36	111.14
3	P	9	HIS	N-CA-C	5.74	118.01	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	59	ARG	N-CA-C	-5.68	104.99	111.07
1	A	495	LEU	N-CA-C	5.67	119.30	112.38
4	Q	22	TYR	N-CA-C	-5.66	100.86	109.30
1	N	217	THR	N-CA-C	-5.62	102.97	110.55
3	P	228	THR	N-CA-C	-5.60	102.17	110.46
3	C	113	GLY	N-CA-C	-5.60	107.47	115.64
3	P	29	SER	N-CA-C	-5.59	105.09	111.07
1	A	445	ASP	N-CA-C	5.59	118.90	111.75
1	N	52	GLN	N-CA-C	-5.58	105.28	111.36
7	G	69	PHE	N-CA-C	5.58	117.80	111.11
1	A	9	SER	N-CA-C	5.55	117.90	110.35
1	A	506	GLU	N-CA-C	-5.50	105.28	111.28
2	O	64	ILE	CB-CA-C	-5.50	104.94	111.81
3	P	256	ILE	N-CA-C	5.49	116.14	110.82
3	C	228	THR	N-CA-C	-5.48	102.35	110.46
1	A	6	TRP	N-CA-C	5.43	120.06	113.38
1	N	237	PHE	N-CA-C	-5.43	105.53	111.82
1	N	170	ASN	N-CA-C	5.41	120.15	113.50
8	H	10	ASN	CA-C-N	5.39	128.41	120.82
8	H	10	ASN	C-N-CA	5.39	128.41	120.82
1	N	495	LEU	N-CA-C	5.37	118.93	112.38
2	O	66	THR	N-CA-C	-5.35	106.06	113.18
5	R	100	THR	CA-C-N	5.33	125.39	119.32
5	R	100	THR	C-N-CA	5.33	125.39	119.32
1	N	101	SER	N-CA-C	-5.31	105.50	111.28
4	D	129	ALA	CA-C-N	5.28	124.97	119.64
4	D	129	ALA	C-N-CA	5.28	124.97	119.64
5	R	76	GLY	CA-C-N	5.25	125.71	120.04
5	R	76	GLY	C-N-CA	5.25	125.71	120.04
2	O	58	ALA	N-CA-C	5.25	119.81	113.41
6	F	95	GLN	N-CA-C	5.24	121.96	110.80
1	N	141	ALA	N-CA-C	5.23	118.92	112.54
11	X	6	ALA	CA-C-N	5.22	125.47	119.83
11	X	6	ALA	C-N-CA	5.22	125.47	119.83
2	B	66	THR	N-CA-C	-5.22	106.24	113.18
1	A	237	PHE	N-CA-C	-5.20	105.73	111.71
3	P	257	TYR	N-CA-C	5.19	116.75	111.14
1	A	66	ILE	N-CA-C	5.19	115.46	110.74
3	C	257	TYR	N-CA-C	5.16	116.72	111.14
7	T	6	GLY	N-CA-C	5.16	125.42	113.18
2	B	92	ASN	CA-C-N	5.15	125.13	120.03
2	B	92	ASN	C-N-CA	5.15	125.13	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	U	10	ASN	CA-C-N	5.14	128.07	120.82
8	U	10	ASN	C-N-CA	5.14	128.07	120.82
4	Q	24	LEU	CA-C-N	5.13	125.41	119.92
4	Q	24	LEU	C-N-CA	5.13	125.41	119.92
10	J	57	HIS	N-CA-C	-5.13	106.78	112.57
10	W	15	ASP	N-CA-C	5.10	117.87	108.58
9	I	21	ILE	N-CA-C	-5.07	105.60	110.72
1	A	119	GLU	CB-CA-C	-5.07	110.72	116.54
7	T	69	PHE	N-CA-C	5.04	117.15	111.11
3	P	59	ARG	N-CA-C	-5.02	105.70	111.07

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	304	TYR	Sidechain
1	N	240	HIS	Sidechain
1	N	304	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	66	0
1	N	4027	0	4001	82	0
2	B	1824	0	1833	33	0
2	O	1824	0	1833	46	0
3	C	2110	0	2027	36	0
3	P	2110	0	2027	46	0
4	D	1195	0	1183	17	0
4	Q	1195	0	1183	22	0
5	E	852	0	845	4	0
5	R	852	0	845	22	0
6	F	748	0	728	9	0
6	S	748	0	728	9	0
7	G	675	0	644	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	T	675	0	644	25	0
8	H	662	0	623	7	0
8	U	662	0	623	13	0
9	I	601	0	613	9	0
9	V	601	0	613	12	0
10	J	460	0	459	7	0
10	W	460	0	459	7	0
11	K	384	0	366	5	0
11	X	384	0	366	4	0
12	L	380	0	380	19	0
12	Y	380	0	380	11	0
13	M	335	0	352	8	0
13	Z	335	0	352	5	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	E	1	0	0	0	0
17	N	1	0	0	0	0
17	P	2	0	0	0	0
18	A	120	0	108	3	0
18	N	120	0	108	3	0
19	A	126	0	220	16	0
19	L	63	0	110	23	0
19	N	63	0	110	8	0
19	Q	63	0	110	7	0
19	Y	63	0	110	18	0
20	A	102	0	152	9	0
20	C	102	0	152	8	0
20	N	102	0	152	10	0
20	P	102	0	152	7	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	14	0
22	O	52	0	80	15	0
23	B	29	0	39	1	0
23	C	58	0	78	7	0
23	J	29	0	39	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	O	29	0	39	1	0
23	P	58	0	78	1	0
23	W	29	0	39	5	0
24	C	33	0	36	2	0
24	M	33	0	38	0	0
24	P	33	0	36	8	0
24	Z	33	0	38	0	0
25	C	106	0	154	11	0
25	G	53	0	77	10	0
25	P	106	0	154	12	0
25	T	53	0	77	9	0
26	C	100	0	156	17	0
26	G	100	0	156	21	0
26	P	100	0	156	18	0
26	T	100	0	156	19	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	A	223	0	0	2	0
28	B	146	0	0	4	0
28	C	102	0	0	2	0
28	D	98	0	0	4	0
28	E	60	0	0	1	0
28	F	85	0	0	1	0
28	G	41	0	0	1	0
28	H	49	0	0	2	0
28	I	44	0	0	4	0
28	J	26	0	0	2	0
28	K	25	0	0	1	0
28	L	23	0	0	0	0
28	M	22	0	0	1	0
28	N	213	0	0	3	0
28	O	116	0	0	1	0
28	P	103	0	0	2	0
28	Q	52	0	0	1	0
28	R	41	0	0	0	0
28	S	69	0	0	3	0
28	T	47	0	0	4	0
28	U	43	0	0	1	0
28	V	25	0	0	1	0
28	W	15	0	0	2	0
28	X	17	0	0	0	0
28	Y	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	Z	14	0	0	1	0
All	All	32450	0	31298	605	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 10.

All (605) 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	23:W:1060:CHD:H152	1.31	1.11
22:O:1230:PSC:H142	22:O:1230:PSC:H343	1.39	1.02
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.42	1.00
10:J:33:ARG:HG2	23:J:60:CHD:H152	1.40	0.99
22:B:230:PSC:H343	22:B:230:PSC:H142	1.40	0.99
7:G:84:LYS:H	7:G:84:LYS:HD2	1.24	0.99
7:T:84:LYS:HD2	7:T:84:LYS:H	1.25	0.96
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.30	0.95
4:D:34:SER:H	4:D:37:GLN:HE21	1.14	0.94
3:P:63:ARG:HE	26:P:1270:CDL:HA22	1.33	0.91
25:C:264:PEK:H161	25:C:264:PEK:H102	1.52	0.91
26:G:269:CDL:H541	26:G:269:CDL:H231	1.52	0.90
6:S:94:HIS:CD2	6:S:95:GLN:H	1.89	0.89
26:T:1269:CDL:H541	26:T:1269:CDL:H231	1.55	0.89
7:G:5:LYS:HB2	25:G:1263:PEK:H362	1.56	0.88
26:P:1270:CDL:H191	26:P:1270:CDL:H642	1.55	0.88
2:O:41:ILE:HD13	22:O:1230:PSC:H342	1.54	0.88
12:L:20:ARG:HH22	19:L:522:TGL:HC61	1.39	0.87
26:C:270:CDL:H191	26:C:270:CDL:H642	1.56	0.86
25:P:1264:PEK:H102	25:P:1264:PEK:H161	1.57	0.86
7:G:31:CYS:SG	26:G:269:CDL:H532	2.16	0.86
19:A:521:TGL:H102	19:A:521:TGL:H281	1.57	0.86
28:C:4303:HOH:O	6:F:1:ALA:HB2	1.74	0.86
8:H:43:MET:HE1	8:U:43:MET:HE1	1.57	0.86
7:T:31:CYS:SG	26:T:1269:CDL:H532	2.15	0.86
19:N:1521:TGL:H281	19:N:1521:TGL:H102	1.58	0.84
1:A:278:MET:SD	7:T:5:LYS:HB3	2.18	0.83
7:T:5:LYS:HG3	25:T:263:PEK:H383	1.61	0.82
19:Y:1522:TGL:HC62	19:Y:1522:TGL:HC22	1.62	0.82
19:L:522:TGL:HC62	19:L:522:TGL:HC22	1.61	0.82
19:N:1521:TGL:H102	19:N:1521:TGL:C28	2.11	0.81
12:L:24:MET:SD	19:L:522:TGL:H162	2.22	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:67:PHE:HE1	26:C:270:CDL:H1	1.46	0.80
3:P:67:PHE:HE1	26:P:1270:CDL:H1	1.47	0.80
19:A:521:TGL:H102	19:A:521:TGL:C28	2.12	0.80
4:D:147:LYS:HG2	28:D:4622:HOH:O	1.81	0.79
1:N:514:LYS:HE2	28:S:3395:HOH:O	1.82	0.79
7:G:5:LYS:HB3	1:N:278:MET:SD	2.24	0.78
1:N:1:FME:HCN	1:N:4:ASN:H	1.49	0.78
13:M:42:LYS:HE3	13:M:42:LYS:HA	1.65	0.78
1:A:472:ILE:HG21	19:L:522:TGL:HA92	1.65	0.77
26:G:269:CDL:H622	20:P:1268:PGV:H152	1.65	0.77
1:N:472:ILE:HG21	19:Y:1522:TGL:HA92	1.65	0.76
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.69	0.75
7:T:5:LYS:HD2	25:T:263:PEK:H371	1.67	0.75
19:A:521:TGL:H241	19:A:521:TGL:H201	1.70	0.74
26:G:269:CDL:H522	26:G:269:CDL:H202	1.69	0.74
7:G:5:LYS:HG3	25:G:1263:PEK:H383	1.67	0.74
19:N:1521:TGL:H241	19:N:1521:TGL:H201	1.69	0.73
19:Y:1522:TGL:HC41	28:Y:4411:HOH:O	1.88	0.73
6:F:8:THR:OG1	6:F:11:GLU:HG3	1.88	0.72
26:T:1269:CDL:H522	26:T:1269:CDL:H202	1.72	0.72
12:Y:13:PHE:HA	19:Y:1522:TGL:HC31	1.70	0.72
3:C:160:LEU:HD13	23:C:271:CHD:H181	1.69	0.72
5:R:89:LEU:O	5:R:93:LEU:HG	1.90	0.72
7:G:84:LYS:H	7:G:84:LYS:CD	1.97	0.72
3:P:50:ASN:ND2	3:P:54:MET:HE2	2.05	0.72
22:O:1230:PSC:H071	9:V:10:ARG:HE	1.54	0.72
3:P:160:LEU:HD13	23:P:1271:CHD:H181	1.71	0.71
12:L:13:PHE:HA	19:L:522:TGL:HC31	1.72	0.71
6:S:94:HIS:CG	6:S:95:GLN:H	2.09	0.70
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.74	0.70
12:L:20:ARG:NH2	19:L:522:TGL:HC61	2.06	0.70
7:T:3:ALA:HB1	25:T:263:PEK:H382	1.73	0.70
1:A:1:FME:HE2	1:A:1:FME:HA	1.74	0.69
28:B:4845:HOH:O	4:D:21:ASP:HB2	1.91	0.69
26:G:269:CDL:H541	26:G:269:CDL:C23	2.23	0.69
1:N:334:TRP:CZ3	19:Q:1523:TGL:HA51	2.28	0.69
6:F:85:CYS:SG	6:F:87:THR:HG23	2.33	0.69
6:F:92:VAL:HG23	6:F:92:VAL:O	1.94	0.68
19:Y:1522:TGL:H242	19:Y:1522:TGL:H202	1.76	0.68
19:L:522:TGL:H242	19:L:522:TGL:H202	1.76	0.67
3:P:34:TRP:CZ2	24:P:1272:DMU:H29	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:81:ILE:HG12	9:V:7:PRO:HG2	1.77	0.67
1:N:390:MET:HE2	1:N:413:HIS:HE1	1.60	0.67
26:P:1270:CDL:H391	28:P:4551:HOH:O	1.95	0.67
26:T:1269:CDL:H172	26:T:1269:CDL:H511	1.77	0.67
7:T:38:HIS:NE2	26:T:1269:CDL:H111	2.10	0.66
20:C:267:PGV:H172	26:C:270:CDL:H662	1.76	0.66
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.78	0.65
1:N:296:GLY:HA2	8:U:23:GLN:OE1	1.96	0.65
26:T:1269:CDL:H541	26:T:1269:CDL:C23	2.26	0.65
20:C:268:PGV:H152	26:T:1269:CDL:H622	1.79	0.65
26:G:269:CDL:HB32	1:N:304:TYR:HD1	1.60	0.65
8:H:8:ILE:HG21	28:H:4749:HOH:O	1.97	0.65
3:P:168:THR:HG22	25:P:1265:PEK:H14	1.79	0.64
11:K:24:PHE:O	11:K:28:VAL:HG12	1.96	0.64
6:S:94:HIS:CD2	6:S:95:GLN:N	2.64	0.64
26:G:269:CDL:H511	26:G:269:CDL:H172	1.78	0.64
3:C:168:THR:HG22	25:C:265:PEK:H14	1.80	0.64
3:C:40:MET:O	3:C:44:MET:HG2	1.98	0.64
1:N:53:ILE:O	1:N:57:VAL:HG23	1.98	0.64
3:P:168:THR:CG2	25:P:1265:PEK:H14	2.27	0.64
1:A:177:SER:H	1:A:180:GLN:HE21	1.46	0.63
12:L:20:ARG:HH22	19:L:522:TGL:CC6	2.10	0.63
19:N:1521:TGL:H161	2:O:7:LEU:HD11	1.81	0.63
20:N:1524:PGV:H152	20:N:1524:PGV:H321	1.79	0.63
2:B:56:MET:HG2	22:B:230:PSC:H211	1.80	0.63
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.63	0.63
22:B:230:PSC:C07	9:I:10:ARG:HH21	2.12	0.63
10:J:7:GLU:HG3	28:J:4635:HOH:O	1.98	0.63
1:N:378:HIS:O	1:N:382:SER:HB2	1.99	0.62
3:P:210:ILE:HG23	20:P:1267:PGV:H102	1.80	0.62
1:A:321:PHE:CD2	22:B:230:PSC:H341	2.34	0.62
12:L:20:ARG:HH12	19:L:522:TGL:HC61	1.65	0.62
3:C:168:THR:CG2	25:C:265:PEK:H14	2.30	0.62
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.82	0.62
22:O:1230:PSC:H21	22:O:1230:PSC:H222	1.80	0.62
1:N:76:GLY:O	1:N:80:ASN:HB2	1.98	0.62
19:Q:1523:TGL:HC21	19:Q:1523:TGL:HG11	1.80	0.62
20:A:524:PGV:H152	20:A:524:PGV:H321	1.82	0.62
1:N:151:HIS:CD2	25:P:1264:PEK:H382	2.34	0.62
4:D:34:SER:H	4:D:37:GLN:NE2	1.93	0.61
20:P:1267:PGV:H161	20:P:1267:PGV:H12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:53:THR:HG22	28:S:4719:HOH:O	1.99	0.61
19:A:523:TGL:HC21	19:A:523:TGL:HG11	1.83	0.61
6:F:64:GLU:O	6:F:65:ASP:HB2	2.00	0.61
1:N:169:ILE:HD11	1:N:189:MET:SD	2.40	0.61
20:C:267:PGV:H12	20:C:267:PGV:H161	1.81	0.61
1:N:472:ILE:HG21	19:Y:1522:TGL:CA9	2.31	0.60
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.83	0.60
22:B:230:PSC:H222	22:B:230:PSC:H21	1.83	0.60
3:C:34:TRP:CZ2	24:C:272:DMU:H29	2.36	0.60
1:N:321:PHE:CD2	22:O:1230:PSC:H341	2.36	0.60
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.83	0.60
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.37	0.60
3:P:40:MET:O	3:P:44:MET:HG2	2.01	0.60
20:P:1268:PGV:H062	28:U:4194:HOH:O	2.01	0.60
1:A:1:FME:HE3	12:L:3:TYR:HE1	1.67	0.60
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.83	0.60
2:B:91:ASN:HD21	2:B:183:THR:HG21	1.65	0.59
1:A:484:THR:HB	13:M:2:THR:OG1	2.03	0.59
20:A:604:PGV:H182	3:C:28:THR:HG22	1.85	0.59
7:G:3:ALA:HB1	25:G:1263:PEK:H382	1.85	0.59
2:B:41:ILE:HD13	22:B:230:PSC:H342	1.84	0.59
3:C:210:ILE:HG23	20:C:267:PGV:H102	1.83	0.59
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.68	0.59
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.68	0.59
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.33	0.59
1:A:177:SER:H	1:A:180:GLN:NE2	2.01	0.58
3:C:50:ASN:ND2	3:C:54:MET:HE2	2.16	0.58
5:R:78:HIS:CD2	9:V:12:LEU:HD13	2.38	0.58
5:R:48:ILE:O	5:R:52:LEU:HG	2.03	0.58
1:A:390:MET:HE2	1:A:413:HIS:HE1	1.68	0.58
19:A:521:TGL:HA82	19:A:521:TGL:H222	1.85	0.58
7:G:2:SER:O	25:G:1263:PEK:H322	2.03	0.58
22:O:1230:PSC:C07	9:V:10:ARG:HE	2.17	0.58
3:P:51:MET:HB3	26:P:1270:CDL:H622	1.85	0.58
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.86	0.58
1:A:377:PHE:CD1	18:A:516:HEA:HAD1	2.39	0.58
1:N:51:ASP:OD1	2:O:206:PHE:HE1	1.86	0.57
2:B:62:GLU:O	2:B:66:THR:HB	2.04	0.57
3:C:54:MET:HE1	20:C:267:PGV:H141	1.86	0.57
1:A:282:PHE:HA	7:T:4:ALA:CB	2.34	0.57
1:N:449:MET:SD	2:O:5:MET:HG2	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:481:GLU:HB2	13:Z:4:LYS:HE2	1.85	0.57
26:P:1270:CDL:H642	26:P:1270:CDL:C19	2.31	0.57
19:A:521:TGL:HC22	28:I:2383:HOH:O	2.04	0.57
6:F:90:LYS:HD2	28:F:4237:HOH:O	2.05	0.57
2:B:49:LYS:HE2	28:E:4310:HOH:O	2.03	0.57
25:C:265:PEK:H231	7:G:21:PHE:CD2	2.40	0.57
4:D:34:SER:O	4:D:38:LYS:HG3	2.05	0.57
1:A:282:PHE:HZ	26:T:1269:CDL:H761	1.70	0.57
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.87	0.57
4:Q:122:ARG:HG2	4:Q:126:MET:HE2	1.87	0.57
28:B:4901:HOH:O	25:P:1265:PEK:H031	2.04	0.56
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.87	0.56
2:O:224:ALA:O	2:O:227:LEU:HG	2.05	0.56
24:P:1272:DMU:H25	25:P:1264:PEK:H341	1.87	0.56
20:P:1267:PGV:H172	26:P:1270:CDL:H662	1.88	0.56
12:Y:12:PRO:HB2	19:Y:1522:TGL:HG2	1.87	0.56
22:B:230:PSC:H072	9:I:10:ARG:HH21	1.69	0.56
26:C:270:CDL:H642	26:C:270:CDL:C19	2.31	0.56
1:N:44:PRO:HG2	4:Q:111:PHE:CZ	2.40	0.56
19:N:1521:TGL:H222	19:N:1521:TGL:HA82	1.87	0.56
8:H:43:MET:CE	8:U:43:MET:HE1	2.33	0.55
5:E:84:TYR:O	5:E:88:GLU:HG2	2.06	0.55
11:X:24:PHE:O	11:X:28:VAL:HG12	2.06	0.55
20:N:1524:PGV:H311	13:Z:16:ALA:HA	1.89	0.55
1:N:171:MET:HG2	3:P:8:TYR:CE1	2.42	0.55
1:A:1:FME:HCN	1:A:4:ASN:H	1.71	0.55
1:A:304:TYR:HD1	26:T:1269:CDL:HB32	1.72	0.55
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.89	0.55
10:W:40:LEU:HD12	23:W:1060:CHD:H183	1.87	0.55
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.40	0.55
1:A:378:HIS:O	1:A:382:SER:HB2	2.07	0.54
12:Y:24:MET:HA	12:Y:24:MET:HE2	1.89	0.54
1:A:17:THR:OG1	19:L:522:TGL:H281	2.07	0.54
1:N:71:MET:HE1	1:N:195:LEU:HD21	1.90	0.54
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.90	0.54
20:A:524:PGV:H062	28:M:2160:HOH:O	2.08	0.54
2:B:78:LEU:HD12	26:T:1269:CDL:H351	1.90	0.54
1:N:369:ASP:C	1:N:438:ARG:HG3	2.33	0.54
22:O:1230:PSC:H142	22:O:1230:PSC:C34	2.27	0.54
20:A:524:PGV:H311	13:M:16:ALA:HA	1.89	0.54
3:C:34:TRP:HZ2	24:C:272:DMU:H29	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:86:MET:HE3	28:K:4855:HOH:O	2.08	0.54
8:U:49:ASP:O	8:U:52:VAL:HG22	2.08	0.54
4:Q:33:LEU:HB2	4:Q:38:LYS:HG2	1.89	0.54
4:D:20:ARG:HG3	28:D:4203:HOH:O	2.06	0.53
1:A:240:HIS:O	1:A:243:VAL:HG22	2.08	0.53
3:P:34:TRP:HZ2	24:P:1272:DMU:H29	1.73	0.53
19:Q:1523:TGL:H363	28:V:4756:HOH:O	2.09	0.53
8:U:7:LYS:O	8:U:8:ILE:HG22	2.08	0.53
1:N:165:ILE:O	1:N:169:ILE:HG12	2.08	0.53
9:V:65:LYS:O	11:X:54:ARG:NH1	2.41	0.53
22:B:230:PSC:H142	22:B:230:PSC:C34	2.28	0.53
2:O:83:ILE:O	2:O:87:MET:HG3	2.09	0.53
7:T:3:ALA:O	7:T:4:ALA:HB2	2.09	0.53
3:C:50:ASN:HD22	3:C:51:MET:HE2	1.73	0.53
7:G:84:LYS:HD2	7:G:84:LYS:N	2.09	0.53
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.91	0.53
7:G:3:ALA:O	7:G:4:ALA:HB2	2.09	0.53
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.44	0.53
3:P:67:PHE:CE1	26:P:1270:CDL:H1	2.35	0.52
3:C:156:ARG:HE	23:C:271:CHD:H232	1.74	0.52
25:P:1264:PEK:H102	25:P:1264:PEK:C16	2.34	0.52
7:T:2:SER:O	25:T:263:PEK:H322	2.09	0.52
1:A:472:ILE:HG21	19:L:522:TGL:CA9	2.35	0.52
1:A:406:ASN:HD21	20:A:524:PGV:C2	2.23	0.52
1:A:502:TYR:CD1	12:L:2:HIS:HD2	2.28	0.52
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.90	0.52
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.44	0.52
2:O:56:MET:HA	22:O:1230:PSC:H202	1.91	0.52
10:W:2:GLU:HA	28:W:4707:HOH:O	2.08	0.52
12:L:20:ARG:NH1	19:L:522:TGL:HC61	2.24	0.52
19:A:521:TGL:H161	2:B:7:LEU:HD11	1.92	0.52
1:A:377:PHE:O	1:A:381:LEU:HB3	2.10	0.51
3:C:63:ARG:NE	26:C:270:CDL:HA22	2.13	0.51
7:T:84:LYS:H	7:T:84:LYS:CD	2.05	0.51
22:B:230:PSC:H12	22:B:230:PSC:H322	1.93	0.51
1:N:112:LEU:HG	28:N:3073:HOH:O	2.11	0.51
25:C:265:PEK:C38	26:G:269:CDL:H273	2.41	0.51
7:G:5:LYS:HD2	25:G:1263:PEK:H371	1.93	0.51
2:B:23:PHE:CZ	2:B:80:SER:HB2	2.45	0.51
1:N:422:ASN:HB3	19:N:1521:TGL:H242	1.93	0.51
1:A:472:ILE:HD13	19:L:522:TGL:HA91	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:267:PGV:H182	26:C:270:CDL:H673	1.92	0.51
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.93	0.51
1:N:310:MET:HE1	2:O:76:ILE:HB	1.92	0.51
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.92	0.51
19:L:522:TGL:HC21	19:L:522:TGL:OA1	2.10	0.51
3:C:80:ARG:NH1	25:T:263:PEK:H032	2.25	0.51
1:N:472:ILE:HD13	19:Y:1522:TGL:HA91	1.93	0.51
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.46	0.50
1:N:406:ASN:HD21	20:N:1524:PGV:C2	2.24	0.50
1:N:87:ILE:O	1:N:173:PRO:HD3	2.11	0.50
22:O:1230:PSC:H322	22:O:1230:PSC:H12	1.94	0.50
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.94	0.50
25:G:1263:PEK:H042	3:P:77:LYS:HZ1	1.76	0.50
2:O:84:LEU:HA	2:O:87:MET:HE2	1.92	0.50
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.47	0.50
4:D:130:PRO:HG2	4:D:131:ILE:HD12	1.94	0.50
2:O:82:ARG:HH11	2:O:86:MET:HE1	1.77	0.50
1:A:290:HIS:CD2	1:A:291:HIS:CD2	2.99	0.50
5:R:78:HIS:HD2	9:V:12:LEU:HD13	1.76	0.50
4:Q:58:GLU:O	4:Q:62:LEU:HG	2.12	0.50
19:N:1521:TGL:HC22	28:Q:3383:HOH:O	2.12	0.49
2:B:41:ILE:O	2:B:45:MET:HG2	2.12	0.49
10:W:50:LEU:O	10:W:50:LEU:HD22	2.12	0.49
1:A:334:TRP:CZ3	19:A:523:TGL:HA51	2.47	0.49
25:G:1263:PEK:H042	3:P:77:LYS:NZ	2.26	0.49
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.95	0.49
20:N:1524:PGV:H062	28:Z:3160:HOH:O	2.12	0.49
1:N:177:SER:H	1:N:180:GLN:NE2	2.11	0.49
26:T:1269:CDL:H231	26:T:1269:CDL:C54	2.35	0.49
1:A:1:FME:HE3	12:L:3:TYR:CE1	2.47	0.49
2:B:91:ASN:ND2	2:B:183:THR:HG21	2.28	0.49
3:P:207:HIS:HD2	3:P:241:TYR:OH	1.95	0.49
3:C:51:MET:HB3	26:C:270:CDL:H622	1.94	0.49
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.94	0.49
7:G:2:SER:OG	25:G:1263:PEK:H301	2.13	0.49
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.13	0.49
12:L:20:ARG:HH22	19:L:522:TGL:HC32	1.78	0.49
1:N:28:MET:HE3	12:Y:29:PHE:CD2	2.48	0.49
1:N:177:SER:H	1:N:180:GLN:HE21	1.60	0.49
2:O:57:ASP:H	22:O:1230:PSC:H201	1.78	0.49
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:157:LYS:NZ	25:C:265:PEK:H052	2.27	0.48
23:C:271:CHD:H161	28:C:4708:HOH:O	2.12	0.48
1:N:405:LEU:HD23	1:N:475:ALA:HB2	1.93	0.48
20:N:1266:PGV:H182	3:P:28:THR:HG22	1.95	0.48
7:T:84:LYS:HD2	7:T:84:LYS:N	2.10	0.48
4:D:127:LYS:HD2	28:I:2391:HOH:O	2.14	0.48
1:N:449:MET:SD	2:O:5:MET:CG	3.01	0.48
1:N:462:LEU:HG	1:N:466:MET:HE2	1.94	0.48
8:H:60:TYR:CD1	8:H:60:TYR:C	2.91	0.48
19:L:522:TGL:H231	19:L:522:TGL:H272	1.96	0.48
2:O:68:LEU:CB	2:O:69:PRO:HD3	2.44	0.48
3:P:250:LEU:HD22	26:T:1269:CDL:C67	2.43	0.48
1:A:76:GLY:O	1:A:80:ASN:HB2	2.13	0.48
5:R:37:VAL:HG11	5:R:70:VAL:HG21	1.95	0.48
4:D:33:LEU:HD22	4:D:37:GLN:HB3	1.94	0.48
3:P:34:TRP:CE2	24:P:1272:DMU:H29	2.49	0.48
26:G:269:CDL:HB32	1:N:304:TYR:CD1	2.45	0.48
5:R:105:GLY:O	5:R:108:LYS:HG2	2.13	0.48
6:S:51:SER:O	6:S:94:HIS:N	2.46	0.48
7:T:45:PRO:HD2	28:T:3152:HOH:O	2.13	0.48
25:P:1265:PEK:C38	26:T:1269:CDL:H273	2.43	0.48
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.14	0.48
26:C:270:CDL:H632	26:C:270:CDL:H602	1.59	0.48
2:O:203:ASN:N	2:O:203:ASN:HD22	2.12	0.48
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.96	0.48
3:P:34:TRP:NE1	24:P:1272:DMU:H29	2.29	0.48
4:Q:57:VAL:O	4:Q:61:ARG:HG2	2.14	0.48
19:Y:1522:TGL:H202	19:Y:1522:TGL:C24	2.43	0.48
1:A:310:MET:HE2	1:A:356:ILE:HG23	1.96	0.48
1:A:422:ASN:HB3	19:A:521:TGL:H242	1.96	0.48
26:G:269:CDL:H761	1:N:282:PHE:HZ	1.78	0.48
9:I:35:TYR:C	9:I:37:PHE:H	2.22	0.48
2:O:139:ASP:OD2	2:O:140:ASN:N	2.46	0.48
6:S:85:CYS:SG	6:S:87:THR:HG23	2.54	0.48
26:T:1269:CDL:H322	26:T:1269:CDL:HA62	1.96	0.48
10:J:1:PHE:H1	10:J:1:PHE:HD1	1.61	0.48
1:N:377:PHE:CD1	18:N:516:HEA:HAD1	2.49	0.48
3:C:54:MET:HE3	26:C:270:CDL:H612	1.96	0.47
7:G:17:ARG:HD2	28:G:2309:HOH:O	2.14	0.47
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.78	0.47
1:A:87:ILE:O	1:A:173:PRO:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:524:PGV:H302	13:M:19:LEU:HD23	1.95	0.47
19:Y:1522:TGL:H231	19:Y:1522:TGL:H272	1.95	0.47
1:A:44:PRO:HG2	4:D:111:PHE:CZ	2.50	0.47
1:A:321:PHE:CZ	22:B:230:PSC:H171	2.50	0.47
6:F:92:VAL:O	6:F:92:VAL:CG2	2.61	0.47
19:L:522:TGL:H202	19:L:522:TGL:C24	2.41	0.47
9:V:35:TYR:C	9:V:37:PHE:H	2.23	0.47
23:C:271:CHD:H12A	23:C:271:CHD:H112	1.78	0.47
11:K:42:PRO:HG2	11:K:47:ARG:HE	1.80	0.47
2:O:41:ILE:CD1	22:O:1230:PSC:H342	2.35	0.47
19:Y:1522:TGL:H361	19:Y:1522:TGL:HB91	1.96	0.47
1:A:390:MET:HE2	1:A:413:HIS:CE1	2.48	0.47
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.96	0.47
28:O:4280:HOH:O	8:U:61:LYS:HD2	2.14	0.47
26:G:269:CDL:H351	2:O:78:LEU:HD12	1.96	0.47
1:N:68:PHE:HE2	1:N:112:LEU:CD1	2.28	0.47
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.50	0.47
4:Q:101:HIS:HD2	4:Q:102:TYR:CD2	2.33	0.47
4:Q:127:LYS:O	4:Q:130:PRO:HD3	2.15	0.47
5:R:8:ASP:HB3	9:V:10:ARG:CZ	2.44	0.47
1:A:225:GLY:HA3	3:C:112:LEU:HD21	1.96	0.47
2:B:214:VAL:HB	2:B:215:PRO:CD	2.44	0.47
3:C:156:ARG:HE	23:C:271:CHD:C23	2.28	0.47
3:P:187:THR:HG22	25:P:1264:PEK:H052	1.97	0.47
7:T:2:SER:O	7:T:3:ALA:HB3	2.15	0.47
1:A:306:THR:O	1:A:310:MET:HG3	2.15	0.47
3:C:63:ARG:HE	26:C:270:CDL:CA2	2.15	0.47
2:O:98:LYS:HG2	2:O:153:LEU:HB2	1.97	0.47
3:P:116:TRP:HA	3:P:117:PRO:C	2.39	0.47
12:L:20:ARG:NH2	19:L:522:TGL:HC32	2.30	0.47
1:N:321:PHE:CZ	22:O:1230:PSC:H171	2.50	0.47
7:T:2:SER:OG	25:T:263:PEK:H301	2.14	0.47
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.97	0.46
22:O:1230:PSC:C07	9:V:10:ARG:HH21	2.28	0.46
3:P:132:LEU:O	3:P:136:VAL:HG23	2.16	0.46
3:C:116:TRP:HA	3:C:117:PRO:C	2.40	0.46
7:T:33:LEU:HD12	28:T:4821:HOH:O	2.14	0.46
2:B:164:ALA:O	2:B:194:GLY:HA3	2.14	0.46
26:G:269:CDL:H231	26:G:269:CDL:C54	2.32	0.46
8:H:27:ARG:NH1	28:H:2303:HOH:O	2.47	0.46
1:N:34:SER:HB2	18:N:515:HEA:C2B	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.15	0.46
1:N:115:SER:O	1:N:121:GLY:HA2	2.16	0.46
19:N:1521:TGL:HB91	2:O:32:PHE:HE2	1.79	0.46
5:R:7:THR:HB	5:R:9:GLU:OE2	2.16	0.46
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.97	0.46
3:P:34:TRP:HE1	24:P:1272:DMU:H29	1.80	0.46
6:S:92:VAL:O	6:S:92:VAL:HG23	2.16	0.46
19:A:521:TGL:HC92	28:B:4798:HOH:O	2.14	0.46
12:L:12:PRO:HB2	19:L:522:TGL:HG2	1.97	0.46
4:D:34:SER:N	4:D:37:GLN:HE21	1.96	0.46
7:G:37:LEU:HD21	26:G:269:CDL:H361	1.97	0.46
1:N:390:MET:HE2	1:N:413:HIS:CE1	2.44	0.46
4:Q:101:HIS:HD2	4:Q:102:TYR:CE2	2.34	0.46
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.51	0.46
2:O:62:GLU:O	2:O:66:THR:HB	2.16	0.46
2:O:164:ALA:O	2:O:194:GLY:HA3	2.15	0.46
26:P:1270:CDL:H672	26:P:1270:CDL:H641	1.84	0.46
20:N:1524:PGV:H12	4:Q:87:PHE:CD2	2.51	0.46
2:O:155:SER:O	2:O:174:ALA:HB1	2.15	0.46
3:P:47:LEU:O	3:P:51:MET:HG2	2.16	0.46
4:Q:63:LYS:HG2	4:Q:64:PHE:CE1	2.51	0.46
1:A:406:ASN:HD21	20:A:524:PGV:H22	1.81	0.45
3:C:44:MET:HE2	3:C:44:MET:HA	1.98	0.45
1:N:415:ALA:O	1:N:419:VAL:HG23	2.16	0.45
26:C:270:CDL:H202	26:C:270:CDL:H171	1.79	0.45
19:Y:1522:TGL:HC21	19:Y:1522:TGL:OA1	2.15	0.45
4:D:32:ASN:ND2	28:D:4451:HOH:O	2.45	0.45
23:O:229:CHD:H12	23:O:229:CHD:H212	1.98	0.45
4:Q:24:LEU:HD12	5:R:30:ARG:HA	1.98	0.45
5:R:12:ASP:HA	5:R:47:ILE:HD11	1.98	0.45
19:L:522:TGL:H361	19:L:522:TGL:HB91	1.98	0.45
4:D:88:PHE:HZ	13:M:19:LEU:HD21	1.80	0.45
26:G:269:CDL:H322	26:G:269:CDL:HA62	1.97	0.45
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.17	0.45
7:G:4:ALA:CB	1:N:282:PHE:HA	2.47	0.45
12:L:22:LEU:O	12:L:26:THR:HB	2.17	0.45
2:O:93:PRO:HG3	2:O:151:ARG:HB2	1.98	0.45
3:C:47:LEU:O	3:C:51:MET:HG2	2.17	0.45
1:N:240:HIS:HB3	1:N:241:PRO:HD3	1.99	0.45
1:N:400:PHE:HB3	19:Y:1522:TGL:H283	1.98	0.45
1:A:240:HIS:HB3	1:A:241:PRO:HD3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:128:LEU:HD11	2:B:134:ARG:HA	1.98	0.45
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.98	0.45
3:P:55:TYR:CE1	26:P:1270:CDL:H161	2.52	0.45
7:T:7:ASP:HB2	28:T:4278:HOH:O	2.16	0.45
12:Y:11:ILE:HD12	12:Y:13:PHE:CE1	2.51	0.45
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.99	0.45
3:P:168:THR:HG21	25:P:1265:PEK:H14	1.99	0.45
26:P:1270:CDL:H602	26:P:1270:CDL:H632	1.59	0.45
19:L:522:TGL:HC62	19:L:522:TGL:CC2	2.33	0.45
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.51	0.45
26:T:1269:CDL:H571	26:T:1269:CDL:H771	1.99	0.45
20:C:267:PGV:H12	20:C:267:PGV:C16	2.45	0.44
26:G:269:CDL:H601	26:G:269:CDL:H571	1.57	0.44
9:I:2:THR:HG22	9:I:3:ALA:N	2.32	0.44
26:P:1270:CDL:H202	26:P:1270:CDL:H171	1.77	0.44
19:Q:1523:TGL:H242	19:Q:1523:TGL:H212	1.78	0.44
19:Y:1522:TGL:HB31	19:Y:1522:TGL:HB61	1.81	0.44
3:P:34:TRP:HE1	24:P:1272:DMU:C57	2.30	0.44
3:C:213:THR:HG23	26:C:270:CDL:H762	1.98	0.44
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.17	0.44
4:D:9:GLU:CD	4:D:9:GLU:H	2.25	0.44
12:L:20:ARG:CZ	19:L:522:TGL:HC61	2.47	0.44
1:N:62:ALA:HB2	18:N:515:HEA:HBD1	1.98	0.44
2:O:100:MET:SD	2:O:155:SER:HB3	2.57	0.44
1:A:115:SER:O	1:A:121:GLY:HA2	2.17	0.44
4:Q:118:LYS:HB3	11:X:53:TRP:HB3	1.98	0.44
19:A:523:TGL:HC22	19:A:523:TGL:HC51	1.89	0.44
3:P:213:THR:HG23	26:P:1270:CDL:H762	2.00	0.44
12:Y:42:HIS:NE2	12:Y:46:LYS:HD2	2.33	0.44
1:A:344:PHE:CD1	1:A:344:PHE:C	2.95	0.44
1:N:407:ASP:O	1:N:411:LYS:HG3	2.18	0.44
2:O:56:MET:HA	22:O:1230:PSC:C20	2.47	0.44
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.99	0.44
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.17	0.44
1:A:347:LEU:HD13	1:A:383:MET:SD	2.57	0.44
1:A:449:MET:SD	2:B:5:MET:HG2	2.57	0.44
7:G:5:LYS:HD3	1:N:278:MET:HB3	2.00	0.44
7:G:50:TYR:HB3	7:G:52:HIS:CE1	2.52	0.44
1:A:165:ILE:O	1:A:169:ILE:HG12	2.17	0.44
20:A:524:PGV:H321	20:A:524:PGV:C15	2.48	0.44
28:N:3339:HOH:O	6:S:87:THR:HG21	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:67:PHE:HE1	26:P:1270:CDL:C1	2.25	0.44
5:R:5:HIS:HB3	5:R:6:GLU:H	1.58	0.44
7:G:2:SER:O	7:G:3:ALA:HB3	2.18	0.43
2:O:216:LEU:O	2:O:219:PHE:HB3	2.18	0.43
4:D:75:THR:HB	28:D:2332:HOH:O	2.18	0.43
8:H:43:MET:HE1	8:U:43:MET:CE	2.38	0.43
1:N:400:PHE:HB3	19:Y:1522:TGL:C28	2.48	0.43
5:R:63:SER:O	5:R:67:ILE:HG13	2.19	0.43
7:T:5:LYS:HD2	25:T:263:PEK:C37	2.44	0.43
26:T:1269:CDL:H571	26:T:1269:CDL:H601	1.56	0.43
8:U:58:ARG:HA	8:U:58:ARG:HD2	1.80	0.43
2:B:52:HIS:HE1	22:B:230:PSC:H02	1.83	0.43
26:C:270:CDL:H672	26:C:270:CDL:H641	1.84	0.43
1:N:5:ARG:O	1:N:9:SER:HB2	2.18	0.43
1:N:376:HIS:O	1:N:380:VAL:HG22	2.19	0.43
2:O:52:HIS:HE1	22:O:1230:PSC:H212	1.83	0.43
4:Q:138:TRP:CH2	11:X:50:PRO:HG2	2.54	0.43
5:R:57:ARG:HH11	5:R:57:ARG:HG3	1.84	0.43
1:N:409:TRP:CE2	20:N:1524:PGV:H61	2.53	0.43
5:R:86:ILE:HD13	5:R:86:ILE:HA	1.76	0.43
2:B:14:SER:HB3	2:B:168:LEU:HD23	2.01	0.43
26:G:269:CDL:H212	1:N:311:ILE:HD12	2.01	0.43
13:M:37:LEU:HA	13:M:37:LEU:HD23	1.79	0.43
13:M:42:LYS:HA	13:M:42:LYS:CE	2.39	0.43
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.06	0.43
3:P:41:THR:O	3:P:45:ILE:HG13	2.18	0.43
3:P:112:LEU:HD13	3:P:118:PRO:HG3	2.01	0.43
5:R:80:GLU:H	5:R:80:GLU:CD	2.27	0.43
8:U:39:CYS:O	8:U:43:MET:HG2	2.18	0.43
10:W:36:MET:HB3	23:W:1060:CHD:H181	2.01	0.43
26:C:270:CDL:H661	26:C:270:CDL:H242	2.01	0.43
3:P:187:THR:HB	7:T:68:THR:HG21	2.01	0.43
26:P:1270:CDL:H273	28:P:4551:HOH:O	2.17	0.43
1:A:229:ILE:HD11	2:B:175:ILE:CD1	2.48	0.43
20:N:1524:PGV:H321	20:N:1524:PGV:C15	2.46	0.43
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.92	0.43
1:A:488:THR:HB	1:A:495:LEU:HD13	2.01	0.42
2:O:59:GLN:O	2:O:59:GLN:HG3	2.19	0.42
3:P:50:ASN:HD22	3:P:51:MET:HE2	1.84	0.42
23:B:1086:CHD:H212	23:B:1086:CHD:H12	2.01	0.42
25:C:265:PEK:H371	26:G:269:CDL:H261	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.19	0.42
5:R:82:TYR:N	5:R:83:PRO:CD	2.82	0.42
1:A:430:PHE:HE1	19:A:521:TGL:HB21	1.84	0.42
1:A:377:PHE:CE2	1:A:378:HIS:CE1	3.07	0.42
1:N:113:LEU:CD1	19:Y:1522:TGL:H292	2.49	0.42
1:N:406:ASN:HD21	20:N:1524:PGV:H21	1.84	0.42
26:P:1270:CDL:H242	26:P:1270:CDL:H661	2.02	0.42
7:T:5:LYS:CB	25:T:263:PEK:H362	2.32	0.42
3:C:187:THR:HG22	25:C:264:PEK:H052	2.01	0.42
1:N:344:PHE:CD1	1:N:344:PHE:C	2.97	0.42
1:N:459:PHE:HB3	4:Q:92:THR:HG23	2.01	0.42
3:P:54:MET:HE1	20:P:1267:PGV:H141	2.01	0.42
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.72	0.42
5:R:99:SER:HB2	5:R:104:LEU:HD21	2.01	0.42
1:A:136:LEU:HD11	28:B:4860:HOH:O	2.20	0.42
2:B:56:MET:HA	22:B:230:PSC:H202	2.02	0.42
26:G:269:CDL:H571	26:G:269:CDL:H771	2.02	0.42
1:N:292:MET:O	1:N:295:VAL:HG22	2.20	0.42
25:P:1265:PEK:H371	26:T:1269:CDL:H261	2.02	0.42
19:Q:1523:TGL:HG11	19:Q:1523:TGL:CC2	2.48	0.42
10:W:30:ILE:O	10:W:34:VAL:HG23	2.20	0.42
2:B:81:LEU:HD13	26:T:1269:CDL:H122	2.01	0.42
3:C:164:PHE:CD1	23:C:271:CHD:H192	2.54	0.42
1:N:3:ILE:HG23	1:N:7:LEU:HD22	2.02	0.42
1:N:289:ALA:HB3	1:N:305:PHE:CD2	2.53	0.42
2:O:15:PRO:CD	2:O:185:MET:HE3	2.50	0.42
28:A:4044:HOH:O	12:L:3:TYR:HB3	2.19	0.42
5:E:105:GLY:O	5:E:108:LYS:HG2	2.19	0.42
9:I:2:THR:CG2	9:I:3:ALA:N	2.82	0.42
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.50	0.42
1:N:225:GLY:HA3	3:P:112:LEU:HD21	2.02	0.42
12:Y:24:MET:HE1	19:Y:1522:TGL:H162	2.02	0.42
19:A:523:TGL:H212	19:A:523:TGL:H242	1.77	0.42
12:L:35:ALA:HB3	12:L:36:PRO:HD3	2.01	0.42
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.49	0.42
2:O:15:PRO:HD3	2:O:185:MET:HE3	2.01	0.42
19:Q:1523:TGL:HB81	19:Q:1523:TGL:H122	2.01	0.42
10:J:50:LEU:HD22	10:J:50:LEU:O	2.20	0.41
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.91	0.41
2:O:217:LYS:HA	2:O:217:LYS:HE2	2.01	0.41
12:L:11:ILE:CG2	19:L:522:TGL:H271	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:FME:HA	1:A:1:FME:CE	2.46	0.41
1:A:136:LEU:HD12	28:A:4243:HOH:O	2.19	0.41
26:G:269:CDL:H181	26:G:269:CDL:H152	1.94	0.41
18:A:515:HEA:HHC	18:A:515:HEA:H11	1.87	0.41
2:B:82:ARG:NH1	2:B:86:MET:HE1	2.35	0.41
3:C:173:PHE:CD2	3:C:173:PHE:C	2.97	0.41
25:C:265:PEK:H383	26:G:269:CDL:H273	2.01	0.41
26:G:269:CDL:H221	1:N:286:ILE:CD1	2.51	0.41
9:I:1:SAC:OAC	9:I:1:SAC:HB2	2.20	0.41
1:N:297:MET:HB2	28:N:4474:HOH:O	2.21	0.41
8:U:60:TYR:CD1	8:U:60:TYR:C	2.99	0.41
1:A:304:TYR:CD1	26:T:1269:CDL:HB32	2.53	0.41
3:C:223:LEU:HD21	23:C:271:CHD:C18	2.50	0.41
26:C:270:CDL:H561	26:C:270:CDL:H532	1.74	0.41
1:N:17:THR:OG1	19:Y:1522:TGL:H281	2.20	0.41
2:O:82:ARG:NH1	2:O:86:MET:HE1	2.35	0.41
8:U:64:CYS:HA	8:U:65:PRO:HD3	1.97	0.41
19:A:521:TGL:H201	19:A:521:TGL:C24	2.46	0.41
2:B:65:TRP:CZ3	22:B:230:PSC:H331	2.55	0.41
10:J:40:LEU:HD12	23:J:60:CHD:H183	2.03	0.41
1:N:381:LEU:O	1:N:385:ALA:HB3	2.20	0.41
9:V:58:LYS:O	9:V:62:GLU:HG3	2.19	0.41
2:B:78:LEU:HD12	2:B:78:LEU:HA	1.88	0.41
2:B:98:LYS:HE3	2:B:98:LYS:HB2	1.90	0.41
9:I:44:LYS:NZ	28:I:4743:HOH:O	2.53	0.41
10:J:14:GLU:HG3	28:J:4760:HOH:O	2.21	0.41
1:N:468:MET:O	1:N:472:ILE:HG13	2.20	0.41
25:P:1265:PEK:H201	28:T:4510:HOH:O	2.19	0.41
4:Q:52:SER:OG	4:Q:55:GLU:HG3	2.21	0.41
8:U:57:ARG:HA	8:U:60:TYR:CE2	2.56	0.41
23:W:1060:CHD:H212	23:W:1060:CHD:H161	1.73	0.41
1:A:334:TRP:CZ2	2:B:46:LEU:HB3	2.56	0.41
1:A:334:TRP:HH2	2:B:46:LEU:HD13	1.84	0.41
19:A:523:TGL:H122	19:A:523:TGL:HB81	2.03	0.41
11:K:42:PRO:HG2	11:K:47:ARG:NE	2.35	0.41
12:L:2:HIS:HB3	12:L:3:TYR:H	1.55	0.41
2:B:59:GLN:C	2:B:60:GLU:HG3	2.46	0.41
2:B:168:LEU:HD13	2:B:184:LEU:HG	2.03	0.41
25:C:264:PEK:H102	25:C:264:PEK:C16	2.36	0.41
25:C:264:PEK:H041	7:G:70:PHE:HB2	2.03	0.41
7:G:2:SER:OG	25:G:1263:PEK:H291	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:5:ALA:HB3	28:I:4611:HOH:O	2.21	0.41
23:J:60:CHD:H212	23:J:60:CHD:H161	1.74	0.41
1:N:363:LEU:HD23	1:N:363:LEU:HA	1.87	0.41
24:P:1272:DMU:H30	24:P:1272:DMU:O1	2.21	0.41
20:P:1267:PGV:H182	26:P:1270:CDL:H673	2.01	0.41
26:P:1270:CDL:H352	26:P:1270:CDL:H162	2.03	0.41
4:Q:48:TRP:CH2	5:R:56:ARG:HA	2.56	0.41
7:T:21:PHE:HD2	7:T:25:LEU:HD12	1.85	0.41
1:A:510:TYR:CD1	1:A:510:TYR:C	2.99	0.41
22:B:230:PSC:C07	9:I:10:ARG:HE	2.34	0.41
11:K:43:SER:HA	11:K:44:PRO:HD3	1.97	0.41
3:P:184:ALA:HA	3:P:185:PRO:HD2	1.94	0.41
4:Q:36:SER:O	4:Q:39:ALA:HB3	2.20	0.41
23:W:1060:CHD:H211	28:W:4516:HOH:O	2.20	0.41
1:A:38:ARG:HD2	18:A:515:HEA:OMA	2.22	0.40
1:A:406:ASN:HD21	20:A:524:PGV:H21	1.86	0.40
25:G:1263:PEK:H182	3:P:98:PHE:CD2	2.56	0.40
13:M:37:LEU:O	13:M:41:LYS:HG3	2.21	0.40
2:O:5:MET:HE2	2:O:5:MET:HB3	1.89	0.40
2:O:46:LEU:HD12	19:Q:1523:TGL:H271	2.03	0.40
3:P:230:ASN:HB2	28:S:3287:HOH:O	2.21	0.40
10:W:50:LEU:HD22	10:W:50:LEU:C	2.46	0.40
1:A:246:LEU:HD13	1:A:381:LEU:HD11	2.03	0.40
19:A:523:TGL:HG11	19:A:523:TGL:CC2	2.49	0.40
26:C:270:CDL:H162	26:C:270:CDL:H352	2.02	0.40
6:F:82:CYS:HA	6:F:83:PRO:HD3	1.95	0.40
2:O:122:MET:SD	2:O:206:PHE:HB3	2.62	0.40
2:O:217:LYS:HE2	2:O:217:LYS:CA	2.52	0.40
3:P:42:LEU:HD23	3:P:42:LEU:HA	1.94	0.40
4:Q:71:MET:HE1	5:R:66:ARG:NH2	2.37	0.40
1:A:351:GLY:C	1:A:380:VAL:HG13	2.47	0.40
1:A:399:LEU:HB2	1:A:494:TRP:CZ3	2.55	0.40
4:D:118:LYS:HB3	11:K:53:TRP:HB3	2.02	0.40
7:G:11:TPO:O	7:G:11:TPO:CG2	2.68	0.40
10:J:29:ASN:H	10:J:29:ASN:HD22	1.68	0.40
3:C:99:TRP:CE2	20:C:268:PGV:H232	2.57	0.40
8:H:49:ASP:O	8:H:52:VAL:HG22	2.21	0.40
20:N:1524:PGV:H202	20:N:1524:PGV:H011	1.94	0.40
3:P:31:LEU:HA	3:P:31:LEU:HD23	1.86	0.40
5:R:81:ILE:HD11	9:V:8:GLN:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	499 (98%)	13 (2%)	0	100	100
1	N	512/514 (100%)	500 (98%)	12 (2%)	0	100	100
2	B	225/227 (99%)	212 (94%)	11 (5%)	2 (1%)	14	10
2	O	225/227 (99%)	211 (94%)	13 (6%)	1 (0%)	30	28
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
5	E	103/109 (94%)	100 (97%)	3 (3%)	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	88 (92%)	5 (5%)	3 (3%)	3	1
6	S	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	3	1
7	G	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	0	0
7	T	81/85 (95%)	66 (82%)	8 (10%)	7 (9%)	0	0
8	H	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	9	6
8	U	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	9	6
9	I	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
9	V	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
10	J	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3504/3614 (97%)	3354 (96%)	125 (4%)	25 (1%)	18	15

