



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:07 am BST

PDB ID : 2EIL
Title : Cadmium ion binding structure of bovine heart cytochrome C oxidase in the fully oxidized 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

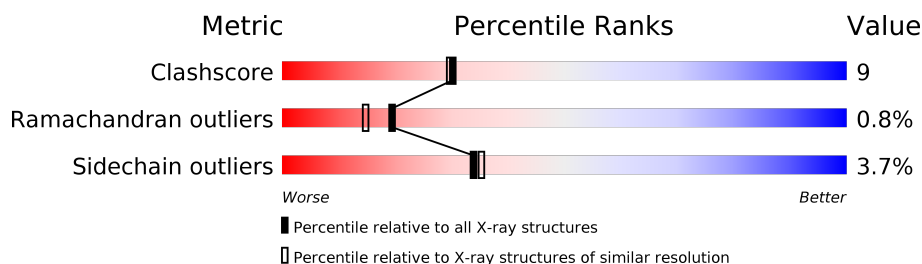
1 Overall quality at a glance i

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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (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 on 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	86% 13% .
1	N	514	82% 16% .
2	B	227	78% 19% .
2	O	227	73% 24% .
3	C	261	85% 15% .
3	P	261	84% 15% .
4	D	147	88% 10% .
4	Q	147	73% 24% .

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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
18	HEA	A	515	X	-	-	-
18	HEA	A	516	X	-	-	-
18	HEA	N	515	X	-	-	-
18	HEA	N	516	X	-	-	-
19	TGL	L	522	-	-	X	-
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CHD	P	1271	X	-	-	-
23	CHD	W	1060	X	-	-	-
24	DMU	C	272	X	-	-	-
24	DMU	M	526	X	-	-	-
24	DMU	P	1272	X	-	-	-
24	DMU	Z	1526	X	-	-	-
26	CDL	T	1269	-	-	X	-
9	SAC	V	1	-	X	-	-

2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 32357 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 (three-letter code: 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 (three-letter code: 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		

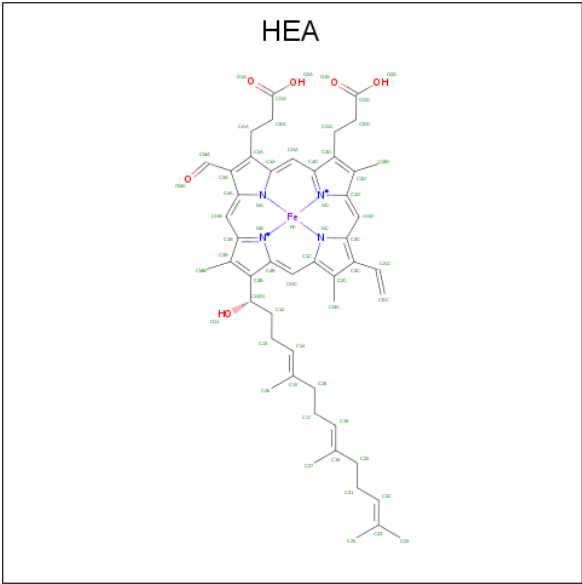
- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

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 (three-letter code: CD) (formula: Cd).

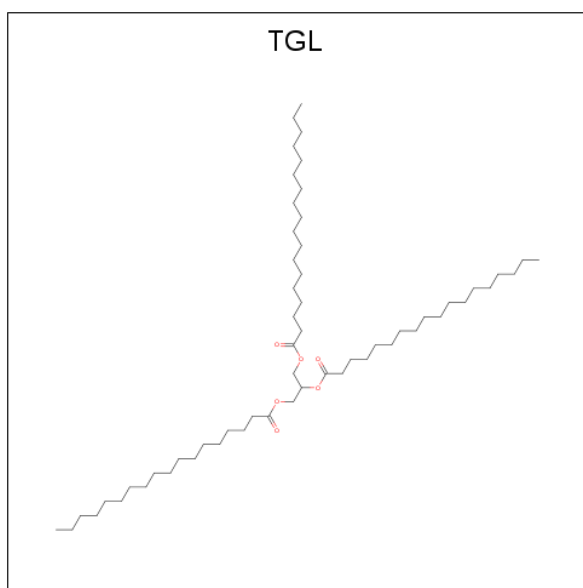
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	P	1	Total	Cd	0	0
			1	1		
17	A	1	Total	Cd	0	0
			1	1		
17	C	1	Total	Cd	0	0
			1	1		

- Molecule 18 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



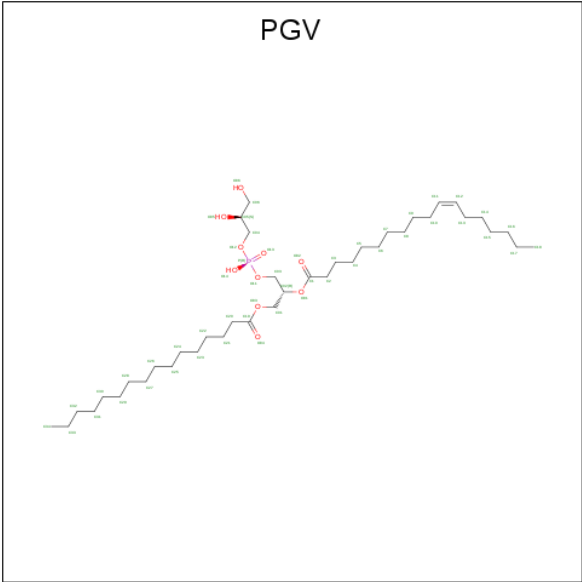
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
18	A	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
18	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0
18	N	1	Total 60	C 49	Fe 1	N 4	O 6	0	0

- Molecule 19 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: $C_{57}H_{110}O_6$).



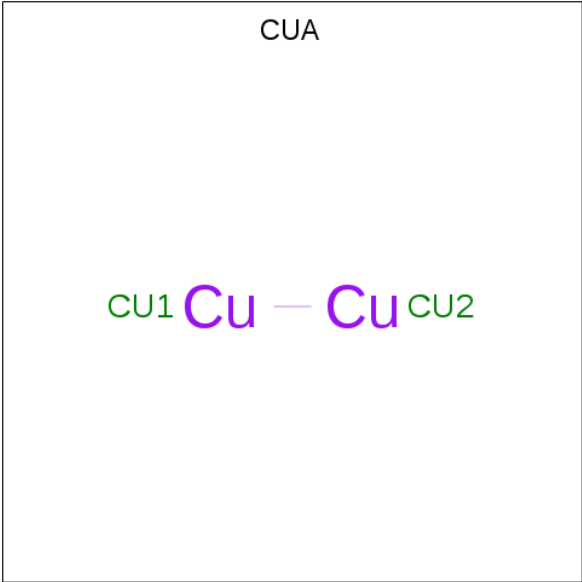
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	Q	1	Total	C	O	0	0
			63	57	6		

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



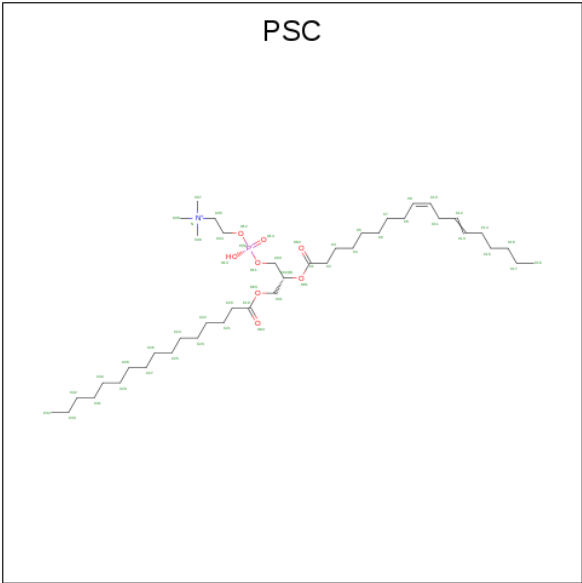
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0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

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: 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-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C₄₂H₈₁NO₈P).



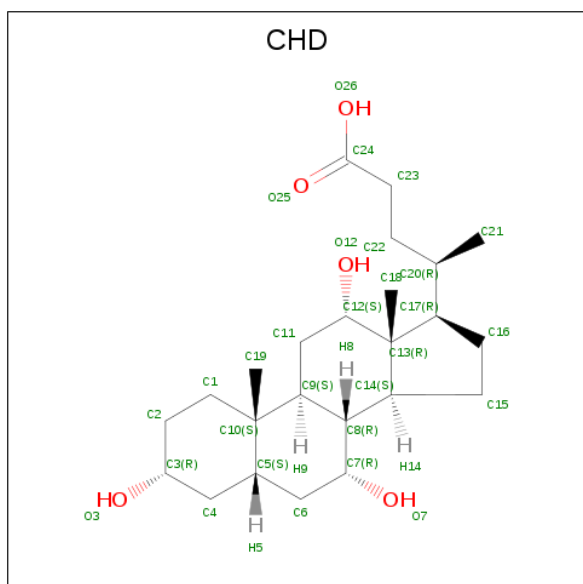
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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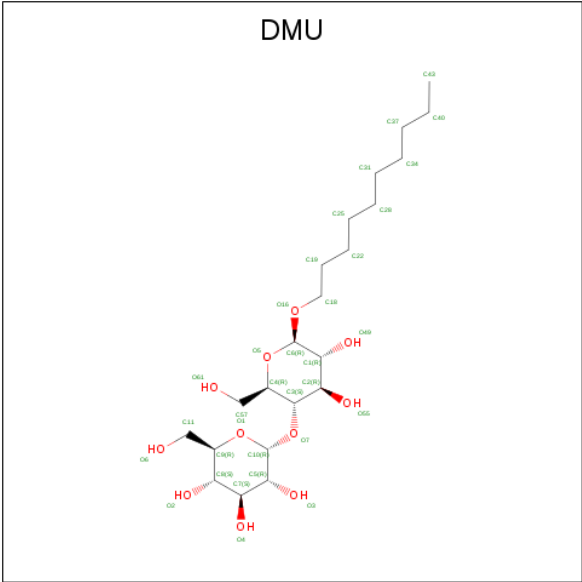
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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



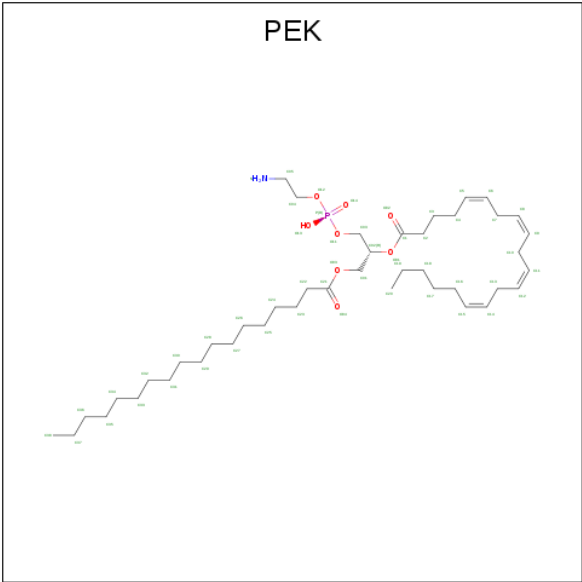
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		
23	J	1	Total	C	O	0	0
			29	24	5		
23	O	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	W	1	Total	C	O	0	0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

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



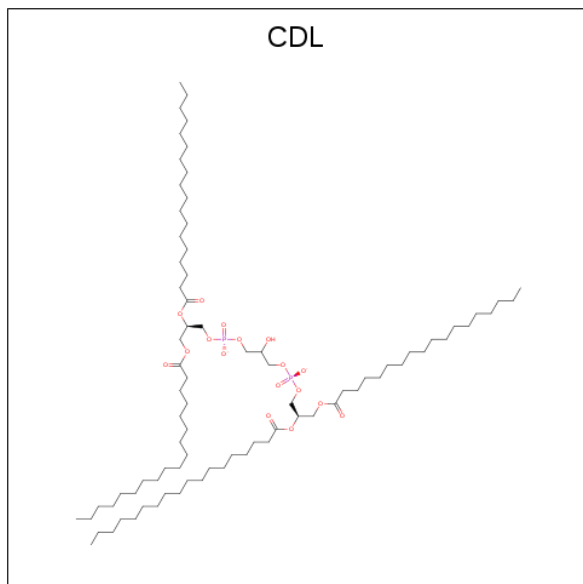
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			33	22	11		
24	M	1	Total	C	O	0	0
			33	22	11		
24	P	1	Total	C	O	0	0
			33	22	11		
24	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: 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 (three-letter code: 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 (three-letter code: ZN) (formula: Zn).

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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	220	Total 220	O 220	0	0
28	B	128	Total 128	O 128	0	0
28	C	103	Total 103	O 103	0	0
28	D	90	Total 90	O 90	0	0
28	E	58	Total 58	O 58	0	0
28	F	75	Total 75	O 75	0	0
28	G	42	Total 42	O 42	0	0
28	H	44	Total 44	O 44	0	0
28	I	45	Total 45	O 45	0	0
28	J	21	Total 21	O 21	0	0
28	K	24	Total 24	O 24	0	0
28	L	20	Total 20	O 20	0	0
28	M	21	Total 21	O 21	0	0
28	N	198	Total 198	O 198	0	0
28	O	118	Total 118	O 118	0	0
28	P	94	Total 94	O 94	0	0
28	Q	53	Total 53	O 53	0	0
28	R	43	Total 43	O 43	0	0

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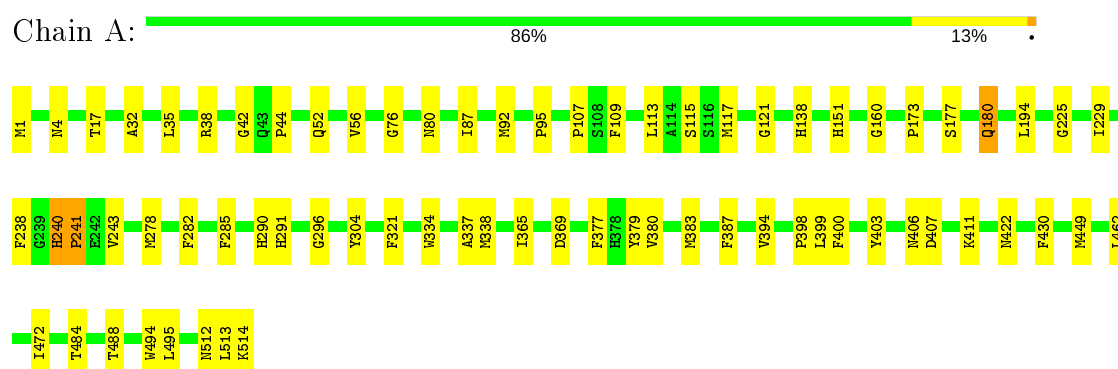
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	S	62	Total 62	O 62	0	0
28	T	44	Total 44	O 44	0	0
28	U	38	Total 38	O 38	0	0
28	V	23	Total 23	O 23	0	0
28	W	16	Total 16	O 16	0	0
28	X	16	Total 16	O 16	0	0
28	Y	15	Total 15	O 15	0	0
28	Z	13	Total 13	O 13	0	0

3 Residue-property plots

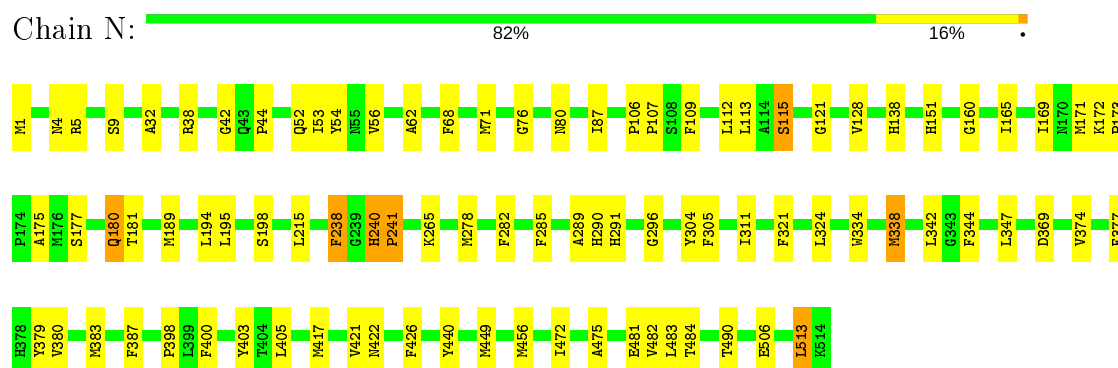
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