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER
6	S	94	HIS
6	S	95	GLN
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
7	T	39	SER
2	B	60	GLU
7	G	3	ALA
7	G	40	GLY
8	H	8	ILE
2	O	60	GLU
7	T	3	ALA
7	T	40	GLY
8	U	8	ILE
6	F	94	HIS
6	S	96	LEU
6	F	96	LEU
7	G	6	GLY
7	T	6	GLY
2	B	92	ASN

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%)	415 (97%)	11 (3%)	40	46
1	N	426/426 (100%)	415 (97%)	11 (3%)	40	46
2	B	210/210 (100%)	201 (96%)	9 (4%)	26	27
2	O	210/210 (100%)	197 (94%)	13 (6%)	16	14
3	C	224/226 (99%)	218 (97%)	6 (3%)	39	45
3	P	224/226 (99%)	219 (98%)	5 (2%)	45	53
4	D	128/129 (99%)	126 (98%)	2 (2%)	55	64
4	Q	128/129 (99%)	124 (97%)	4 (3%)	35	39
5	E	92/95 (97%)	89 (97%)	3 (3%)	33	37
5	R	92/95 (97%)	89 (97%)	3 (3%)	33	37
6	F	81/81 (100%)	79 (98%)	2 (2%)	42	48
6	S	81/81 (100%)	78 (96%)	3 (4%)	30	33
7	G	67/68 (98%)	63 (94%)	4 (6%)	17	15
7	T	67/68 (98%)	65 (97%)	2 (3%)	36	41
8	H	71/75 (95%)	68 (96%)	3 (4%)	26	28
8	U	71/75 (95%)	70 (99%)	1 (1%)	59	67
9	I	57/57 (100%)	56 (98%)	1 (2%)	51	60
9	V	57/57 (100%)	54 (95%)	3 (5%)	20	19
10	J	49/50 (98%)	48 (98%)	1 (2%)	48	56
10	W	49/50 (98%)	48 (98%)	1 (2%)	48	56
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	46
11	X	39/46 (85%)	37 (95%)	2 (5%)	21	21
12	L	39/40 (98%)	37 (95%)	2 (5%)	21	21
12	Y	39/40 (98%)	38 (97%)	1 (3%)	40	46
13	M	37/38 (97%)	33 (89%)	4 (11%)	6	4
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	4
All	All	3040/3082 (99%)	2938 (97%)	102 (3%)	32	35

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	112	LEU
1	A	138	HIS

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Mol	Chain	Res	Type
1	A	180	GLN
1	A	297	MET
1	A	369	ASP
1	A	380	VAL
1	A	486	ASP
1	A	504	THR
1	A	512	ASN
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	115	ASP
2	B	167	SER
3	C	77	LYS
3	C	127	LEU
3	C	159	MET
3	C	179	SER
3	C	192	VAL
3	C	230	ASN
4	D	4	SER
4	D	51	LEU
5	E	70	VAL
5	E	80	GLU
5	E	90	ARG
6	F	48	LEU
6	F	95	GLN
7	G	17	ARG
7	G	33	LEU
7	G	36	TRP
7	G	84	LYS
8	H	8	ILE
8	H	29	CYS
8	H	60	TYR
9	I	8	GLN
10	J	50	LEU
11	K	54	ARG
12	L	2	HIS
12	L	26	THR

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Mol	Chain	Res	Type
13	M	4	LYS
13	M	13	LYS
13	M	34	LEU
13	M	42	LYS
1	N	38	ARG
1	N	115	SER
1	N	138	HIS
1	N	180	GLN
1	N	297	MET
1	N	369	ASP
1	N	380	VAL
1	N	394	VAL
1	N	484	THR
1	N	504	THR
1	N	513	LEU
2	O	33	LEU
2	O	60	GLU
2	O	66	THR
2	O	68	LEU
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	167	SER
2	O	205	SER
2	O	217	LYS
3	P	17	PRO
3	P	77	LYS
3	P	127	LEU
3	P	159	MET
3	P	230	ASN
4	Q	8	SER
4	Q	9	GLU
4	Q	51	LEU
4	Q	121	LYS
5	R	16	VAL
5	R	77	PRO
5	R	80	GLU
6	S	48	LEU
6	S	53	THR

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Mol	Chain	Res	Type
6	S	94	HIS
7	T	26	PRO
7	T	43	GLU
8	U	61	LYS
9	V	8	GLN
9	V	29	LEU
9	V	61	GLU
10	W	50	LEU
11	X	20	SER
11	X	54	ARG
12	Y	26	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 (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	10	GLN
2	B	52	HIS
2	B	91	ASN
2	B	181	GLN
3	C	3	HIS
3	C	50	ASN
3	C	68	GLN
3	C	76	GLN
3	C	161	GLN
4	D	32	ASN
4	D	37	GLN
4	D	76	ASN
4	D	109	HIS
4	D	119	GLN
4	D	143	ASN
5	E	94	ASN
7	G	34	ASN
7	G	71	HIS
9	I	53	ASN

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Mol	Chain	Res	Type
10	J	29	ASN
11	K	35	GLN
1	N	151	HIS
1	N	178	GLN
1	N	180	GLN
1	N	406	ASN
1	N	512	ASN
2	O	52	HIS
2	O	91	ASN
2	O	181	GLN
2	O	203	ASN
3	P	50	ASN
3	P	68	GLN
3	P	161	GLN
3	P	207	HIS
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN
6	S	80	GLN
6	S	88	HIS
10	W	57	HIS
13	Z	36	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	$\# Z > 2$
2	FME	O	1	2	8,9,10	0.69	0	8,9,11	2.33	2 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FME	B	1	2	8,9,10	0.65	0	8,9,11	1.73	2 (25%)
7	TPO	G	11	7	8,10,11	1.64	1 (12%)	10,14,16	1.11	1 (10%)
9	SAC	V	1	9	7,8,9	2.84	2 (28%)	7,9,11	1.95	3 (42%)
1	FME	N	1	1	8,9,10	0.78	0	8,9,11	1.51	1 (12%)
7	TPO	T	11	7	8,10,11	1.49	2 (25%)	10,14,16	1.02	1 (10%)
1	FME	A	1	1	8,9,10	0.65	0	8,9,11	0.99	0
9	SAC	I	1	9	7,8,9	2.89	2 (28%)	7,9,11	1.59	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FME	O	1	2	-	2/7/9/11	-
2	FME	B	1	2	-	1/7/9/11	-
7	TPO	G	11	7	-	5/9/11/13	-
9	SAC	V	1	9	-	3/7/8/10	-
1	FME	N	1	1	-	4/7/9/11	-
7	TPO	T	11	7	-	4/9/11/13	-
1	FME	A	1	1	-	3/7/9/11	-
9	SAC	I	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	I	1	SAC	OAC-C1A	5.66	1.35	1.23
9	V	1	SAC	CA-N	5.20	1.54	1.46
9	I	1	SAC	CA-N	4.96	1.53	1.46
9	V	1	SAC	OAC-C1A	4.95	1.34	1.23
7	G	11	TPO	CB-CA	3.25	1.60	1.53
7	T	11	TPO	CB-CA	2.27	1.58	1.53
7	T	11	TPO	P-O1P	2.08	1.56	1.50

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	FME	C-CA-N	5.07	119.29	109.50
2	O	1	FME	CA-N-CN	-3.98	116.71	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	C-CA-N	3.74	116.72	109.50
1	N	1	FME	CA-N-CN	-3.51	117.42	122.82
9	V	1	SAC	C2A-C1A-N	3.30	121.59	116.12
2	B	1	FME	CA-N-CN	-2.76	118.58	122.82
9	I	1	SAC	C-CA-N	-2.66	104.36	109.50
9	V	1	SAC	OAC-C1A-C2A	-2.39	117.80	122.05
9	V	1	SAC	C-CA-N	-2.37	104.93	109.50
7	T	11	TPO	O3P-P-OG1	2.08	113.97	105.85
7	G	11	TPO	O3P-P-OG1	2.08	113.95	105.85

There are no chirality outliers.

All (25) 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
7	G	11	TPO	O-C-CA-CB
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
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
7	T	11	TPO	O-C-CA-CB
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	CB-CA-N-C1A
9	I	1	SAC	OAC-C1A-N-CA
9	I	1	SAC	C2A-C1A-N-CA
1	A	1	FME	C-CA-CB-CG
7	G	11	TPO	CB-OG1-P-O2P
1	N	1	FME	CA-CB-CG-SD
2	O	1	FME	CB-CG-SD-CE

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	1	0
1	N	1	FME	1	0
7	T	11	TPO	1	0
1	A	1	FME	5	0
9	I	1	SAC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 58 ligands modelled in this entry, 14 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
18	HEA	N	515	1	67,67,67	1.05	3 (4%)	81,103,103	1.14	5 (6%)
23	CHD	W	1060	-	32,32,32	1.41	3 (9%)	51,51,51	3.55	26 (50%)
18	HEA	N	516	1	67,67,67	1.21	5 (7%)	81,103,103	1.29	6 (7%)
26	CDL	P	1270	-	99,99,99	0.91	5 (5%)	105,111,111	1.02	7 (6%)
23	CHD	C	525	-	32,32,32	0.92	1 (3%)	51,51,51	1.87	14 (27%)
26	CDL	C	270	-	99,99,99	0.86	4 (4%)	105,111,111	1.02	6 (5%)
25	PEK	T	263	-	52,52,52	1.82	10 (19%)	55,57,57	1.17	5 (9%)
23	CHD	C	271	-	32,32,32	1.00	1 (3%)	51,51,51	3.69	25 (49%)
19	TGL	A	523	-	62,62,62	0.78	1 (1%)	65,65,65	1.29	11 (16%)
25	PEK	C	264	-	52,52,52	1.41	4 (7%)	55,57,57	1.22	5 (9%)
25	PEK	C	265	-	52,52,52	1.63	10 (19%)	55,57,57	1.14	6 (10%)
20	PGV	N	1524	-	50,50,50	1.06	4 (8%)	53,56,56	0.94	3 (5%)
24	DMU	M	526	-	34,34,34	3.34	8 (23%)	45,45,45	4.04	20 (44%)
23	CHD	J	60	-	32,32,32	1.36	3 (9%)	51,51,51	3.52	29 (56%)
23	CHD	B	1086	-	32,32,32	0.75	0	51,51,51	1.77	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	PGV	A	524	-	50,50,50	1.07	3 (6%)	53,56,56	0.96	3 (5%)
24	DMU	Z	1526	-	34,34,34	3.25	9 (26%)	45,45,45	3.97	20 (44%)
20	PGV	A	604	-	50,50,50	0.87	1 (2%)	53,56,56	0.75	1 (1%)
23	CHD	O	229	-	32,32,32	0.72	0	51,51,51	1.74	12 (23%)
23	CHD	P	1271	-	32,32,32	0.94	1 (3%)	51,51,51	3.61	26 (50%)
20	PGV	C	268	-	50,50,50	1.19	3 (6%)	53,56,56	0.82	0
19	TGL	L	522	-	62,62,62	1.14	6 (9%)	65,65,65	1.73	14 (21%)
24	DMU	C	272	-	34,34,34	2.83	12 (35%)	45,45,45	4.20	19 (42%)
26	CDL	T	1269	-	99,99,99	0.98	7 (7%)	105,111,111	0.98	7 (6%)
18	HEA	A	516	1	67,67,67	1.32	7 (10%)	81,103,103	1.28	10 (12%)
19	TGL	A	521	-	62,62,62	0.74	1 (1%)	65,65,65	1.45	9 (13%)
25	PEK	P	1264	-	52,52,52	1.49	5 (9%)	55,57,57	1.17	6 (10%)
18	HEA	A	515	1	67,67,67	1.07	6 (8%)	81,103,103	1.14	4 (4%)
24	DMU	P	1272	-	34,34,34	2.87	12 (35%)	45,45,45	4.06	19 (42%)
22	PSC	B	230	-	51,51,51	1.23	3 (5%)	57,59,59	0.91	1 (1%)
21	CUA	B	228	2	0,1,1	-	-	-	-	-
25	PEK	P	1265	-	52,52,52	1.64	10 (19%)	55,57,57	1.14	6 (10%)
20	PGV	N	1266	-	50,50,50	0.90	2 (4%)	53,56,56	0.83	3 (5%)
19	TGL	Q	1523	-	62,62,62	0.82	1 (1%)	65,65,65	1.26	6 (9%)
21	CUA	O	228	2	0,1,1	-	-	-	-	-
20	PGV	P	1267	-	50,50,50	0.82	1 (2%)	53,56,56	0.87	1 (1%)
26	CDL	G	269	-	99,99,99	1.00	7 (7%)	105,111,111	0.97	6 (5%)
19	TGL	N	1521	-	62,62,62	0.74	1 (1%)	65,65,65	1.44	9 (13%)
22	PSC	O	1230	-	51,51,51	1.24	3 (5%)	57,59,59	0.92	1 (1%)
25	PEK	G	1263	-	52,52,52	1.79	10 (19%)	55,57,57	1.16	5 (9%)
20	PGV	C	267	-	50,50,50	0.84	1 (2%)	53,56,56	0.97	3 (5%)
19	TGL	Y	1522	-	62,62,62	1.17	5 (8%)	65,65,65	1.71	14 (21%)
20	PGV	P	1268	-	50,50,50	1.16	2 (4%)	53,56,56	0.86	0
23	CHD	P	1525	-	32,32,32	0.91	1 (3%)	51,51,51	1.80	12 (23%)

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
18	HEA	N	515	1	-	3/36/76/76	-
23	CHD	W	1060	-	5/5/12/12	8/9/74/74	0/4/4/4
18	HEA	N	516	1	-	7/36/76/76	-
26	CDL	P	1270	-	-	68/110/110/110	-
23	CHD	C	525	-	-	0/9/74/74	0/4/4/4
26	CDL	C	270	-	-	67/110/110/110	-
25	PEK	T	263	-	-	29/56/56/56	-
23	CHD	C	271	-	5/5/12/12	8/9/74/74	0/4/4/4
19	TGL	A	523	-	-	13/65/65/65	-
25	PEK	C	264	-	-	26/56/56/56	-
25	PEK	C	265	-	-	17/56/56/56	-
24	DMU	M	526	-	5/5/10/10	10/19/59/59	0/2/2/2
20	PGV	N	1524	-	-	33/55/55/55	-
23	CHD	J	60	-	5/5/12/12	8/9/74/74	0/4/4/4
23	CHD	B	1086	-	-	2/9/74/74	0/4/4/4
20	PGV	A	524	-	-	33/55/55/55	-
24	DMU	Z	1526	-	5/5/10/10	10/19/59/59	0/2/2/2
20	PGV	A	604	-	-	13/55/55/55	-
23	CHD	O	229	-	-	2/9/74/74	0/4/4/4
23	CHD	P	1271	-	5/5/12/12	8/9/74/74	0/4/4/4
20	PGV	C	268	-	-	35/55/55/55	-
19	TGL	L	522	-	-	16/65/65/65	-
24	DMU	C	272	-	6/6/10/10	8/19/59/59	0/2/2/2
26	CDL	T	1269	-	-	60/110/110/110	-
18	HEA	A	516	1	-	7/36/76/76	-
19	TGL	A	521	-	-	14/65/65/65	-
25	PEK	P	1264	-	-	24/56/56/56	-
24	DMU	P	1272	-	6/6/10/10	9/19/59/59	0/2/2/2
18	HEA	A	515	1	-	3/36/76/76	-
22	PSC	B	230	-	-	39/55/55/55	-
25	PEK	P	1265	-	-	17/56/56/56	-
20	PGV	N	1266	-	-	13/55/55/55	-
19	TGL	Q	1523	-	-	14/65/65/65	-
20	PGV	P	1267	-	-	16/55/55/55	-
26	CDL	G	269	-	-	60/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TGL	N	1521	-	-	14/65/65/65	-
22	PSC	O	1230	-	-	39/55/55/55	-
25	PEK	G	1263	-	-	29/56/56/56	-
20	PGV	C	267	-	-	17/55/55/55	-
19	TGL	Y	1522	-	-	16/65/65/65	-
20	PGV	P	1268	-	-	35/55/55/55	-
23	CHD	P	1525	-	-	0/9/74/74	0/4/4/4

All (182) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	526	DMU	O7-C3	-8.53	1.22	1.43
24	Z	1526	DMU	O7-C3	-8.08	1.23	1.43
24	M	526	DMU	O16-C6	-7.91	1.27	1.40
24	Z	1526	DMU	O16-C6	-7.74	1.27	1.40
24	M	526	DMU	O5-C4	-6.81	1.27	1.44
24	M	526	DMU	O1-C9	-6.70	1.28	1.44
24	M	526	DMU	O16-C18	-6.69	1.24	1.43
24	Z	1526	DMU	O16-C18	-6.50	1.25	1.43
24	Z	1526	DMU	O5-C4	-6.49	1.28	1.44
24	P	1272	DMU	O16-C6	-6.47	1.29	1.40
24	Z	1526	DMU	O1-C9	-6.43	1.28	1.44
24	P	1272	DMU	O1-C9	-6.41	1.28	1.44
24	M	526	DMU	O7-C10	-6.36	1.23	1.41
24	P	1272	DMU	O7-C3	-6.31	1.27	1.43
24	Z	1526	DMU	O7-C10	-6.27	1.24	1.41
24	C	272	DMU	O16-C6	-6.22	1.29	1.40
24	P	1272	DMU	O16-C18	-6.14	1.26	1.43
24	C	272	DMU	O1-C9	-6.07	1.29	1.44
24	C	272	DMU	O7-C3	-6.05	1.28	1.43
24	C	272	DMU	O16-C18	-6.00	1.26	1.43
24	M	526	DMU	O1-C10	-5.64	1.27	1.41
24	C	272	DMU	O5-C4	-5.23	1.31	1.44
24	Z	1526	DMU	O1-C10	-5.21	1.28	1.41
25	P	1264	PEK	C15-C14	5.00	1.60	1.31
24	Z	1526	DMU	O5-C6	-4.96	1.29	1.41
19	Y	1522	TGL	OG2-CB1	4.94	1.48	1.34
25	G	1263	PEK	C12-C11	4.93	1.59	1.31
25	C	264	PEK	C15-C14	4.90	1.59	1.31
24	M	526	DMU	O5-C6	-4.89	1.29	1.41
25	T	263	PEK	C12-C11	4.79	1.58	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	P	1272	DMU	O7-C10	-4.71	1.28	1.41
24	P	1272	DMU	O5-C4	-4.71	1.32	1.44
19	L	522	TGL	OG2-CB1	4.66	1.47	1.34
23	W	1060	CHD	C13-C17	4.66	1.63	1.55
25	T	263	PEK	C6-C5	4.65	1.58	1.31
18	A	516	HEA	FE-NC	4.63	2.10	1.95
20	P	1268	PGV	C12-C11	4.59	1.57	1.31
18	N	516	HEA	FE-NA	4.54	2.10	1.95
25	C	264	PEK	C12-C11	4.54	1.57	1.31
24	P	1272	DMU	O1-C10	-4.54	1.30	1.41
25	G	1263	PEK	C6-C5	4.52	1.57	1.31
20	C	268	PGV	C12-C11	4.49	1.57	1.31
24	C	272	DMU	O7-C10	-4.49	1.29	1.41
25	P	1265	PEK	C12-C11	4.48	1.57	1.31
25	P	1264	PEK	C12-C11	4.47	1.57	1.31
25	C	265	PEK	C12-C11	4.45	1.56	1.31
25	C	265	PEK	C15-C14	4.43	1.56	1.31
25	C	265	PEK	C9-C8	4.37	1.56	1.31
22	O	1230	PSC	C10-C9	4.35	1.56	1.31
23	J	60	CHD	C13-C17	4.35	1.62	1.55
22	B	230	PSC	C10-C9	4.33	1.56	1.31
24	C	272	DMU	O1-C10	-4.33	1.30	1.41
22	O	1230	PSC	C13-C12	4.32	1.56	1.31
25	G	1263	PEK	C9-C8	4.31	1.56	1.31
25	P	1265	PEK	C9-C8	4.29	1.56	1.31
25	P	1265	PEK	C15-C14	4.26	1.55	1.31
25	T	263	PEK	C9-C8	4.24	1.55	1.31
25	P	1265	PEK	C6-C5	4.18	1.55	1.31
25	C	265	PEK	C6-C5	4.17	1.55	1.31
25	P	1264	PEK	C9-C8	4.15	1.55	1.31
25	T	263	PEK	C15-C14	4.15	1.55	1.31
20	N	1266	PGV	C12-C11	4.14	1.55	1.31
25	G	1263	PEK	C15-C14	4.13	1.55	1.31
24	C	272	DMU	O5-C6	-4.11	1.31	1.41
18	A	516	HEA	FE-NA	4.09	2.08	1.95
25	C	264	PEK	C6-C5	4.08	1.54	1.31
22	B	230	PSC	C13-C12	4.07	1.54	1.31
20	N	1524	PGV	C12-C11	4.05	1.54	1.31
20	A	604	PGV	C12-C11	4.02	1.54	1.31
24	P	1272	DMU	O5-C6	-3.93	1.31	1.41
20	A	524	PGV	C12-C11	3.89	1.53	1.31
25	C	264	PEK	C9-C8	3.87	1.53	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	263	PEK	O03-C21	3.86	1.44	1.33
25	P	1264	PEK	C6-C5	3.83	1.53	1.31
19	Y	1522	TGL	OG1-CA1	3.82	1.44	1.33
25	T	263	PEK	C03-C02	3.62	1.62	1.50
25	G	1263	PEK	O03-C21	3.56	1.43	1.33
25	G	1263	PEK	C03-C02	3.56	1.61	1.50
18	N	515	HEA	C11-C3B	-3.47	1.47	1.51
26	T	1269	CDL	CB6-CB4	3.33	1.61	1.50
25	G	1263	PEK	C01-C02	3.32	1.61	1.50
20	P	1267	PGV	C12-C11	3.30	1.50	1.31
18	A	515	HEA	FE-ND	3.24	2.04	1.94
19	L	522	TGL	OG1-CA1	3.24	1.42	1.33
25	T	263	PEK	C01-C02	3.22	1.60	1.50
20	C	267	PGV	C12-C11	3.16	1.49	1.31
26	G	269	CDL	CB6-CB4	3.15	1.60	1.50
25	P	1264	PEK	C2-C1	3.05	1.59	1.50
20	P	1268	PGV	O01-C1	2.96	1.42	1.34
20	A	524	PGV	O03-C19	2.95	1.41	1.33
18	A	515	HEA	FE-NA	2.91	2.04	1.95
25	T	263	PEK	P-O11	2.88	1.70	1.59
25	T	263	PEK	C2-C1	2.87	1.59	1.50
19	L	522	TGL	CG1-CG2	2.85	1.59	1.50
18	N	516	HEA	FE-NC	2.85	2.04	1.95
26	G	269	CDL	C11-CA5	2.84	1.59	1.50
18	A	516	HEA	C4D-ND	2.83	1.44	1.38
18	N	516	HEA	FE-ND	-2.81	1.86	1.94
25	P	1265	PEK	O03-C21	2.80	1.41	1.33
20	C	268	PGV	O01-C1	2.78	1.42	1.34
19	Y	1522	TGL	CG1-CG2	2.77	1.59	1.50
25	C	265	PEK	C03-C02	2.73	1.59	1.50
26	P	1270	CDL	CA6-CA4	2.70	1.59	1.50
20	N	1524	PGV	O03-C19	2.69	1.41	1.33
25	G	1263	PEK	P-O11	2.66	1.69	1.59
23	W	1060	CHD	C8-C7	2.66	1.58	1.53
18	N	516	HEA	C4D-ND	2.65	1.44	1.38
18	N	516	HEA	CMA-C3A	-2.64	1.39	1.45
18	A	515	HEA	FE-NB	-2.62	1.86	1.94
24	C	272	DMU	C3-C4	2.62	1.60	1.52
24	P	1272	DMU	C6-C1	2.62	1.60	1.52
24	P	1272	DMU	C3-C4	2.61	1.60	1.52
26	T	1269	CDL	CB2-C1	2.61	1.59	1.51
26	G	269	CDL	OA6-CA5	2.60	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	C	271	CHD	C13-C14	2.60	1.59	1.55
25	C	265	PEK	O03-C21	2.59	1.40	1.33
24	C	272	DMU	C6-C1	2.57	1.60	1.52
19	N	1521	TGL	OG2-CB1	2.57	1.41	1.34
25	P	1265	PEK	C01-C02	2.57	1.58	1.50
22	O	1230	PSC	C2-C1	2.56	1.58	1.50
26	C	270	CDL	CA6-CA4	2.56	1.58	1.50
22	B	230	PSC	C2-C1	2.55	1.58	1.50
23	W	1060	CHD	C20-C17	2.55	1.58	1.54
26	T	1269	CDL	C11-CA5	2.51	1.58	1.50
25	P	1265	PEK	P-O11	2.51	1.69	1.59
25	P	1265	PEK	C03-C02	2.48	1.58	1.50
18	A	515	HEA	C4B-C3B	-2.48	1.40	1.44
18	N	515	HEA	CMA-C3A	-2.47	1.39	1.45
26	P	1270	CDL	OA8-CA7	2.46	1.40	1.33
23	J	60	CHD	C20-C17	2.46	1.58	1.54
26	P	1270	CDL	C31-CA7	2.45	1.57	1.50
18	A	516	HEA	CMA-C3A	-2.45	1.39	1.45
26	T	1269	CDL	CA6-CA4	2.43	1.58	1.50
20	N	1266	PGV	C01-C02	2.41	1.58	1.50
25	C	265	PEK	C01-C02	2.41	1.58	1.50
26	T	1269	CDL	OA6-CA5	2.41	1.41	1.34
25	C	265	PEK	P-O11	2.38	1.68	1.59
24	Z	1526	DMU	C8-C9	2.35	1.58	1.53
23	P	1271	CHD	C13-C14	2.35	1.59	1.55
26	G	269	CDL	CB2-C1	2.35	1.59	1.51
20	N	1524	PGV	C20-C19	2.33	1.57	1.50
26	G	269	CDL	CA6-CA4	2.33	1.58	1.50
26	P	1270	CDL	CA3-CA4	2.31	1.58	1.50
26	C	270	CDL	CA3-CA4	2.30	1.58	1.50
26	T	1269	CDL	CB3-CB4	2.30	1.58	1.50
25	G	1263	PEK	P-O12	2.30	1.68	1.59
20	A	524	PGV	C20-C19	2.29	1.57	1.50
26	G	269	CDL	CB3-CB4	2.27	1.57	1.50
26	P	1270	CDL	CB2-C1	2.26	1.58	1.51
18	N	515	HEA	C1C-C2C	2.25	1.48	1.43
23	J	60	CHD	C8-C7	2.25	1.57	1.53
20	C	268	PGV	C04-C05	2.23	1.58	1.51
19	A	521	TGL	OG2-CB1	2.23	1.40	1.34
25	C	265	PEK	P-O12	2.21	1.68	1.59
23	C	525	CHD	C13-C12	-2.20	1.51	1.54
24	C	272	DMU	C7-C5	2.19	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	265	PEK	C22-C21	2.18	1.57	1.50
26	C	270	CDL	OA8-CA7	2.18	1.39	1.33
18	A	515	HEA	CMA-C3A	-2.16	1.40	1.45
18	A	516	HEA	C20-C19	2.16	1.55	1.51
19	Y	1522	TGL	CC2-CC1	2.15	1.56	1.50
19	Y	1522	TGL	CG3-CG2	2.13	1.57	1.50
18	A	515	HEA	C11-C3B	-2.13	1.48	1.51
26	C	270	CDL	CB2-C1	2.11	1.58	1.51
25	P	1265	PEK	P-O12	2.11	1.67	1.59
19	Q	1523	TGL	CG3-CG2	2.11	1.57	1.50
25	T	263	PEK	P-O12	2.11	1.67	1.59
18	A	516	HEA	CMB-C2B	2.10	1.55	1.50
24	C	272	DMU	C2-C3	2.10	1.58	1.52
25	P	1265	PEK	C22-C21	2.09	1.56	1.50
19	A	523	TGL	OG3-CC1	2.09	1.39	1.33
25	G	1263	PEK	C2-C1	2.09	1.56	1.50
19	L	522	TGL	CG3-CG2	2.08	1.57	1.50
26	G	269	CDL	C71-CB7	2.06	1.56	1.50
19	L	522	TGL	CC2-CC1	2.06	1.56	1.50
20	N	1524	PGV	C03-C02	2.06	1.57	1.50
24	P	1272	DMU	C8-C9	2.05	1.57	1.53
23	P	1525	CHD	C8-C9	2.05	1.57	1.53
26	T	1269	CDL	C71-CB7	2.04	1.56	1.50
19	L	522	TGL	CC3-CC2	2.03	1.59	1.52
18	A	516	HEA	CMD-C2D	2.02	1.54	1.50
24	P	1272	DMU	C8-C7	2.02	1.57	1.52

All (396) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	272	DMU	O16-C6-C1	11.70	126.04	108.27
24	M	526	DMU	C10-C5-C7	10.24	131.56	110.01
24	Z	1526	DMU	C10-C5-C7	10.10	131.26	110.01
23	C	271	CHD	C17-C13-C14	9.86	110.00	100.11
23	W	1060	CHD	C17-C13-C14	9.84	109.98	100.11
23	J	60	CHD	C17-C13-C14	9.82	109.97	100.11
24	P	1272	DMU	O16-C6-C1	9.81	123.17	108.27
23	P	1271	CHD	C10-C9-C8	9.75	122.71	111.84
23	P	1271	CHD	C17-C13-C14	9.50	109.64	100.11
23	C	271	CHD	C10-C9-C8	9.47	122.40	111.84
24	C	272	DMU	C1-C2-C3	9.30	130.78	109.68
24	P	1272	DMU	C1-C2-C3	9.19	130.54	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	271	CHD	C19-C10-C9	-9.07	98.99	111.18
24	C	272	DMU	C6-O5-C4	8.79	130.89	113.72
24	C	272	DMU	O1-C9-C11	8.71	128.01	106.44
24	P	1272	DMU	C6-O5-C4	8.39	130.11	113.72
23	P	1271	CHD	C19-C10-C9	-8.33	99.98	111.18
23	P	1271	CHD	C17-C13-C12	-8.28	110.22	117.67
24	P	1272	DMU	O1-C9-C11	8.09	126.48	106.44
23	C	271	CHD	C17-C13-C12	-8.03	110.44	117.67
23	W	1060	CHD	C13-C17-C20	7.93	129.09	119.48
23	J	60	CHD	C13-C17-C20	7.82	128.95	119.48
24	M	526	DMU	C8-C7-C5	-7.81	97.13	110.83
24	Z	1526	DMU	C8-C7-C5	-7.69	97.33	110.83
24	M	526	DMU	O1-C9-C8	7.68	123.54	109.70
24	C	272	DMU	O5-C4-C3	7.56	125.35	109.72
24	M	526	DMU	O5-C4-C57	7.43	124.86	106.44
24	Z	1526	DMU	O1-C9-C8	7.42	123.06	109.70
24	Z	1526	DMU	O5-C4-C57	7.38	124.73	106.44
24	P	1272	DMU	O7-C3-C4	7.35	128.75	109.48
24	M	526	DMU	C6-O5-C4	7.26	127.89	113.72
24	M	526	DMU	O1-C9-C11	7.24	124.38	106.44
24	Z	1526	DMU	O1-C9-C11	7.23	124.35	106.44
24	M	526	DMU	C7-C8-C9	7.14	123.17	110.23
24	Z	1526	DMU	C7-C8-C9	7.10	123.11	110.23
24	P	1272	DMU	C18-O16-C6	7.09	125.80	113.68
24	Z	1526	DMU	C6-O5-C4	6.98	127.35	113.72
24	Z	1526	DMU	O5-C6-O16	6.97	126.52	110.04
24	Z	1526	DMU	O5-C4-C3	6.77	123.71	109.72
24	M	526	DMU	O5-C6-O16	6.71	125.91	110.04
23	W	1060	CHD	C6-C5-C10	6.68	119.77	112.66
24	P	1272	DMU	O5-C4-C3	6.67	123.52	109.72
24	M	526	DMU	O5-C4-C3	6.64	123.44	109.72
24	P	1272	DMU	O5-C4-C57	6.57	122.72	106.44
24	C	272	DMU	O7-C3-C4	6.57	126.71	109.48
23	C	271	CHD	C1-C10-C5	6.46	117.02	107.75
23	J	60	CHD	C10-C9-C8	6.34	118.90	111.84
24	C	272	DMU	C18-O16-C6	6.33	124.49	113.68
23	C	271	CHD	C4-C3-C2	6.18	118.16	110.62
23	P	1271	CHD	C1-C10-C5	6.15	116.58	107.75
23	W	1060	CHD	C10-C9-C8	6.15	118.69	111.84
23	C	271	CHD	C4-C5-C10	6.08	119.14	112.66
24	C	272	DMU	O7-C3-C2	6.08	122.69	107.23
23	J	60	CHD	C4-C3-C2	6.05	118.00	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	1060	CHD	C4-C3-C2	6.05	118.00	110.62
24	M	526	DMU	O7-C3-C2	6.01	122.50	107.23
23	W	1060	CHD	C18-C13-C14	-6.01	101.79	111.20
23	C	271	CHD	C14-C13-C12	5.95	112.86	107.42
23	W	1060	CHD	C11-C9-C10	5.92	119.71	113.70
23	J	60	CHD	C6-C5-C10	5.86	118.89	112.66
23	P	1271	CHD	C14-C13-C12	5.83	112.75	107.42
23	P	1271	CHD	C4-C5-C10	5.81	118.84	112.66
24	P	1272	DMU	O7-C3-C2	5.80	121.97	107.23
24	C	272	DMU	O5-C4-C57	5.72	120.61	106.44
24	C	272	DMU	O7-C10-C5	5.72	122.16	108.09
24	M	526	DMU	C18-O16-C6	5.69	123.41	113.68
23	J	60	CHD	C15-C14-C8	-5.68	110.57	118.36
23	W	1060	CHD	C15-C14-C8	-5.67	110.58	118.36
23	J	60	CHD	C18-C13-C14	-5.66	102.34	111.20
23	P	1271	CHD	C4-C3-C2	5.62	117.47	110.62
24	P	1272	DMU	O1-C9-C8	5.60	119.79	109.70
24	Z	1526	DMU	O7-C3-C2	5.56	121.35	107.23
24	C	272	DMU	C10-O1-C9	5.56	124.57	113.72
23	J	60	CHD	C11-C9-C10	5.52	119.30	113.70
24	C	272	DMU	C8-C7-C5	5.37	120.25	110.83
24	P	1272	DMU	O5-C6-C1	5.36	121.39	110.37
24	M	526	DMU	O16-C6-C1	5.33	116.37	108.27
24	P	1272	DMU	C10-O1-C9	5.32	124.11	113.72
24	P	1272	DMU	O7-C10-C5	5.32	121.17	108.09
23	C	525	CHD	C13-C17-C20	5.32	125.92	119.48
23	C	525	CHD	C14-C13-C12	-5.30	102.57	107.42
24	Z	1526	DMU	C18-O16-C6	5.28	122.70	113.68
23	P	1271	CHD	C15-C14-C8	-5.28	111.11	118.36
23	C	271	CHD	C9-C8-C7	5.26	118.47	111.86
23	P	1525	CHD	C13-C17-C20	5.18	125.76	119.48
23	P	1271	CHD	C9-C8-C7	5.18	118.38	111.86
23	C	271	CHD	C15-C14-C8	-5.15	111.29	118.36
19	A	521	TGL	CG2-OG2-CB1	5.10	130.00	117.80
24	Z	1526	DMU	O16-C6-C1	5.08	115.99	108.27
24	C	272	DMU	O1-C9-C8	5.02	118.74	109.70
23	W	1060	CHD	C1-C10-C5	4.98	114.89	107.75
19	N	1521	TGL	CG2-OG2-CB1	4.91	129.56	117.80
19	L	522	TGL	C12-C11-C10	-4.78	90.22	114.37
19	Y	1522	TGL	C12-C11-C10	-4.76	90.31	114.37
23	B	1086	CHD	C15-C14-C13	-4.70	98.99	103.54
23	J	60	CHD	C1-C10-C5	4.64	114.41	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Y	1522	TGL	CB9-CB8-CB7	-4.62	91.02	114.37
23	J	60	CHD	C5-C6-C7	4.60	119.87	114.40
23	J	60	CHD	C2-C1-C10	4.55	120.42	112.74
19	L	522	TGL	CB9-CB8-CB7	-4.52	91.51	114.37
24	Z	1526	DMU	C6-C1-C2	4.51	119.49	110.01
23	B	1086	CHD	C16-C17-C13	-4.50	99.18	103.54
23	P	1525	CHD	C14-C13-C12	-4.45	103.35	107.42
23	O	229	CHD	C16-C17-C13	-4.43	99.24	103.54
23	W	1060	CHD	C2-C1-C10	4.36	120.10	112.74
23	J	60	CHD	O12-C12-C13	4.35	118.36	111.02
23	W	1060	CHD	O12-C12-C13	4.31	118.30	111.02
23	C	271	CHD	C19-C10-C1	-4.30	101.47	108.31
24	M	526	DMU	C6-C1-C2	4.29	119.03	110.01
23	W	1060	CHD	C9-C8-C7	4.19	117.13	111.86
23	J	60	CHD	C13-C14-C8	4.13	119.95	114.72
19	A	521	TGL	CG1-OG1-CA1	-4.13	102.02	117.12
23	W	1060	CHD	C13-C14-C8	4.12	119.94	114.72
19	N	1521	TGL	CG1-OG1-CA1	-4.11	102.09	117.12
23	W	1060	CHD	C5-C6-C7	4.11	119.29	114.40
24	Z	1526	DMU	O7-C10-O1	4.09	121.45	110.69
23	J	60	CHD	C14-C8-C7	4.08	117.27	111.85
23	C	525	CHD	C15-C14-C8	-4.07	112.78	118.36
19	Y	1522	TGL	C15-CC9-CC8	4.07	134.94	114.37
24	C	272	DMU	O5-C6-C1	4.06	118.72	110.37
24	P	1272	DMU	O7-C10-O1	4.06	121.37	110.69
23	J	60	CHD	C9-C8-C7	4.05	116.96	111.86
24	C	272	DMU	O7-C10-O1	4.04	121.33	110.69
23	C	271	CHD	C18-C13-C12	-4.04	105.01	109.06
19	L	522	TGL	C15-CC9-CC8	4.03	134.73	114.37
24	P	1272	DMU	C8-C7-C5	4.01	117.87	110.83
23	W	1060	CHD	C14-C8-C7	3.96	117.10	111.85
23	J	60	CHD	C5-C4-C3	3.95	118.66	112.71
23	W	1060	CHD	C5-C4-C3	3.93	118.64	112.71
23	O	229	CHD	C10-C9-C8	3.92	116.20	111.84
23	P	1525	CHD	C15-C14-C8	-3.88	113.04	118.36
25	T	263	PEK	P-O11-C03	3.86	143.45	121.35
24	M	526	DMU	O7-C10-C5	3.84	117.53	108.09
19	Y	1522	TGL	C16-C15-CC9	3.82	133.67	114.37
23	P	1525	CHD	C1-C10-C5	3.82	113.23	107.75
23	C	271	CHD	C9-C11-C12	3.81	119.28	114.29
24	M	526	DMU	C10-O7-C3	3.81	127.00	117.98
19	L	522	TGL	C16-C15-CC9	3.80	133.59	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	1263	PEK	P-O11-C03	3.75	142.85	121.35
19	A	523	TGL	CG3-OG3-CC1	3.68	130.58	117.12
23	P	1271	CHD	C19-C10-C1	-3.63	102.54	108.31
23	B	1086	CHD	C15-C14-C8	-3.62	113.39	118.36
25	G	1263	PEK	O03-C01-C02	3.62	118.84	108.40
19	L	522	TGL	CC3-CC2-CC1	3.62	126.97	113.69
24	Z	1526	DMU	O7-C3-C4	3.59	118.89	109.48
19	Q	1523	TGL	CG3-OG3-CC1	3.58	130.20	117.12
25	T	263	PEK	O03-C01-C02	3.57	118.68	108.40
23	J	60	CHD	C11-C12-C13	3.56	114.88	111.26
23	P	1271	CHD	C9-C11-C12	3.54	118.92	114.29
24	C	272	DMU	C2-C3-C4	-3.53	103.10	110.93
23	O	229	CHD	C15-C14-C13	-3.53	100.12	103.54
23	J	60	CHD	C6-C5-C4	3.51	115.24	111.23
19	L	522	TGL	CG2-OG2-CB1	3.51	126.21	117.80
26	P	1270	CDL	PA1-OA5-CA3	3.51	141.49	121.35
19	L	522	TGL	C11-C10-CB9	3.50	132.06	114.37
23	O	229	CHD	C15-C14-C8	-3.47	113.60	118.36
23	P	1271	CHD	C14-C8-C7	3.46	116.44	111.85
24	M	526	DMU	O5-C6-C1	3.44	117.45	110.37
19	Y	1522	TGL	C11-C10-CB9	3.44	131.74	114.37
26	C	270	CDL	PA1-OA5-CA3	3.42	140.94	121.35
20	A	524	PGV	C02-O01-C1	3.40	125.94	117.80
19	Y	1522	TGL	CC3-CC2-CC1	3.39	126.13	113.69
24	Z	1526	DMU	O5-C6-C1	3.37	117.29	110.37
25	C	264	PEK	O03-C21-C22	-3.37	101.57	111.83
24	C	272	DMU	C10-O7-C3	3.36	125.95	117.98
23	W	1060	CHD	C16-C15-C14	3.36	111.72	105.14
23	P	1525	CHD	C11-C12-C13	-3.36	107.85	111.26
23	P	1525	CHD	C14-C8-C9	-3.33	105.10	109.75
23	C	271	CHD	C14-C8-C7	3.32	116.26	111.85
23	J	60	CHD	C1-C2-C3	3.31	114.86	110.48
24	P	1272	DMU	C10-O7-C3	3.31	125.81	117.98
19	Y	1522	TGL	CG2-OG2-CB1	3.31	125.71	117.80
23	C	525	CHD	C10-C9-C8	3.29	115.50	111.84
18	N	516	HEA	C3C-C4C-NC	3.28	112.56	109.80
24	M	526	DMU	O7-C10-O1	3.28	119.33	110.69
20	N	1524	PGV	C02-O01-C1	3.27	125.63	117.80
23	O	229	CHD	C5-C6-C7	3.27	118.29	114.40
25	C	265	PEK	P-O11-C03	3.24	139.91	121.35
23	W	1060	CHD	C6-C5-C4	3.23	114.92	111.23
23	O	229	CHD	C5-C4-C3	3.22	117.57	112.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Z	1526	DMU	C10-O7-C3	3.21	125.59	117.98
24	M	526	DMU	O7-C3-C4	3.21	117.89	109.48
23	W	1060	CHD	C1-C2-C3	3.20	114.72	110.48
23	W	1060	CHD	C11-C12-C13	3.19	114.51	111.26
23	W	1060	CHD	C18-C13-C12	-3.18	105.88	109.06
23	J	60	CHD	C16-C15-C14	3.17	111.35	105.14
23	P	1271	CHD	C18-C13-C12	-3.17	105.88	109.06
23	P	1271	CHD	C5-C4-C3	3.16	117.47	112.71
26	C	270	CDL	OB6-CB5-C51	-3.15	104.67	111.48
25	P	1265	PEK	P-O11-C03	3.14	139.36	121.35
23	J	60	CHD	C14-C8-C9	3.14	114.13	109.75
23	B	1086	CHD	C10-C9-C8	3.12	115.32	111.84
23	P	1271	CHD	C5-C6-C7	3.10	118.08	114.40
18	N	516	HEA	C27-C19-C20	3.10	120.61	115.23
23	B	1086	CHD	C1-C10-C5	3.09	112.18	107.75
18	A	515	HEA	C26-C15-C16	3.07	120.56	115.23
23	J	60	CHD	C15-C16-C17	3.07	111.15	105.14
22	O	1230	PSC	C01-O03-C19	-3.06	105.92	117.12
23	P	1525	CHD	C10-C9-C8	3.06	115.25	111.84
26	P	1270	CDL	CB6-OB8-CB7	-3.05	105.96	117.12
19	L	522	TGL	CC4-CC3-CC2	3.05	124.34	113.13
23	B	1086	CHD	C1-C2-C3	3.04	114.50	110.48
18	A	516	HEA	CMB-C2B-C3B	-3.03	124.41	130.28
19	A	521	TGL	CG3-OG3-CC1	3.03	128.19	117.12
23	W	1060	CHD	C15-C16-C17	3.02	111.05	105.14
18	A	515	HEA	C3C-C2C-C1C	-3.02	103.61	107.17
23	C	525	CHD	C14-C8-C9	-3.01	105.54	109.75
19	Q	1523	TGL	CG1-OG1-CA1	-3.01	106.13	117.12
23	W	1060	CHD	C14-C8-C9	3.01	113.95	109.75
19	Y	1522	TGL	CC4-CC3-CC2	2.99	124.09	113.13
26	C	270	CDL	CB6-OB8-CB7	-2.97	106.24	117.12
23	C	271	CHD	C15-C16-C17	2.97	110.96	105.14
23	O	229	CHD	C1-C10-C5	2.97	112.01	107.75
24	M	526	DMU	C10-O1-C9	2.97	119.52	113.72
19	Q	1523	TGL	OG2-CG2-CG3	2.96	118.96	108.34
18	N	515	HEA	C26-C15-C16	2.96	120.36	115.23
25	P	1264	PEK	C3-C2-C1	-2.95	102.89	113.69
25	C	264	PEK	C3-C2-C1	-2.95	102.90	113.69
23	C	525	CHD	C1-C10-C5	2.93	111.95	107.75
23	B	1086	CHD	C5-C4-C3	2.93	117.12	112.71
19	N	1521	TGL	CG3-OG3-CC1	2.92	127.79	117.12
23	J	60	CHD	C18-C13-C12	-2.91	106.15	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	1269	CDL	C23-C22-C21	2.90	129.05	114.37
22	B	230	PSC	C01-O03-C19	-2.90	106.52	117.12
19	A	523	TGL	CB3-CB2-CB1	2.90	124.31	113.69
23	P	1271	CHD	C1-C2-C3	2.88	114.30	110.48
23	C	271	CHD	C1-C10-C9	2.88	115.81	111.34
23	C	271	CHD	C1-C2-C3	2.87	114.28	110.48
20	C	267	PGV	O01-C1-C2	-2.86	105.29	111.48
25	G	1263	PEK	C02-O01-C1	2.86	124.63	117.80
23	W	1060	CHD	C9-C11-C12	2.86	118.03	114.29
19	A	523	TGL	OG1-CG1-CG2	2.85	116.61	108.40
23	B	1086	CHD	C9-C11-C12	2.84	118.01	114.29
26	P	1270	CDL	OB6-CB5-C51	-2.84	105.34	111.48
25	P	1265	PEK	C11-C10-C9	2.84	126.00	112.02
26	T	1269	CDL	C22-C21-C20	2.84	128.70	114.37
19	A	523	TGL	CG1-OG1-CA1	-2.83	106.76	117.12
23	B	1086	CHD	C17-C13-C14	2.83	102.95	100.11
24	Z	1526	DMU	O7-C10-C5	2.83	115.04	108.09
26	G	269	CDL	C22-C21-C20	2.82	128.60	114.37
26	G	269	CDL	C23-C22-C21	2.81	128.56	114.37
25	C	265	PEK	C11-C10-C9	2.78	125.72	112.02
25	T	263	PEK	C02-O01-C1	2.76	124.40	117.80
23	P	1271	CHD	C15-C16-C17	2.75	110.53	105.14
23	P	1271	CHD	C9-C10-C5	2.75	112.33	108.51
19	A	523	TGL	OG2-CG2-CG3	2.74	118.17	108.34
23	P	1525	CHD	C1-C2-C3	2.74	114.11	110.48
25	P	1265	PEK	P-O12-C04	2.73	134.28	121.26
23	J	60	CHD	C19-C10-C1	-2.73	103.97	108.31
23	P	1271	CHD	C2-C1-C10	2.73	117.34	112.74
23	C	271	CHD	C5-C6-C7	2.73	117.64	114.40
26	C	270	CDL	OB6-CB5-OB7	2.71	130.04	123.70
19	L	522	TGL	C20-CA9-CA8	2.70	128.01	114.37
23	C	525	CHD	C5-C6-C7	2.70	117.61	114.40
25	C	265	PEK	P-O12-C04	2.69	134.07	121.26
25	P	1264	PEK	O03-C01-C02	-2.68	100.66	108.40
25	C	264	PEK	C23-C22-C21	-2.68	103.87	113.69
23	W	1060	CHD	C19-C10-C1	-2.68	104.05	108.31
24	C	272	DMU	O1-C10-C5	2.67	115.86	110.37
23	O	229	CHD	C1-C2-C3	2.66	114.01	110.48
23	C	271	CHD	C16-C15-C14	2.66	110.36	105.14
19	Y	1522	TGL	C13-C12-C11	2.65	127.77	114.37
23	P	1271	CHD	C11-C9-C10	2.64	116.39	113.70
23	P	1271	CHD	C16-C15-C14	2.64	110.32	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Q	1523	TGL	CB3-CB2-CB1	2.62	123.30	113.69
18	A	516	HEA	C4A-C3A-C2A	-2.61	104.55	106.81
25	P	1264	PEK	O03-C21-C22	-2.61	103.88	111.83
24	P	1272	DMU	O1-C10-C5	2.60	115.72	110.37
20	P	1267	PGV	C9-C10-C11	-2.59	98.10	112.60
23	C	271	CHD	C5-C4-C3	2.58	116.59	112.71
23	O	229	CHD	C17-C13-C14	2.58	102.70	100.11
24	M	526	DMU	C1-C2-C3	2.57	115.52	109.68
23	C	271	CHD	C11-C9-C10	2.57	116.31	113.70
23	P	1271	CHD	C1-C10-C9	2.56	115.31	111.34
26	G	269	CDL	C20-C19-C18	2.56	127.30	114.37
19	L	522	TGL	C13-C12-C11	2.55	127.24	114.37
26	T	1269	CDL	C20-C19-C18	2.53	127.13	114.37
23	C	271	CHD	C9-C10-C5	2.52	112.02	108.51
26	P	1270	CDL	OB6-CB5-OB7	2.52	129.60	123.70
23	P	1271	CHD	C11-C12-C13	2.51	113.82	111.26
19	Y	1522	TGL	C20-CA9-CA8	2.51	127.06	114.37
19	Y	1522	TGL	C10-CB9-CB8	2.51	127.06	114.37
23	O	229	CHD	C9-C11-C12	2.50	117.56	114.29
19	L	522	TGL	OG1-CG1-CG2	2.49	115.58	108.40
20	N	1266	PGV	O01-C1-C2	-2.49	106.09	111.48
23	B	1086	CHD	C14-C8-C9	-2.49	106.28	109.75
18	A	515	HEA	C26-C15-C14	-2.48	117.25	123.63
23	C	271	CHD	C2-C1-C10	2.48	116.93	112.74
19	A	521	TGL	CG3-CG2-CG1	2.48	117.57	111.78
26	C	270	CDL	OA8-CA6-CA4	2.48	115.54	108.40
19	N	1521	TGL	OG2-CG2-CG3	2.47	117.22	108.34
19	A	521	TGL	CA8-CA7-CA6	-2.47	101.86	114.37
18	N	515	HEA	C3C-C2C-C1C	-2.47	104.26	107.17
19	N	1521	TGL	CA8-CA7-CA6	-2.46	101.92	114.37
25	P	1264	PEK	C23-C22-C21	-2.46	104.69	113.69
20	N	1524	PGV	C3-C2-C1	-2.46	104.69	113.69
23	P	1525	CHD	C5-C6-C7	2.45	117.32	114.40
18	N	515	HEA	C3C-C4C-NC	2.45	111.86	109.80
23	J	60	CHD	C9-C11-C12	2.45	117.49	114.29
24	Z	1526	DMU	C10-O1-C9	2.44	118.49	113.72
18	N	516	HEA	CMB-C2B-C3B	-2.44	125.56	130.28
23	O	229	CHD	C19-C10-C1	-2.44	104.43	108.31
25	C	265	PEK	C24-C23-C22	2.44	122.08	113.13
19	L	522	TGL	C10-CB9-CB8	2.43	126.63	114.37
19	Y	1522	TGL	OG1-CG1-CG2	2.43	115.39	108.40
23	W	1060	CHD	C19-C10-C5	-2.42	106.39	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Z	1526	DMU	C1-C2-C3	2.42	115.16	109.68
23	C	525	CHD	C11-C12-C13	-2.40	108.83	111.26
20	C	267	PGV	C9-C10-C11	-2.40	99.18	112.60
25	P	1265	PEK	C03-C02-C01	2.40	117.37	111.78
25	T	263	PEK	P-O12-C04	2.39	132.65	121.26
18	A	516	HEA	C4B-NB-C1B	-2.39	102.38	105.21
19	A	521	TGL	OG2-CG2-CG3	2.39	116.90	108.34
23	J	60	CHD	C19-C10-C5	-2.38	106.46	110.44
20	N	1266	PGV	C01-O03-C19	-2.38	108.41	117.12
18	A	516	HEA	C21-C20-C19	2.38	121.07	113.19
25	C	264	PEK	O03-C21-O04	2.38	129.57	123.63
23	P	1525	CHD	C19-C10-C9	-2.37	107.98	111.18
23	C	525	CHD	C9-C11-C12	2.37	117.40	114.29
23	O	229	CHD	C14-C8-C9	-2.37	106.44	109.75
25	G	1263	PEK	P-O12-C04	2.37	132.53	121.26
26	C	270	CDL	C52-C51-CB5	-2.36	105.05	113.69
19	Q	1523	TGL	OG1-CG1-CG2	2.36	115.20	108.40
19	A	523	TGL	OG2-CG2-CG1	2.36	116.80	108.34
26	P	1270	CDL	OA8-CA6-CA4	2.36	115.19	108.40
19	N	1521	TGL	C10-CB9-CB8	2.35	126.22	114.37
20	A	524	PGV	O01-C02-C03	2.34	116.75	108.34
20	A	524	PGV	C3-C2-C1	-2.34	105.11	113.69
23	P	1525	CHD	C11-C9-C10	2.33	116.07	113.70
18	A	516	HEA	C1D-ND-C4D	-2.33	102.45	105.21
18	A	516	HEA	C27-C19-C20	2.33	119.27	115.23
19	Q	1523	TGL	OG2-CG2-CG1	2.32	116.68	108.34
24	P	1272	DMU	C2-C3-C4	-2.32	105.78	110.93
19	L	522	TGL	CC7-CC6-CC5	2.31	126.06	114.37
23	B	1086	CHD	C14-C13-C12	-2.31	105.31	107.42
25	C	265	PEK	C03-C02-C01	2.29	117.14	111.78
26	T	1269	CDL	C19-C18-C17	2.29	125.97	114.37
20	N	1524	PGV	O01-C02-C03	2.29	116.56	108.34
25	C	265	PEK	O03-C01-C02	2.29	115.00	108.40
18	N	516	HEA	C17-C18-C19	2.29	132.86	127.62
26	G	269	CDL	C19-C18-C17	2.28	125.92	114.37
19	N	1521	TGL	CG3-CG2-CG1	2.28	117.11	111.78
24	P	1272	DMU	O5-C6-O16	2.28	115.43	110.04
26	P	1270	CDL	C52-C51-CB5	-2.27	105.39	113.69
25	P	1265	PEK	O03-C01-C02	2.26	114.92	108.40
18	A	516	HEA	C3C-C4C-NC	2.26	111.70	109.80
23	J	60	CHD	C4-C5-C10	2.26	115.07	112.66
18	A	516	HEA	CMC-C2C-C3C	2.26	131.87	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	515	HEA	CHC-C4B-NB	2.25	127.15	124.37
18	N	516	HEA	O11-C11-C3B	-2.25	107.13	111.26
19	A	521	TGL	C10-CB9-CB8	2.25	125.75	114.37
23	C	271	CHD	C11-C12-C13	2.24	113.54	111.26
23	P	1271	CHD	C6-C5-C4	2.24	113.78	111.23
25	C	264	PEK	O01-C1-C2	-2.23	106.66	111.48
25	P	1265	PEK	C24-C23-C22	2.23	121.31	113.13
25	T	263	PEK	C03-C02-C01	2.22	116.95	111.78
24	C	272	DMU	O5-C6-O16	2.20	115.24	110.04
25	P	1264	PEK	O03-C21-O04	2.20	129.12	123.63
23	C	271	CHD	C6-C5-C10	2.19	114.99	112.66
23	C	525	CHD	C19-C10-C9	-2.19	108.23	111.18
20	A	604	PGV	O01-C1-C2	-2.17	106.79	111.48
18	A	515	HEA	C3A-C2A-C1A	2.17	109.10	107.05
26	T	1269	CDL	OB8-CB6-CB4	2.17	114.64	108.40
23	C	525	CHD	C18-C13-C12	2.16	111.22	109.06
25	G	1263	PEK	C03-C02-C01	2.16	116.81	111.78
23	C	525	CHD	C11-C9-C10	2.15	115.88	113.70
23	J	60	CHD	C1-C10-C9	2.15	114.67	111.34
19	Y	1522	TGL	CC7-CC6-CC5	2.14	125.16	114.37
26	T	1269	CDL	OB8-CB7-C71	-2.13	105.34	111.83
18	N	516	HEA	C21-C20-C19	2.13	120.24	113.19
20	C	267	PGV	C3-C2-C1	-2.12	105.92	113.69
23	C	525	CHD	C6-C5-C10	2.12	114.91	112.66
26	G	269	CDL	OB8-CB7-C71	-2.11	105.41	111.83
20	N	1266	PGV	O03-C01-C02	2.11	114.47	108.40
19	A	521	TGL	OG1-CG1-CG2	2.10	114.46	108.40
19	N	1521	TGL	CA6-CA5-CA4	-2.10	103.76	114.37
19	N	1521	TGL	OG1-CG1-CG2	2.09	114.42	108.40
26	G	269	CDL	OB8-CB6-CB4	2.08	114.40	108.40
18	A	516	HEA	C26-C15-C16	2.07	118.83	115.23
19	A	523	TGL	CC3-CC2-CC1	-2.07	106.10	113.69
18	A	516	HEA	C3C-C2C-C1C	-2.07	104.73	107.17
26	P	1270	CDL	C82-C81-C80	2.06	124.78	114.37
19	A	523	TGL	CG2-OG2-CB1	2.06	122.72	117.80
25	P	1264	PEK	C24-C23-C22	-2.05	105.58	113.13
23	P	1525	CHD	C9-C11-C12	2.05	116.97	114.29
18	N	515	HEA	C26-C15-C14	-2.04	118.38	123.63
23	J	60	CHD	C19-C10-C9	-2.04	108.43	111.18
19	A	523	TGL	CB4-CB3-CB2	2.04	120.63	113.13
19	A	523	TGL	CB8-CB7-CB6	2.04	124.67	114.37
19	A	521	TGL	CA6-CA5-CA4	-2.04	104.08	114.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Y	1522	TGL	OG2-CB1-OB1	2.03	128.44	123.70
23	P	1271	CHD	C18-C13-C14	-2.02	108.03	111.20
19	L	522	TGL	OG2-CB1-OB1	2.02	128.44	123.70
19	A	523	TGL	CA3-CA2-CA1	-2.02	106.28	113.69
23	C	525	CHD	C1-C2-C3	2.02	113.15	110.48
26	T	1269	CDL	C83-C82-C81	2.00	124.48	114.37