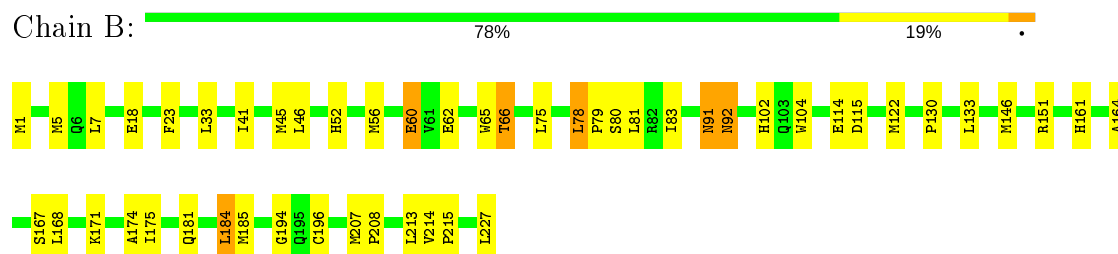
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 1: Cytochrome c oxidase subunit 1

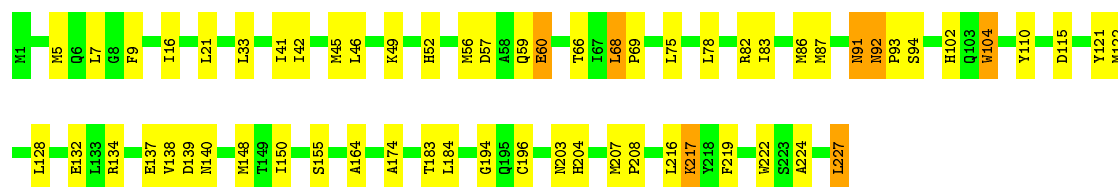


• Molecule 2: Cytochrome c oxidase subunit 2




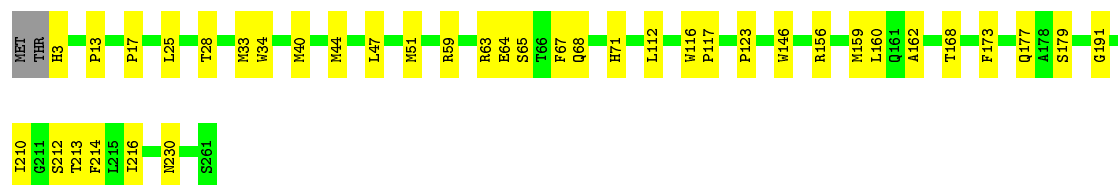
• Molecule 2: Cytochrome c oxidase subunit 2

Chain O:  73% 24%




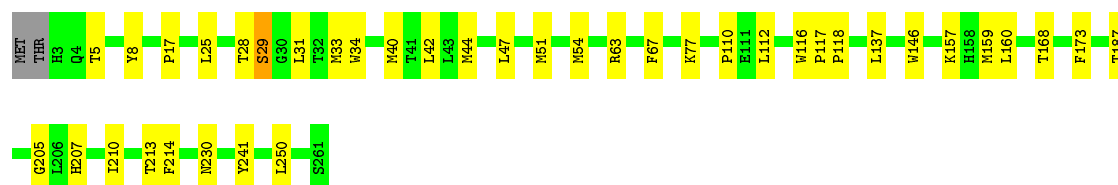
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C:  85% 15%




• Molecule 3: Cytochrome c oxidase subunit 3

Chain P:  84% 15%



• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D:  88% 10%




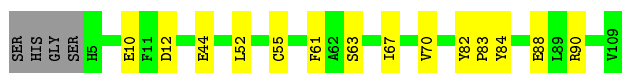
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q:  73% 24%

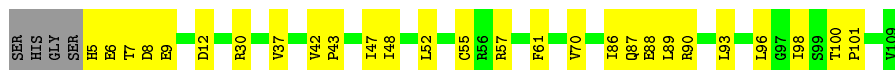


• Molecule 5: Cytochrome c oxidase polypeptide Va

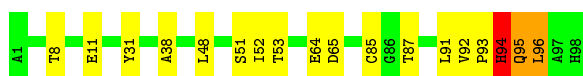
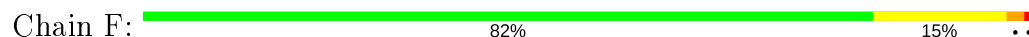
Chain E:  83% 13%



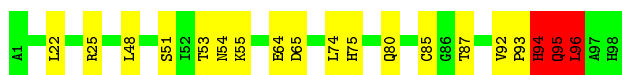
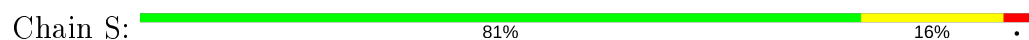
- Molecule 5: Cytochrome c oxidase polypeptide Va



- Molecule 6: Cytochrome c oxidase polypeptide Vb



- Molecule 6: Cytochrome c oxidase polypeptide Vb



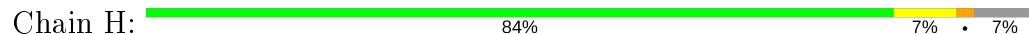
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart



- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1



- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1





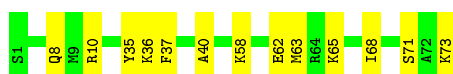
- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I: 90% 8%



- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V: 82% 18%



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain J: 90% 7%



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain W: 85% 12%



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K: 79% 9% 13%



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X: 75% 11% 13%



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L: 77% 21%



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y: 74% 21% ..



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M: 74% 15% • 7%



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain Z: 57% 37% 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	183.38Å 205.90Å 178.18Å 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 , 0.231	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32357	wwPDB-VP
Average B, all atoms (Å ²)	40.0	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: ZN, TPO, CHD, TGL, CDL, PSC, PEK, MG, CD, PGV, SAC, DMU, CUA, NA, FME, CU, 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	0.55	0/4156	0.70	0/5678
1	N	0.55	2/4156 (0.0%)	0.67	0/5678
2	B	0.53	0/1860	0.78	1/2534 (0.0%)
2	O	0.55	0/1860	0.81	2/2534 (0.1%)
3	C	0.57	0/2197	0.62	0/3005
3	P	0.53	0/2197	0.63	0/3005
4	D	0.54	0/1229	0.69	1/1658 (0.1%)
4	Q	0.57	0/1229	0.67	1/1658 (0.1%)
5	E	0.56	0/871	0.70	0/1182
5	R	0.54	0/871	0.72	1/1182 (0.1%)
6	F	0.52	0/765	0.83	2/1038 (0.2%)
6	S	0.53	0/765	0.83	2/1038 (0.2%)
7	G	0.58	1/690 (0.1%)	0.74	1/937 (0.1%)
7	T	0.59	0/690	0.76	2/937 (0.2%)
8	H	0.52	0/682	0.68	0/921
8	U	0.50	0/682	0.67	0/921
9	I	0.54	0/605	0.63	0/802
9	V	0.54	0/605	0.61	0/802
10	J	0.51	0/471	0.65	0/636
10	W	0.51	0/471	0.66	0/636
11	K	0.56	0/398	0.69	0/546
11	X	0.53	0/398	0.66	0/546
12	L	0.53	0/393	0.57	0/526
12	Y	0.54	0/393	0.63	0/526
13	M	0.55	0/345	0.65	0/470
13	Z	0.52	0/345	0.64	0/470
All	All	0.54	3/29324 (0.0%)	0.70	13/39866 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	1
8	U	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	506	GLU	CB-CG	5.12	1.61	1.52
1	N	506	GLU	CG-CD	5.09	1.59	1.51
7	G	31	CYS	CB-SG	-5.02	1.73	1.81