All (42) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
24	P	1272	DMU	C10
24	P	1272	DMU	C6
24	P	1272	DMU	C5
24	P	1272	DMU	C4
24	P	1272	DMU	C2
24	Z	1526	DMU	C9
24	Z	1526	DMU	C2
24	Z	1526	DMU	C5
24	Z	1526	DMU	C6
24	Z	1526	DMU	C4

All (850) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	524	PGV	C04-O12-P-O11
20	A	524	PGV	C04-O12-P-O13
20	A	524	PGV	C04-O12-P-O14
20	A	524	PGV	C02-C03-O11-P
20	A	524	PGV	C05-C04-O12-P
20	A	524	PGV	C04-C05-C06-O06
20	A	524	PGV	O02-C1-O01-C02
20	A	524	PGV	C20-C19-O03-C01
20	C	268	PGV	C04-O12-P-O11
20	C	268	PGV	C04-O12-P-O13
20	C	268	PGV	C04-O12-P-O14
20	C	268	PGV	O05-C05-C06-O06
20	N	1524	PGV	C04-O12-P-O11
20	N	1524	PGV	C04-O12-P-O13
20	N	1524	PGV	C04-O12-P-O14
20	N	1524	PGV	C02-C03-O11-P
20	N	1524	PGV	C05-C04-O12-P
20	N	1524	PGV	C04-C05-C06-O06
20	N	1524	PGV	O02-C1-O01-C02
20	N	1524	PGV	C20-C19-O03-C01
20	P	1268	PGV	C04-O12-P-O11
20	P	1268	PGV	C04-O12-P-O13
20	P	1268	PGV	C04-O12-P-O14
22	B	230	PSC	C03-O11-P-O14
22	B	230	PSC	C04-O12-P-O14
22	O	1230	PSC	C03-O11-P-O14
22	O	1230	PSC	C04-O12-P-O11
22	O	1230	PSC	C04-O12-P-O14

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Mol	Chain	Res	Type	Atoms
23	J	60	CHD	C16-C17-C20-C21
23	J	60	CHD	C16-C17-C20-C22
23	W	1060	CHD	C16-C17-C20-C21
23	W	1060	CHD	C16-C17-C20-C22
24	M	526	DMU	O5-C6-O16-C18
24	Z	1526	DMU	O5-C6-O16-C18
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-O14
25	G	1263	PEK	O12-C04-C05-N
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
26	G	269	CDL	OB6-CB4-CB6-OB8
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

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Mol	Chain	Res	Type	Atoms
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
26	T	1269	CDL	OB6-CB4-CB6-OB8
20	A	524	PGV	O04-C19-O03-C01
20	N	1524	PGV	O04-C19-O03-C01
19	A	523	TGL	OC1-CC1-OG3-CG3
19	Q	1523	TGL	OC1-CC1-OG3-CG3
19	A	521	TGL	OB1-CB1-OG2-CG2
19	N	1521	TGL	OB1-CB1-OG2-CG2
22	B	230	PSC	O02-C1-O01-C02
22	O	1230	PSC	O02-C1-O01-C02
26	C	270	CDL	OA7-CA5-OA6-CA4
26	P	1270	CDL	OA7-CA5-OA6-CA4
19	A	521	TGL	CB2-CB1-OG2-CG2
19	N	1521	TGL	CB2-CB1-OG2-CG2
20	A	524	PGV	C2-C1-O01-C02
20	N	1524	PGV	C2-C1-O01-C02
19	A	523	TGL	CC2-CC1-OG3-CG3
19	Q	1523	TGL	CC2-CC1-OG3-CG3
26	G	269	CDL	C31-CA7-OA8-CA6
26	T	1269	CDL	C31-CA7-OA8-CA6
26	C	270	CDL	C80-C81-C82-C83
24	C	272	DMU	O6-C11-C9-O1
24	P	1272	DMU	O6-C11-C9-O1
19	A	521	TGL	OA1-CA1-OG1-CG1
19	L	522	TGL	OA1-CA1-OG1-CG1
19	N	1521	TGL	OA1-CA1-OG1-CG1
19	Y	1522	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	C40-C41-C42-C43
26	G	269	CDL	C20-C21-C22-C23
26	P	1270	CDL	C40-C41-C42-C43
26	P	1270	CDL	C60-C61-C62-C63
26	P	1270	CDL	C80-C81-C82-C83
26	T	1269	CDL	C77-C78-C79-C80
19	A	521	TGL	C16-C15-CC9-CC8
26	C	270	CDL	C57-C58-C59-C60
26	C	270	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
26	C	270	CDL	C77-C78-C79-C80
26	G	269	CDL	C17-C18-C19-C20
26	G	269	CDL	C40-C41-C42-C43
26	G	269	CDL	C57-C58-C59-C60
26	G	269	CDL	C77-C78-C79-C80
26	G	269	CDL	C80-C81-C82-C83
26	P	1270	CDL	C57-C58-C59-C60
26	T	1269	CDL	C17-C18-C19-C20
26	T	1269	CDL	C20-C21-C22-C23
26	T	1269	CDL	C40-C41-C42-C43
26	T	1269	CDL	C57-C58-C59-C60
26	G	269	CDL	O1-C1-CA2-OA2
26	T	1269	CDL	O1-C1-CA2-OA2
19	A	521	TGL	CA2-CA1-OG1-CG1
19	N	1521	TGL	CA2-CA1-OG1-CG1
19	N	1521	TGL	C16-C15-CC9-CC8
26	P	1270	CDL	C37-C38-C39-C40
22	B	230	PSC	C2-C1-O01-C02
22	O	1230	PSC	C2-C1-O01-C02
26	C	270	CDL	C20-C21-C22-C23
26	G	269	CDL	C37-C38-C39-C40
26	P	1270	CDL	C20-C21-C22-C23
26	P	1270	CDL	C77-C78-C79-C80
26	T	1269	CDL	C37-C38-C39-C40
26	T	1269	CDL	C80-C81-C82-C83
26	C	270	CDL	C37-C38-C39-C40
26	T	1269	CDL	C60-C61-C62-C63
19	Y	1522	TGL	C21-C20-CA9-CA8
19	L	522	TGL	C21-C20-CA9-CA8
26	C	270	CDL	C17-C18-C19-C20
26	G	269	CDL	C60-C61-C62-C63
26	P	1270	CDL	C17-C18-C19-C20
19	A	523	TGL	C21-C20-CA9-CA8
19	Q	1523	TGL	C21-C20-CA9-CA8
19	Y	1522	TGL	CA2-CA1-OG1-CG1
19	A	523	TGL	C11-C10-CB9-CB8
19	Q	1523	TGL	C11-C10-CB9-CB8
23	W	1060	CHD	C17-C20-C22-C23
19	N	1521	TGL	C21-C20-CA9-CA8
19	Q	1523	TGL	C16-C15-CC9-CC8
19	A	521	TGL	C21-C20-CA9-CA8
19	A	521	TGL	C11-C10-CB9-CB8

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Mol	Chain	Res	Type	Atoms
19	A	523	TGL	C16-C15-CC9-CC8
19	L	522	TGL	C16-C15-CC9-CC8
19	N	1521	TGL	C11-C10-CB9-CB8
19	Y	1522	TGL	C16-C15-CC9-CC8
20	A	524	PGV	O12-C04-C05-C06
20	N	1524	PGV	O12-C04-C05-C06
19	L	522	TGL	CA2-CA1-OG1-CG1
22	B	230	PSC	C20-C19-O03-C01
22	O	1230	PSC	C20-C19-O03-C01
19	Y	1522	TGL	C11-C10-CB9-CB8
23	W	1060	CHD	C13-C17-C20-C22
19	L	522	TGL	C11-C10-CB9-CB8
24	C	272	DMU	C1-C6-O16-C18
23	W	1060	CHD	C21-C20-C22-C23
20	A	524	PGV	O12-C04-C05-O05
20	N	1524	PGV	O12-C04-C05-O05
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
22	B	230	PSC	O04-C19-O03-C01
22	O	1230	PSC	O04-C19-O03-C01
24	P	1272	DMU	C3-C4-C57-O61
24	M	526	DMU	O5-C4-C57-O61
23	W	1060	CHD	C13-C17-C20-C21
23	J	60	CHD	C13-C17-C20-C22
23	J	60	CHD	C17-C20-C22-C23
24	C	272	DMU	C3-C4-C57-O61
23	J	60	CHD	C21-C20-C22-C23
24	Z	1526	DMU	O5-C4-C57-O61
20	P	1268	PGV	O05-C05-C06-O06
24	M	526	DMU	O6-C11-C9-C8
23	J	60	CHD	C13-C17-C20-C21
20	A	524	PGV	C19-C20-C21-C22
20	N	1524	PGV	C19-C20-C21-C22
22	B	230	PSC	C1-C2-C3-C4
24	Z	1526	DMU	O6-C11-C9-C8
22	O	1230	PSC	C1-C2-C3-C4
20	C	268	PGV	O12-C04-C05-O05
20	P	1268	PGV	O12-C04-C05-O05
24	M	526	DMU	O16-C18-C19-C22
24	Z	1526	DMU	O16-C18-C19-C22

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Mol	Chain	Res	Type	Atoms
19	A	523	TGL	CA2-CA1-OG1-CG1
19	L	522	TGL	CC3-CC4-CC5-CC6
19	Q	1523	TGL	CA2-CA1-OG1-CG1
20	P	1268	PGV	C2-C1-O01-C02
26	T	1269	CDL	C11-CA5-OA6-CA4
25	G	1263	PEK	C28-C29-C30-C31
25	T	263	PEK	C28-C29-C30-C31
22	B	230	PSC	C20-C21-C22-C23
22	O	1230	PSC	C20-C21-C22-C23
19	A	523	TGL	OA1-CA1-OG1-CG1
19	Q	1523	TGL	OA1-CA1-OG1-CG1
26	C	270	CDL	CB7-C71-C72-C73
26	G	269	CDL	CA5-C11-C12-C13
26	P	1270	CDL	CB7-C71-C72-C73
26	T	1269	CDL	CA5-C11-C12-C13
26	G	269	CDL	OA7-CA5-OA6-CA4
26	T	1269	CDL	OA7-CA5-OA6-CA4
20	C	268	PGV	O12-C04-C05-C06
20	P	1268	PGV	O12-C04-C05-C06
26	G	269	CDL	CA2-C1-CB2-OB2
26	T	1269	CDL	CA2-C1-CB2-OB2
23	C	271	CHD	C17-C20-C22-C23
20	C	268	PGV	C2-C1-O01-C02
26	G	269	CDL	C11-CA5-OA6-CA4
19	Y	1522	TGL	CC3-CC4-CC5-CC6
20	C	268	PGV	O02-C1-O01-C02
20	P	1268	PGV	O02-C1-O01-C02
24	P	1272	DMU	C1-C6-O16-C18
24	P	1272	DMU	O5-C4-C57-O61
19	A	521	TGL	OC1-CC1-OG3-CG3
20	C	268	PGV	C04-C05-C06-O06
20	P	1268	PGV	C04-C05-C06-O06
23	C	271	CHD	C21-C20-C22-C23
24	Z	1526	DMU	C3-C4-C57-O61
23	P	1271	CHD	C17-C20-C22-C23
25	G	1263	PEK	O03-C01-C02-O01
19	N	1521	TGL	OC1-CC1-OG3-CG3
20	N	1524	PGV	C4-C5-C6-C7
22	B	230	PSC	C29-C30-C31-C32
22	O	1230	PSC	C29-C30-C31-C32
26	T	1269	CDL	C58-C59-C60-C61
20	C	268	PGV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
20	N	1266	PGV	C6-C7-C8-C9
20	P	1268	PGV	C22-C23-C24-C25
22	O	1230	PSC	C2-C3-C4-C5
26	C	270	CDL	C51-C52-C53-C54
26	G	269	CDL	C58-C59-C60-C61
20	A	604	PGV	C6-C7-C8-C9
20	C	268	PGV	C13-C14-C15-C16
22	B	230	PSC	C2-C3-C4-C5
20	P	1268	PGV	C13-C14-C15-C16
26	C	270	CDL	C13-C14-C15-C16
26	C	270	CDL	C59-C60-C61-C62
26	P	1270	CDL	C51-C52-C53-C54
20	A	524	PGV	O05-C05-C06-O06
20	N	1524	PGV	O05-C05-C06-O06
20	C	268	PGV	C24-C25-C26-C27
20	P	1268	PGV	C24-C25-C26-C27
26	P	1270	CDL	C13-C14-C15-C16
26	P	1270	CDL	C59-C60-C61-C62
20	A	524	PGV	C4-C5-C6-C7
26	C	270	CDL	C16-C17-C18-C19
26	P	1270	CDL	C16-C17-C18-C19
25	T	263	PEK	C1-C2-C3-C4
25	C	265	PEK	C25-C26-C27-C28
25	P	1265	PEK	C25-C26-C27-C28
26	T	1269	CDL	C56-C57-C58-C59
26	T	1269	CDL	C72-C73-C74-C75
26	T	1269	CDL	C73-C74-C75-C76
26	G	269	CDL	C56-C57-C58-C59
26	G	269	CDL	C72-C73-C74-C75
20	N	1524	PGV	C24-C25-C26-C27
26	G	269	CDL	C13-C14-C15-C16
26	G	269	CDL	C73-C74-C75-C76
20	P	1268	PGV	C1-C2-C3-C4
19	L	522	TGL	CB4-CB5-CB6-CB7
19	Y	1522	TGL	CB4-CB5-CB6-CB7
19	Y	1522	TGL	CC2-CC3-CC4-CC5
24	Z	1526	DMU	C25-C28-C31-C34
25	G	1263	PEK	C29-C30-C31-C32
25	T	263	PEK	C29-C30-C31-C32
26	G	269	CDL	C79-C80-C81-C82
26	T	1269	CDL	C13-C14-C15-C16
26	T	1269	CDL	C79-C80-C81-C82

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Mol	Chain	Res	Type	Atoms
20	A	524	PGV	C24-C25-C26-C27
23	P	1271	CHD	C21-C20-C22-C23
24	M	526	DMU	C25-C28-C31-C34
26	C	270	CDL	C73-C74-C75-C76
26	C	270	CDL	CA5-C11-C12-C13
26	P	1270	CDL	CA5-C11-C12-C13
20	P	1268	PGV	C3-C4-C5-C6
26	C	270	CDL	C55-C56-C57-C58
26	C	270	CDL	C74-C75-C76-C77
26	P	1270	CDL	C55-C56-C57-C58
26	P	1270	CDL	C73-C74-C75-C76
25	C	264	PEK	C22-C21-O03-C01
25	P	1264	PEK	C22-C21-O03-C01
20	A	604	PGV	C29-C30-C31-C32
20	C	268	PGV	C3-C4-C5-C6
25	G	1263	PEK	C27-C28-C29-C30
25	T	263	PEK	C27-C28-C29-C30
20	C	268	PGV	C1-C2-C3-C4
25	C	265	PEK	C21-C22-C23-C24
25	G	1263	PEK	C1-C2-C3-C4
25	P	1265	PEK	C21-C22-C23-C24
19	A	521	TGL	CB6-CB7-CB8-CB9
20	A	604	PGV	C23-C24-C25-C26
20	N	1266	PGV	C23-C24-C25-C26
20	N	1266	PGV	C29-C30-C31-C32
20	N	1524	PGV	C28-C29-C30-C31
26	C	270	CDL	OB7-CB5-OB6-CB4
26	P	1270	CDL	OB7-CB5-OB6-CB4
20	A	524	PGV	C28-C29-C30-C31
25	P	1264	PEK	C23-C24-C25-C26
26	P	1270	CDL	C74-C75-C76-C77
19	Y	1522	TGL	CC2-CC1-OG3-CG3
25	C	264	PEK	C23-C24-C25-C26
25	C	264	PEK	C31-C32-C33-C34
20	C	267	PGV	C22-C23-C24-C25
26	P	1270	CDL	C75-C76-C77-C78
20	C	268	PGV	C27-C28-C29-C30
20	P	1267	PGV	C22-C23-C24-C25
20	P	1268	PGV	C27-C28-C29-C30
26	C	270	CDL	C51-CB5-OB6-CB4
26	P	1270	CDL	C51-CB5-OB6-CB4
25	P	1264	PEK	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
25	T	263	PEK	C25-C26-C27-C28
25	G	1263	PEK	C25-C26-C27-C28
26	P	1270	CDL	C72-C73-C74-C75
20	C	267	PGV	C11-C10-C9-C8
20	P	1267	PGV	C11-C10-C9-C8
22	B	230	PSC	C13-C14-C15-C16
22	O	1230	PSC	C13-C14-C15-C16
26	C	270	CDL	C72-C73-C74-C75
26	C	270	CDL	C75-C76-C77-C78
19	N	1521	TGL	CB6-CB7-CB8-CB9
20	N	1524	PGV	C22-C23-C24-C25
24	C	272	DMU	C25-C28-C31-C34
25	P	1265	PEK	C16-C17-C18-C19
20	A	524	PGV	C22-C23-C24-C25
25	C	265	PEK	C31-C32-C33-C34
22	B	230	PSC	C04-C05-N-C08
22	O	1230	PSC	C04-C05-N-C08
20	P	1267	PGV	C7-C8-C9-C10
22	B	230	PSC	C22-C23-C24-C25
25	P	1265	PEK	C31-C32-C33-C34
26	C	270	CDL	C18-C19-C20-C21
20	C	267	PGV	C7-C8-C9-C10
26	P	1270	CDL	C18-C19-C20-C21
24	P	1272	DMU	C25-C28-C31-C34
25	T	263	PEK	O03-C01-C02-O01
25	C	265	PEK	C29-C30-C31-C32
20	C	267	PGV	C13-C14-C15-C16
25	P	1265	PEK	C29-C30-C31-C32
20	N	1266	PGV	C7-C8-C9-C10
20	N	1266	PGV	C5-C6-C7-C8
20	P	1267	PGV	C13-C14-C15-C16
20	P	1268	PGV	C25-C26-C27-C28
25	C	265	PEK	C16-C17-C18-C19
25	C	264	PEK	C25-C26-C27-C28
20	A	604	PGV	C5-C6-C7-C8
20	C	268	PGV	C25-C26-C27-C28
26	T	1269	CDL	CB5-C51-C52-C53
20	P	1267	PGV	C25-C26-C27-C28
24	M	526	DMU	C3-C4-C57-O61
19	L	522	TGL	CC2-CC3-CC4-CC5
20	A	604	PGV	C7-C8-C9-C10
26	P	1270	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
20	P	1268	PGV	C12-C13-C14-C15
25	G	1263	PEK	C15-C16-C17-C18
25	P	1264	PEK	C16-C17-C18-C19
26	G	269	CDL	C82-C83-C84-C85
25	G	1263	PEK	C01-C02-C03-O11
25	T	263	PEK	C01-C02-C03-O11
26	C	270	CDL	OB5-CB3-CB4-CB6
26	G	269	CDL	OA5-CA3-CA4-CA6
26	P	1270	CDL	OB5-CB3-CB4-CB6
25	P	1264	PEK	C35-C36-C37-C38
20	P	1268	PGV	C28-C29-C30-C31
25	C	264	PEK	C22-C23-C24-C25
26	C	270	CDL	C11-C12-C13-C14
26	T	1269	CDL	C43-C44-C45-C46
24	Z	1526	DMU	O6-C11-C9-O1
20	C	268	PGV	C28-C29-C30-C31
26	G	269	CDL	C21-C22-C23-C24
26	G	269	CDL	C43-C44-C45-C46
25	P	1264	PEK	O04-C21-O03-C01
20	C	267	PGV	C25-C26-C27-C28
22	O	1230	PSC	C22-C23-C24-C25
26	C	270	CDL	C36-C37-C38-C39
26	C	270	CDL	C64-C65-C66-C67
26	P	1270	CDL	C64-C65-C66-C67
25	G	1263	PEK	C26-C27-C28-C29
25	T	263	PEK	C26-C27-C28-C29
26	T	1269	CDL	C21-C22-C23-C24
26	T	1269	CDL	C82-C83-C84-C85
19	A	521	TGL	CC2-CC1-OG3-CG3
18	A	516	HEA	C4D-C3D-CAD-CBD
25	P	1264	PEK	C22-C23-C24-C25
26	G	269	CDL	CB5-C51-C52-C53
22	B	230	PSC	O03-C01-C02-C03
22	O	1230	PSC	O03-C01-C02-C03
25	C	264	PEK	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

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Mol	Chain	Res	Type	Atoms
25	T	263	PEK	C34-C35-C36-C37
20	A	524	PGV	C12-C13-C14-C15
20	C	268	PGV	C12-C13-C14-C15
20	P	1268	PGV	C11-C10-C9-C8
25	G	1263	PEK	C34-C35-C36-C37
26	C	270	CDL	C71-C72-C73-C74
26	P	1270	CDL	C71-C72-C73-C74
19	L	522	TGL	CC2-CC1-OG3-CG3
25	C	264	PEK	C16-C17-C18-C19
26	C	270	CDL	C32-C33-C34-C35
26	P	1270	CDL	C36-C37-C38-C39
25	P	1264	PEK	C25-C26-C27-C28
26	C	270	CDL	C61-C62-C63-C64
26	P	1270	CDL	C61-C62-C63-C64
26	P	1270	CDL	C32-C33-C34-C35
25	C	264	PEK	C35-C36-C37-C38
20	C	268	PGV	C30-C31-C32-C33
26	C	270	CDL	C63-C64-C65-C66
26	G	269	CDL	C33-C34-C35-C36
26	T	1269	CDL	C33-C34-C35-C36
20	A	524	PGV	C03-C02-O01-C1
20	N	1524	PGV	C03-C02-O01-C1
20	P	1268	PGV	C30-C31-C32-C33
26	G	269	CDL	C53-C54-C55-C56
26	P	1270	CDL	C42-C43-C44-C45
26	P	1270	CDL	C63-C64-C65-C66
18	N	515	HEA	C17-C18-C19-C27
20	C	268	PGV	C11-C10-C9-C8
20	N	1524	PGV	C12-C13-C14-C15
22	O	1230	PSC	C14-C15-C16-C17
26	C	270	CDL	C42-C43-C44-C45
22	B	230	PSC	C14-C15-C16-C17
26	G	269	CDL	C41-C42-C43-C44
26	T	1269	CDL	C53-C54-C55-C56
25	C	264	PEK	O04-C21-O03-C01
19	N	1521	TGL	CC2-CC1-OG3-CG3
24	M	526	DMU	C34-C37-C40-C43
26	P	1270	CDL	C78-C79-C80-C81
20	A	524	PGV	C5-C6-C7-C8
26	T	1269	CDL	C41-C42-C43-C44
22	B	230	PSC	C23-C24-C25-C26
22	O	1230	PSC	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
24	Z	1526	DMU	C22-C25-C28-C31
22	O	1230	PSC	C27-C28-C29-C30
24	M	526	DMU	C22-C25-C28-C31
20	N	1266	PGV	C30-C31-C32-C33
26	C	270	CDL	C78-C79-C80-C81
25	T	263	PEK	C22-C21-O03-C01
20	P	1267	PGV	C15-C16-C17-C18
20	N	1524	PGV	C5-C6-C7-C8
20	C	267	PGV	C15-C16-C17-C18
20	A	604	PGV	C30-C31-C32-C33
22	B	230	PSC	C27-C28-C29-C30
25	G	1263	PEK	C2-C3-C4-C5
26	C	270	CDL	C44-C45-C46-C47
26	P	1270	CDL	C44-C45-C46-C47
24	Z	1526	DMU	C34-C37-C40-C43
18	A	515	HEA	C17-C18-C19-C27
25	P	1265	PEK	C32-C33-C34-C35
25	P	1264	PEK	C1-C2-C3-C4
25	C	264	PEK	C27-C28-C29-C30
26	G	269	CDL	C15-C16-C17-C18
20	C	268	PGV	C31-C32-C33-C34
25	T	263	PEK	O04-C21-O03-C01
26	G	269	CDL	C31-C32-C33-C34
25	G	1263	PEK	C22-C21-O03-C01
22	B	230	PSC	C24-C25-C26-C27
18	N	516	HEA	C4D-C3D-CAD-CBD
20	A	524	PGV	C26-C27-C28-C29
22	B	230	PSC	C3-C4-C5-C6
22	O	1230	PSC	C24-C25-C26-C27
25	G	1263	PEK	C30-C31-C32-C33
19	L	522	TGL	OB1-CB1-OG2-CG2
26	T	1269	CDL	C71-C72-C73-C74
25	G	1263	PEK	O04-C21-O03-C01
20	N	1524	PGV	C26-C27-C28-C29
22	O	1230	PSC	C3-C4-C5-C6
25	T	263	PEK	C30-C31-C32-C33
26	G	269	CDL	C35-C36-C37-C38
26	T	1269	CDL	C31-C32-C33-C34
25	C	265	PEK	C32-C33-C34-C35
20	P	1268	PGV	C31-C32-C33-C34
26	T	1269	CDL	C44-C45-C46-C47
20	C	268	PGV	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
25	P	1264	PEK	C24-C25-C26-C27
26	P	1270	CDL	C39-C40-C41-C42
26	T	1269	CDL	C35-C36-C37-C38
25	P	1264	PEK	C17-C18-C19-C20
26	T	1269	CDL	OA5-CA3-CA4-CA6
20	C	268	PGV	C23-C24-C25-C26
26	C	270	CDL	C39-C40-C41-C42
26	C	270	CDL	C84-C85-C86-C87
26	G	269	CDL	C44-C45-C46-C47
26	P	1270	CDL	C84-C85-C86-C87
26	G	269	CDL	C71-C72-C73-C74
20	P	1268	PGV	C23-C24-C25-C26
20	P	1268	PGV	C14-C15-C16-C17
25	C	264	PEK	C24-C25-C26-C27
26	G	269	CDL	C14-C15-C16-C17
20	P	1267	PGV	C23-C24-C25-C26
25	P	1264	PEK	C26-C27-C28-C29
25	P	1264	PEK	C27-C28-C29-C30
26	G	269	CDL	CA3-CA4-CA6-OA8
26	T	1269	CDL	CA3-CA4-CA6-OA8
25	C	264	PEK	C17-C18-C19-C20
19	A	521	TGL	C12-C13-C14-C29
20	C	268	PGV	C5-C6-C7-C8
26	T	1269	CDL	C14-C15-C16-C17
20	P	1268	PGV	C5-C6-C7-C8
20	P	1268	PGV	C4-C5-C6-C7
24	Z	1526	DMU	C28-C31-C34-C37
19	Y	1522	TGL	OB1-CB1-OG2-CG2
26	C	270	CDL	OB5-CB3-CB4-OB6
26	P	1270	CDL	OA5-CA3-CA4-OA6
26	P	1270	CDL	OB5-CB3-CB4-OB6
25	C	264	PEK	C32-C33-C34-C35
19	N	1521	TGL	C12-C13-C14-C29
20	C	268	PGV	C4-C5-C6-C7
25	T	263	PEK	C15-C16-C17-C18
20	C	268	PGV	C15-C16-C17-C18
20	A	604	PGV	C4-C5-C6-C7
25	C	264	PEK	C26-C27-C28-C29
20	C	267	PGV	C23-C24-C25-C26
22	B	230	PSC	O03-C01-C02-O01
22	O	1230	PSC	O03-C01-C02-O01
22	B	230	PSC	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
22	O	1230	PSC	C9-C10-C11-C12
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	P	1265	PEK	C12-C13-C14-C15
25	T	263	PEK	C6-C7-C8-C9
26	T	1269	CDL	C19-C20-C21-C22
25	C	265	PEK	C17-C18-C19-C20
20	P	1268	PGV	C15-C16-C17-C18
26	T	1269	CDL	C15-C16-C17-C18
26	C	270	CDL	C34-C35-C36-C37
26	G	269	CDL	C19-C20-C21-C22
26	C	270	CDL	C38-C39-C40-C41
26	P	1270	CDL	C38-C39-C40-C41
26	P	1270	CDL	C34-C35-C36-C37
25	T	263	PEK	C2-C3-C4-C5
24	C	272	DMU	C22-C25-C28-C31
23	C	271	CHD	C13-C17-C20-C22
23	P	1271	CHD	C13-C17-C20-C22
20	C	267	PGV	C31-C32-C33-C34
25	C	264	PEK	C1-C2-C3-C4
20	P	1267	PGV	C31-C32-C33-C34
19	Y	1522	TGL	CC7-CC8-CC9-C15
23	C	271	CHD	C13-C17-C20-C21
24	P	1272	DMU	C22-C25-C28-C31
25	P	1265	PEK	C17-C18-C19-C20
18	A	516	HEA	C2D-C3D-CAD-CBD
20	C	268	PGV	C20-C19-O03-C01
20	C	268	PGV	O04-C19-O03-C01
26	G	269	CDL	C24-C25-C26-C27
23	P	1271	CHD	C13-C17-C20-C21
19	L	522	TGL	CC7-CC8-CC9-C15
20	N	1266	PGV	C4-C5-C6-C7
25	P	1264	PEK	C32-C33-C34-C35
20	P	1268	PGV	C26-C27-C28-C29
25	G	1263	PEK	C16-C17-C18-C19
26	C	270	CDL	OA5-CA3-CA4-OA6
24	P	1272	DMU	C34-C37-C40-C43

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Mol	Chain	Res	Type	Atoms
24	P	1272	DMU	O5-C6-O16-C18
20	A	524	PGV	O03-C01-C02-C03
20	N	1524	PGV	O03-C01-C02-C03
19	A	523	TGL	CA9-C20-C21-C22
26	P	1270	CDL	C43-C44-C45-C46
26	T	1269	CDL	OA6-CA4-CA6-OA8
19	Q	1523	TGL	CA9-C20-C21-C22
20	C	268	PGV	C26-C27-C28-C29
20	P	1268	PGV	O04-C19-O03-C01
22	O	1230	PSC	C04-C05-N-C07
26	C	270	CDL	C43-C44-C45-C46
26	T	1269	CDL	C24-C25-C26-C27
26	C	270	CDL	C24-C25-C26-C27
20	C	267	PGV	C20-C21-C22-C23
20	P	1268	PGV	C20-C19-O03-C01
20	A	524	PGV	C11-C10-C9-C8
20	P	1267	PGV	C20-C21-C22-C23
20	P	1267	PGV	C24-C25-C26-C27
26	P	1270	CDL	C24-C25-C26-C27
26	T	1269	CDL	C54-C55-C56-C57
22	O	1230	PSC	C31-C32-C33-C34
23	P	1271	CHD	C16-C17-C20-C21
22	B	230	PSC	C31-C32-C33-C34
22	B	230	PSC	C04-C05-N-C07
23	C	271	CHD	C16-C17-C20-C21
26	C	270	CDL	OA5-CA3-CA4-CA6
22	O	1230	PSC	C11-C12-C13-C14
24	M	526	DMU	C28-C31-C34-C37
26	G	269	CDL	CB4-CB3-OB5-PB2
26	G	269	CDL	C54-C55-C56-C57
23	C	271	CHD	C16-C17-C20-C22
25	G	1263	PEK	O01-C02-C03-O11
25	T	263	PEK	O01-C02-C03-O11
25	C	264	PEK	C2-C1-O01-C02
25	P	1264	PEK	C2-C1-O01-C02
22	O	1230	PSC	C04-C05-N-C06
24	M	526	DMU	O6-C11-C9-O1
20	C	267	PGV	C24-C25-C26-C27
23	P	1271	CHD	C16-C17-C20-C22
20	A	604	PGV	C25-C26-C27-C28
19	A	523	TGL	OG2-CG2-CG3-OG3
19	Q	1523	TGL	OG2-CG2-CG3-OG3

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Mol	Chain	Res	Type	Atoms
20	A	524	PGV	O03-C01-C02-O01
20	N	1524	PGV	O03-C01-C02-O01
25	C	264	PEK	O03-C01-C02-O01
25	P	1264	PEK	O03-C01-C02-O01
26	C	270	CDL	OB6-CB4-CB6-OB8
26	G	269	CDL	OA6-CA4-CA6-OA8
26	P	1270	CDL	OB6-CB4-CB6-OB8
25	C	265	PEK	C30-C31-C32-C33
19	Y	1522	TGL	OC1-CC1-OG3-CG3
25	T	263	PEK	C16-C17-C18-C19
20	A	524	PGV	C03-O11-P-O13
20	N	1524	PGV	C03-O11-P-O13
22	B	230	PSC	C03-O11-P-O12
22	B	230	PSC	C03-O11-P-O13
22	B	230	PSC	C04-O12-P-O11
22	B	230	PSC	C04-O12-P-O13
22	B	230	PSC	C04-C05-N-C06
22	O	1230	PSC	C03-O11-P-O12
22	O	1230	PSC	C03-O11-P-O13
22	O	1230	PSC	C04-O12-P-O13
25	G	1263	PEK	C03-O11-P-O13
25	P	1264	PEK	O12-C04-C05-N
25	T	263	PEK	C03-O11-P-O13
26	C	270	CDL	CB2-OB2-PB2-OB5
26	P	1270	CDL	CB2-OB2-PB2-OB5
19	Y	1522	TGL	CC5-CC6-CC7-CC8
22	B	230	PSC	C4-C5-C6-C7
22	O	1230	PSC	C4-C5-C6-C7
20	C	267	PGV	C02-C03-O11-P
20	P	1267	PGV	C02-C03-O11-P
25	G	1263	PEK	C02-C03-O11-P
25	T	263	PEK	C02-C03-O11-P
26	T	1269	CDL	CB4-CB3-OB5-PB2
26	T	1269	CDL	C64-C65-C66-C67
25	T	263	PEK	C21-C22-C23-C24
26	G	269	CDL	C64-C65-C66-C67
25	P	1265	PEK	C30-C31-C32-C33
26	G	269	CDL	CB7-C71-C72-C73
25	G	1263	PEK	C21-C22-C23-C24
20	N	1524	PGV	C20-C21-C22-C23
20	N	1266	PGV	C25-C26-C27-C28
20	A	524	PGV	C01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
20	N	1524	PGV	C01-C02-C03-O11
26	P	1270	CDL	OA5-CA3-CA4-CA6
20	N	1266	PGV	C26-C27-C28-C29
20	A	524	PGV	C20-C21-C22-C23
26	T	1269	CDL	CB7-C71-C72-C73
26	T	1269	CDL	OA5-CA3-CA4-OA6
25	P	1265	PEK	C35-C36-C37-C38
25	C	265	PEK	C35-C36-C37-C38
26	T	1269	CDL	C36-C37-C38-C39
24	C	272	DMU	C34-C37-C40-C43
22	B	230	PSC	C11-C12-C13-C14
26	G	269	CDL	C36-C37-C38-C39
20	P	1267	PGV	C1-C2-C3-C4
18	N	516	HEA	C2D-C3D-CAD-CBD
26	T	1269	CDL	CA7-C31-C32-C33
20	C	267	PGV	C1-C2-C3-C4
20	N	1524	PGV	C11-C10-C9-C8
25	G	1263	PEK	C31-C32-C33-C34
26	C	270	CDL	C52-C53-C54-C55
23	C	271	CHD	C22-C23-C24-O26
20	P	1268	PGV	O01-C02-C03-O11
20	N	1266	PGV	C9-C10-C11-C12
20	P	1267	PGV	C11-C12-C13-C14
25	T	263	PEK	C31-C32-C33-C34
26	G	269	CDL	CA7-C31-C32-C33
23	P	1271	CHD	C22-C23-C24-O26
20	A	604	PGV	C9-C10-C11-C12
20	C	267	PGV	C11-C12-C13-C14
25	C	265	PEK	C3-C4-C5-C6
25	P	1265	PEK	C3-C4-C5-C6
20	A	604	PGV	C26-C27-C28-C29
19	A	521	TGL	CG2-CG3-OG3-CC1
20	A	524	PGV	C25-C26-C27-C28
26	G	269	CDL	C12-C13-C14-C15
18	N	516	HEA	CAD-CBD-CGD-O2D
26	T	1269	CDL	C12-C13-C14-C15
26	P	1270	CDL	C76-C77-C78-C79
23	C	271	CHD	C22-C23-C24-O25
23	P	1271	CHD	C22-C23-C24-O25
26	P	1270	CDL	C23-C24-C25-C26
19	L	522	TGL	CC5-CC6-CC7-CC8
26	C	270	CDL	C76-C77-C78-C79

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Mol	Chain	Res	Type	Atoms
20	C	267	PGV	C29-C30-C31-C32
25	T	263	PEK	C32-C33-C34-C35
20	A	604	PGV	O03-C19-C20-C21
19	A	521	TGL	CG1-CG2-OG2-CB1
19	A	523	TGL	CG1-CG2-OG2-CB1
19	Q	1523	TGL	CG1-CG2-OG2-CB1
22	B	230	PSC	C03-C02-O01-C1
22	O	1230	PSC	C03-C02-O01-C1
18	N	516	HEA	CAD-CBD-CGD-O1D
26	C	270	CDL	C23-C24-C25-C26
20	C	268	PGV	O01-C02-C03-O11
18	A	516	HEA	CAD-CBD-CGD-O1D
23	O	229	CHD	C22-C23-C24-O26
25	G	1263	PEK	C32-C33-C34-C35
18	A	516	HEA	CAD-CBD-CGD-O2D
18	N	515	HEA	CAD-CBD-CGD-O1D
18	N	516	HEA	CAA-CBA-CGA-O1A
23	B	1086	CHD	C22-C23-C24-O26
20	P	1268	PGV	C01-C02-C03-O11
20	P	1267	PGV	C29-C30-C31-C32
26	P	1270	CDL	C52-C53-C54-C55
25	C	265	PEK	O03-C01-C02-O01
25	P	1265	PEK	O03-C01-C02-O01
18	A	516	HEA	CAA-CBA-CGA-O1A
25	C	264	PEK	C11-C10-C9-C8
25	C	265	PEK	C12-C13-C14-C15
25	T	263	PEK	C33-C34-C35-C36
18	A	515	HEA	CAD-CBD-CGD-O1D
20	N	1266	PGV	O03-C19-C20-C21
20	P	1268	PGV	C7-C8-C9-C10
23	B	1086	CHD	C22-C23-C24-O25
23	O	229	CHD	C22-C23-C24-O25
26	C	270	CDL	C56-C57-C58-C59
22	B	230	PSC	C15-C16-C17-C18
26	P	1270	CDL	C56-C57-C58-C59
26	T	1269	CDL	C52-C53-C54-C55
25	G	1263	PEK	C33-C34-C35-C36
26	C	270	CDL	C1-CA2-OA2-PA1
26	P	1270	CDL	C1-CA2-OA2-PA1
18	A	516	HEA	CAA-CBA-CGA-O2A
19	N	1521	TGL	C13-C14-C29-C30
19	A	521	TGL	C13-C14-C29-C30

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Mol	Chain	Res	Type	Atoms
20	N	1524	PGV	C25-C26-C27-C28
22	O	1230	PSC	C15-C16-C17-C18
26	G	269	CDL	C38-C39-C40-C41
26	G	269	CDL	OA5-CA3-CA4-OA6
19	L	522	TGL	CB5-CB6-CB7-CB8
18	N	515	HEA	CAD-CBD-CGD-O2D
26	G	269	CDL	C52-C53-C54-C55
24	P	1272	DMU	C4-C3-O7-C10
18	N	516	HEA	CAA-CBA-CGA-O2A
20	A	604	PGV	C11-C12-C13-C14
20	C	268	PGV	C01-C02-C03-O11
20	P	1268	PGV	O03-C01-C02-O01
18	A	515	HEA	CAD-CBD-CGD-O2D
19	L	522	TGL	OG2-CB1-CB2-CB3
25	G	1263	PEK	C3-C4-C5-C6
25	T	263	PEK	C3-C4-C5-C6
20	P	1268	PGV	C02-C03-O11-P
20	C	268	PGV	C7-C8-C9-C10
20	A	524	PGV	C7-C8-C9-C10
19	Y	1522	TGL	OG2-CB1-CB2-CB3
26	P	1270	CDL	C22-C23-C24-C25
20	N	1266	PGV	C11-C12-C13-C14
20	P	1267	PGV	C9-C10-C11-C12
22	B	230	PSC	C7-C8-C9-C10
25	T	263	PEK	C14-C15-C16-C17
18	A	516	HEA	C26-C15-C16-C17
19	N	1521	TGL	CG2-CG3-OG3-CC1
19	Y	1522	TGL	CB5-CB6-CB7-CB8
19	N	1521	TGL	CG1-CG2-OG2-CB1
20	C	267	PGV	C9-C10-C11-C12
25	G	1263	PEK	C14-C15-C16-C17
26	T	1269	CDL	C38-C39-C40-C41
22	O	1230	PSC	C7-C8-C9-C10
20	C	267	PGV	C05-C04-O12-P
20	C	268	PGV	C02-C03-O11-P
20	C	268	PGV	C05-C04-O12-P
26	C	270	CDL	C22-C23-C24-C25
20	N	1266	PGV	C19-C20-C21-C22
20	A	524	PGV	C9-C10-C11-C12
20	N	1524	PGV	C9-C10-C11-C12
25	P	1264	PEK	C3-C4-C5-C6
20	N	1524	PGV	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
20	C	268	PGV	O03-C01-C02-O01
19	L	522	TGL	OC1-CC1-OG3-CG3
22	B	230	PSC	C12-C13-C14-C15
22	O	1230	PSC	C12-C13-C14-C15
22	B	230	PSC	O03-C19-C20-C21
22	O	1230	PSC	O03-C19-C20-C21
25	P	1264	PEK	O01-C1-C2-C3
26	C	270	CDL	C52-C51-CB5-OB6
22	B	230	PSC	C01-C02-C03-O11
25	C	264	PEK	C29-C30-C31-C32
20	A	524	PGV	O01-C1-C2-C3
20	N	1524	PGV	O01-C1-C2-C3
25	C	264	PEK	C3-C4-C5-C6
20	P	1268	PGV	C05-C04-O12-P
26	P	1270	CDL	C52-C51-CB5-OB6
24	C	272	DMU	O5-C6-O16-C18
19	L	522	TGL	OG3-CC1-CC2-CC3
25	C	264	PEK	O02-C1-O01-C02
20	P	1267	PGV	C14-C15-C16-C17
25	C	264	PEK	O01-C1-C2-C3
26	C	270	CDL	C32-C31-CA7-OA8
26	C	270	CDL	C82-C83-C84-C85
19	A	523	TGL	C21-C22-C23-C24
19	A	523	TGL	OG2-CB1-CB2-CB3
26	P	1270	CDL	C32-C31-CA7-OA8
19	Q	1523	TGL	C21-C22-C23-C24
26	P	1270	CDL	C83-C84-C85-C86
23	J	60	CHD	C22-C23-C24-O25
23	W	1060	CHD	C22-C23-C24-O25
23	J	60	CHD	C22-C23-C24-O26
23	W	1060	CHD	C22-C23-C24-O26
18	N	516	HEA	C26-C15-C16-C17
26	T	1269	CDL	C39-C40-C41-C42
25	P	1265	PEK	C34-C35-C36-C37
19	Q	1523	TGL	OG2-CB1-CB2-CB3
25	P	1264	PEK	C29-C30-C31-C32
22	O	1230	PSC	C01-C02-C03-O11
26	G	269	CDL	C39-C40-C41-C42
25	C	265	PEK	C26-C27-C28-C29
20	C	267	PGV	C14-C15-C16-C17
19	Y	1522	TGL	OG3-CC1-CC2-CC3
26	P	1270	CDL	C82-C83-C84-C85

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Mol	Chain	Res	Type	Atoms
24	C	272	DMU	O5-C4-C57-O61
26	P	1270	CDL	C12-C11-CA5-OA6
20	A	604	PGV	C19-C20-C21-C22
25	C	264	PEK	C02-C03-O11-P
19	Q	1523	TGL	OC1-CC1-CC2-CC3
26	T	1269	CDL	C59-C60-C61-C62
22	B	230	PSC	O01-C1-C2-C3
22	O	1230	PSC	O01-C1-C2-C3
26	C	270	CDL	C12-C11-CA5-OA6
19	A	523	TGL	OC1-CC1-CC2-CC3
25	C	264	PEK	O02-C1-C2-C3
19	Q	1523	TGL	OB1-CB1-CB2-CB3
20	N	1524	PGV	O02-C1-C2-C3
26	C	270	CDL	C32-C31-CA7-OA9
26	P	1270	CDL	C32-C31-CA7-OA9
20	A	524	PGV	O02-C1-C2-C3
22	B	230	PSC	O04-C19-C20-C21
22	O	1230	PSC	O04-C19-C20-C21
26	C	270	CDL	C83-C84-C85-C86
22	B	230	PSC	O02-C1-C2-C3
22	O	1230	PSC	O02-C1-C2-C3
26	P	1270	CDL	C52-C51-CB5-OB7
25	P	1264	PEK	O02-C1-C2-C3
26	G	269	CDL	C11-C12-C13-C14

There are no ring outliers.

38 monomers are involved in 274 short contacts:

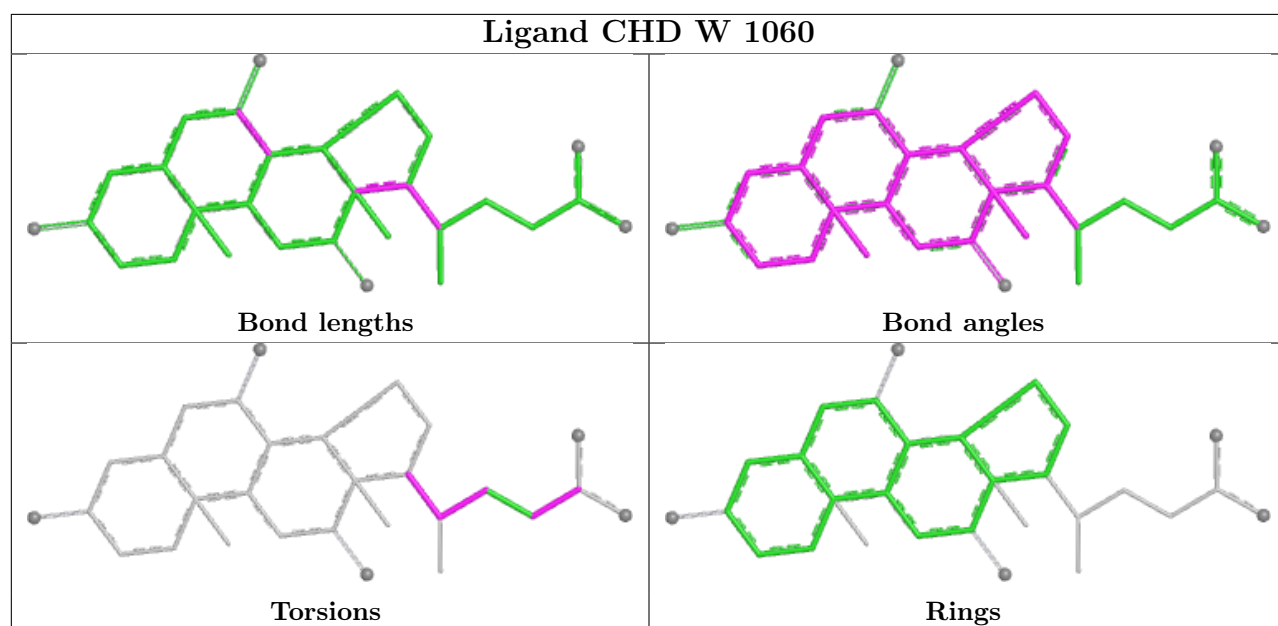
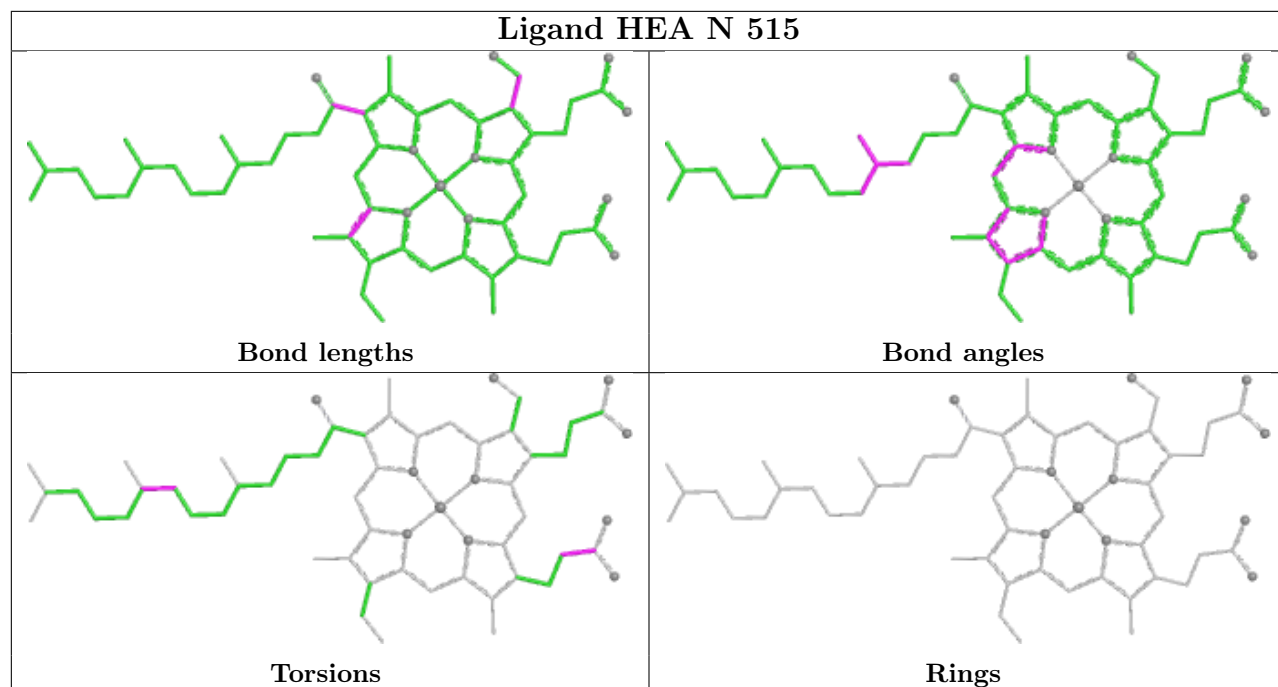
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	N	515	HEA	2	0
23	W	1060	CHD	5	0
18	N	516	HEA	1	0
26	P	1270	CDL	18	0
26	C	270	CDL	17	0
25	T	263	PEK	9	0
23	C	271	CHD	7	0
19	A	523	TGL	6	0
25	C	264	PEK	4	0
25	C	265	PEK	7	0
20	N	1524	PGV	9	0
23	J	60	CHD	3	0
23	B	1086	CHD	1	0

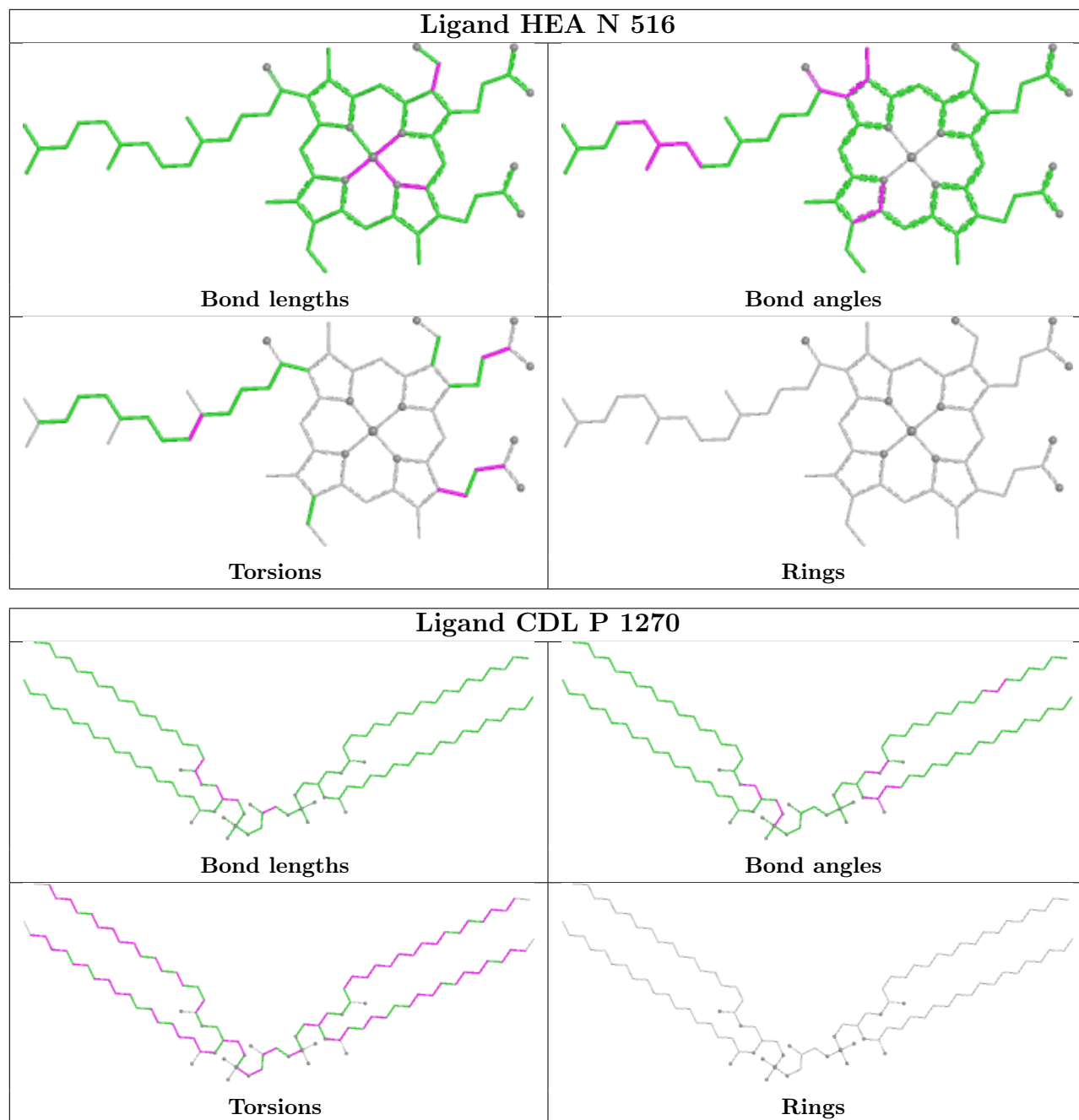
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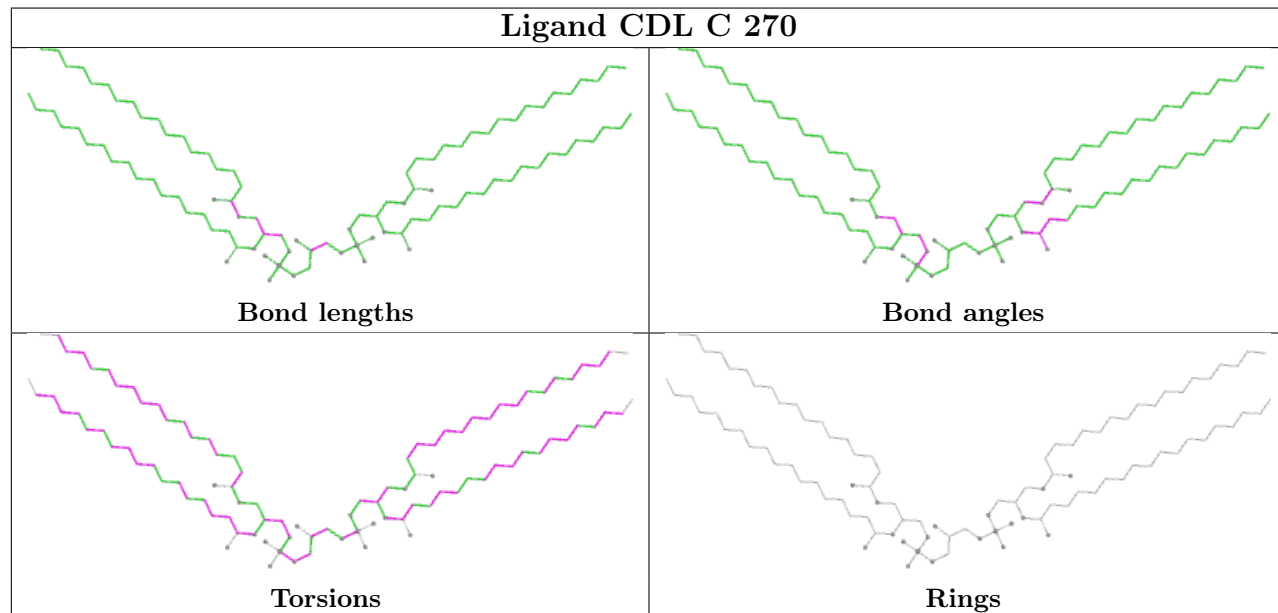
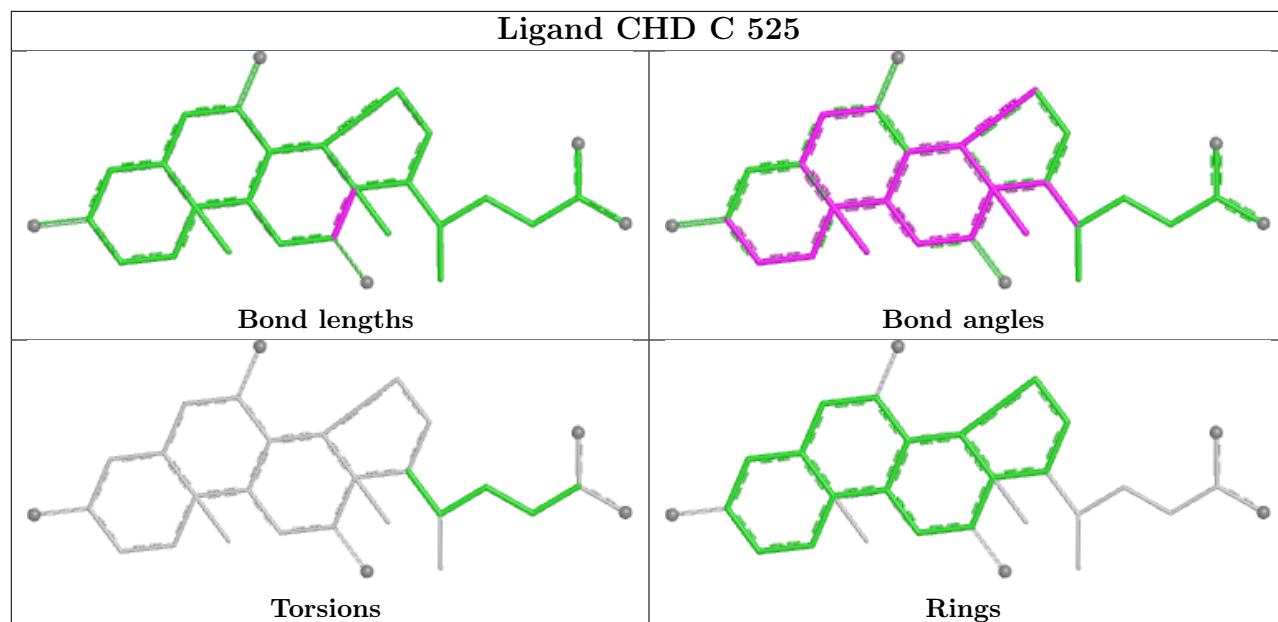
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	524	PGV	8	0
20	A	604	PGV	1	0
23	O	229	CHD	1	0
23	P	1271	CHD	1	0
20	C	268	PGV	2	0
19	L	522	TGL	23	0
24	C	272	DMU	2	0
26	T	1269	CDL	19	0
18	A	516	HEA	1	0
19	A	521	TGL	10	0
25	P	1264	PEK	5	0
18	A	515	HEA	2	0
24	P	1272	DMU	8	0
22	B	230	PSC	14	0
25	P	1265	PEK	7	0
20	N	1266	PGV	1	0
19	Q	1523	TGL	7	0
20	P	1267	PGV	5	0
26	G	269	CDL	21	0
19	N	1521	TGL	8	0
22	O	1230	PSC	15	0
25	G	1263	PEK	10	0
20	C	267	PGV	6	0
19	Y	1522	TGL	18	0
20	P	1268	PGV	2	0