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	33	LEU	CA-CB-CG	6.75	130.82	115.30
6	F	94	HIS	N-CA-C	6.51	128.58	111.00
6	S	94	HIS	N-CA-C	6.27	127.93	111.00
2	O	227	LEU	CA-CB-CG	6.11	129.35	115.30
4	D	133	GLY	N-CA-C	5.72	127.40	113.10
4	Q	133	GLY	N-CA-C	5.58	127.06	113.10
6	F	93	PRO	N-CA-C	5.39	126.13	112.10
5	R	42	VAL	N-CA-C	-5.38	96.49	111.00
2	B	184	LEU	CA-CB-CG	5.34	127.58	115.30
7	G	6	GLY	N-CA-C	5.24	126.19	113.10
2	O	104	TRP	N-CA-CB	-5.22	101.20	110.60
6	S	93	PRO	N-CA-C	5.15	125.48	112.10
7	T	6	GLY	N-CA-C	5.09	125.83	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain
8	U	11	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	60	0
1	N	4027	0	4001	78	0
2	B	1824	0	1833	32	0
2	O	1824	0	1833	41	0
3	C	2110	0	2027	32	0
3	P	2110	0	2027	36	0
4	D	1195	0	1183	13	0
4	Q	1195	0	1183	27	0
5	E	852	0	845	7	0
5	R	852	0	845	16	0
6	F	748	0	728	9	0
6	S	748	0	728	14	0
7	G	675	0	644	25	0
7	T	675	0	644	31	0
8	H	662	0	623	6	0
8	U	662	0	623	12	0
9	I	601	0	613	5	0
9	V	601	0	613	10	0
10	J	460	0	459	5	0
10	W	460	0	459	6	0
11	K	384	0	366	2	0
11	X	384	0	366	5	0
12	L	380	0	380	15	0
12	Y	380	0	380	10	0
13	M	335	0	352	6	0
13	Z	335	0	352	10	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	P	1	0	0	0	0
18	A	120	0	108	4	0
18	N	120	0	108	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	A	63	0	110	9	0
19	D	63	0	110	4	0
19	L	63	0	110	24	0
19	N	126	0	220	24	0
19	Q	63	0	110	5	0
20	A	102	0	152	10	0
20	C	102	0	152	7	0
20	N	51	0	76	1	0
20	P	102	0	152	6	0
20	Z	51	0	76	6	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	15	0
22	O	52	0	80	15	0
23	B	29	0	39	0	0
23	C	58	0	78	4	0
23	J	29	0	39	2	0
23	O	29	0	39	0	0
23	P	58	0	78	2	0
23	W	29	0	39	3	0
24	C	33	0	36	3	0
24	M	33	0	38	1	0
24	P	33	0	37	5	0
24	Z	33	0	38	0	0
25	C	106	0	154	12	0
25	G	53	0	77	7	0
25	P	106	0	154	16	0
25	T	53	0	77	9	0
26	C	100	0	156	18	0
26	G	100	0	156	18	0
26	P	100	0	156	16	0
26	T	100	0	156	22	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	A	220	0	0	4	0
28	B	128	0	0	2	0
28	C	103	0	0	1	0
28	D	90	0	0	2	0
28	E	58	0	0	1	0
28	F	75	0	0	0	0
28	G	42	0	0	6	0
28	H	44	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	I	45	0	0	3	0
28	J	21	0	0	2	0
28	K	24	0	0	1	0
28	L	20	0	0	1	0
28	M	21	0	0	1	0
28	N	198	0	0	3	0
28	O	118	0	0	2	0
28	P	94	0	0	1	0
28	Q	53	0	0	1	0
28	R	43	0	0	0	0
28	S	62	0	0	2	0
28	T	44	0	0	3	0
28	U	38	0	0	0	0
28	V	23	0	0	1	0
28	W	16	0	0	0	0
28	X	16	0	0	0	0
28	Y	15	0	0	1	0
28	Z	13	0	0	1	0
All	All	32357	0	31299	579	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (579) 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)
22:O:1230:PSC:H142	22:O:1230:PSC:H343	1.29	1.09
22:B:230:PSC:H343	22:B:230:PSC:H142	1.31	1.05
10:W:33:ARG:HG2	23:W:1060:CHD:H152	1.31	1.05
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.23	1.04
7:T:84:LYS:H	7:T:84:LYS:HD2	1.23	0.99
4:D:34:SER:H	4:D:37:GLN:HE21	1.07	0.98
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.43	0.97
3:P:63:ARG:HE	26:P:1270:CDL:HA22	1.27	0.97
19:N:1521:TGL:H281	19:N:1521:TGL:H102	1.48	0.95
7:G:84:LYS:HD2	7:G:84:LYS:H	1.30	0.95
19:A:521:TGL:H281	19:A:521:TGL:H102	1.50	0.93
19:L:522:TGL:HC62	19:L:522:TGL:HC22	1.52	0.92
7:G:5:LYS:HB2	25:G:1263:PEK:H362	1.52	0.91
26:P:1270:CDL:H642	26:P:1270:CDL:H191	1.53	0.91
26:G:269:CDL:H541	26:G:269:CDL:H231	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:1522:TGL:HC62	19:N:1522:TGL:HC22	1.55	0.89
25:C:264:PEK:H102	25:C:264:PEK:H161	1.55	0.88
26:C:270:CDL:H642	26:C:270:CDL:H191	1.54	0.88
26:T:1269:CDL:H541	26:T:1269:CDL:H231	1.57	0.87
10:J:33:ARG:HG2	23:J:60:CHD:H152	1.57	0.86
7:T:31:CYS:SG	26:T:1269:CDL:H532	2.14	0.86
19:N:1521:TGL:C28	19:N:1521:TGL:H102	2.08	0.83
25:P:1264:PEK:H102	25:P:1264:PEK:H161	1.59	0.83
6:S:94:HIS:CD2	6:S:95:GLN:H	1.97	0.83
2:O:41:ILE:HD13	22:O:1230:PSC:H342	1.62	0.82
1:N:472:ILE:HG21	19:N:1522:TGL:HA92	1.61	0.81
19:A:521:TGL:H102	19:A:521:TGL:C28	2.11	0.80
1:A:278:MET:SD	7:T:5:LYS:HB3	2.21	0.79
9:I:1:SAC:HA	28:I:4751:HOH:O	1.82	0.79
13:M:42:LYS:HE3	13:M:42:LYS:HA	1.66	0.78
1:A:472:ILE:HG21	19:L:522:TGL:HA92	1.66	0.78
12:L:20:ARG:HH22	19:L:522:TGL:HC61	1.50	0.77
1:N:112:LEU:HG	28:N:3073:HOH:O	1.84	0.77
26:G:269:CDL:H622	20:P:1268:PGV:H152	1.65	0.76
19:N:1522:TGL:HC31	12:Y:13:PHE:HA	1.65	0.76
6:S:94:HIS:CG	6:S:95:GLN:H	2.03	0.76
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.69	0.75
12:L:13:PHE:HA	19:L:522:TGL:HC31	1.67	0.75
3:P:67:PHE:HE1	26:P:1270:CDL:H1	1.51	0.75
1:N:334:TRP:CZ3	19:Q:1523:TGL:HA51	2.22	0.74
7:G:31:CYS:SG	26:G:269:CDL:H532	2.27	0.74
19:L:522:TGL:H242	19:L:522:TGL:H202	1.69	0.74
7:T:5:LYS:HG3	25:T:263:PEK:H383	1.70	0.74
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.36	0.74
19:N:1521:TGL:H201	19:N:1521:TGL:H241	1.69	0.73
2:O:224:ALA:O	2:O:227:LEU:HG	1.88	0.73
19:N:1522:TGL:H242	19:N:1522:TGL:H202	1.70	0.73
12:L:24:MET:SD	19:L:522:TGL:H162	2.29	0.73
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.71	0.73
19:A:521:TGL:H201	19:A:521:TGL:H241	1.72	0.71
3:P:34:TRP:CZ2	24:P:1272:DMU:H29	2.25	0.71
7:T:84:LYS:H	7:T:84:LYS:CD	2.02	0.71
5:R:89:LEU:O	5:R:93:LEU:HG	1.91	0.70
12:L:20:ARG:HH12	19:L:522:TGL:HC61	1.56	0.70
26:G:269:CDL:C23	26:G:269:CDL:H541	2.22	0.70
3:C:67:PHE:HE1	26:C:270:CDL:H1	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:268:PGV:H152	26:T:1269:CDL:H622	1.75	0.69
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.74	0.69
4:D:34:SER:H	4:D:37:GLN:NE2	1.87	0.69
26:G:269:CDL:H522	26:G:269:CDL:H202	1.75	0.69
7:G:84:LYS:H	7:G:84:LYS:CD	2.00	0.68
22:B:230:PSC:C34	22:B:230:PSC:H142	2.17	0.68
7:T:5:LYS:HD2	25:T:263:PEK:H371	1.74	0.68
19:N:1521:TGL:H161	2:O:7:LEU:HD11	1.76	0.68
20:Z:1524:PGV:H321	20:Z:1524:PGV:H152	1.75	0.68
1:A:321:PHE:CD2	22:B:230:PSC:H341	2.29	0.67
7:T:3:ALA:HB1	25:T:263:PEK:H382	1.76	0.67
20:P:1267:PGV:H12	20:P:1267:PGV:H161	1.75	0.67
1:N:449:MET:SD	2:O:5:MET:HG2	2.34	0.67
7:T:45:PRO:HD2	28:T:3152:HOH:O	1.95	0.67
6:S:94:HIS:CD2	6:S:95:GLN:N	2.64	0.66
22:O:1230:PSC:H222	22:O:1230:PSC:H21	1.76	0.66
1:N:1:FME:HCN	1:N:4:ASN:H	1.60	0.66
7:G:5:LYS:HG3	25:G:1263:PEK:H383	1.76	0.66
20:C:267:PGV:H172	26:C:270:CDL:H662	1.77	0.66
22:B:230:PSC:C07	9:I:10:ARG:HH21	2.08	0.65
7:G:5:LYS:HB3	1:N:278:MET:SD	2.36	0.65
26:T:1269:CDL:H522	26:T:1269:CDL:H202	1.79	0.65
20:C:267:PGV:H12	20:C:267:PGV:H161	1.76	0.65
26:T:1269:CDL:H541	26:T:1269:CDL:C23	2.26	0.64
1:N:321:PHE:CD2	22:O:1230:PSC:H341	2.32	0.64
2:B:41:ILE:HD13	22:B:230:PSC:H342	1.78	0.64
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.61	0.64
3:C:34:TRP:CZ2	24:C:272:DMU:H29	2.32	0.64
6:F:92:VAL:O	6:F:92:VAL:HG23	1.97	0.64
1:N:151:HIS:CD2	25:P:1264:PEK:H382	2.33	0.64
1:N:113:LEU:CD1	19:N:1522:TGL:H292	2.28	0.64
1:N:54:TYR:HB2	28:N:3113:HOH:O	1.97	0.64
19:N:1521:TGL:HC92	28:Q:4513:HOH:O	1.98	0.64
1:N:347:LEU:HD13	1:N:383:MET:SD	2.38	0.64
22:B:230:PSC:H21	22:B:230:PSC:H222	1.80	0.64
1:N:472:ILE:HG21	19:N:1522:TGL:CA9	2.27	0.64
22:O:1230:PSC:H071	9:V:10:ARG:HE	1.62	0.63
5:E:84:TYR:O	5:E:88:GLU:HG2	1.98	0.63
3:P:160:LEU:HD13	23:P:1271:CHD:H181	1.81	0.63
20:A:524:PGV:H152	20:A:524:PGV:H321	1.80	0.63
12:L:9:LYS:HG3	28:L:4708:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:1230:PSC:H142	22:O:1230:PSC:C34	2.16	0.63
26:T:1269:CDL:H172	26:T:1269:CDL:H511	1.81	0.63
18:N:515:HEA:HMC1	18:N:515:HEA:HBC1	1.81	0.63
26:P:1270:CDL:H642	26:P:1270:CDL:C19	2.29	0.62
1:N:53:ILE:HD11	12:Y:40:VAL:HG13	1.82	0.62
12:L:20:ARG:NH2	19:L:522:TGL:HC61	2.14	0.62
8:H:23:GLN:HG3	28:H:4576:HOH:O	2.00	0.61
26:G:269:CDL:H511	26:G:269:CDL:H172	1.82	0.61
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.01	0.61
1:A:379:TYR:O	1:A:383:MET:HB2	2.00	0.61
2:B:56:MET:HG2	22:B:230:PSC:H211	1.82	0.61
3:C:34:TRP:HZ2	24:C:272:DMU:H29	1.64	0.61
20:A:524:PGV:H062	28:M:2160:HOH:O	2.01	0.61
3:P:210:ILE:HG23	20:P:1267:PGV:H102	1.83	0.60
4:Q:101:HIS:HD2	4:Q:102:TYR:CD2	2.19	0.60
7:G:2:SER:O	25:G:1263:PEK:H322	2.01	0.60
10:J:7:GLU:HG3	28:J:4786:HOH:O	2.00	0.60
26:C:270:CDL:C19	26:C:270:CDL:H642	2.29	0.60
20:C:267:PGV:H182	26:C:270:CDL:H673	1.83	0.60
3:C:160:LEU:HD13	23:C:271:CHD:H181	1.81	0.60
26:C:270:CDL:H431	28:J:4770:HOH:O	2.01	0.60
1:A:484:THR:HB	13:M:2:THR:OG1	2.02	0.60
1:A:334:TRP:CZ3	19:D:523:TGL:HA51	2.37	0.60
2:B:114:GLU:HG3	2:B:227:LEU:HD11	1.83	0.60
1:A:472:ILE:HG21	19:L:522:TGL:CA9	2.32	0.60
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.68	0.59
18:A:515:HEA:HMC1	18:A:515:HEA:HBC1	1.83	0.59
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.00	0.59
3:C:210:ILE:HG23	20:C:267:PGV:H102	1.84	0.59
3:P:34:TRP:HZ2	24:P:1272:DMU:H29	1.64	0.59
4:D:34:SER:N	4:D:37:GLN:HE21	1.90	0.59
1:N:87:ILE:O	1:N:173:PRO:HD3	2.02	0.59
24:P:1272:DMU:H25	25:P:1264:PEK:H341	1.83	0.59
1:N:472:ILE:HD13	19:N:1522:TGL:HA91	1.83	0.59
2:O:217:LYS:HE2	2:O:217:LYS:HA	1.85	0.59
25:C:265:PEK:C38	26:G:269:CDL:H273	2.34	0.58
25:P:1265:PEK:C38	26:T:1269:CDL:H273	2.33	0.58
12:L:20:ARG:NH1	19:L:522:TGL:HC61	2.19	0.58
26:P:1270:CDL:H112	28:P:4729:HOH:O	2.04	0.57
1:A:177:SER:H	1:A:180:GLN:HE21	1.51	0.57
12:L:20:ARG:HH22	19:L:522:TGL:HC32	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:MET:HG2	28:C:4095:HOH:O	2.05	0.57
2:O:56:MET:HA	22:O:1230:PSC:H202	1.87	0.57
1:A:17:THR:OG1	19:L:522:TGL:H281	2.04	0.57
8:H:49:ASP:O	8:H:52:VAL:HG22	2.05	0.57
6:S:22:LEU:HD12	28:S:4738:HOH:O	2.03	0.57
1:A:87:ILE:O	1:A:173:PRO:HD3	2.05	0.57
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.87	0.57
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.39	0.57
1:N:449:MET:SD	2:O:5:MET:CG	2.92	0.56
6:S:75:HIS:H	6:S:80:GLN:HE22	1.53	0.56
7:T:38:HIS:NE2	26:T:1269:CDL:H111	2.20	0.56
19:Q:1523:TGL:HC21	19:Q:1523:TGL:HG11	1.86	0.56
7:T:2:SER:O	25:T:263:PEK:H322	2.05	0.56
1:A:472:ILE:HD13	19:L:522:TGL:HA91	1.88	0.56
6:F:64:GLU:O	6:F:65:ASP:HB2	2.05	0.56
7:G:45:PRO:HD2	28:G:2152:HOH:O	2.04	0.56
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.88	0.56
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.88	0.56
2:O:41:ILE:CD1	22:O:1230:PSC:H342	2.34	0.56
28:B:4533:HOH:O	25:P:1265:PEK:H031	2.05	0.56
2:B:78:LEU:HD12	26:T:1269:CDL:H351	1.88	0.56
25:C:265:PEK:H383	26:G:269:CDL:H273	1.87	0.55
1:N:1:FME:HE3	28:Y:4681:HOH:O	2.06	0.55
1:N:44:PRO:HG2	4:Q:111:PHE:CZ	2.42	0.55
5:R:12:ASP:HA	5:R:47:ILE:HD11	1.89	0.55
12:L:20:ARG:HH22	19:L:522:TGL:CC6	2.18	0.55
3:P:47:LEU:O	3:P:51:MET:HG2	2.07	0.55
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.89	0.55
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.41	0.55
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.87	0.55
3:C:168:THR:HG22	25:C:265:PEK:H14	1.88	0.55
5:R:37:VAL:HG11	5:R:70:VAL:HG21	1.88	0.55
1:A:282:PHE:HA	7:T:4:ALA:CB	2.37	0.55
19:D:523:TGL:HC21	19:D:523:TGL:HG11	1.89	0.55
6:S:92:VAL:HG23	6:S:92:VAL:O	2.07	0.55
22:B:230:PSC:H12	22:B:230:PSC:H322	1.89	0.54
7:G:3:ALA:HB1	25:G:1263:PEK:H382	1.89	0.54
20:Z:1524:PGV:H062	28:Z:3160:HOH:O	2.05	0.54
3:C:168:THR:CG2	25:C:265:PEK:H14	2.38	0.54
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.88	0.54
2:O:59:GLN:O	2:O:59:GLN:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:321:PHE:CZ	22:O:1230:PSC:H171	2.43	0.54
12:L:20:ARG:NH2	19:L:522:TGL:HC32	2.23	0.54
22:B:230:PSC:H072	9:I:10:ARG:HH21	1.71	0.54
25:C:265:PEK:H231	7:G:21:PHE:CD2	2.43	0.54
2:O:9:PHE:HB2	2:O:21:LEU:HD21	1.90	0.54
1:N:115:SER:O	1:N:121:GLY:HA2	2.08	0.54
8:U:20:PHE:HE2	8:U:27:ARG:HG2	1.71	0.54
1:A:449:MET:SD	2:B:5:MET:HG2	2.47	0.54
7:G:5:LYS:HD2	25:G:1263:PEK:H371	1.90	0.54
26:G:269:CDL:HB32	1:N:304:TYR:HD1	1.73	0.53
1:N:165:ILE:O	1:N:169:ILE:HG12	2.07	0.53
2:O:57:ASP:H	22:O:1230:PSC:H201	1.72	0.53
19:L:522:TGL:HC21	19:L:522:TGL:OA1	2.08	0.53
4:Q:58:GLU:O	4:Q:62:LEU:HG	2.09	0.53
6:S:85:CYS:SG	6:S:87:THR:HG23	2.48	0.53
1:N:42:GLY:HA3	4:Q:104:TYR:OH	2.07	0.53
1:N:405:LEU:HD23	1:N:475:ALA:HB2	1.89	0.53
25:C:264:PEK:H102	25:C:264:PEK:C16	2.36	0.53
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.44	0.53
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.90	0.53
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.91	0.53
1:N:379:TYR:O	1:N:383:MET:HB2	2.08	0.53
25:P:1265:PEK:H383	26:T:1269:CDL:H273	1.91	0.52
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.39	0.52
11:X:24:PHE:O	11:X:28:VAL:HG12	2.09	0.52
1:A:383:MET:O	1:A:387:PHE:HB2	2.09	0.52
19:L:522:TGL:C24	19:L:522:TGL:H202	2.37	0.52
1:A:406:ASN:HD21	20:A:524:PGV:C2	2.23	0.52
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.91	0.52
2:O:56:MET:HA	22:O:1230:PSC:C20	2.39	0.52
7:G:3:ALA:O	7:G:4:ALA:HB2	2.10	0.52
4:Q:82:VAL:O	4:Q:86:MET:HG3	2.10	0.52
7:T:3:ALA:O	7:T:4:ALA:HB2	2.10	0.52
19:A:521:TGL:H161	2:B:7:LEU:HD11	1.91	0.52
19:A:521:TGL:HA82	19:A:521:TGL:H222	1.92	0.52
22:O:1230:PSC:H322	22:O:1230:PSC:H12	1.92	0.52
12:Y:42:HIS:NE2	12:Y:46:LYS:HD2	2.25	0.52
1:N:456:MET:HG2	4:Q:96:LEU:HD13	1.91	0.51
6:F:8:THR:OG1	6:F:11:GLU:HG3	2.10	0.51
19:N:1522:TGL:H202	19:N:1522:TGL:C24	2.39	0.51
6:S:87:THR:HG21	28:S:3339:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.10	0.51
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.41	0.51
2:O:68:LEU:CB	2:O:69:PRO:HD3	2.41	0.51
20:P:1267:PGV:H172	26:P:1270:CDL:H662	1.92	0.51
19:N:1521:TGL:H222	19:N:1521:TGL:HA82	1.92	0.51
1:N:169:ILE:HD11	1:N:189:MET:SD	2.49	0.51
1:N:177:SER:H	1:N:180:GLN:NE2	2.09	0.51
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.10	0.51
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.75	0.51
8:U:57:ARG:HA	8:U:60:TYR:CE2	2.45	0.51
28:A:4493:HOH:O	19:D:523:TGL:HG2	2.09	0.51
5:R:48:ILE:O	5:R:52:LEU:HG	2.10	0.51
2:B:81:LEU:HD13	26:T:1269:CDL:H122	1.93	0.51
2:O:91:ASN:HD21	2:O:183:THR:HG21	1.76	0.51
2:O:46:LEU:HD12	19:Q:1523:TGL:H271	1.92	0.51
8:H:27:ARG:NH1	28:H:2303:HOH:O	2.43	0.51
7:T:84:LYS:N	7:T:84:LYS:HD2	2.07	0.50
1:A:321:PHE:CZ	22:B:230:PSC:H171	2.47	0.50
7:G:50:TYR:HB3	7:G:52:HIS:CE1	2.46	0.50
1:N:76:GLY:O	1:N:80:ASN:HB2	2.11	0.50
8:U:57:ARG:HA	8:U:60:TYR:CD2	2.45	0.50
13:Z:16:ALA:HA	20:Z:1524:PGV:H311	1.94	0.50
2:O:83:ILE:O	2:O:87:MET:HG3	2.12	0.50
20:P:1267:PGV:H182	26:P:1270:CDL:H673	1.93	0.50
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.12	0.50
1:A:35:LEU:HD11	1:A:462:LEU:HD13	1.94	0.50
3:P:67:PHE:CE1	26:P:1270:CDL:H1	2.41	0.50
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.94	0.50
2:B:1:FME:SD	2:B:133:LEU:HD11	2.52	0.49
3:P:168:THR:HG22	25:P:1265:PEK:H14	1.95	0.49
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.94	0.49
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.11	0.49
1:N:290:HIS:CD2	1:N:291:HIS:CD2	2.99	0.49
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.94	0.49
1:N:374:VAL:HA	1:N:377:PHE:CE1	2.48	0.49
1:N:177:SER:H	1:N:180:GLN:HE21	1.58	0.49
3:P:157:LYS:NZ	25:P:1265:PEK:H052	2.28	0.49
1:A:115:SER:O	1:A:121:GLY:HA2	2.13	0.49
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.46	0.49
1:A:377:PHE:CD1	18:A:516:HEA:HAD1	2.47	0.49
19:N:1522:TGL:HC21	19:N:1522:TGL:OA1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.78	0.49
3:C:40:MET:O	3:C:44:MET:HG2	2.11	0.49
11:K:24:PHE:O	11:K:28:VAL:HG12	2.13	0.49
1:N:481:GLU:HB2	13:Z:4:LYS:HE2	1.95	0.49
2:B:102:HIS:O	2:B:104:TRP:HA	2.13	0.48
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.78	0.48
4:D:127:LYS:HD2	28:I:2391:HOH:O	2.12	0.48
8:U:7:LYS:O	8:U:8:ILE:HG22	2.13	0.48
5:E:10:GLU:HB3	28:E:4759:HOH:O	2.13	0.48
6:F:85:CYS:SG	6:F:87:THR:HG23	2.53	0.48
9:I:22:VAL:O	9:I:26:MET:HG2	2.13	0.48
20:A:524:PGV:H311	13:M:16:ALA:HA	1.94	0.48
1:N:171:MET:HG2	3:P:8:TYR:CE1	2.47	0.48
4:Q:138:TRP:CH2	11:X:50:PRO:HG2	2.48	0.48
1:A:160:GLY:HA3	28:A:2064:HOH:O	2.14	0.48
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.00	0.48
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.48	0.48
8:H:8:ILE:HB	28:H:4704:HOH:O	2.14	0.48
4:Q:52:SER:OG	4:Q:55:GLU:HG3	2.12	0.48
1:N:417:MET:O	1:N:421:VAL:HG22	2.13	0.48
18:A:515:HEA:H122	18:A:515:HEA:HHC	1.94	0.48
20:A:604:PGV:H182	3:C:28:THR:HG22	1.95	0.48
1:N:383:MET:O	1:N:387:PHE:HB2	2.13	0.48
2:B:65:TRP:CZ3	22:B:230:PSC:H331	2.48	0.48
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.95	0.48
3:P:205:GLY:HA3	25:P:1264:PEK:H181	1.96	0.48
2:B:1:FME:SD	2:B:133:LEU:CD1	3.01	0.48
1:N:62:ALA:HB2	18:N:515:HEA:HBD1	1.94	0.48
2:O:68:LEU:HD23	22:O:1230:PSC:H182	1.94	0.48
5:R:86:ILE:HA	5:R:86:ILE:HD13	1.73	0.48
10:W:40:LEU:HD12	23:W:1060:CHD:H183	1.96	0.48
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.44	0.48
4:D:34:SER:O	4:D:38:LYS:HG3	2.14	0.47
7:G:2:SER:OG	25:G:1263:PEK:H301	2.14	0.47
26:T:1269:CDL:HA62	26:T:1269:CDL:H322	1.96	0.47
2:B:164:ALA:O	2:B:194:GLY:HA3	2.13	0.47
1:N:71:MET:HE3	1:N:195:LEU:HD21	1.96	0.47
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.96	0.47
7:T:12:GLY:HA3	28:T:3274:HOH:O	2.14	0.47
7:T:2:SER:OG	25:T:263:PEK:H301	2.13	0.47
2:B:56:MET:HA	22:B:230:PSC:H202	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:8:HIS:ND1	25:T:263:PEK:H312	2.29	0.47
10:W:50:LEU:HD22	10:W:50:LEU:O	2.15	0.47
3:C:51:MET:SD	26:C:270:CDL:H622	2.53	0.47
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.79	0.47
11:K:42:PRO:HG2	11:K:47:ARG:NE	2.29	0.47
3:P:51:MET:HB3	26:P:1270:CDL:H622	1.96	0.47
5:R:8:ASP:HB3	9:V:10:ARG:CZ	2.44	0.47
22:O:1230:PSC:C07	9:V:10:ARG:HE	2.28	0.47
20:P:1267:PGV:H12	20:P:1267:PGV:C16	2.42	0.47
1:N:426:PHE:CZ	19:N:1521:TGL:HA62	2.50	0.47
25:P:1265:PEK:H231	7:T:21:PHE:CD2	2.50	0.47
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.96	0.47
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.15	0.47
2:O:82:ARG:HG2	2:O:86:MET:HE1	1.95	0.47
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.97	0.47
1:A:42:GLY:HA3	4:D:104:TYR:OH	2.15	0.47
5:E:52:LEU:O	5:E:55:CYS:HB2	2.15	0.47
1:N:400:PHE:HB3	19:N:1522:TGL:H283	1.97	0.47
1:N:422:ASN:HB3	19:N:1521:TGL:H242	1.97	0.47
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.50	0.47
9:V:65:LYS:O	11:X:54:ARG:NH1	2.44	0.47
1:A:177:SER:H	1:A:180:GLN:NE2	2.13	0.46
2:B:23:PHE:CZ	2:B:80:SER:HB2	2.50	0.46
1:A:113:LEU:CD1	19:L:522:TGL:H292	2.45	0.46
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.15	0.46
12:Y:2:HIS:ND1	12:Y:3:TYR:N	2.62	0.46
1:N:513:LEU:HD22	1:N:513:LEU:HA	1.72	0.46
18:N:515:HEA:H122	18:N:515:HEA:HHC	1.98	0.46
1:N:215:LEU:HD11	25:P:1264:PEK:H271	1.97	0.46
4:Q:127:LYS:O	4:Q:130:PRO:HD3	2.15	0.46
1:A:488:THR:HB	1:A:495:LEU:HD13	1.98	0.46
13:Z:11:SER:OG	13:Z:14:GLU:HG3	2.14	0.46
28:A:4241:HOH:O	4:D:20:ARG:HG3	2.15	0.46
23:P:1271:CHD:H12A	23:P:1271:CHD:H112	1.66	0.46
1:A:304:TYR:HD1	26:T:1269:CDL:HB32	1.81	0.46
4:Q:118:LYS:HB3	11:X:53:TRP:HB3	1.96	0.46
19:N:1522:TGL:H361	19:N:1522:TGL:HB91	1.97	0.46
26:T:1269:CDL:H231	26:T:1269:CDL:C54	2.37	0.46
1:A:406:ASN:HD21	20:A:524:PGV:H21	1.81	0.46
20:Z:1524:PGV:C15	20:Z:1524:PGV:H321	2.44	0.46
1:N:440:TYR:HE2	2:O:204:HIS:CE1	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Y:20:ARG:HB3	12:Y:20:ARG:HH11	1.81	0.46
2:B:52:HIS:HE1	22:B:230:PSC:H02	1.81	0.46
10:J:29:ASN:HD22	10:J:29:ASN:H	1.63	0.46
1:N:377:PHE:HA	1:N:380:VAL:HG22	1.97	0.46
3:P:187:THR:HB	7:T:68:THR:HG21	1.97	0.46
4:Q:68:PHE:HA	4:Q:71:MET:HG2	1.98	0.46
2:B:56:MET:HA	22:B:230:PSC:C20	2.46	0.45
7:G:12:GLY:HA3	28:G:2274:HOH:O	2.14	0.45
1:N:160:GLY:HA3	28:N:3064:HOH:O	2.15	0.45
1:A:113:LEU:O	1:A:117:MET:HG2	2.15	0.45
4:D:86:MET:HE3	28:K:4516:HOH:O	2.15	0.45
26:G:269:CDL:H571	26:G:269:CDL:H601	1.55	0.45
2:O:164:ALA:O	2:O:194:GLY:HA3	2.16	0.45
26:P:1270:CDL:H602	26:P:1270:CDL:H632	1.60	0.45
7:T:5:LYS:CB	25:T:263:PEK:H362	2.31	0.45
28:H:4673:HOH:O	8:U:46:LYS:HD3	2.16	0.45
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.99	0.45
2:B:41:ILE:O	2:B:45:MET:HG2	2.16	0.45
2:B:78:LEU:HA	2:B:78:LEU:HD12	1.76	0.45
3:C:47:LEU:O	3:C:51:MET:HG2	2.16	0.45
6:S:94:HIS:CG	6:S:95:GLN:N	2.79	0.45
19:A:521:TGL:HC22	28:I:2383:HOH:O	2.16	0.45
25:C:265:PEK:H383	26:G:269:CDL:C27	2.47	0.45
19:L:522:TGL:H272	19:L:522:TGL:H231	1.99	0.45
12:L:2:HIS:HE1	12:L:5:GLU:OE1	2.00	0.45
13:M:42:LYS:HA	13:M:42:LYS:CE	2.38	0.45
19:N:1522:TGL:HG2	12:Y:12:PRO:HB2	1.98	0.45
24:P:1272:DMU:O1	24:P:1272:DMU:H30	2.16	0.45
5:R:87:GLN:HG2	5:R:88:GLU:N	2.31	0.45
7:T:2:SER:O	7:T:3:ALA:HB3	2.17	0.45
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.99	0.45
26:C:270:CDL:H202	26:C:270:CDL:H171	1.76	0.45
4:D:31:LYS:HE3	28:D:4485:HOH:O	2.16	0.45
1:N:68:PHE:CE2	1:N:112:LEU:HD13	2.48	0.45
4:Q:130:PRO:HG2	4:Q:131:ILE:HD12	1.99	0.45
1:A:365:ILE:HD11	28:A:4177:HOH:O	2.15	0.45
1:N:128:VAL:HG12	1:N:128:VAL:O	2.17	0.45
1:N:400:PHE:HB3	19:N:1522:TGL:C28	2.47	0.45
5:R:52:LEU:O	5:R:55:CYS:HB2	2.16	0.45
26:P:1270:CDL:H171	26:P:1270:CDL:H202	1.75	0.45
26:T:1269:CDL:H571	26:T:1269:CDL:H601	1.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.84	0.45
10:W:30:ILE:O	10:W:34:VAL:HG23	2.17	0.45
2:B:91:ASN:HD22	2:B:92:ASN:N	2.15	0.45
25:C:265:PEK:H031	28:O:4625:HOH:O	2.17	0.45
6:F:51:SER:HB2	6:F:91:LEU:HD11	1.99	0.45
23:C:271:CHD:H222	23:C:271:CHD:H162	1.72	0.44
19:D:523:TGL:H242	19:D:523:TGL:H212	1.74	0.44
25:P:1265:PEK:H383	26:T:1269:CDL:C27	2.47	0.44
1:A:240:HIS:O	1:A:243:VAL:HG22	2.17	0.44
2:B:146:MET:HA	2:B:213:LEU:HD12	1.99	0.44
2:B:214:VAL:HB	2:B:215:PRO:CD	2.46	0.44
2:O:52:HIS:HE1	22:O:1230:PSC:H212	1.82	0.44
4:D:56:LYS:HB3	5:E:61:PHE:CE2	2.52	0.44
23:J:60:CHD:H212	23:J:60:CHD:H161	1.74	0.44
19:N:1522:TGL:H272	19:N:1522:TGL:H231	1.98	0.44
3:P:157:LYS:HZ1	25:P:1265:PEK:H052	1.82	0.44
19:Q:1523:TGL:H361	28:V:4566:HOH:O	2.17	0.44
2:B:161:HIS:HB2	2:B:174:ALA:HB3	1.99	0.44
5:E:63:SER:O	5:E:67:ILE:HG13	2.18	0.44
2:O:41:ILE:O	2:O:45:MET:HG2	2.16	0.44
25:P:1264:PEK:H102	25:P:1264:PEK:C16	2.38	0.44
3:C:65:SER:HB3	3:C:71:HIS:CE1	2.53	0.44
6:S:51:SER:O	6:S:94:HIS:N	2.50	0.44
2:B:62:GLU:O	2:B:66:THR:HB	2.18	0.44
3:C:3:HIS:HE1	6:F:31:TYR:OH	2.00	0.44
26:G:269:CDL:HA62	26:G:269:CDL:H322	1.99	0.44
3:P:63:ARG:NE	26:P:1270:CDL:HA22	2.11	0.44
3:P:34:TRP:CE2	24:P:1272:DMU:H29	2.52	0.44
26:G:269:CDL:C54	26:G:269:CDL:H231	2.35	0.44
7:G:4:ALA:CB	1:N:282:PHE:HA	2.48	0.44
1:N:5:ARG:O	1:N:9:SER:HB2	2.17	0.44
4:Q:131:ILE:N	4:Q:131:ILE:HD12	2.32	0.44
10:W:9:GLN:O	10:W:13:GLN:HG3	2.17	0.44
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.84	0.44
20:A:524:PGV:C15	20:A:524:PGV:H321	2.47	0.44
10:J:50:LEU:HD22	10:J:50:LEU:O	2.17	0.44
26:G:269:CDL:H761	1:N:282:PHE:HZ	1.83	0.44
1:N:482:VAL:HG13	13:Z:1:ILE:HD11	1.99	0.44
3:C:213:THR:HG23	26:C:270:CDL:H762	1.99	0.43
7:G:84:LYS:N	7:G:84:LYS:HD2	2.13	0.43
19:Q:1523:TGL:H212	19:Q:1523:TGL:H242	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:48:TRP:HB2	5:R:96:LEU:O	2.17	0.43
1:A:32:ALA:HB3	12:L:36:PRO:HG2	2.00	0.43
6:S:22:LEU:O	6:S:25:ARG:HB3	2.18	0.43
3:C:116:TRP:HA	3:C:117:PRO:C	2.38	0.43
2:O:216:LEU:O	2:O:219:PHE:HB3	2.19	0.43
26:T:1269:CDL:H571	26:T:1269:CDL:H771	2.00	0.43
7:T:17:ARG:HD2	28:T:3309:HOH:O	2.19	0.43
4:D:75:THR:HB	28:D:2332:HOH:O	2.19	0.43
6:F:52:ILE:HA	6:F:94:HIS:HA	2.01	0.43
1:N:240:HIS:HB3	1:N:241:PRO:HD3	2.01	0.43
1:N:52:GLN:O	1:N:56:VAL:HG23	2.18	0.43
7:G:5:LYS:HD3	1:N:278:MET:HB3	2.00	0.43
3:P:54:MET:HE3	26:P:1270:CDL:H612	2.01	0.43
2:B:168:LEU:HD13	2:B:184:LEU:HG	2.01	0.43
7:G:17:ARG:HD2	28:G:2309:HOH:O	2.17	0.43
1:N:398:PRO:HA	1:N:403:TYR:O	2.19	0.43
2:O:42:ILE:O	2:O:46:LEU:HG	2.18	0.43
1:N:175:ALA:CB	1:N:513:LEU:HD23	2.49	0.43
4:Q:24:LEU:HD12	5:R:30:ARG:HA	2.01	0.43
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.54	0.43
1:N:113:LEU:HD12	19:N:1522:TGL:H292	1.99	0.43
4:Q:101:HIS:HD2	4:Q:102:TYR:CE2	2.36	0.43
26:T:1269:CDL:H152	26:T:1269:CDL:H181	1.93	0.43
26:T:1269:CDL:H222	26:T:1269:CDL:H251	1.93	0.43
3:C:51:MET:HB3	26:C:270:CDL:H622	2.01	0.43
2:O:196:CYS:HB2	2:O:207:MET:HG3	2.01	0.43
4:Q:131:ILE:H	4:Q:131:ILE:HD12	1.84	0.43
1:A:399:LEU:HB2	1:A:494:TRP:CZ3	2.54	0.42
26:C:270:CDL:H532	26:C:270:CDL:H561	1.77	0.42
24:C:272:DMU:H41	28:G:4668:HOH:O	2.19	0.42
2:O:150:ILE:HD12	2:O:184:LEU:HD22	2.00	0.42
2:O:155:SER:O	2:O:174:ALA:HB1	2.19	0.42
3:P:116:TRP:HA	3:P:117:PRO:C	2.38	0.42
6:S:64:GLU:O	6:S:65:ASP:HB2	2.18	0.42
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	2.01	0.42
26:C:270:CDL:H602	26:C:270:CDL:H632	1.57	0.42
12:L:20:ARG:CZ	19:L:522:TGL:HC61	2.49	0.42
26:G:269:CDL:H212	1:N:311:ILE:HD12	2.01	0.42
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.49	0.42
13:Z:32:TRP:CZ3	13:Z:40:TYR:OH	2.71	0.42
1:A:422:ASN:HB3	19:A:521:TGL:H242	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:112:LEU:HD13	3:P:118:PRO:HG3	2.02	0.42
8:U:9:LYS:HB3	8:U:10:ASN:H	1.64	0.42
9:V:36:LYS:HA	9:V:40:ALA:HB3	2.01	0.42
13:Z:19:LEU:HD23	20:Z:1524:PGV:H322	2.01	0.42
1:A:1:FME:HCN	1:A:4:ASN:HB2	2.02	0.42
26:C:270:CDL:H641	26:C:270:CDL:H672	1.83	0.42
3:P:168:THR:CG2	25:P:1265:PEK:H14	2.48	0.42
5:R:100:THR:HB	5:R:101:PRO:HD2	2.00	0.42
1:A:151:HIS:CD2	25:C:264:PEK:H382	2.54	0.42
1:A:229:ILE:HD11	2:B:175:ILE:CD1	2.49	0.42
1:A:377:PHE:HA	1:A:380:VAL:HG22	2.01	0.42
3:C:156:ARG:HE	23:C:271:CHD:C23	2.33	0.42
23:C:271:CHD:H12A	23:C:271:CHD:H112	1.61	0.42
3:P:250:LEU:HD22	26:T:1269:CDL:C67	2.50	0.42
5:R:5:HIS:HB3	5:R:6:GLU:H	1.67	0.42
9:V:58:LYS:O	9:V:62:GLU:HG3	2.19	0.42
2:B:18:GLU:HB3	28:B:4772:HOH:O	2.19	0.42
20:C:267:PGV:H182	26:C:270:CDL:C67	2.49	0.42
7:G:7:ASP:O	7:G:9:GLY:N	2.52	0.42
18:A:516:HEA:HMB1	18:A:516:HEA:H11	1.87	0.42
3:C:212:SER:O	3:C:216:ILE:HG13	2.20	0.42
25:C:265:PEK:H292	28:O:4283:HOH:O	2.19	0.42
3:P:137:LEU:HD23	3:P:137:LEU:HA	1.84	0.42
8:U:49:ASP:O	8:U:52:VAL:HG22	2.20	0.42
1:A:240:HIS:HB3	1:A:241:PRO:HD3	2.02	0.42
1:A:406:ASN:HD21	20:A:524:PGV:H22	1.84	0.42
4:Q:33:LEU:HA	4:Q:37:GLN:NE2	2.35	0.42
2:O:222:TRP:HB2	9:V:71:SER:HB2	2.01	0.42
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	2.02	0.42
22:B:230:PSC:H221	22:B:230:PSC:H251	1.79	0.42
26:P:1270:CDL:HB21	26:P:1270:CDL:CB3	2.50	0.42
23:W:1060:CHD:H161	23:W:1060:CHD:H212	1.77	0.42
10:W:31:LEU:HD12	10:W:31:LEU:HA	1.90	0.42
19:L:522:TGL:H361	19:L:522:TGL:HB91	2.02	0.42
1:N:344:PHE:C	1:N:344:PHE:CD1	2.93	0.42
2:O:128:LEU:HD22	2:O:132:GLU:HB3	2.02	0.42
12:L:12:PRO:HB2	19:L:522:TGL:HG2	2.02	0.41
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.54	0.41
3:P:213:THR:HG23	26:P:1270:CDL:H762	2.02	0.41
8:U:36:PHE:CD1	8:U:57:ARG:HB2	2.54	0.41
8:U:64:CYS:HA	8:U:65:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:ASP:O	1:A:411:LYS:HG3	2.21	0.41
3:C:117:PRO:HG3	3:C:123:PRO:HG2	2.02	0.41
3:C:191:GLY:HA3	28:G:2163:HOH:O	2.20	0.41
1:N:198:SER:HB2	1:N:238:PHE:HA	2.02	0.41
25:G:1263:PEK:H042	3:P:77:LYS:NZ	2.35	0.41
5:R:57:ARG:HH11	5:R:57:ARG:HG3	1.85	0.41
6:S:55:LYS:HA	6:S:74:LEU:O	2.20	0.41
1:A:398:PRO:HA	1:A:403:TYR:O	2.21	0.41
20:A:524:PGV:H011	20:A:524:PGV:H202	1.92	0.41
2:B:79:PRO:O	2:B:83:ILE:HG13	2.20	0.41
3:C:59:ARG:HG3	26:C:270:CDL:H512	2.01	0.41
1:N:289:ALA:HB3	1:N:305:PHE:CG	2.55	0.41
1:A:1:FME:HA	1:A:1:FME:CE	2.51	0.41
26:G:269:CDL:HB32	1:N:304:TYR:CD1	2.53	0.41
12:L:35:ALA:HB3	12:L:36:PRO:HD3	2.01	0.41
19:N:1522:TGL:HB61	19:N:1522:TGL:HB31	1.85	0.41
3:P:173:PHE:CD2	3:P:173:PHE:C	2.94	0.41
4:Q:36:SER:O	4:Q:39:ALA:HB3	2.20	0.41
19:L:522:TGL:HB61	19:L:522:TGL:HB31	1.85	0.41
20:N:1266:PGV:H182	3:P:28:THR:HG22	2.03	0.41
3:P:31:LEU:HD23	3:P:31:LEU:HA	1.77	0.41
1:A:44:PRO:HG2	4:D:111:PHE:CZ	2.55	0.41
1:A:76:GLY:O	1:A:80:ASN:HB2	2.21	0.41
26:P:1270:CDL:H651	26:P:1270:CDL:C77	2.51	0.41
13:M:17:ILE:O	13:M:21:VAL:HG23	2.20	0.41
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.89	0.41
7:T:48:ILE:HA	7:T:49:PRO:HD3	1.82	0.41
1:A:92:MET:O	1:A:95:PRO:HD3	2.20	0.41
26:G:269:CDL:H732	26:G:269:CDL:H762	1.97	0.41
8:H:60:TYR:C	8:H:60:TYR:CD1	2.93	0.41
10:J:31:LEU:HA	10:J:31:LEU:HD12	1.84	0.41
2:O:121:TYR:O	2:O:138:VAL:HA	2.20	0.41
4:Q:20:ARG:HD2	4:Q:72:ASN:OD1	2.20	0.41
7:T:31:CYS:HG	26:T:1269:CDL:H532	1.85	0.41
20:A:524:PGV:H061	20:A:524:PGV:P	2.61	0.41
3:C:210:ILE:HD13	20:C:267:PGV:H301	2.02	0.41
26:C:270:CDL:CB3	26:C:270:CDL:HB21	2.50	0.41
9:I:15:ARG:HD3	9:I:15:ARG:C	2.41	0.41
2:O:132:GLU:HB3	2:O:137:GLU:HG3	2.03	0.41
2:O:139:ASP:OD2	2:O:140:ASN:N	2.54	0.41
4:Q:33:LEU:HB2	4:Q:38:LYS:CG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:35:TYR:C	9:V:37:PHE:H	2.24	0.41
9:V:73:LYS:HE3	9:V:73:LYS:HB3	1.85	0.41
1:A:35:LEU:HA	1:A:35:LEU:HD23	1.94	0.41
3:C:63:ARG:NE	26:C:270:CDL:HA22	2.08	0.41
7:T:7:ASP:O	7:T:9:GLY:N	2.54	0.41
1:A:225:GLY:HA3	3:C:112:LEU:HD21	2.02	0.40
1:N:338:MET:O	1:N:342:LEU:HG	2.21	0.40
2:O:102:HIS:O	2:O:104:TRP:HA	2.21	0.40
7:G:12:GLY:CA	28:G:2274:HOH:O	2.69	0.40
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.74	0.40
5:R:7:THR:HB	5:R:9:GLU:OE2	2.21	0.40
7:T:3:ALA:HB1	25:T:263:PEK:C38	2.48	0.40
20:Z:1524:PGV:H061	20:Z:1524:PGV:P	2.61	0.40
26:G:269:CDL:H222	26:G:269:CDL:H251	1.94	0.40
7:G:7:ASP:O	1:N:169:ILE:HD12	2.21	0.40
7:T:3:ALA:O	7:T:4:ALA:CB	2.69	0.40
3:P:187:THR:CB	7:T:68:THR:HG21	2.52	0.40
1:A:282:PHE:HZ	26:T:1269:CDL:H761	1.86	0.40
1:A:52:GLN:O	1:A:56:VAL:HG23	2.21	0.40
4:D:98:TRP:CD2	24:M:526:DMU:H10	2.56	0.40
7:G:2:SER:O	7:G:3:ALA:HB3	2.21	0.40
5:R:61:PHE:HE1	5:R:98:ILE:HA	1.86	0.40
1:A:400:PHE:HB3	19:L:522:TGL:H283	2.04	0.40
19:A:521:TGL:H201	19:A:521:TGL:C24	2.48	0.40
1:A:430:PHE:HE1	19:A:521:TGL:HB21	1.85	0.40
3:C:173:PHE:CD2	3:C:173:PHE:C	2.94	0.40
25:C:264:PEK:H32	25:C:264:PEK:H71	2.04	0.40
25:P:1264:PEK:H32	25:P:1264:PEK:H71	2.03	0.40
3:P:40:MET:O	3:P:44:MET:HG2	2.21	0.40
4:Q:107:ILE:HD13	11:X:39:GLU:HB2	2.04	0.40
8:U:58:ARG:HD2	8:U:58:ARG:HA	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	495 (97%)	17 (3%)	0	100	100
1	N	512/514 (100%)	497 (97%)	15 (3%)	0	100	100
2	B	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	17	12
2	O	225/227 (99%)	208 (92%)	15 (7%)	2 (1%)	17	12
3	C	257/261 (98%)	252 (98%)	5 (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%)	139 (98%)	3 (2%)	0	100	100
5	E	103/109 (94%)	103 (100%)	0	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%)	4	1
6	S	96/98 (98%)	88 (92%)	5 (5%)	3 (3%)	4	1
7	G	81/85 (95%)	64 (79%)	10 (12%)	7 (9%)	1	0
7	T	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	1	0
8	H	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	5	2
8	U	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	5	2
9	I	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
9	V	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
10	J	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
10	W	56/59 (95%)	54 (96%)	2 (4%)	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%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	1 (2%)	0	100	100
All	All	3504/3614 (97%)	3343 (95%)	133 (4%)	28 (1%)	19	15