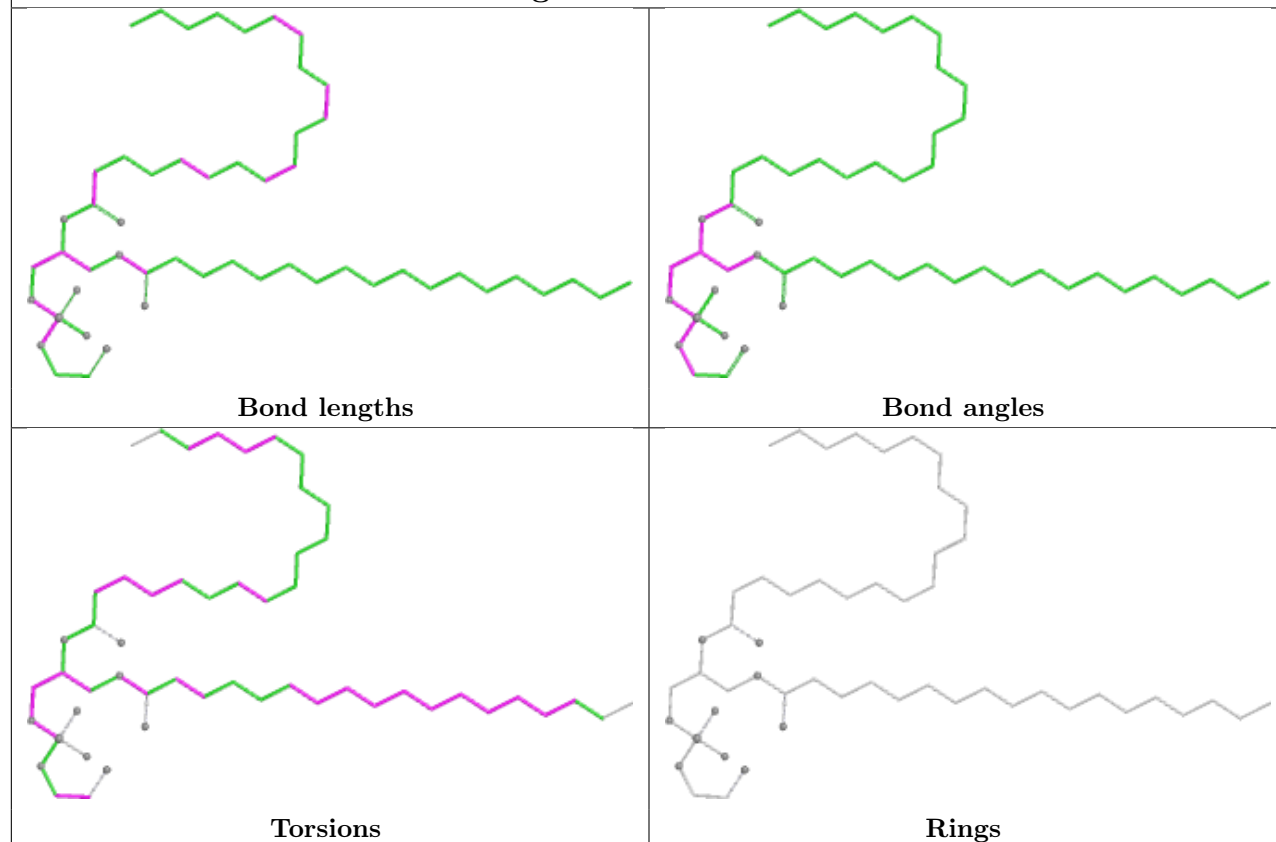
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



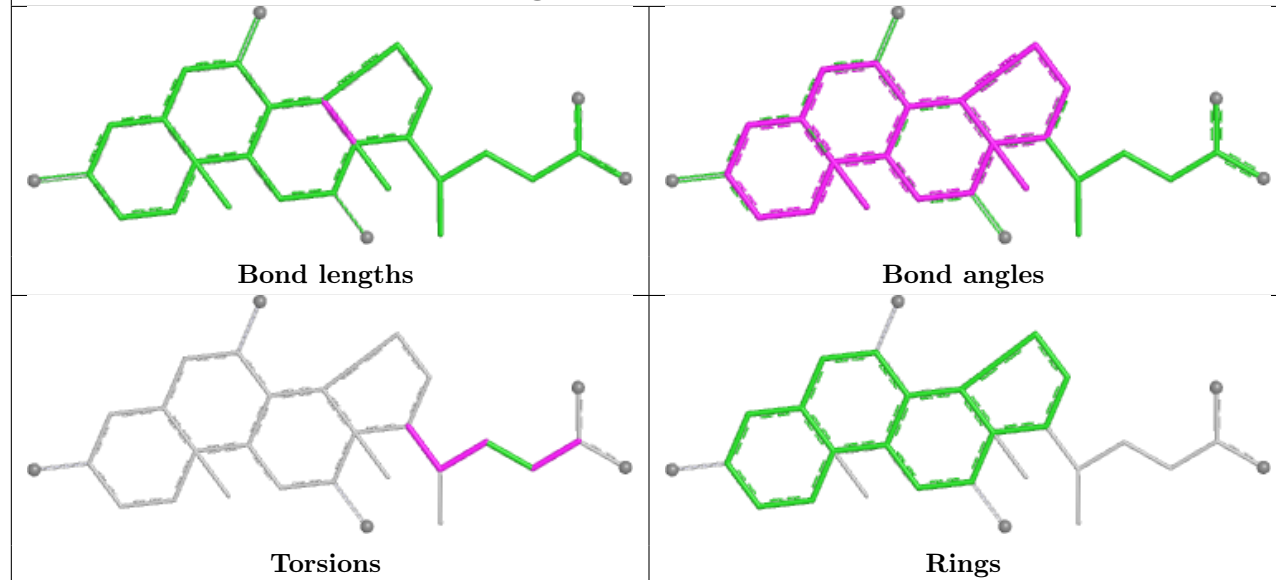


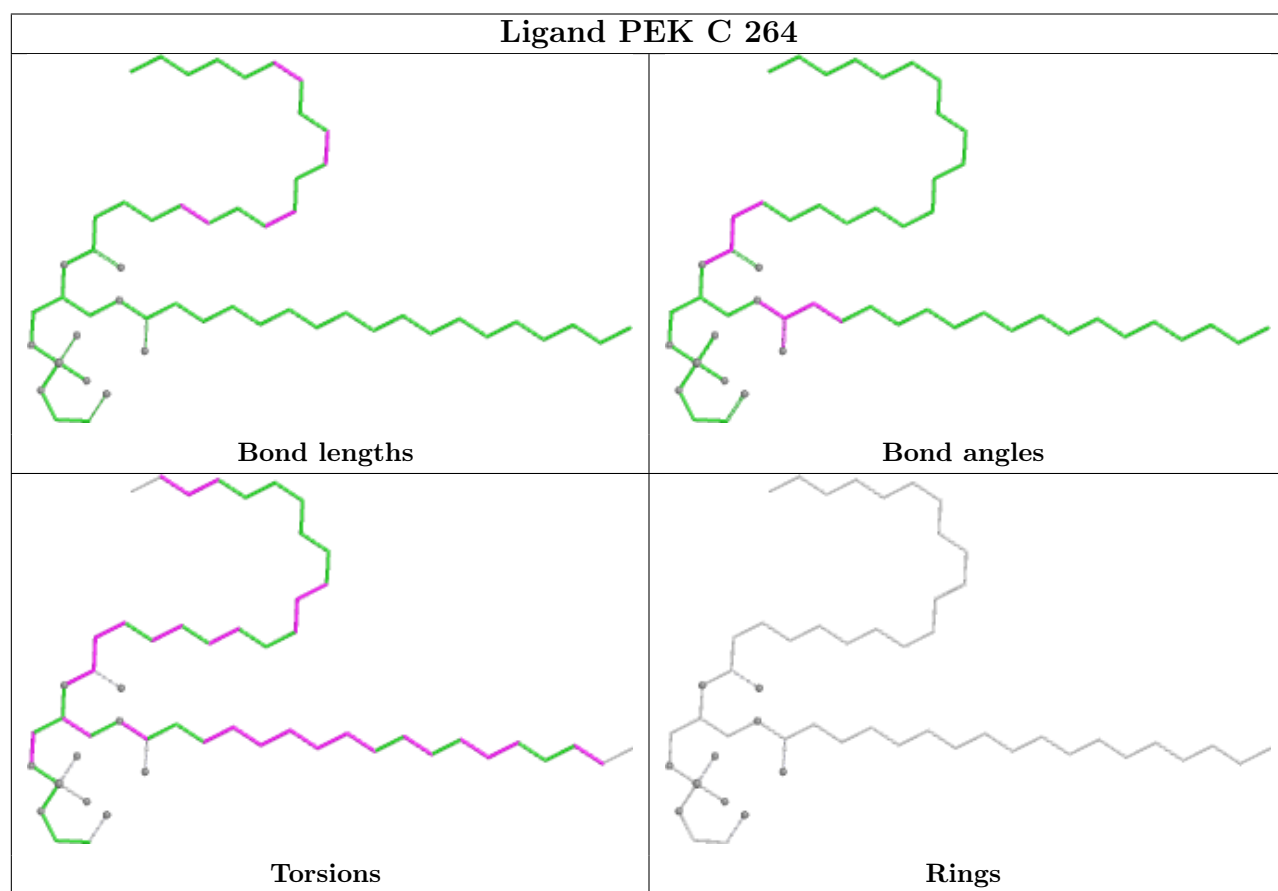
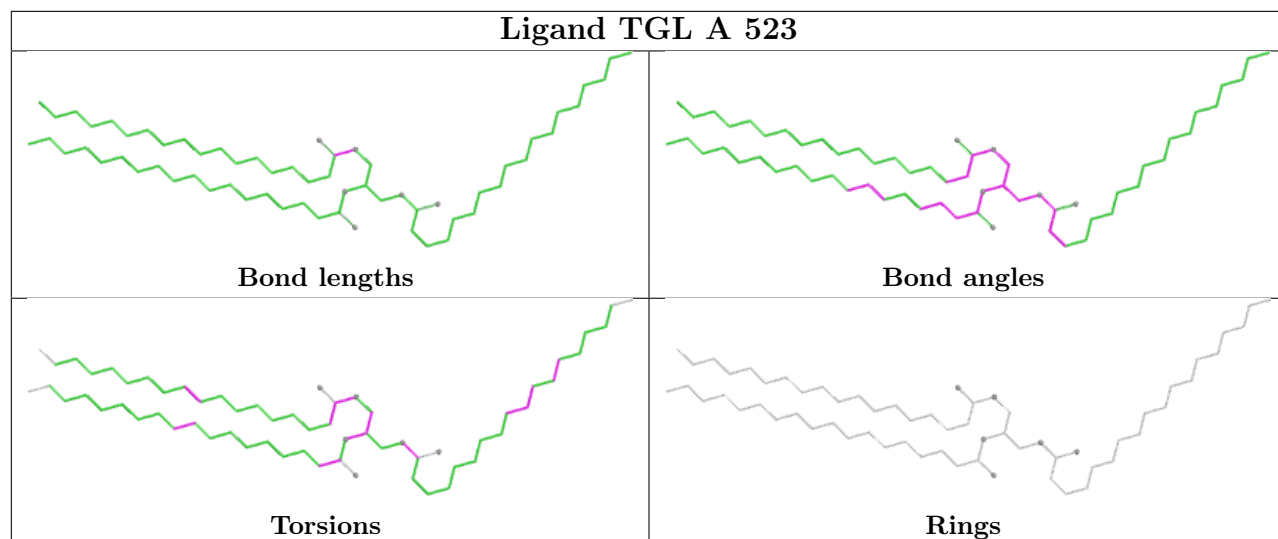


Ligand PEK T 263

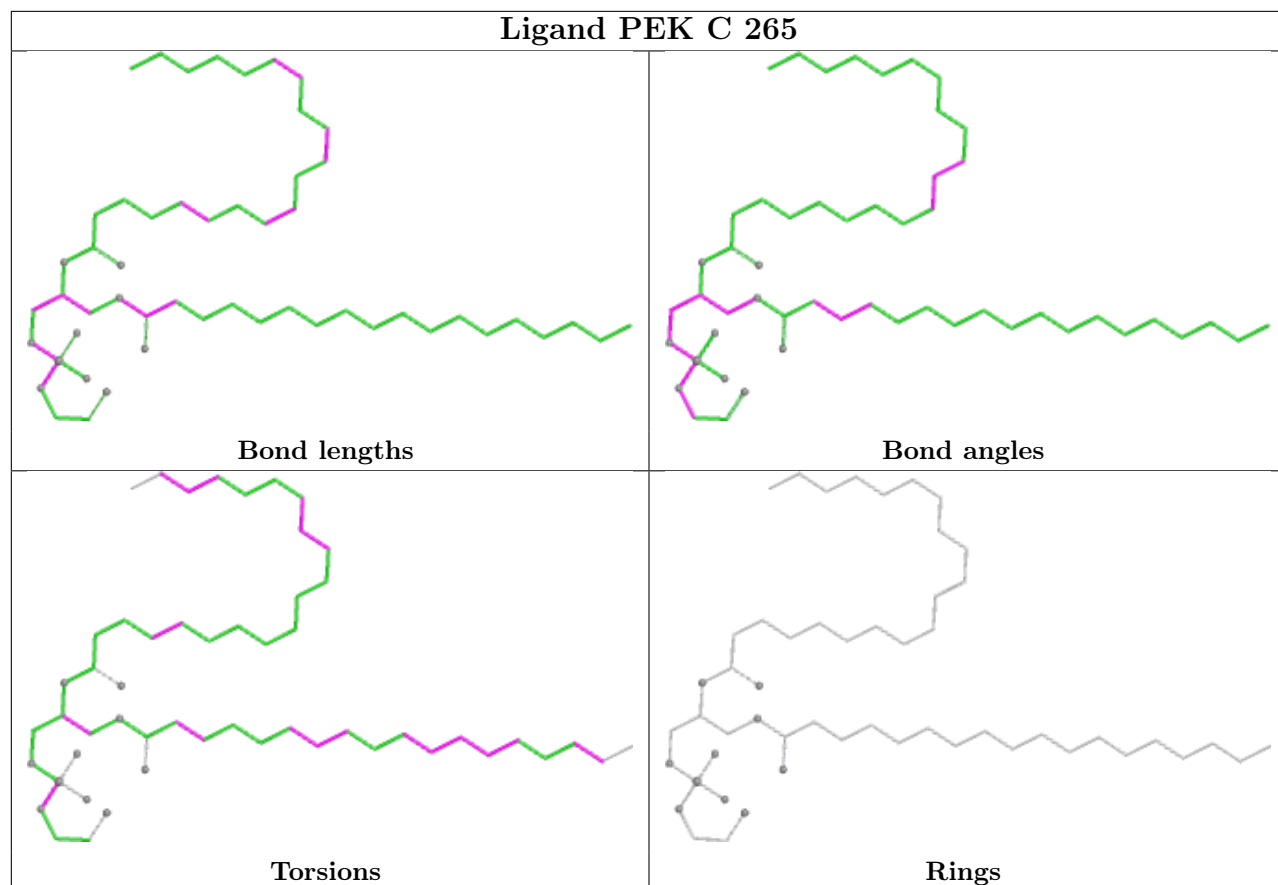


Ligand CHD C 271

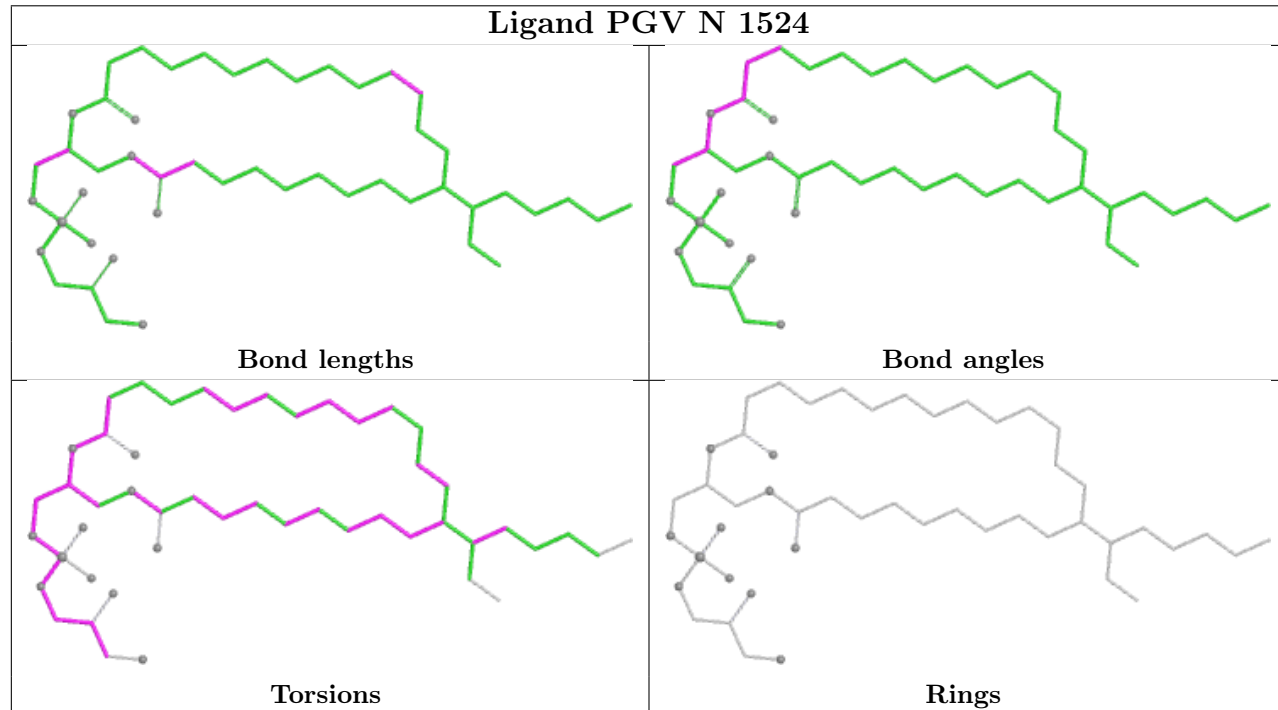




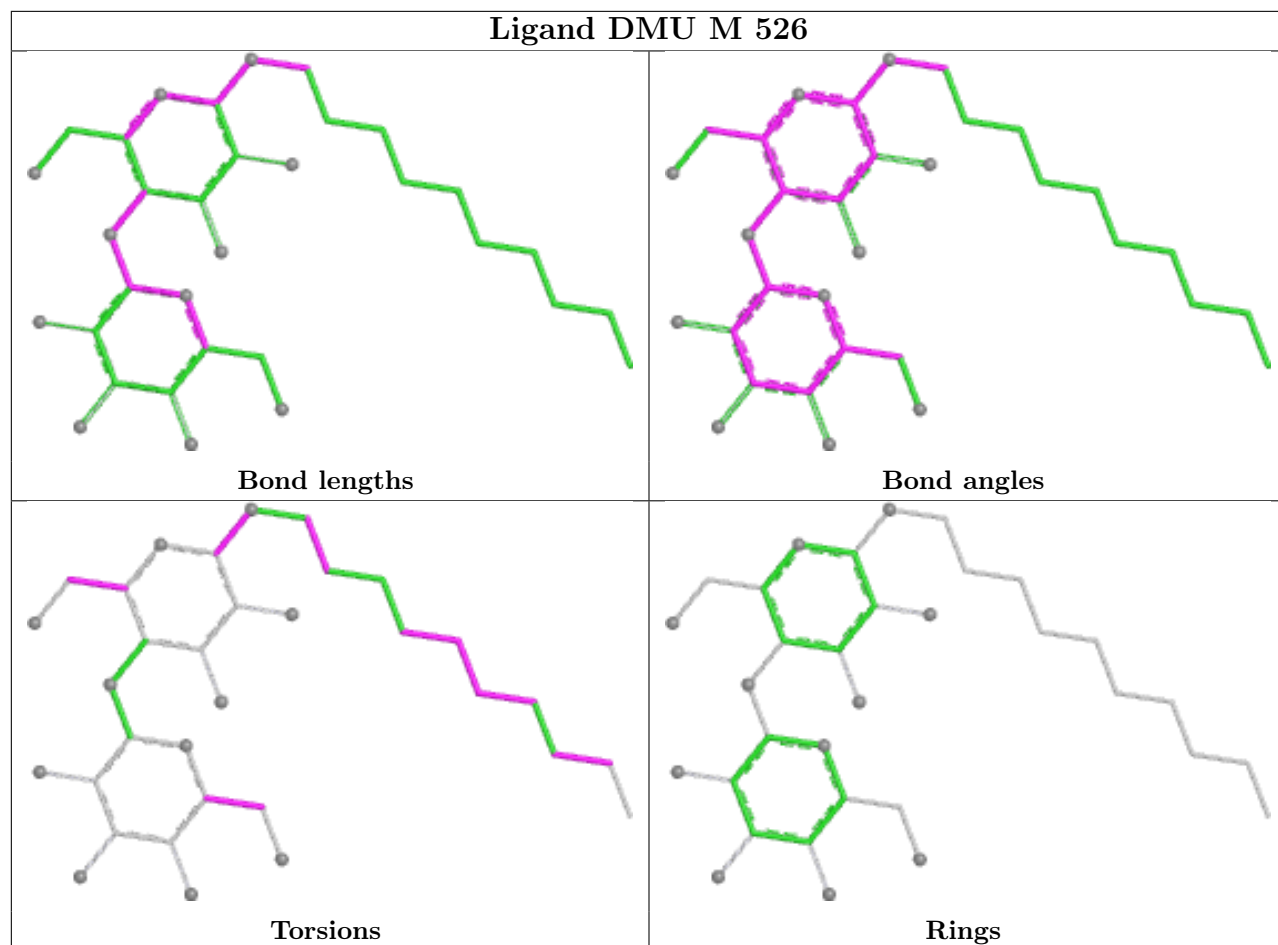
Ligand PEK C 265



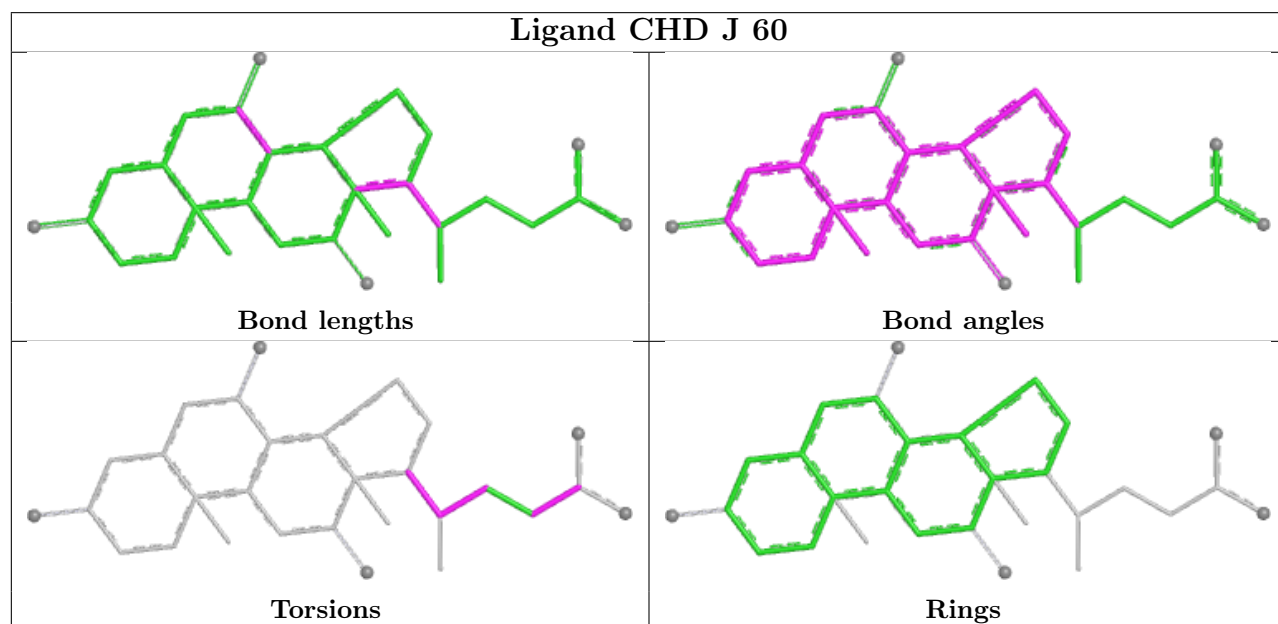
Ligand PGV N 1524



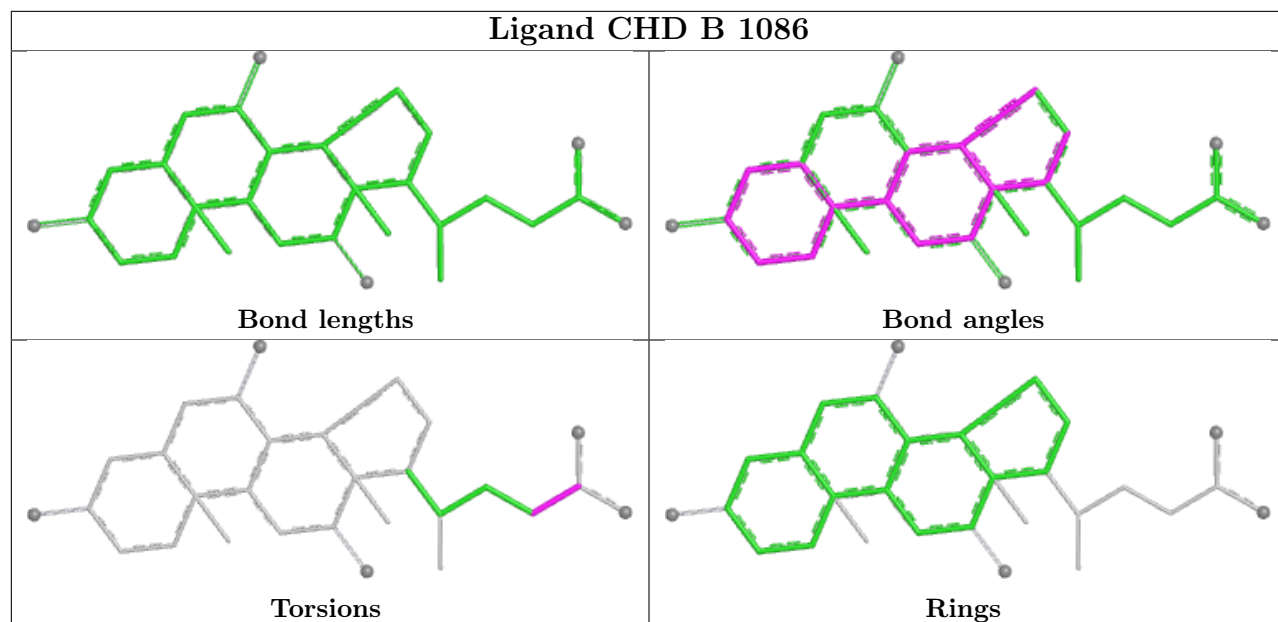
Ligand DMU M 526



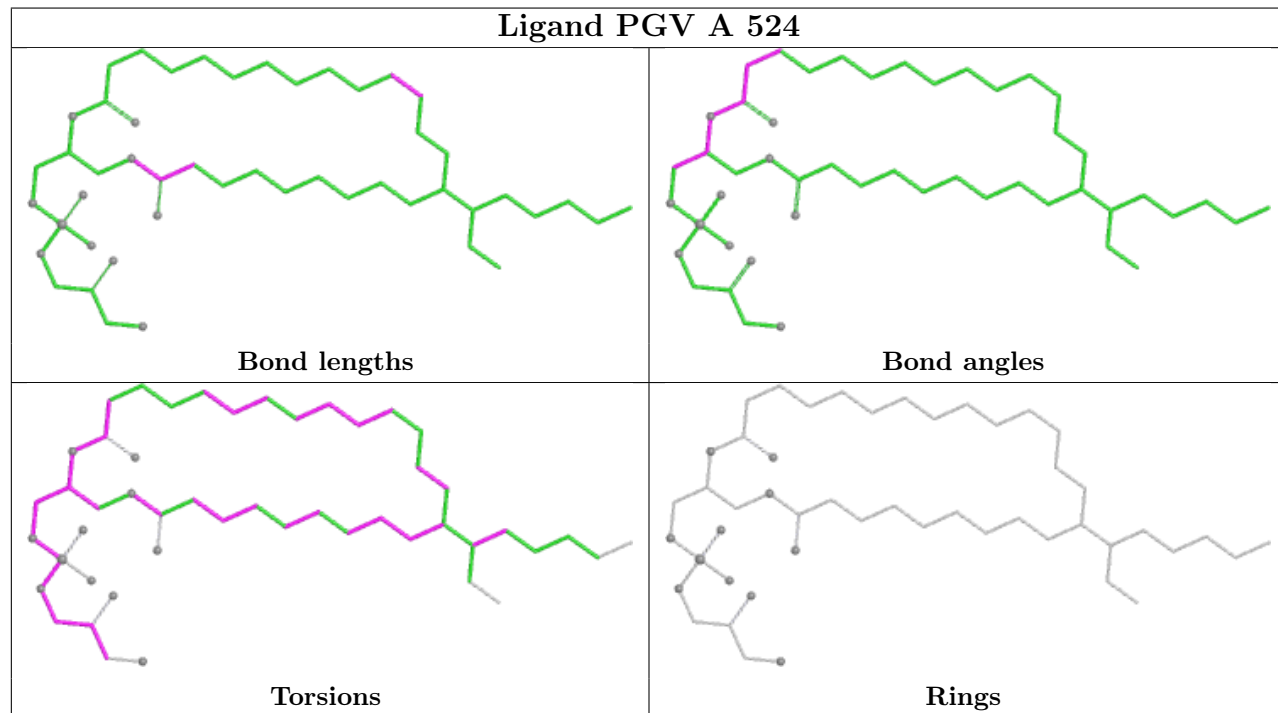
Ligand CHD J 60



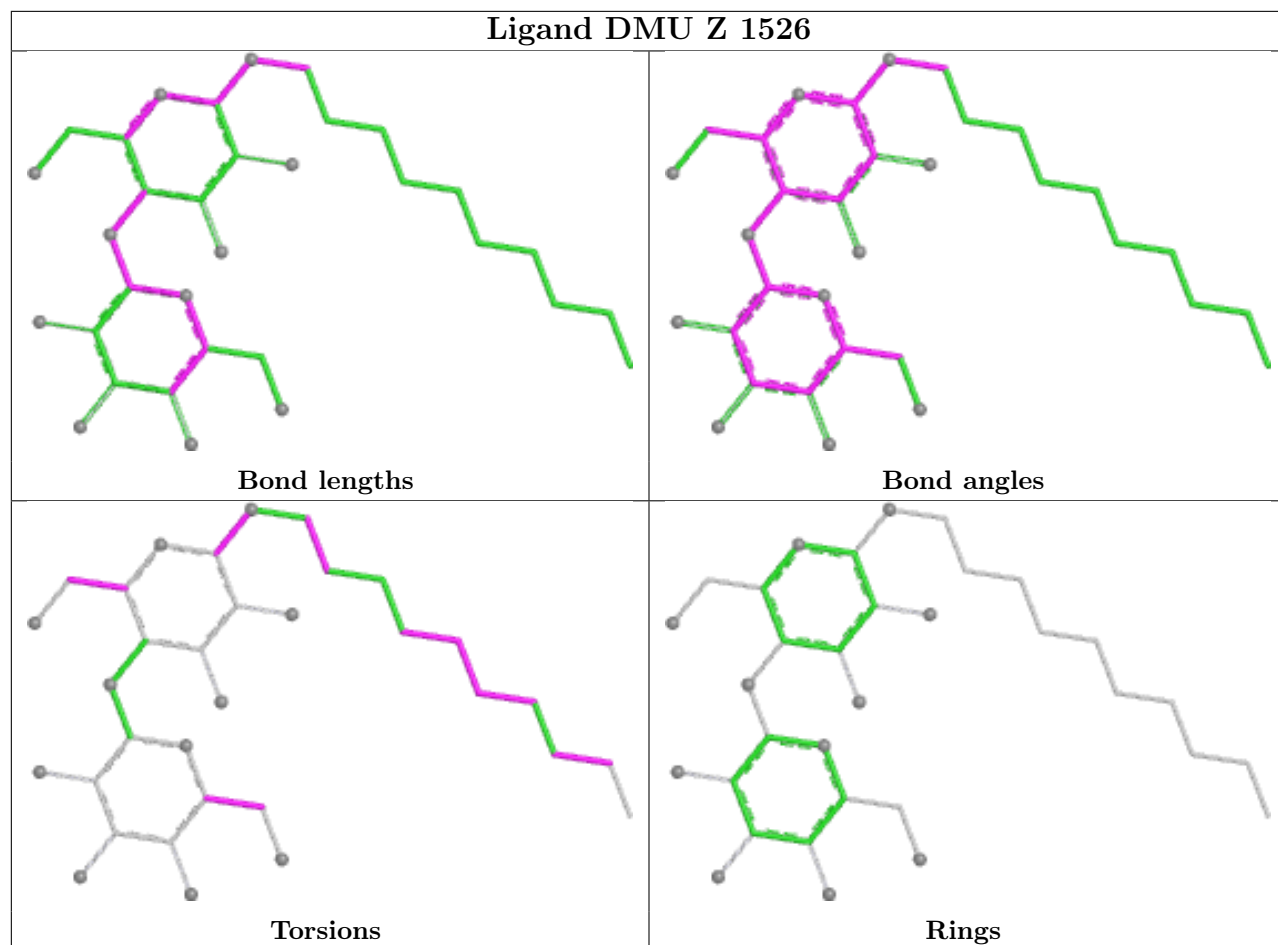
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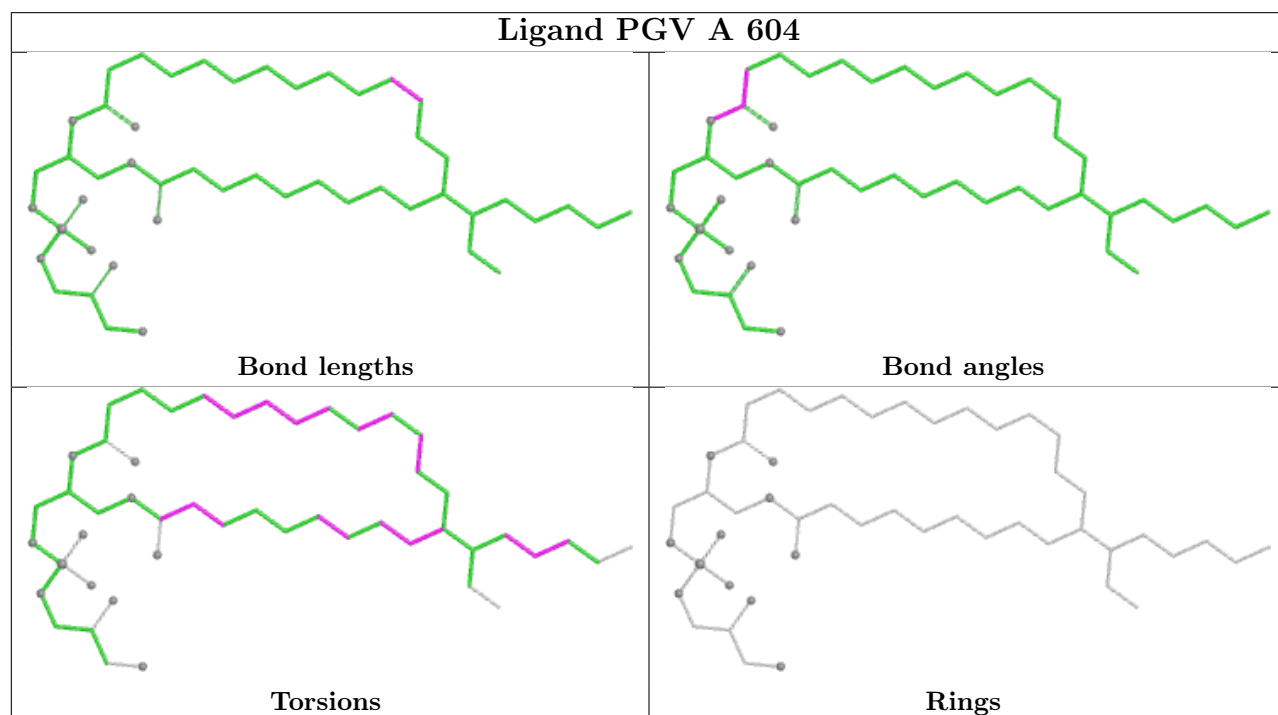
Ligand PGV A 524

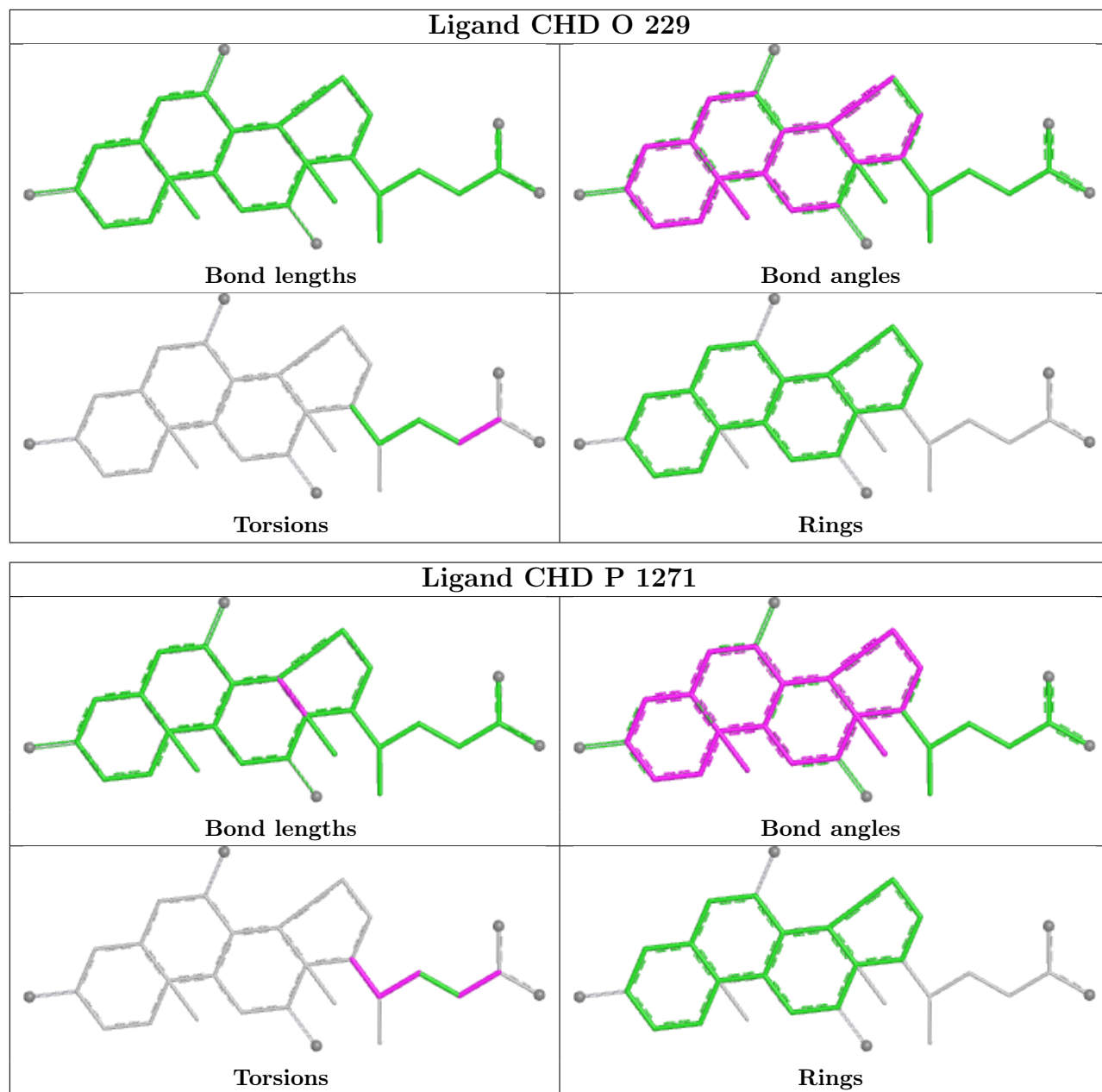


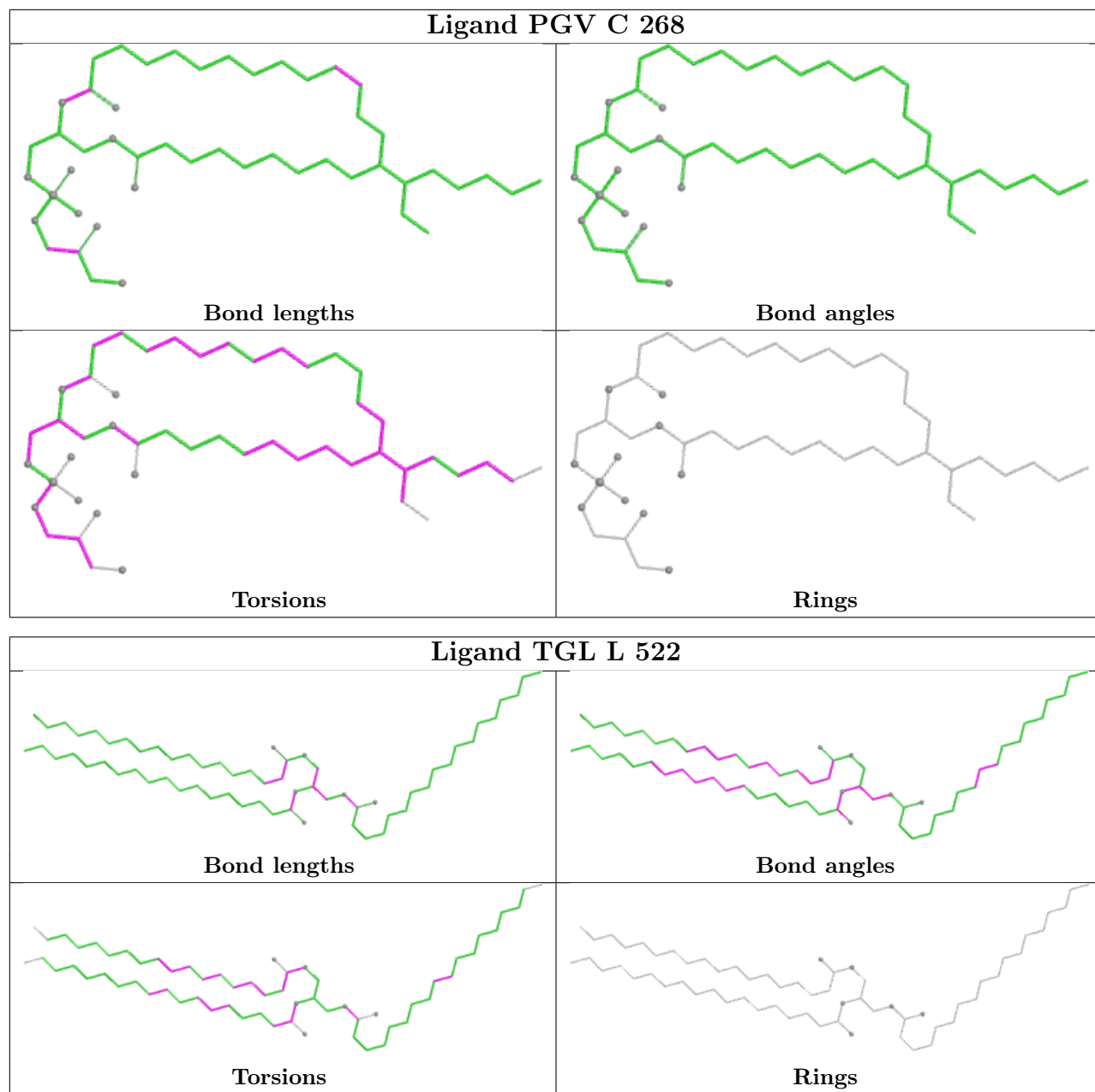
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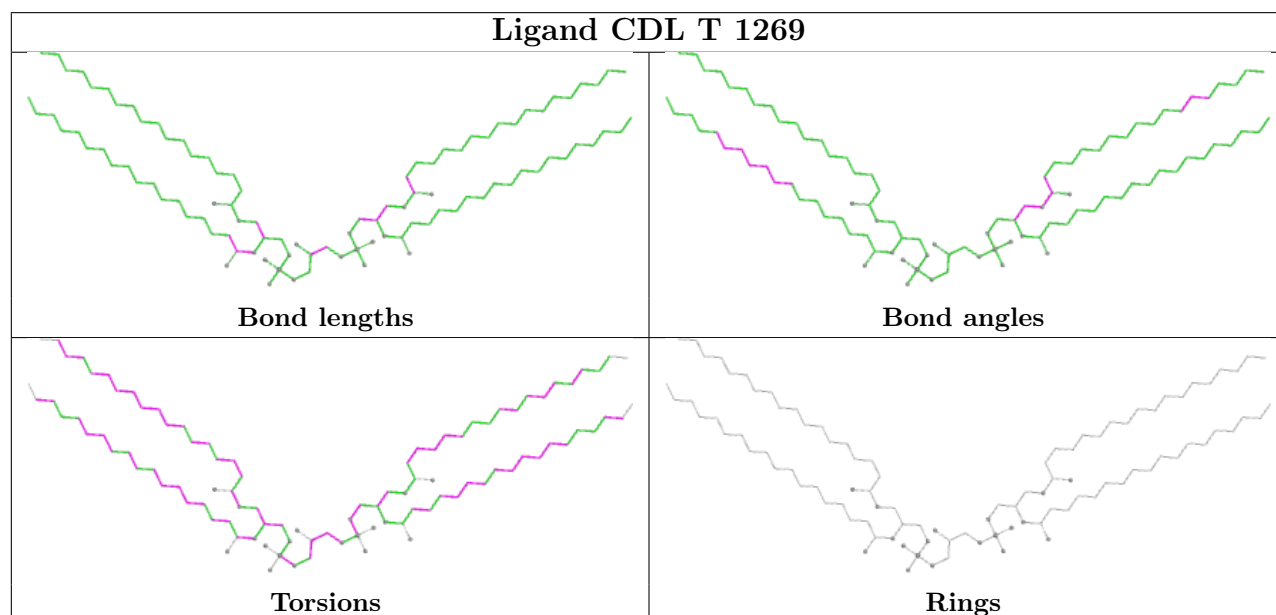
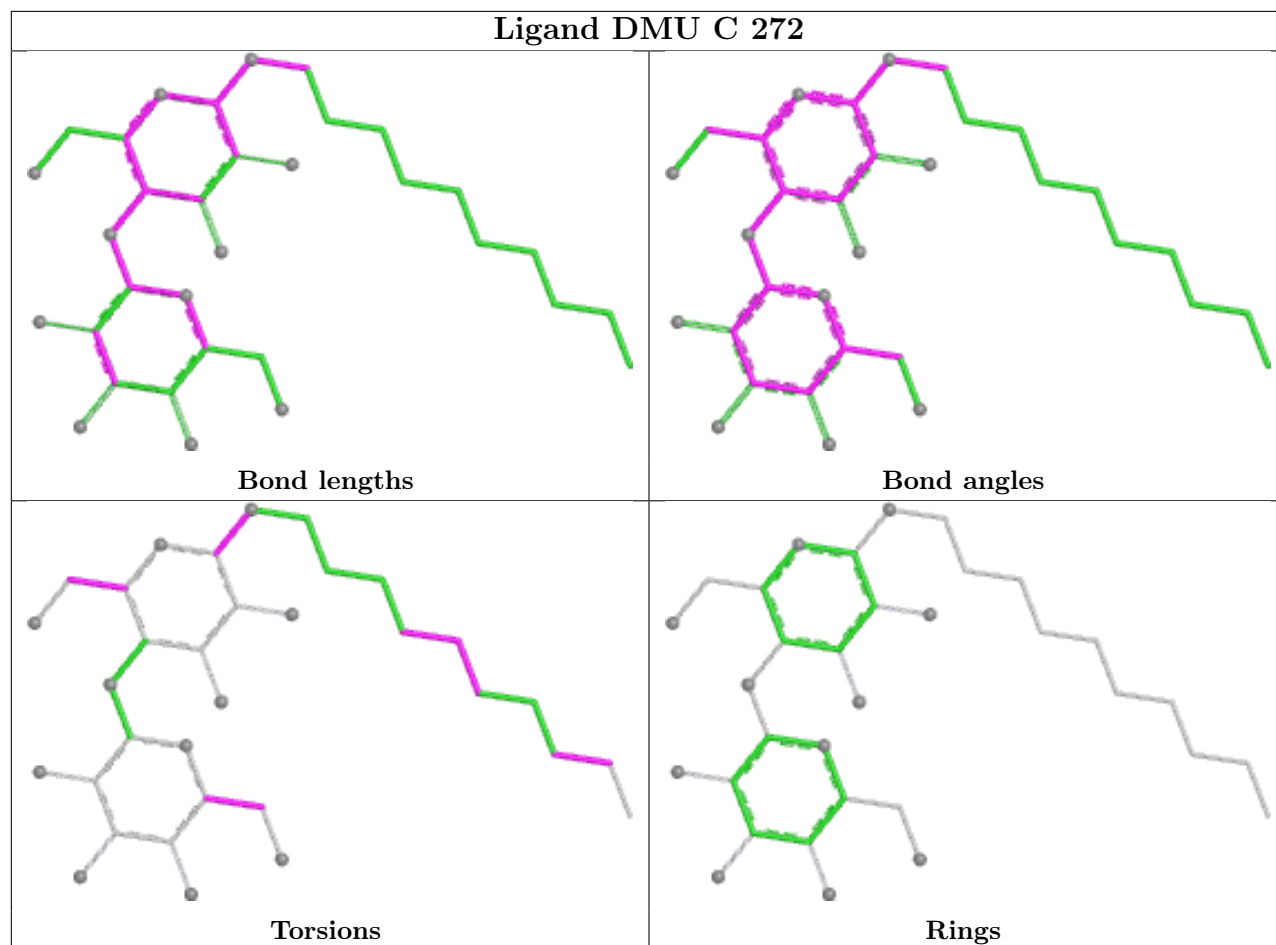


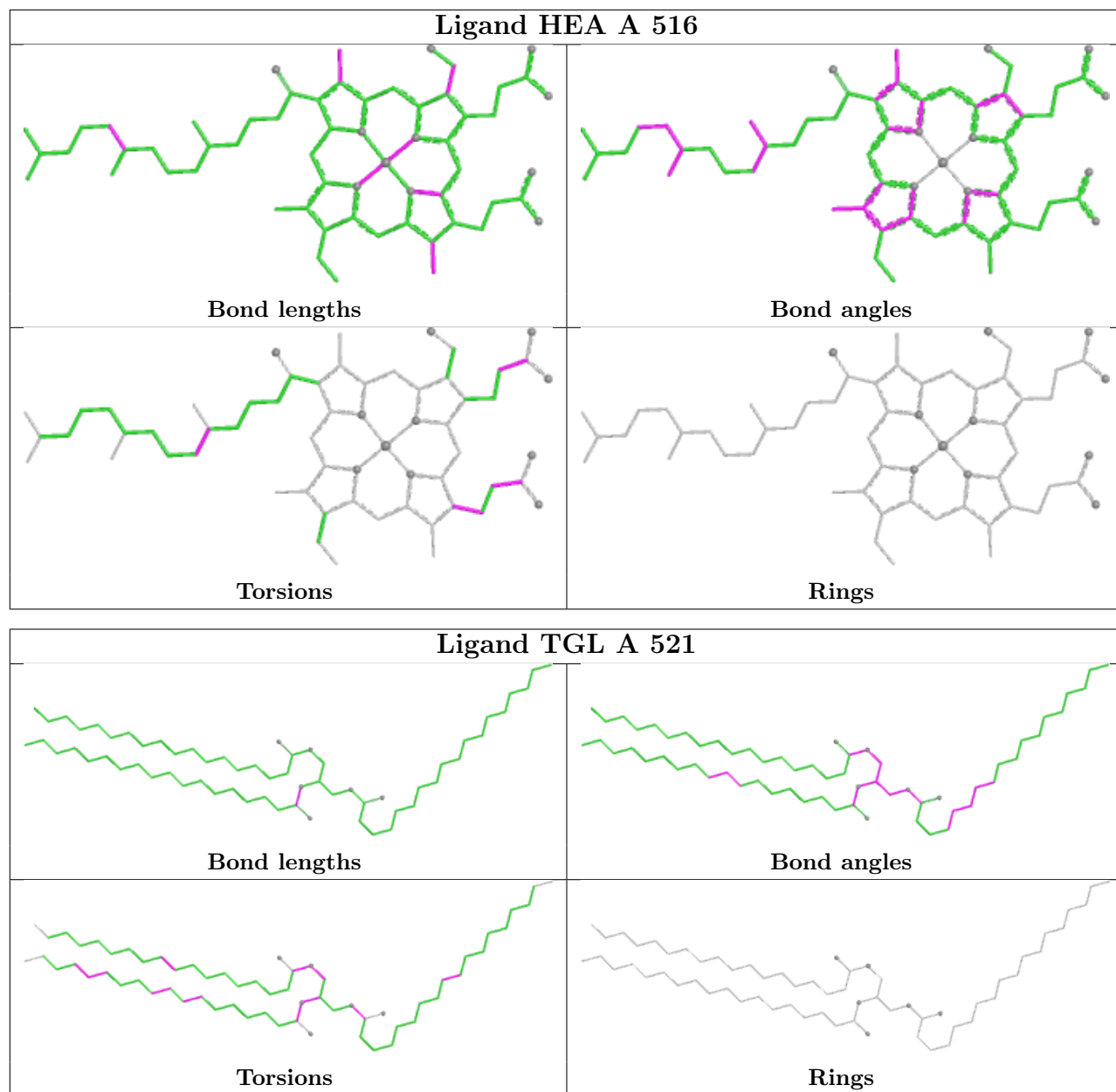
Ligand PGV A 604

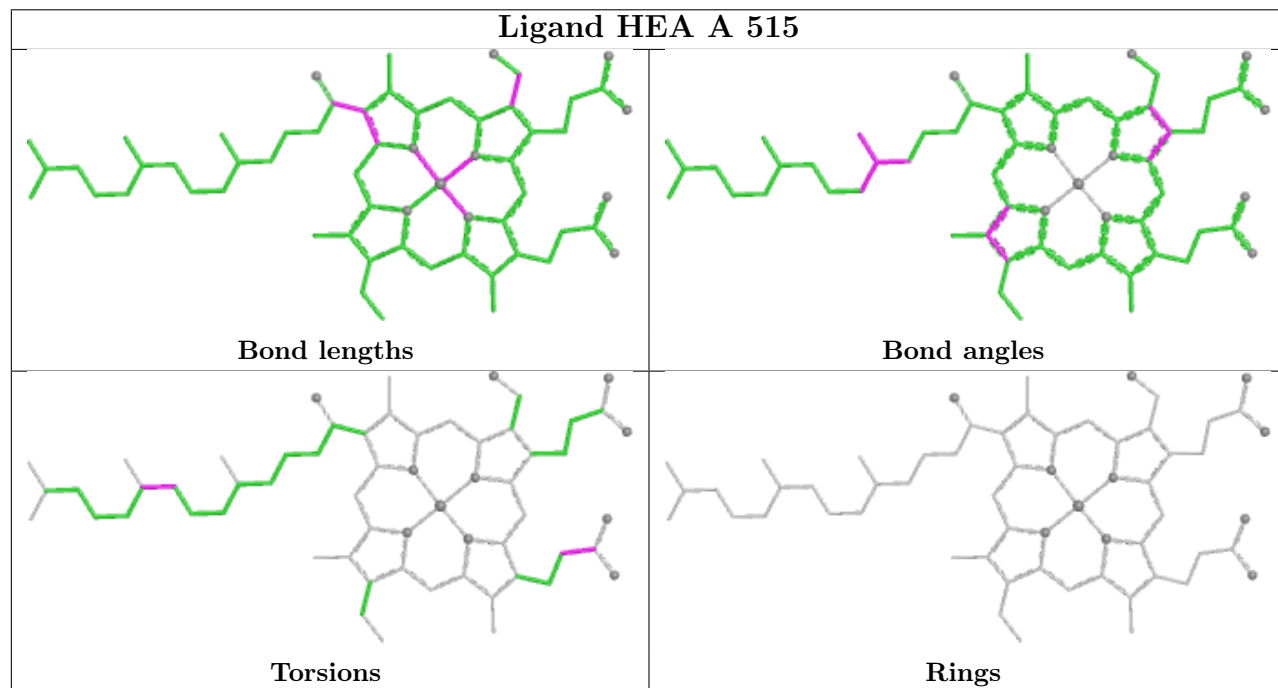
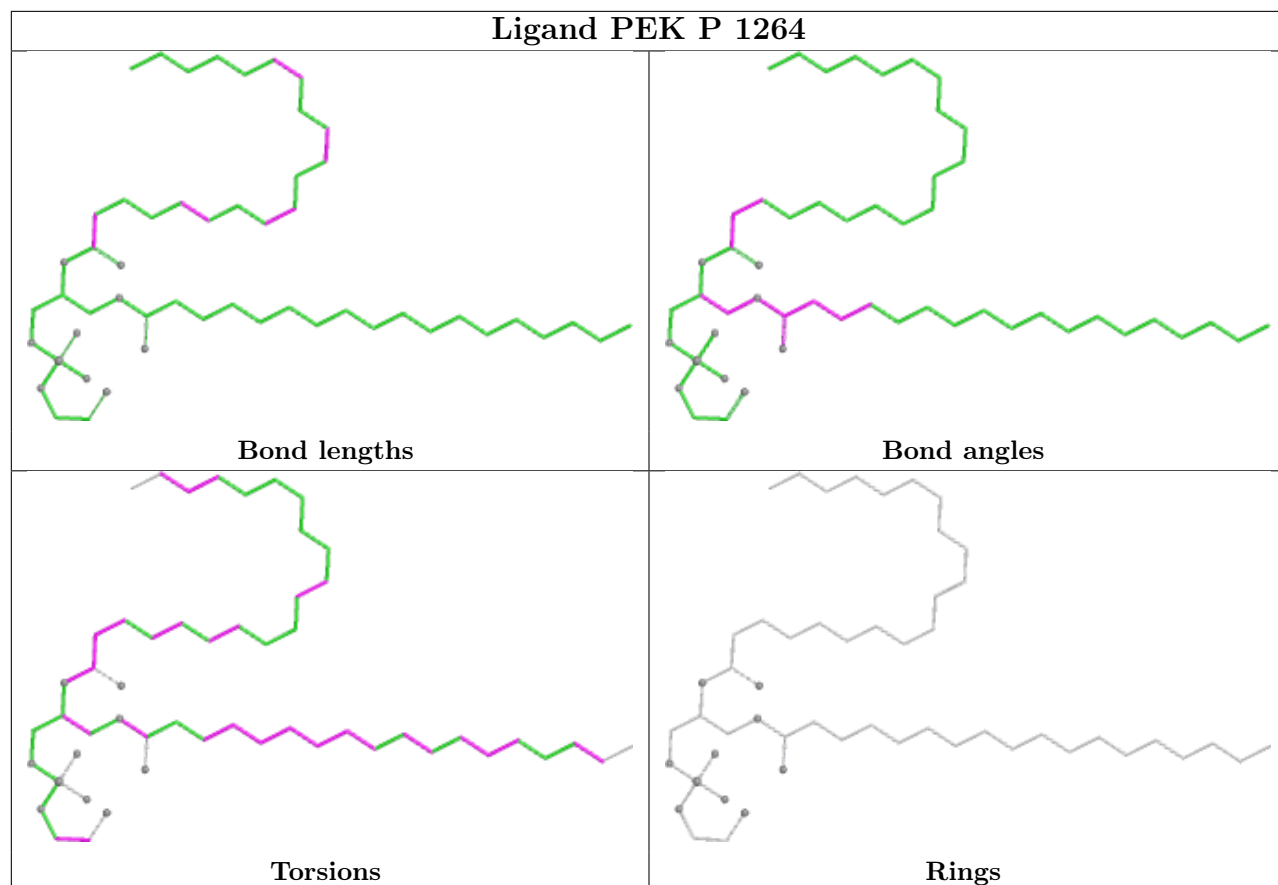