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
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
6	F	95	GLN
7	G	3	ALA
7	G	40	GLY
8	H	8	ILE
8	H	46	LYS
2	O	60	GLU
7	T	3	ALA
7	T	40	GLY
8	U	46	LYS
6	F	94	HIS
6	F	96	LEU
8	U	8	ILE
6	S	96	LEU
2	B	92	ASN
7	G	6	GLY
7	T	6	GLY
2	O	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%)	416 (98%)	10 (2%)	50	55
1	N	426/426 (100%)	415 (97%)	11 (3%)	46	50
2	B	210/210 (100%)	199 (95%)	11 (5%)	23	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	O	210/210 (100%)	198 (94%)	12 (6%)	20	18
3	C	224/226 (99%)	218 (97%)	6 (3%)	44	48
3	P	224/226 (99%)	218 (97%)	6 (3%)	44	48
4	D	128/129 (99%)	126 (98%)	2 (2%)	62	69
4	Q	128/129 (99%)	125 (98%)	3 (2%)	50	55
5	E	92/95 (97%)	90 (98%)	2 (2%)	52	57
5	R	92/95 (97%)	91 (99%)	1 (1%)	73	79
6	F	81/81 (100%)	78 (96%)	3 (4%)	34	35
6	S	81/81 (100%)	76 (94%)	5 (6%)	18	15
7	G	67/68 (98%)	61 (91%)	6 (9%)	9	6
7	T	67/68 (98%)	60 (90%)	7 (10%)	7	4
8	H	71/75 (95%)	69 (97%)	2 (3%)	43	47
8	U	71/75 (95%)	68 (96%)	3 (4%)	30	30
9	I	57/57 (100%)	54 (95%)	3 (5%)	22	20
9	V	57/57 (100%)	56 (98%)	1 (2%)	59	65
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	60
10	W	49/50 (98%)	48 (98%)	1 (2%)	55	60
11	K	39/46 (85%)	38 (97%)	1 (3%)	46	50
11	X	39/46 (85%)	37 (95%)	2 (5%)	24	22
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	50
12	Y	39/40 (98%)	38 (97%)	1 (3%)	46	50
13	M	37/38 (97%)	32 (86%)	5 (14%)	4	2
13	Z	37/38 (97%)	32 (86%)	5 (14%)	4	2
All	All	3040/3082 (99%)	2929 (96%)	111 (4%)	34	35

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN
1	A	238	PHE
1	A	241	PRO

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Mol	Chain	Res	Type
1	A	338	MET
1	A	369	ASP
1	A	512	ASN
1	A	513	LEU
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	130	PRO
2	B	167	SER
2	B	171	LYS
2	B	185	MET
3	C	13	PRO
3	C	17	PRO
3	C	159	MET
3	C	179	SER
3	C	214	PHE
3	C	230	ASN
4	D	4	SER
4	D	51	LEU
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
6	F	53	THR
6	F	96	LEU
7	G	17	ARG
7	G	18	PHE
7	G	36	TRP
7	G	43	GLU
7	G	54	ARG
7	G	84	LYS
8	H	29	CYS
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
9	I	37	PHE
10	J	50	LEU
11	K	54	ARG
12	L	26	THR

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Mol	Chain	Res	Type
13	M	4	LYS
13	M	12	PRO
13	M	34	LEU
13	M	37	LEU
13	M	42	LYS
1	N	38	ARG
1	N	109	PHE
1	N	115	SER
1	N	138	HIS
1	N	180	GLN
1	N	238	PHE
1	N	241	PRO
1	N	338	MET
1	N	369	ASP
1	N	484	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	115	ASP
2	O	148	MET
2	O	217	LYS
3	P	17	PRO
3	P	29	SER
3	P	33	MET
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	51	LEU
4	Q	54	ASP
4	Q	121	LYS
5	R	90	ARG
6	S	48	LEU
6	S	53	THR
6	S	54	ASN
6	S	95	GLN

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Mol	Chain	Res	Type
6	S	96	LEU
7	T	17	ARG
7	T	18	PHE
7	T	26	PRO
7	T	33	LEU
7	T	38	HIS
7	T	54	ARG
7	T	84	LYS
8	U	18	SER
8	U	29	CYS
8	U	60	TYR
9	V	8	GLN
10	W	50	LEU
11	X	47	ARG
11	X	54	ARG
12	Y	20	ARG
13	Z	13	LYS
13	Z	34	LEU
13	Z	37	LEU
13	Z	38	ASP
13	Z	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	HIS
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	91	ASN
2	B	181	GLN
2	B	195	GLN
3	C	3	HIS
3	C	50	ASN
3	C	68	GLN
3	C	149	HIS
4	D	37	GLN
4	D	109	HIS
5	E	94	ASN
9	I	8	GLN
9	I	53	ASN
10	J	29	ASN

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Mol	Chain	Res	Type
1	N	99	ASN
1	N	151	HIS
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	22	HIS
2	O	52	HIS
2	O	91	ASN
2	O	181	GLN
2	O	195	GLN
3	P	50	ASN
3	P	68	GLN
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	94	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	$\# Z > 2$
1	FME	N	1	1	8,9,10	0.72	0	7,9,11	1.43	1 (14%)
9	SAC	V	1	9	7,8,9	2.85	2 (28%)	8,9,11	3.08	5 (62%)
2	FME	B	1	2	8,9,10	0.92	0	7,9,11	1.83	2 (28%)
9	SAC	I	1	9	7,8,9	2.51	2 (28%)	8,9,11	3.25	3 (37%)