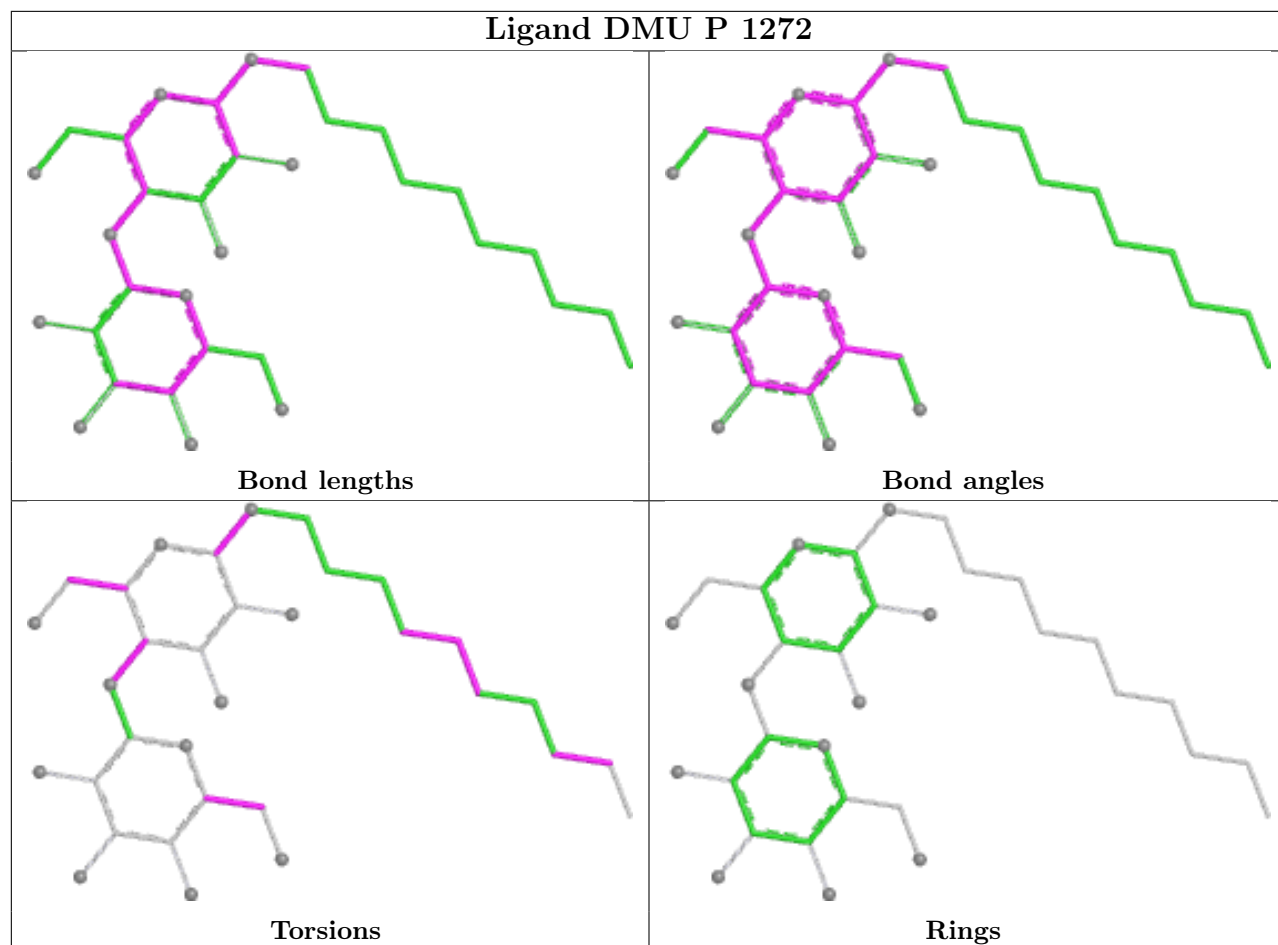




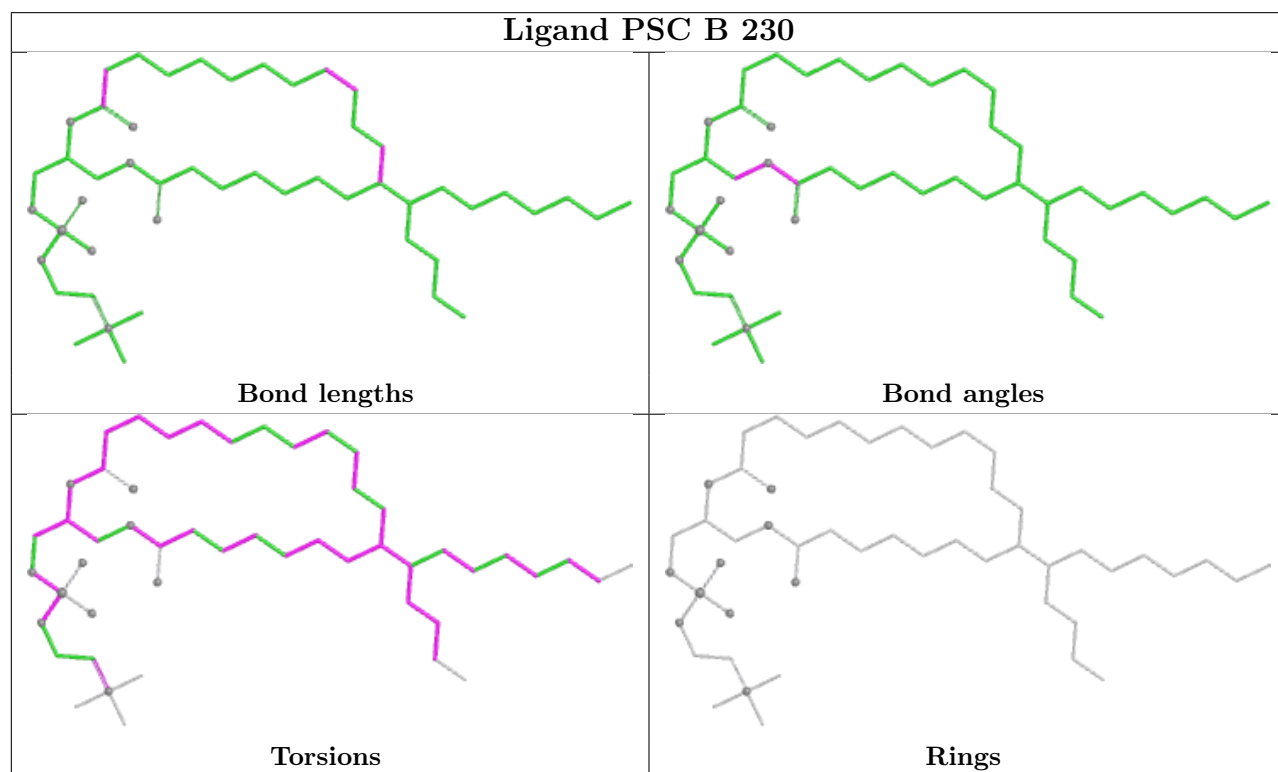




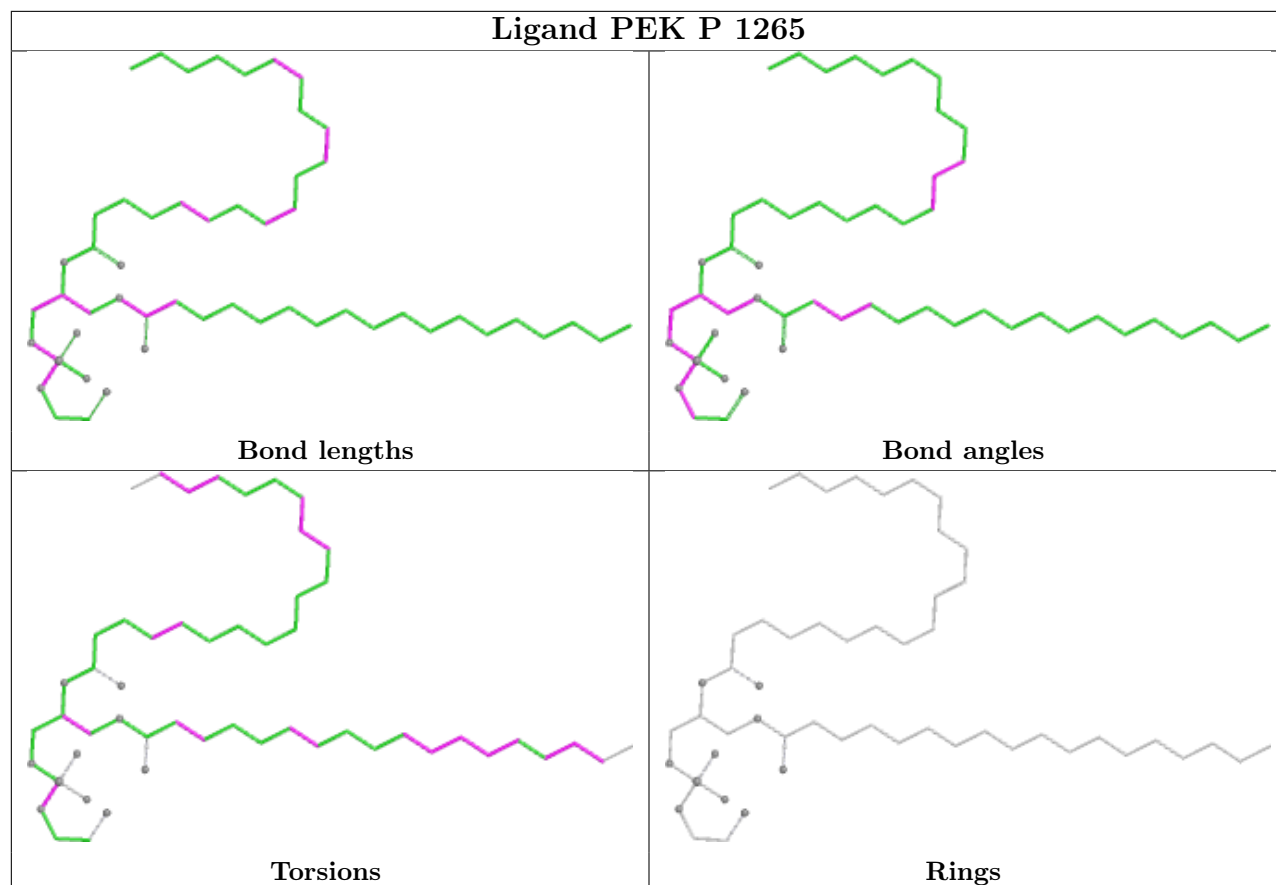
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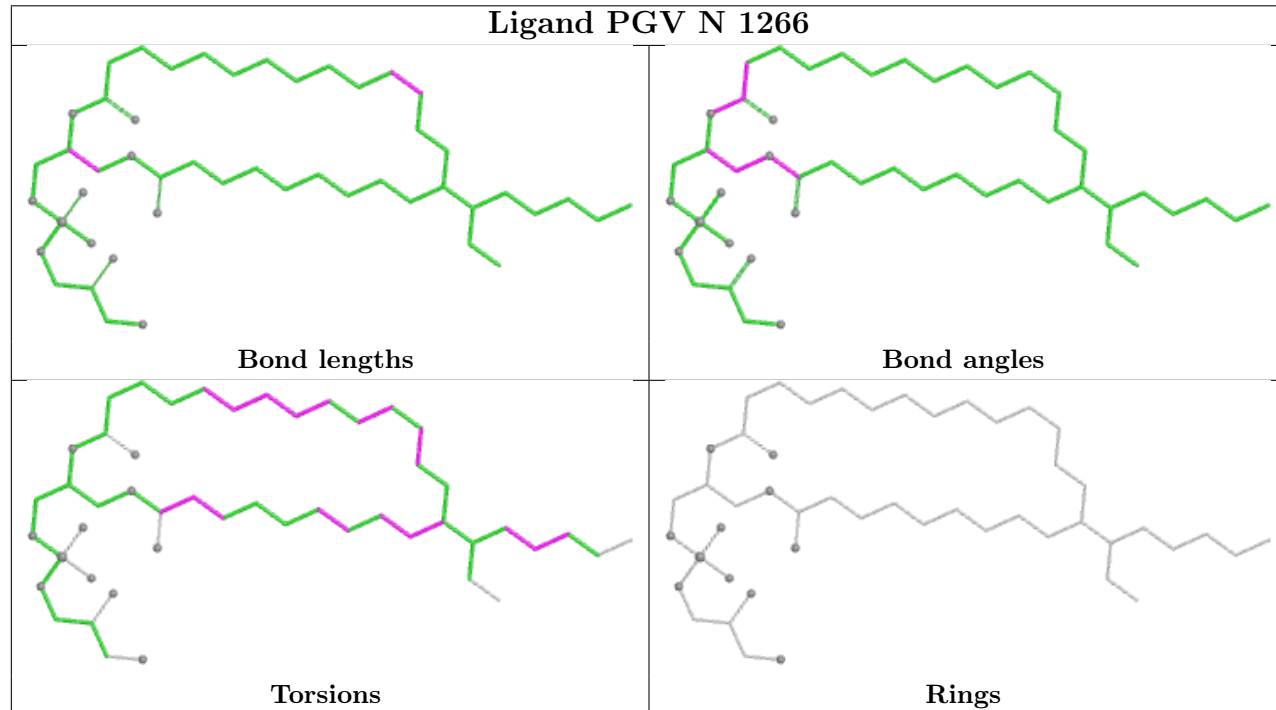
Ligand PSC B 230

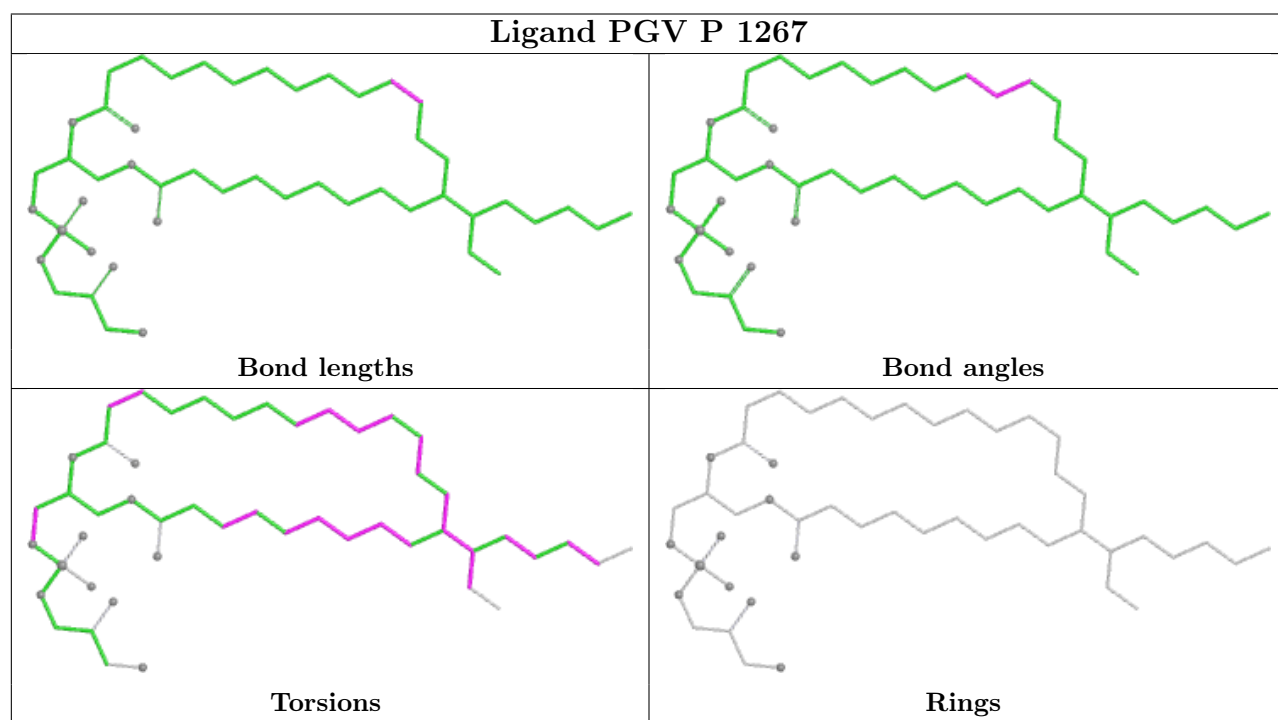
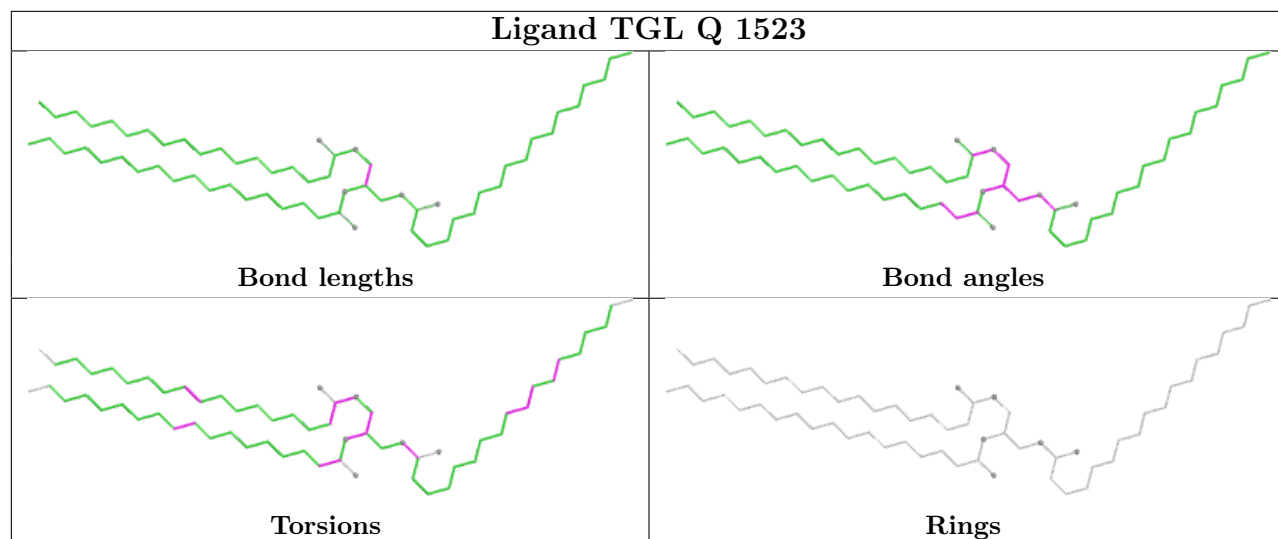


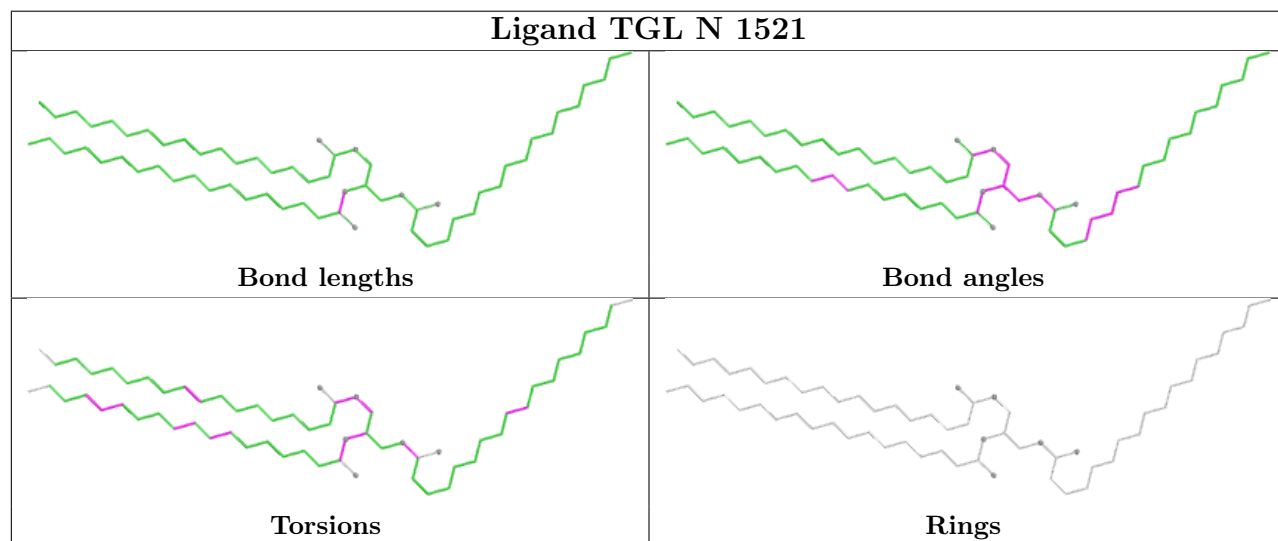
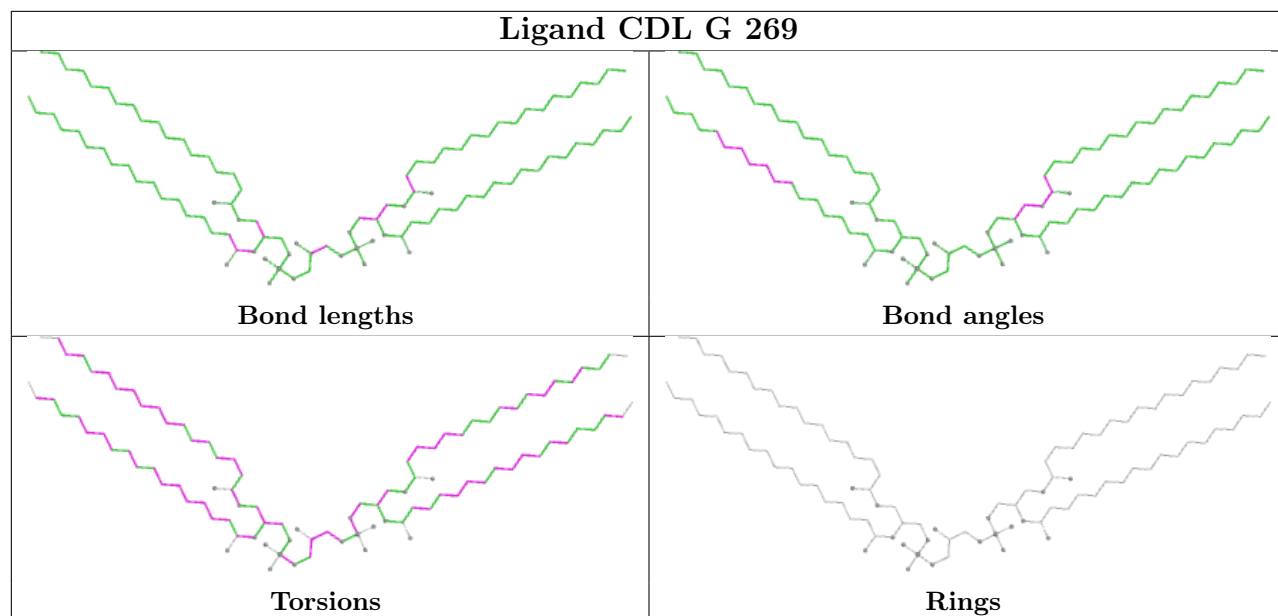
Ligand PEK P 1265

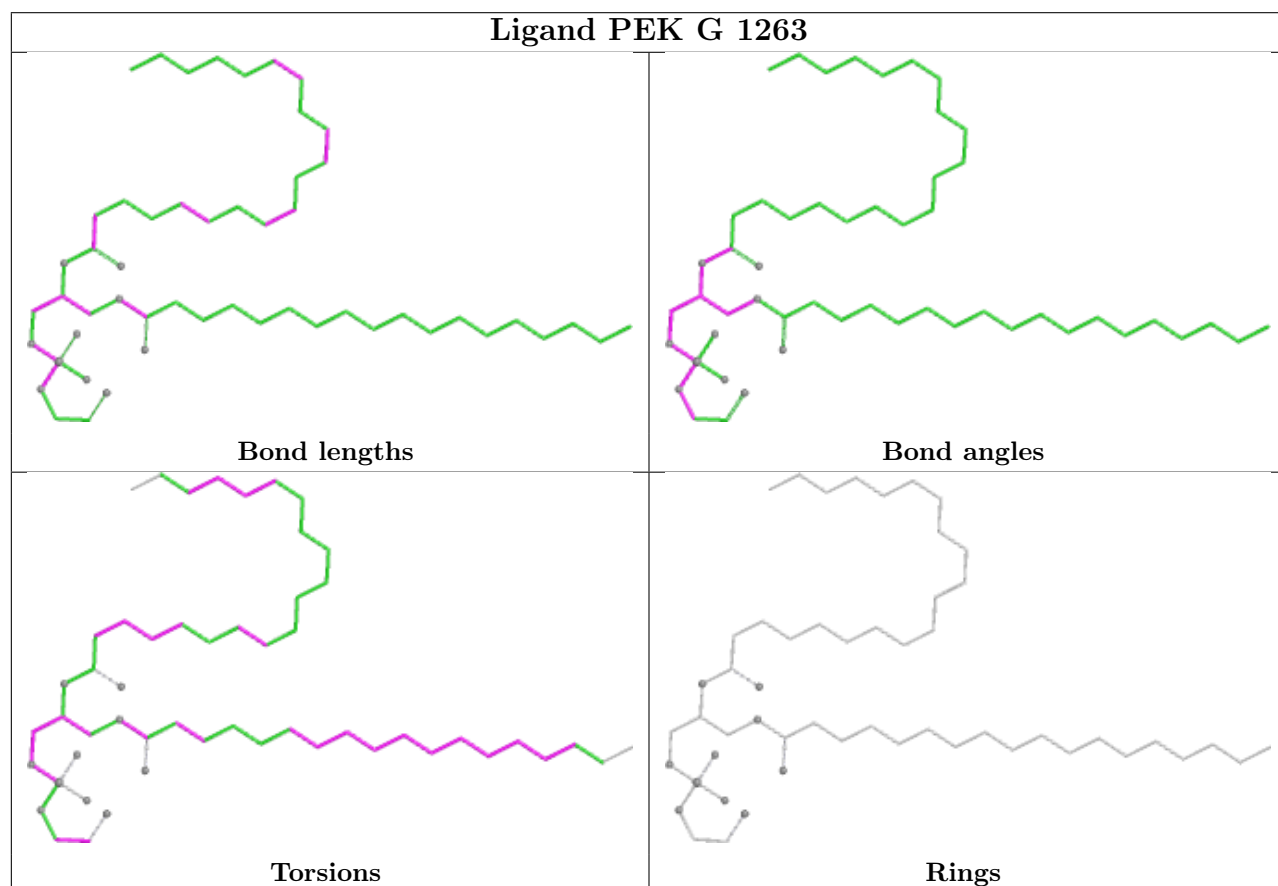
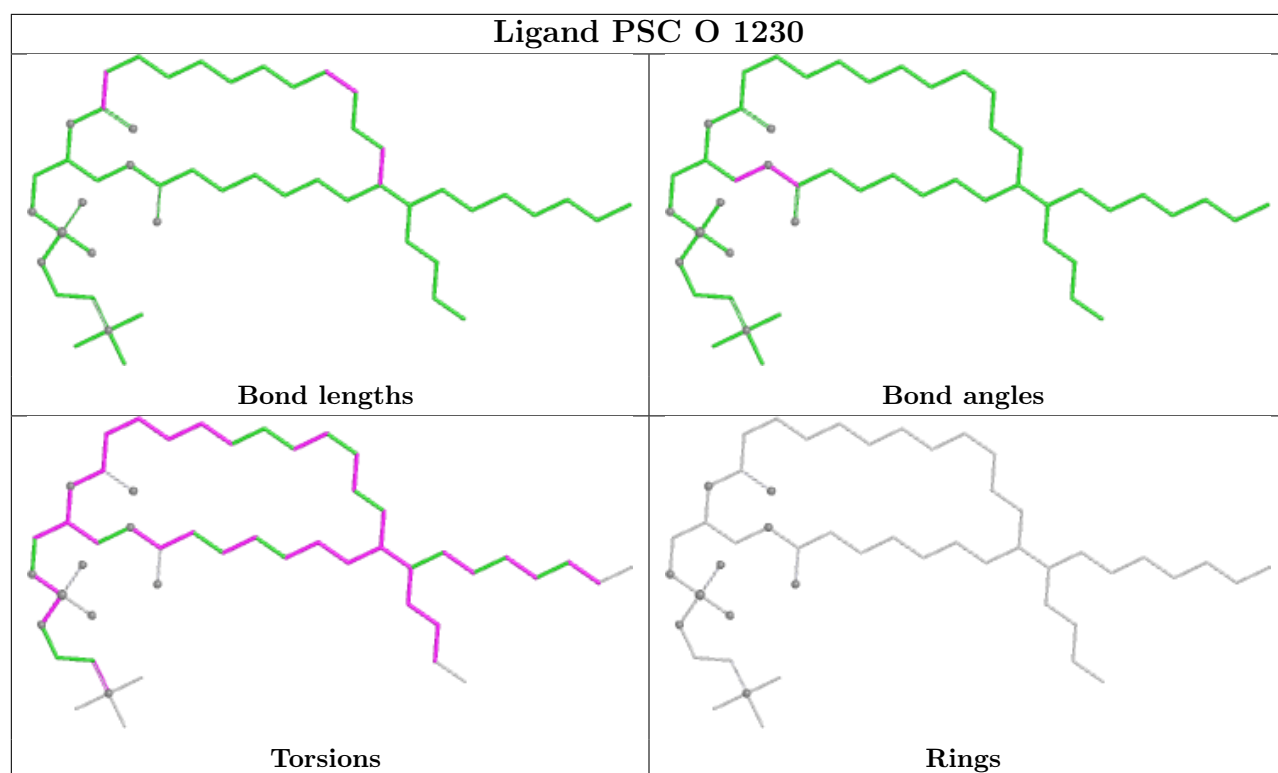


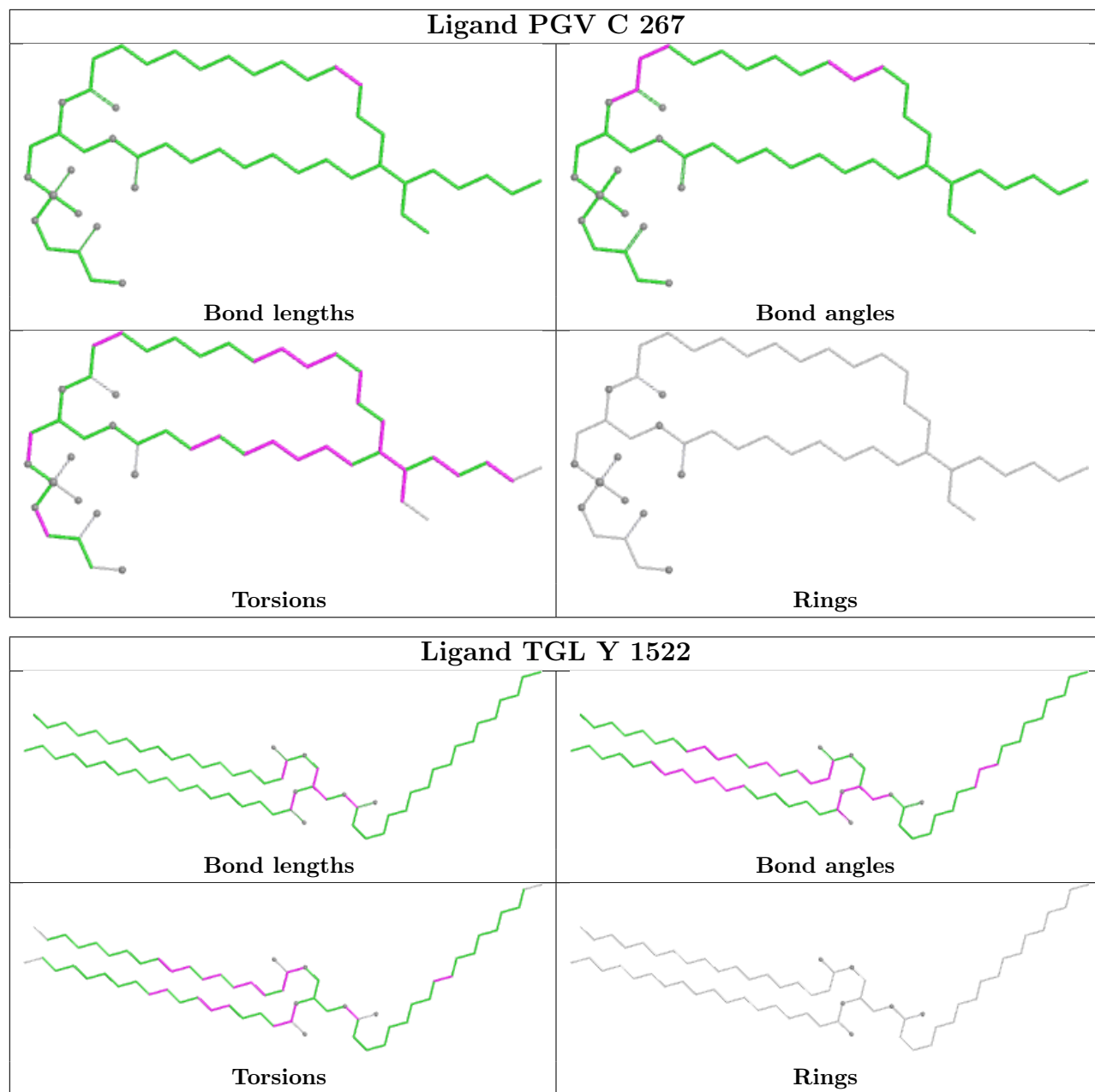
Ligand PGV N 1266

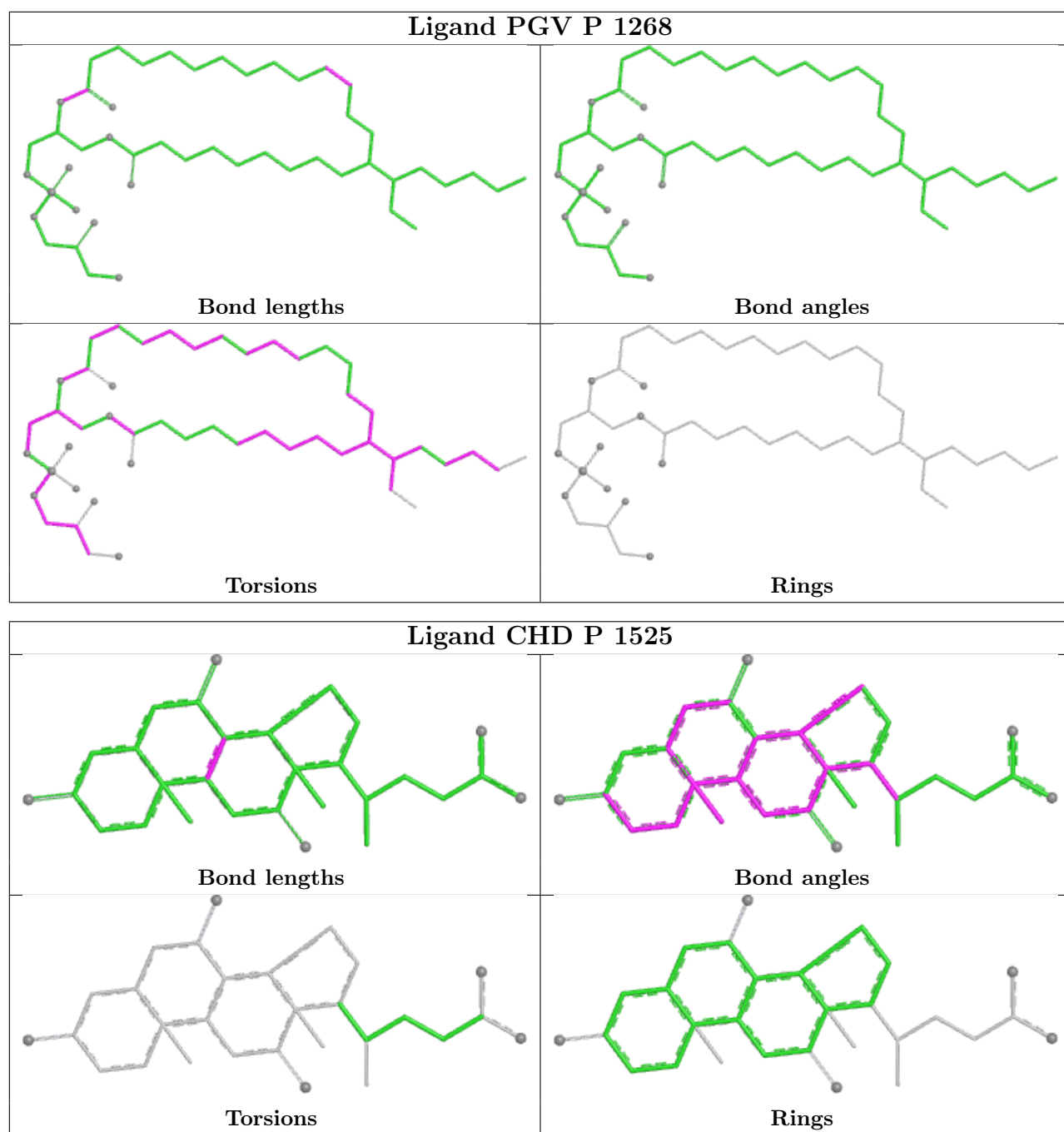












5.7 Other polymers [i](#)

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.