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	0.78	0	7,9,11	1.60	2 (28%)
7	TPO	T	11	7	8,10,11	1.44	2 (25%)	10,14,16	1.03	0
7	TPO	G	11	7	8,10,11	1.68	1 (12%)	10,14,16	1.04	0
1	FME	A	1	1	8,9,10	0.77	0	7,9,11	1.45	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
1	FME	N	1	1	-	4/7/9/11	-
9	SAC	V	1	9	-	3/7/8/10	-
2	FME	B	1	2	-	1/7/9/11	-
9	SAC	I	1	9	-	3/7/8/10	-
2	FME	O	1	2	-	1/7/9/11	-
7	TPO	T	11	7	-	4/9/11/13	-
7	TPO	G	11	7	-	4/9/11/13	-
1	FME	A	1	1	-	3/7/9/11	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	OAC-C1A	5.35	1.35	1.23
9	I	1	SAC	OAC-C1A	5.33	1.35	1.23
9	V	1	SAC	CA-N	4.72	1.53	1.46
9	I	1	SAC	CA-N	3.58	1.51	1.46
7	G	11	TPO	CB-CA	3.16	1.60	1.53
7	T	11	TPO	CB-CA	2.15	1.58	1.53
7	T	11	TPO	P-O1P	2.07	1.57	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	1	SAC	CA-N-C1A	-7.19	109.88	123.15
9	V	1	SAC	CA-N-C1A	-6.43	111.29	123.15
9	I	1	SAC	C-CA-N	-3.55	103.34	109.73
9	I	1	SAC	CB-CA-N	3.39	118.16	110.55
2	B	1	FME	CA-N-CN	-3.30	117.75	122.82
2	O	1	FME	C-CA-N	3.11	115.34	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	1	SAC	C-CA-N	-3.10	104.13	109.73
2	B	1	FME	C-CA-N	3.10	115.33	109.73
9	V	1	SAC	C2A-C1A-N	3.04	121.25	116.10
1	A	1	FME	CA-N-CN	-3.03	118.17	122.82
1	N	1	FME	CA-N-CN	-2.97	118.25	122.82
9	V	1	SAC	CB-CA-N	2.70	116.61	110.55
2	O	1	FME	CA-N-CN	-2.53	118.94	122.82
9	V	1	SAC	OAC-C1A-C2A	-2.38	117.63	122.06

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	CB-CA-N-C1A
2	B	1	FME	O1-CN-N-CA
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
9	I	1	SAC	CB-CA-N-C1A
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	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
1	N	1	FME	CA-CB-CG-SD
1	A	1	FME	CA-CB-CG-SD
7	T	11	TPO	CB-OG1-P-O1P
7	G	11	TPO	CB-OG1-P-O2P

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	N	1	FME	2	0
2	B	1	FME	2	0
9	I	1	SAC	1	0
7	T	11	TPO	1	0
1	A	1	FME	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 55 ligands modelled in this entry, 11 are monoatomic - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	TGL	L	522	-	62,62,62	1.15	6 (9%)	65,65,65	1.73	13 (20%)
26	CDL	G	269	-	99,99,99	1.11	9 (9%)	105,111,111	0.96	7 (6%)
20	PGV	N	1266	-	50,50,50	0.93	4 (8%)	53,56,56	0.79	2 (3%)
20	PGV	P	1267	-	50,50,50	0.80	1 (2%)	53,56,56	0.88	2 (3%)
23	CHD	O	229	-	29,32,32	0.70	0	48,51,51	2.00	15 (31%)
23	CHD	J	60	-	29,32,32	1.24	2 (6%)	48,51,51	3.60	27 (56%)
18	HEA	A	515	1	44,67,67	1.41	6 (13%)	37,103,103	1.79	12 (32%)
25	PEK	P	1264	-	52,52,52	1.45	6 (11%)	55,57,57	1.13	5 (9%)
22	PSC	B	230	-	51,51,51	1.24	5 (9%)	57,59,59	0.93	2 (3%)
25	PEK	P	1265	-	52,52,52	1.64	10 (19%)	55,57,57	1.13	6 (10%)
26	CDL	P	1270	-	99,99,99	0.91	6 (6%)	105,111,111	0.99	5 (4%)
19	TGL	D	523	-	62,62,62	0.88	3 (4%)	65,65,65	1.44	8 (12%)
19	TGL	A	521	-	62,62,62	0.73	0	65,65,65	1.52	14 (21%)
23	CHD	B	1086	-	29,32,32	0.66	0	48,51,51	1.85	13 (27%)
23	CHD	P	1525	-	29,32,32	0.81	1 (3%)	48,51,51	1.96	13 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CDL	T	1269	-	99,99,99	1.09	8 (8%)	105,111,111	0.99	8 (7%)
24	DMU	C	272	-	34,34,34	2.76	14 (41%)	45,45,45	4.08	19 (42%)
23	CHD	P	1271	-	29,32,32	0.83	0	48,51,51	3.70	23 (47%)
18	HEA	N	516	1	44,67,67	1.61	6 (13%)	37,103,103	1.36	6 (16%)
20	PGV	A	604	-	50,50,50	0.80	1 (2%)	53,56,56	0.80	2 (3%)
24	DMU	P	1272	-	34,34,34	2.77	15 (44%)	45,45,45	3.93	18 (40%)
18	HEA	N	515	1	44,67,67	1.52	6 (13%)	37,103,103	1.73	13 (35%)
23	CHD	C	271	-	29,32,32	0.97	1 (3%)	48,51,51	3.69	24 (50%)
20	PGV	C	268	-	50,50,50	1.31	6 (12%)	53,56,56	0.86	1 (1%)
20	PGV	A	524	-	50,50,50	1.23	5 (10%)	53,56,56	1.03	4 (7%)
24	DMU	M	526	-	34,34,34	3.33	8 (23%)	45,45,45	3.77	19 (42%)
19	TGL	N	1522	-	62,62,62	1.28	6 (9%)	65,65,65	1.70	14 (21%)
21	CUA	B	228	2	0,1,1	0.00	-	-	-	-
25	PEK	C	265	-	52,52,52	1.68	11 (21%)	55,57,57	1.17	6 (10%)
25	PEK	T	263	-	52,52,52	1.94	13 (25%)	55,57,57	1.22	6 (10%)
20	PGV	Z	1524	-	50,50,50	1.24	4 (8%)	53,56,56	0.97	3 (5%)
22	PSC	O	1230	-	51,51,51	1.22	4 (7%)	57,59,59	0.93	2 (3%)
24	DMU	Z	1526	-	34,34,34	3.23	9 (26%)	45,45,45	3.72	18 (40%)
21	CUA	O	228	2	0,1,1	0.00	-	-	-	-
23	CHD	C	525	-	29,32,32	0.90	1 (3%)	48,51,51	1.94	12 (25%)
25	PEK	C	264	-	52,52,52	1.40	4 (7%)	55,57,57	1.10	5 (9%)
23	CHD	W	1060	-	29,32,32	1.38	3 (10%)	48,51,51	3.68	26 (54%)
20	PGV	C	267	-	50,50,50	0.81	1 (2%)	53,56,56	0.95	4 (7%)
19	TGL	N	1521	-	62,62,62	0.73	1 (1%)	65,65,65	1.47	12 (18%)
26	CDL	C	270	-	99,99,99	0.85	6 (6%)	105,111,111	0.97	5 (4%)
25	PEK	G	1263	-	52,52,52	1.84	11 (21%)	55,57,57	1.22	4 (7%)
18	HEA	A	516	1	44,67,67	1.53	8 (18%)	37,103,103	1.34	6 (16%)
20	PGV	P	1268	-	50,50,50	1.29	5 (10%)	53,56,56	0.87	2 (3%)
19	TGL	Q	1523	-	62,62,62	0.84	4 (6%)	65,65,65	1.42	9 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TGL	L	522	-	-	16/65/65/65	-
26	CDL	G	269	-	-	62/110/110/110	-
20	PGV	N	1266	-	-	12/55/55/55	-
20	PGV	P	1267	-	-	17/55/55/55	-
23	CHD	O	229	-	-	0/7/74/74	0/4/4/4
23	CHD	J	60	-	5/5/12/12	6/7/74/74	0/4/4/4
18	HEA	A	515	1	3/3/7/16	5/24/76/76	-
25	PEK	P	1264	-	-	22/56/56/56	-
22	PSC	B	230	-	-	41/55/55/55	-
25	PEK	P	1265	-	-	21/56/56/56	-
26	CDL	P	1270	-	-	70/110/110/110	-
19	TGL	D	523	-	-	16/65/65/65	-
19	TGL	A	521	-	-	15/65/65/65	-
23	CHD	B	1086	-	-	0/7/74/74	0/4/4/4
23	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
26	CDL	T	1269	-	-	63/110/110/110	-
23	CHD	C	525	-	-	0/7/74/74	0/4/4/4
23	CHD	P	1271	-	5/5/12/12	6/7/74/74	0/4/4/4
18	HEA	N	516	1	3/3/7/16	0/24/76/76	-
20	PGV	A	604	-	-	12/55/55/55	-
24	DMU	P	1272	-	6/6/10/10	9/19/59/59	0/2/2/2
18	HEA	N	515	1	3/3/7/16	5/24/76/76	-
23	CHD	C	271	-	5/5/12/12	6/7/74/74	0/4/4/4
20	PGV	C	268	-	-	34/55/55/55	-
20	PGV	A	524	-	-	34/55/55/55	-
22	PSC	O	1230	-	-	41/55/55/55	-
19	TGL	N	1522	-	-	16/65/65/65	-
25	PEK	C	265	-	-	20/56/56/56	-
25	PEK	T	263	-	-	29/56/56/56	-
20	PGV	Z	1524	-	-	34/55/55/55	-
24	DMU	M	526	-	5/5/10/10	9/19/59/59	0/2/2/2
24	DMU	Z	1526	-	5/5/10/10	10/19/59/59	0/2/2/2
24	DMU	C	272	-	6/6/10/10	9/19/59/59	0/2/2/2
25	PEK	C	264	-	-	21/56/56/56	-
23	CHD	W	1060	-	5/5/12/12	6/7/74/74	0/4/4/4
20	PGV	C	267	-	-	17/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TGL	N	1521	-	-	15/65/65/65	-
26	CDL	C	270	-	-	68/110/110/110	-
25	PEK	G	1263	-	-	30/56/56/56	-
18	HEA	A	516	1	3/3/7/16	0/24/76/76	-
20	PGV	P	1268	-	-	34/55/55/55	-
19	TGL	Q	1523	-	-	15/65/65/65	-

All (220) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	526	DMU	O7-C3	-8.13	1.22	1.43
24	Z	1526	DMU	O7-C3	-7.79	1.23	1.43
24	M	526	DMU	O16-C6	-7.64	1.27	1.40
24	Z	1526	DMU	O16-C6	-7.46	1.27	1.40
24	M	526	DMU	O1-C9	-7.29	1.26	1.44
24	M	526	DMU	O5-C4	-6.98	1.27	1.44
24	Z	1526	DMU	O1-C9	-6.88	1.27	1.44
24	Z	1526	DMU	O5-C4	-6.70	1.28	1.44
24	M	526	DMU	O16-C18	-6.61	1.24	1.43
24	Z	1526	DMU	O16-C18	-6.43	1.25	1.43
18	N	515	HEA	C3B-C11	-6.25	1.48	1.52
24	P	1272	DMU	O16-C18	-6.14	1.25	1.43
24	M	526	DMU	O7-C10	-6.07	1.24	1.41
24	C	272	DMU	O16-C18	-6.06	1.26	1.43
24	M	526	DMU	O1-C10	-5.87	1.26	1.41
24	P	1272	DMU	O7-C3	-5.82	1.28	1.43
18	A	515	HEA	C3B-C11	-5.81	1.48	1.52
24	C	272	DMU	O16-C6	-5.80	1.30	1.40
24	Z	1526	DMU	O7-C10	-5.79	1.25	1.41
19	N	1522	TGL	OG2-CB1	5.78	1.50	1.34
24	P	1272	DMU	O1-C9	-5.71	1.30	1.44
24	P	1272	DMU	O16-C6	-5.42	1.30	1.40
18	N	516	HEA	C3B-C11	-5.37	1.48	1.52
24	C	272	DMU	O5-C4	-5.33	1.31	1.44
24	Z	1526	DMU	O1-C10	-5.33	1.28	1.41
24	C	272	DMU	O1-C9	-5.31	1.31	1.44
24	C	272	DMU	O7-C3	-5.23	1.30	1.43
23	W	1060	CHD	C13-C17	5.07	1.64	1.55
24	M	526	DMU	O5-C6	-4.99	1.29	1.41
25	P	1264	PEK	C15-C14	4.94	1.60	1.31
19	L	522	TGL	OG2-CB1	4.92	1.48	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Z	1526	DMU	O5-C6	-4.84	1.29	1.41
25	C	264	PEK	C15-C14	4.81	1.59	1.31
25	T	263	PEK	C12-C11	4.79	1.59	1.31
25	G	1263	PEK	C12-C11	4.77	1.59	1.31
20	C	268	PGV	C12-C11	4.71	1.59	1.31
20	P	1268	PGV	C12-C11	4.71	1.59	1.31
25	P	1264	PEK	C12-C11	4.68	1.58	1.31
18	A	516	HEA	C3A-C2A	-4.65	1.33	1.40
24	P	1272	DMU	O7-C10	-4.63	1.28	1.41
25	G	1263	PEK	C6-C5	4.54	1.58	1.31
25	T	263	PEK	C6-C5	4.51	1.57	1.31
25	C	264	PEK	C12-C11	4.51	1.57	1.31
25	T	263	PEK	O03-C21	4.45	1.46	1.33
23	J	60	CHD	C13-C17	4.40	1.63	1.55
25	P	1265	PEK	C12-C11	4.35	1.57	1.31
24	C	272	DMU	O5-C6	-4.34	1.30	1.41
25	C	265	PEK	C12-C11	4.34	1.56	1.31
25	C	265	PEK	C15-C14	4.33	1.56	1.31
24	C	272	DMU	O1-C10	-4.29	1.30	1.41
25	G	1263	PEK	C9-C8	4.29	1.56	1.31
25	T	263	PEK	C15-C14	4.24	1.56	1.31
25	C	265	PEK	C9-C8	4.22	1.56	1.31
25	G	1263	PEK	C15-C14	4.22	1.56	1.31
25	T	263	PEK	C9-C8	4.20	1.56	1.31
20	Z	1524	PGV	C12-C11	4.17	1.55	1.31
22	O	1230	PSC	C10-C9	4.16	1.55	1.31
24	P	1272	DMU	O5-C4	-4.16	1.34	1.44
25	P	1265	PEK	C9-C8	4.14	1.55	1.31
19	N	1522	TGL	OG1-CA1	4.13	1.45	1.33
25	T	263	PEK	C03-C02	4.13	1.63	1.50
25	P	1264	PEK	C6-C5	4.12	1.55	1.31
22	B	230	PSC	C10-C9	4.12	1.55	1.31
25	P	1265	PEK	C15-C14	4.11	1.55	1.31
25	C	264	PEK	C6-C5	4.10	1.55	1.31
24	C	272	DMU	O7-C10	-4.10	1.30	1.41
25	P	1265	PEK	C6-C5	4.02	1.55	1.31
22	O	1230	PSC	C13-C12	4.01	1.55	1.31
20	A	524	PGV	C12-C11	4.01	1.55	1.31
25	T	263	PEK	C01-C02	4.00	1.63	1.50
25	G	1263	PEK	C01-C02	3.98	1.62	1.50
20	N	1266	PGV	C12-C11	3.94	1.54	1.31
22	B	230	PSC	C13-C12	3.93	1.54	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	265	PEK	C6-C5	3.92	1.54	1.31
20	A	524	PGV	O03-C19	3.91	1.44	1.33
18	N	516	HEA	C3A-CMA	-3.89	1.37	1.46
25	G	1263	PEK	C03-C02	3.86	1.62	1.50
25	C	264	PEK	C9-C8	3.82	1.53	1.31
18	A	516	HEA	C3A-CMA	-3.80	1.37	1.46
25	P	1264	PEK	C9-C8	3.74	1.53	1.31
20	P	1268	PGV	O01-C1	3.72	1.44	1.34
20	C	268	PGV	O01-C1	3.70	1.44	1.34
24	P	1272	DMU	O1-C10	-3.69	1.32	1.41
24	P	1272	DMU	C6-C1	3.64	1.63	1.52
20	A	604	PGV	C12-C11	3.59	1.52	1.31
26	T	1269	CDL	CB6-CB4	3.57	1.61	1.50
25	G	1263	PEK	O03-C21	3.50	1.43	1.33
20	Z	1524	PGV	O03-C19	3.21	1.42	1.33
26	G	269	CDL	OA6-CA5	3.20	1.43	1.34
26	G	269	CDL	C11-CA5	3.15	1.59	1.50
24	C	272	DMU	C6-C1	3.15	1.61	1.52
18	N	516	HEA	C3A-C2A	-3.14	1.36	1.40
18	A	516	HEA	C3B-C11	-3.13	1.50	1.52
18	N	515	HEA	C3A-CMA	-3.12	1.39	1.46
26	T	1269	CDL	C11-CA5	3.06	1.59	1.50
20	P	1267	PGV	C12-C11	3.06	1.49	1.31
24	P	1272	DMU	C3-C4	3.06	1.61	1.52
25	T	263	PEK	P-O11	3.04	1.71	1.59
24	C	272	DMU	C3-C4	3.03	1.61	1.52
24	P	1272	DMU	C8-C9	3.03	1.59	1.53
25	P	1265	PEK	O03-C21	3.02	1.42	1.33
24	P	1272	DMU	C8-C7	3.02	1.60	1.52
19	L	522	TGL	CG1-CG2	3.01	1.59	1.50
19	N	1522	TGL	CG1-CG2	2.96	1.59	1.50
26	G	269	CDL	CB6-CB4	2.95	1.59	1.50
24	P	1272	DMU	O5-C6	-2.94	1.34	1.41
25	C	265	PEK	C03-C02	2.94	1.59	1.50
25	G	1263	PEK	P-O11	2.93	1.71	1.59
18	N	516	HEA	C4D-ND	2.91	1.42	1.36
18	N	515	HEA	C3A-C2A	-2.90	1.36	1.40
20	C	267	PGV	C12-C11	2.90	1.48	1.31
19	Q	1523	TGL	OG1-CA1	2.88	1.41	1.33
19	D	523	TGL	OG3-CC1	2.87	1.41	1.33
22	O	1230	PSC	C2-C1	2.86	1.59	1.50
20	Z	1524	PGV	C03-C02	2.86	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	516	HEA	C3C-CAC	2.86	1.53	1.47
20	Z	1524	PGV	C20-C19	2.84	1.59	1.50
23	W	1060	CHD	C20-C17	2.84	1.59	1.54
25	P	1264	PEK	C2-C1	2.84	1.59	1.50
20	A	524	PGV	C20-C19	2.76	1.58	1.50
26	P	1270	CDL	CA6-CA4	2.76	1.59	1.50
25	C	265	PEK	C01-C02	2.76	1.59	1.50
25	P	1265	PEK	C01-C02	2.75	1.59	1.50
25	T	263	PEK	C2-C1	2.75	1.58	1.50
25	C	265	PEK	P-O12	2.71	1.70	1.59
25	C	265	PEK	P-O11	2.71	1.70	1.59
24	C	272	DMU	C7-C5	2.70	1.59	1.52
26	P	1270	CDL	C31-CA7	2.69	1.58	1.50
18	N	516	HEA	C1B-NB	2.69	1.41	1.36
18	A	516	HEA	C4D-ND	2.69	1.41	1.36
25	C	265	PEK	O03-C21	2.69	1.41	1.33
25	G	1263	PEK	P-O12	2.67	1.70	1.59
25	T	263	PEK	O01-C1	2.67	1.41	1.34
18	A	515	HEA	C3A-CMA	-2.67	1.40	1.46
24	P	1272	DMU	C7-C5	2.61	1.59	1.52
19	D	523	TGL	CB2-CB1	2.60	1.58	1.50
19	N	1521	TGL	OG2-CB1	2.59	1.41	1.34
18	A	515	HEA	C4D-ND	2.57	1.41	1.36
25	P	1265	PEK	C03-C02	2.54	1.58	1.50
26	T	1269	CDL	CB3-CB4	2.53	1.58	1.50
25	C	265	PEK	C22-C21	2.53	1.58	1.50
25	T	263	PEK	P-O12	2.53	1.69	1.59
19	L	522	TGL	CC2-CC1	2.51	1.58	1.50
18	A	515	HEA	C1C-NC	2.51	1.41	1.36
26	C	270	CDL	CA6-CA4	2.50	1.58	1.50
25	P	1265	PEK	P-O11	2.50	1.69	1.59
19	N	1522	TGL	CA2-CA1	2.50	1.58	1.50
25	P	1265	PEK	P-O12	2.48	1.69	1.59
19	L	522	TGL	OG1-CA1	2.47	1.40	1.33
25	P	1265	PEK	C22-C21	2.45	1.57	1.50
26	G	269	CDL	C71-CB7	2.43	1.57	1.50
19	D	523	TGL	OG1-CA1	2.43	1.40	1.33
26	T	1269	CDL	OA6-CA5	2.43	1.41	1.34
26	P	1270	CDL	CA3-CA4	2.42	1.58	1.50
18	A	515	HEA	C3B-C2B	-2.41	1.33	1.41
18	N	515	HEA	C4C-NC	2.41	1.41	1.36
26	T	1269	CDL	C71-CB7	2.39	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	T	263	PEK	C22-C21	2.39	1.57	1.50
24	P	1272	DMU	C10-C5	2.39	1.59	1.52
18	A	516	HEA	C20-C19	2.39	1.56	1.51
26	T	1269	CDL	CB2-C1	2.38	1.59	1.51
26	G	269	CDL	CB3-CB4	2.38	1.58	1.50
26	P	1270	CDL	PB2-OB2	2.37	1.68	1.59
20	C	268	PGV	P-O12	2.37	1.68	1.59
19	L	522	TGL	CG3-CG2	2.36	1.57	1.50
19	N	1522	TGL	CG3-CG2	2.36	1.57	1.50
19	Q	1523	TGL	CB2-CB1	2.35	1.57	1.50
24	P	1272	DMU	C2-C1	2.35	1.58	1.52
22	B	230	PSC	C2-C1	2.32	1.57	1.50
26	G	269	CDL	PB2-OB2	2.30	1.68	1.59
26	C	270	CDL	CA3-CA4	2.30	1.57	1.50
18	A	515	HEA	C4C-NC	2.29	1.40	1.36
20	P	1268	PGV	P-O12	2.25	1.68	1.59
23	C	525	CHD	C10-C9	-2.24	1.52	1.56
20	C	268	PGV	C04-C05	2.23	1.59	1.51
22	B	230	PSC	P-O12	2.23	1.68	1.59
18	N	516	HEA	C4C-NC	2.23	1.40	1.36
18	N	515	HEA	C1A-C2A	2.22	1.47	1.42
22	O	1230	PSC	P-O12	2.22	1.68	1.59
20	P	1268	PGV	C2-C1	2.22	1.57	1.50
25	C	265	PEK	O01-C1	2.21	1.40	1.34
20	C	268	PGV	P-O11	2.21	1.68	1.59
23	P	1525	CHD	C8-C9	2.21	1.58	1.53
20	N	1266	PGV	C01-C02	2.19	1.57	1.50
23	W	1060	CHD	C8-C7	2.19	1.57	1.53
24	Z	1526	DMU	C8-C9	2.19	1.57	1.53
20	P	1268	PGV	C04-C05	2.18	1.58	1.51
23	J	60	CHD	C20-C17	2.17	1.58	1.54
19	Q	1523	TGL	OG3-CC1	2.16	1.39	1.33
20	N	1266	PGV	C20-C19	2.16	1.57	1.50
24	C	272	DMU	C8-C7	2.16	1.57	1.52
20	C	268	PGV	C2-C1	2.15	1.57	1.50
26	T	1269	CDL	PB2-OB2	2.15	1.68	1.59
24	C	272	DMU	C10-C5	2.14	1.58	1.52
25	P	1264	PEK	O03-C01	-2.14	1.40	1.45
26	G	269	CDL	OB8-CB7	2.13	1.39	1.33
25	G	1263	PEK	O03-C01	2.13	1.50	1.45
23	C	271	CHD	C19-C10	-2.13	1.50	1.54
26	C	270	CDL	CB2-C1	2.12	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	272	DMU	C8-C9	2.12	1.57	1.53
26	P	1270	CDL	CB2-C1	2.12	1.58	1.51
20	A	524	PGV	C03-C02	2.11	1.57	1.50
26	P	1270	CDL	OA8-CA7	2.10	1.39	1.33
18	A	516	HEA	C3B-C2B	-2.10	1.34	1.41
18	N	515	HEA	C1C-NC	2.09	1.40	1.36
26	C	270	CDL	C71-CB7	2.09	1.56	1.50
20	A	524	PGV	P-O12	2.09	1.67	1.59
19	L	522	TGL	CB2-CB1	2.09	1.56	1.50
26	C	270	CDL	PB2-OB2	2.09	1.67	1.59
19	N	1522	TGL	CB2-CB1	2.09	1.56	1.50
26	G	269	CDL	CB2-C1	2.08	1.58	1.51
25	G	1263	PEK	C22-C21	2.08	1.56	1.50
20	N	1266	PGV	O03-C19	2.07	1.39	1.33
26	C	270	CDL	OA8-CA7	2.06	1.39	1.33
19	Q	1523	TGL	CA2-CA1	2.06	1.56	1.50
26	G	269	CDL	C31-CA7	2.04	1.56	1.50
22	B	230	PSC	C01-C02	2.04	1.57	1.50
26	T	1269	CDL	OB6-CB5	2.03	1.40	1.34
25	T	263	PEK	C23-C22	2.01	1.59	1.52
18	A	516	HEA	C1A-C2A	2.00	1.47	1.42

All (415) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	272	DMU	O16-C6-C1	11.34	126.01	108.30
23	P	1271	CHD	C17-C13-C14	10.33	110.50	100.09
23	C	271	CHD	C17-C13-C14	10.25	110.43	100.09
24	P	1272	DMU	O16-C6-C1	10.13	124.12	108.30
23	P	1271	CHD	C10-C9-C8	9.75	122.29	111.82
23	W	1060	CHD	C17-C13-C14	9.41	109.58	100.09
24	C	272	DMU	C1-C2-C3	9.34	131.01	109.68
23	P	1271	CHD	C17-C13-C12	-9.30	109.17	117.67
23	J	60	CHD	C17-C13-C14	9.28	109.45	100.09
23	W	1060	CHD	C13-C17-C20	9.21	130.49	119.50
23	C	271	CHD	C10-C9-C8	9.20	121.69	111.82
24	P	1272	DMU	C1-C2-C3	9.19	130.65	109.68
24	C	272	DMU	O5-C4-C3	9.17	129.09	109.75
23	C	271	CHD	C17-C13-C12	-8.85	109.59	117.67
23	J	60	CHD	C13-C17-C20	8.82	130.02	119.50
24	C	272	DMU	O1-C9-C11	8.52	127.61	106.44
23	C	271	CHD	C19-C10-C9	-8.52	99.45	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1271	CHD	C19-C10-C9	-8.35	99.68	111.18
24	M	526	DMU	C6-O5-C4	7.69	128.79	113.69
24	P	1272	DMU	O1-C9-C11	7.61	125.36	106.44
24	P	1272	DMU	C6-O5-C4	7.44	128.29	113.69
24	P	1272	DMU	O7-C3-C4	7.42	129.77	109.45
23	W	1060	CHD	C10-C9-C8	7.41	119.78	111.82
24	Z	1526	DMU	C6-O5-C4	7.41	128.24	113.69
24	P	1272	DMU	O5-C4-C3	7.37	125.30	109.75
24	M	526	DMU	O1-C9-C8	7.36	123.05	109.69
24	Z	1526	DMU	O1-C9-C11	7.35	124.71	106.44
24	M	526	DMU	O1-C9-C11	7.29	124.56	106.44
24	Z	1526	DMU	O5-C4-C3	7.27	125.08	109.75
24	M	526	DMU	O5-C4-C57	7.18	124.28	106.44
24	C	272	DMU	C6-O5-C4	7.15	127.72	113.69
23	J	60	CHD	C10-C9-C8	7.13	119.47	111.82
24	Z	1526	DMU	O1-C9-C8	7.11	122.60	109.69
23	J	60	CHD	C11-C12-C13	7.02	118.45	111.24
24	Z	1526	DMU	O5-C4-C57	6.90	123.60	106.44
24	M	526	DMU	C18-O16-C6	6.90	125.28	113.84
24	Z	1526	DMU	C18-O16-C6	6.88	125.25	113.84
24	M	526	DMU	O5-C4-C3	6.84	124.17	109.75
24	M	526	DMU	C10-C5-C7	6.81	124.17	110.00
24	Z	1526	DMU	C10-C5-C7	6.68	123.90	110.00
24	C	272	DMU	O7-C3-C4	6.59	127.51	109.45
23	W	1060	CHD	C6-C5-C10	6.54	119.60	112.66
24	M	526	DMU	O7-C3-C2	6.51	124.60	107.28
24	C	272	DMU	O7-C3-C2	6.48	124.51	107.28
23	W	1060	CHD	C11-C12-C13	6.44	117.86	111.24
24	P	1272	DMU	O1-C9-C8	6.17	120.89	109.69
24	Z	1526	DMU	O7-C3-C2	6.06	123.39	107.28
24	C	272	DMU	C18-O16-C6	6.03	123.83	113.84
23	C	271	CHD	C9-C8-C7	5.99	119.03	111.88
24	P	1272	DMU	O5-C4-C57	5.96	121.27	106.44
24	M	526	DMU	C1-C2-C3	5.93	123.22	109.68
23	C	271	CHD	C1-C10-C5	5.92	116.52	107.77
23	C	271	CHD	C4-C5-C10	5.88	118.90	112.66
24	P	1272	DMU	C18-O16-C6	5.86	123.56	113.84
23	P	1271	CHD	C9-C8-C7	5.86	118.88	111.88
24	Z	1526	DMU	O5-C6-O16	5.85	123.82	109.97
24	Z	1526	DMU	C7-C8-C9	5.80	120.58	110.24
23	W	1060	CHD	C4-C3-C2	5.71	117.37	110.55
23	P	1271	CHD	C1-C10-C5	5.67	116.16	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Z	1526	DMU	C1-C2-C3	5.66	122.61	109.68
23	J	60	CHD	C4-C3-C2	5.65	117.30	110.55
24	C	272	DMU	O7-C10-C5	5.62	122.65	108.10
23	C	525	CHD	C14-C13-C12	-5.60	102.19	107.40
23	J	60	CHD	C6-C5-C10	5.59	118.59	112.66
24	M	526	DMU	C7-C8-C9	5.55	120.13	110.24
23	W	1060	CHD	C15-C14-C8	-5.54	110.59	118.33
24	C	272	DMU	O1-C9-C8	5.50	119.69	109.69
23	C	271	CHD	C4-C3-C2	5.50	117.12	110.55
23	J	60	CHD	C15-C14-C8	-5.46	110.69	118.33
24	M	526	DMU	O5-C6-O16	5.39	122.75	109.97
24	M	526	DMU	O16-C6-C1	5.29	116.56	108.30
23	P	1271	CHD	C15-C14-C8	-5.27	110.97	118.33
23	P	1271	CHD	C4-C5-C10	5.25	118.23	112.66
24	P	1272	DMU	C8-C7-C5	5.22	119.94	110.82
23	J	60	CHD	C5-C6-C7	5.12	120.11	114.46
23	C	271	CHD	C15-C14-C8	-5.08	111.22	118.33
23	W	1060	CHD	C5-C6-C7	5.08	120.06	114.46
24	P	1272	DMU	O5-C6-C1	5.07	121.08	110.35
23	P	1271	CHD	C4-C3-C2	5.03	116.56	110.55
23	P	1525	CHD	C13-C17-C20	5.00	125.46	119.50
19	Q	1523	TGL	CG2-OG2-CB1	4.89	129.82	117.79
24	Z	1526	DMU	O16-C6-C1	4.88	115.92	108.30
23	C	271	CHD	C19-C10-C1	-4.87	100.42	108.26
19	N	1522	TGL	CB9-CB8-CB7	-4.87	89.71	114.42
19	A	521	TGL	CG2-OG2-CB1	4.83	129.69	117.79
19	L	522	TGL	C12-C11-C10	-4.76	90.24	114.42
19	N	1522	TGL	C12-C11-C10	-4.74	90.38	114.42
24	P	1272	DMU	O7-C10-C5	4.69	120.26	108.10
23	J	60	CHD	C11-C9-C10	4.68	118.55	113.73
23	W	1060	CHD	C1-C10-C5	4.68	114.68	107.77
24	P	1272	DMU	O7-C3-C2	4.66	119.67	107.28
23	J	60	CHD	C9-C8-C7	4.63	117.41	111.88
23	W	1060	CHD	C11-C9-C10	4.61	118.48	113.73
24	M	526	DMU	O5-C6-C1	4.60	120.08	110.35
19	L	522	TGL	CB9-CB8-CB7	-4.58	91.15	114.42
23	W	1060	CHD	C18-C13-C14	-4.57	104.05	111.21
19	N	1521	TGL	CG2-OG2-CB1	4.54	128.97	117.79
24	C	272	DMU	O5-C4-C57	4.54	117.72	106.44
23	W	1060	CHD	C9-C8-C7	4.51	117.27	111.88
23	P	1525	CHD	C5-C6-C7	4.50	119.43	114.46
23	O	229	CHD	C16-C17-C13	-4.47	99.17	103.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	525	CHD	C13-C17-C20	4.45	124.81	119.50
24	Z	1526	DMU	O5-C6-C1	4.45	119.77	110.35
23	P	1271	CHD	C19-C10-C1	-4.44	101.10	108.26
19	D	523	TGL	CG2-OG2-CB1	4.44	128.72	117.79
24	Z	1526	DMU	C8-C7-C5	-4.43	103.09	110.82
19	A	521	TGL	CG1-OG1-CA1	-4.42	100.75	117.12
23	W	1060	CHD	C13-C14-C8	4.38	120.33	114.74
23	J	60	CHD	C1-C10-C5	4.35	114.20	107.77
19	N	1521	TGL	CG1-OG1-CA1	-4.33	101.09	117.12
23	J	60	CHD	C18-C13-C14	-4.33	104.44	111.21
23	W	1060	CHD	C2-C1-C10	4.27	120.11	112.78
24	C	272	DMU	O5-C6-C1	4.25	119.35	110.35
23	P	1525	CHD	C14-C13-C12	-4.25	103.44	107.40
23	O	229	CHD	C19-C10-C1	-4.24	101.43	108.26
23	C	525	CHD	C10-C9-C8	4.23	116.37	111.82
24	P	1272	DMU	O1-C10-C5	4.23	119.31	110.35
23	J	60	CHD	C13-C14-C8	4.22	120.12	114.74
24	P	1272	DMU	C10-O1-C9	4.21	121.95	113.69
23	J	60	CHD	C2-C1-C10	4.20	119.98	112.78
24	M	526	DMU	C8-C7-C5	-4.18	103.53	110.82
24	C	272	DMU	C10-O1-C9	4.15	121.84	113.69
25	G	1263	PEK	O03-C01-C02	4.13	120.47	108.43
23	C	271	CHD	C14-C13-C12	4.09	111.21	107.40
23	P	1271	CHD	C14-C13-C12	4.05	111.17	107.40
24	C	272	DMU	C2-C3-C4	-4.05	101.65	110.93
19	L	522	TGL	C15-CC9-CC8	4.03	134.87	114.42
19	N	1522	TGL	C15-CC9-CC8	4.02	134.84	114.42
23	C	525	CHD	C5-C6-C7	3.99	118.86	114.46
24	M	526	DMU	O7-C10-C5	3.97	118.39	108.10
24	M	526	DMU	C10-O7-C3	3.95	127.75	117.96
23	O	229	CHD	C10-C9-C8	3.95	116.06	111.82
24	Z	1526	DMU	O7-C3-C4	3.92	120.18	109.45
19	N	1522	TGL	C16-C15-CC9	3.90	134.23	114.42
25	T	263	PEK	P-O11-C03	3.90	144.54	121.68
23	B	1086	CHD	C16-C17-C13	-3.90	99.73	103.55
19	L	522	TGL	C16-C15-CC9	3.88	134.11	114.42
19	L	522	TGL	CC3-CC2-CC1	3.86	127.65	113.62
25	T	263	PEK	O03-C01-C02	3.82	119.56	108.43
25	G	1263	PEK	P-O11-C03	3.73	143.55	121.68
23	W	1060	CHD	C5-C4-C3	3.70	118.19	112.76
23	W	1060	CHD	C14-C8-C7	3.70	116.71	111.81
19	L	522	TGL	CG2-OG2-CB1	3.69	126.87	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	1086	CHD	C15-C14-C8	-3.68	113.19	118.33
18	A	515	HEA	CMB-C2B-C1B	-3.67	122.82	128.46
23	B	1086	CHD	C1-C2-C3	3.61	115.10	110.47
23	B	1086	CHD	C15-C14-C13	-3.61	100.02	103.55
23	P	1271	CHD	C14-C8-C7	3.60	116.58	111.81
24	M	526	DMU	O7-C3-C4	3.58	119.25	109.45
23	B	1086	CHD	C5-C4-C3	3.58	118.01	112.76
23	O	229	CHD	C15-C14-C8	-3.58	113.33	118.33
23	P	1525	CHD	C1-C10-C5	3.57	113.06	107.77
19	L	522	TGL	C11-C10-CB9	3.56	132.47	114.42
23	O	229	CHD	C15-C14-C13	-3.54	100.08	103.55
24	C	272	DMU	O7-C10-O1	3.54	120.56	110.67
23	O	229	CHD	C5-C4-C3	3.54	117.95	112.76
23	P	1525	CHD	C10-C9-C8	3.54	115.62	111.82
18	N	515	HEA	CMB-C2B-C1B	-3.52	123.06	128.46
18	A	516	HEA	CMC-C2C-C1C	-3.49	123.10	128.46
23	P	1525	CHD	C15-C14-C8	-3.49	113.45	118.33
23	J	60	CHD	C5-C4-C3	3.47	117.85	112.76
23	P	1271	CHD	C5-C6-C7	3.47	118.29	114.46
25	C	265	PEK	P-O11-C03	3.46	142.00	121.68
19	N	1522	TGL	C11-C10-CB9	3.46	132.00	114.42
23	J	60	CHD	C1-C2-C3	3.45	114.90	110.47
19	N	1522	TGL	CC3-CC2-CC1	3.44	126.13	113.62
19	N	1522	TGL	CG2-OG2-CB1	3.41	126.19	117.79
23	P	1271	CHD	C1-C10-C9	3.41	116.71	111.35
23	J	60	CHD	C14-C8-C7	3.39	116.31	111.81
23	C	525	CHD	C15-C14-C8	-3.39	113.59	118.33
24	Z	1526	DMU	O7-C10-C5	3.39	116.89	108.10
23	W	1060	CHD	C16-C15-C14	3.39	111.85	105.13
19	D	523	TGL	CG3-OG3-CC1	3.38	129.65	117.12
18	N	515	HEA	C1B-C2B-C3B	3.38	109.35	107.00
23	B	1086	CHD	C19-C10-C1	-3.37	102.83	108.26
26	P	1270	CDL	PA1-OA5-CA3	3.35	141.35	121.68
19	Q	1523	TGL	CG3-OG3-CC1	3.35	129.52	117.12
23	C	271	CHD	C14-C8-C7	3.34	116.24	111.81
19	D	523	TGL	CB3-CB2-CB1	3.34	125.78	113.62
23	P	1271	CHD	C5-C4-C3	3.34	117.66	112.76
24	Z	1526	DMU	O7-C10-O1	3.33	119.97	110.67
23	J	60	CHD	C6-C5-C4	3.32	115.01	111.19
23	B	1086	CHD	C9-C11-C12	3.30	118.66	114.30
19	Q	1523	TGL	OG2-CG2-CG3	3.29	120.31	108.40
23	J	60	CHD	C14-C8-C9	3.27	114.20	109.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	1265	PEK	P-O11-C03	3.27	140.83	121.68
23	W	1060	CHD	C18-C13-C12	-3.27	105.74	109.07
26	C	270	CDL	PA1-OA5-CA3	3.26	140.80	121.68
23	C	271	CHD	C1-C2-C3	3.21	114.59	110.47
19	Q	1523	TGL	CG1-OG1-CA1	-3.20	105.28	117.12
18	A	515	HEA	C1B-C2B-C3B	3.19	109.21	107.00
18	N	515	HEA	C4B-C3B-C2B	-3.17	104.65	106.87
18	N	516	HEA	C27-C19-C20	3.17	120.60	115.27
18	A	516	HEA	CMC-C2C-C3C	3.17	130.60	124.68
18	A	515	HEA	C4B-C3B-C2B	-3.17	104.66	106.87
19	D	523	TGL	OG1-CG1-CG2	3.17	117.65	108.43
25	G	1263	PEK	C02-O01-C1	3.16	125.57	117.79
23	O	229	CHD	C5-C6-C7	3.16	117.94	114.46
23	W	1060	CHD	C14-C8-C9	3.15	114.03	109.71
18	A	515	HEA	C27-C19-C18	-3.12	115.68	123.68
19	D	523	TGL	CG1-OG1-CA1	-3.11	105.59	117.12
23	J	60	CHD	C16-C15-C14	3.10	111.28	105.13
24	C	272	DMU	C8-C7-C5	3.10	116.23	110.82
26	P	1270	CDL	CB6-OB8-CB7	-3.08	105.72	117.12
24	P	1272	DMU	O7-C10-O1	3.08	119.27	110.67
18	A	515	HEA	CMC-C2C-C1C	-3.04	123.79	128.46
20	A	524	PGV	C02-O01-C1	3.03	125.26	117.79
25	P	1264	PEK	C3-C2-C1	-3.03	102.59	113.62
23	B	1086	CHD	C1-C10-C5	3.02	112.24	107.77
23	C	271	CHD	C1-C10-C9	3.02	116.10	111.35
25	C	264	PEK	C3-C2-C1	-3.01	102.67	113.62
23	C	271	CHD	C5-C6-C7	3.01	117.78	114.46
23	W	1060	CHD	C1-C2-C3	3.01	114.33	110.47
24	Z	1526	DMU	C10-O7-C3	3.01	125.41	117.96
19	Q	1523	TGL	CB3-CB2-CB1	3.00	124.55	113.62
25	T	263	PEK	C02-O01-C1	3.00	125.17	117.79
26	P	1270	CDL	OB6-CB5-C51	-2.99	105.05	111.50
23	J	60	CHD	C15-C16-C17	2.99	111.06	105.13
19	A	521	TGL	CG3-CG2-CG1	2.99	118.85	111.79
23	O	229	CHD	C1-C2-C3	2.96	114.27	110.47
23	P	1271	CHD	C15-C16-C17	2.95	110.98	105.13
18	A	515	HEA	CMC-C2C-C3C	2.95	130.19	124.68
19	D	523	TGL	OG2-CG2-CG3	2.94	119.06	108.40
23	C	271	CHD	C6-C5-C10	2.94	115.78	112.66
23	P	1271	CHD	C2-C1-C10	2.92	117.78	112.78
22	O	1230	PSC	C01-O03-C19	-2.92	106.32	117.12
18	N	515	HEA	C27-C19-C18	-2.91	116.22	123.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	1060	CHD	C9-C11-C12	2.91	118.14	114.30
18	A	516	HEA	C27-C19-C20	2.90	120.15	115.27
23	C	271	CHD	C15-C16-C17	2.90	110.87	105.13
22	B	230	PSC	C01-O03-C19	-2.89	106.42	117.12
23	P	1271	CHD	C1-C2-C3	2.89	114.17	110.47
23	W	1060	CHD	C15-C16-C17	2.88	110.84	105.13
26	T	1269	CDL	C23-C22-C21	2.88	129.05	114.42
25	P	1265	PEK	P-O12-C04	2.88	135.77	121.59
25	C	265	PEK	P-O12-C04	2.88	135.75	121.59
18	N	516	HEA	CMC-C2C-C1C	-2.87	124.05	128.46
19	N	1521	TGL	CG3-CG2-CG1	2.85	118.52	111.79
20	Z	1524	PGV	O01-C02-C03	2.83	118.66	108.40
24	M	526	DMU	O7-C10-O1	2.82	118.56	110.67
23	P	1525	CHD	C19-C10-C9	-2.81	107.31	111.18
26	C	270	CDL	CB6-OB8-CB7	-2.80	106.75	117.12
18	N	516	HEA	C3C-C4C-NC	2.79	112.82	109.21
23	O	229	CHD	C1-C10-C5	2.79	111.89	107.77
23	O	229	CHD	C9-C11-C12	2.78	117.97	114.30
19	N	1521	TGL	CG3-OG3-CC1	2.77	127.39	117.12
23	C	271	CHD	C5-C4-C3	2.76	116.81	112.76
19	Q	1523	TGL	OG1-CG1-CG2	2.75	116.44	108.43
23	C	525	CHD	C14-C8-C9	-2.75	105.94	109.71
23	C	525	CHD	C1-C10-C5	2.75	111.83	107.77
23	P	1525	CHD	C6-C5-C4	-2.74	108.04	111.19
25	C	264	PEK	O03-C21-C22	-2.73	103.32	111.91
24	C	272	DMU	C7-C8-C9	2.73	115.10	110.24
19	N	1522	TGL	C13-C12-C11	2.72	128.23	114.42
24	C	272	DMU	O1-C10-C5	2.71	116.09	110.35
26	C	270	CDL	OB6-CB5-C51	-2.71	105.66	111.50
23	C	271	CHD	C16-C15-C14	2.71	110.50	105.13
23	B	1086	CHD	C17-C13-C14	2.70	102.82	100.09
26	G	269	CDL	C23-C22-C21	2.70	128.13	114.42
23	W	1060	CHD	C6-C5-C4	2.70	114.30	111.19
23	O	229	CHD	C14-C13-C12	-2.69	104.89	107.40
26	T	1269	CDL	C22-C21-C20	2.68	128.04	114.42
23	P	1271	CHD	C16-C15-C14	2.68	110.44	105.13
23	O	229	CHD	C17-C13-C14	2.67	102.79	100.09
20	C	267	PGV	O01-C1-C2	-2.67	105.75	111.50
19	A	521	TGL	CA3-CA2-CA1	-2.67	103.92	113.62
26	G	269	CDL	C22-C21-C20	2.66	127.95	114.42
23	O	229	CHD	O3-C3-C4	-2.66	104.56	109.85
23	C	525	CHD	C19-C10-C9	-2.65	107.53	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	522	TGL	C13-C12-C11	2.64	127.81	114.42
23	P	1271	CHD	C6-C5-C10	2.64	115.46	112.66
23	J	60	CHD	C4-C5-C10	2.62	115.44	112.66
23	C	271	CHD	C2-C1-C10	2.62	117.27	112.78
25	P	1265	PEK	C11-C10-C9	2.60	124.82	112.02
25	C	265	PEK	C24-C23-C22	2.60	122.53	113.19
18	N	515	HEA	C17-C18-C19	-2.59	121.42	127.66
20	A	524	PGV	O01-C02-C03	2.59	117.78	108.40
23	B	1086	CHD	C10-C9-C8	2.59	114.60	111.82
19	L	522	TGL	C20-CA9-CA8	2.58	127.54	114.42
20	C	267	PGV	C9-C10-C11	-2.57	97.69	112.43
23	C	271	CHD	C9-C10-C5	2.57	112.19	108.58
19	A	521	TGL	CG3-OG3-CC1	2.56	126.61	117.12
19	D	523	TGL	OG2-CG2-CG1	2.55	117.63	108.40
25	C	265	PEK	C11-C10-C9	2.55	124.57	112.02
18	N	516	HEA	C26-C15-C16	2.55	119.55	115.27
18	N	515	HEA	CMD-C2D-C3D	2.54	129.72	124.94
20	P	1267	PGV	C9-C10-C11	-2.53	97.93	112.43
19	A	521	TGL	OG1-CG1-CG2	2.52	115.78	108.43
20	C	268	PGV	C02-O01-C1	-2.51	111.61	117.79
23	C	525	CHD	C5-C4-C3	2.51	116.44	112.76
26	P	1270	CDL	OB6-CB5-OB7	2.50	129.74	123.70
26	G	269	CDL	C20-C19-C18	2.48	127.04	114.42
23	P	1525	CHD	C1-C2-C3	2.48	113.64	110.47
19	N	1522	TGL	CC4-CC3-CC2	2.47	122.06	113.19
25	T	263	PEK	P-O12-C04	2.46	133.72	121.59
25	G	1263	PEK	P-O12-C04	2.45	133.67	121.59
19	N	1522	TGL	C20-CA9-CA8	2.45	126.88	114.42
18	N	515	HEA	CMC-C2C-C1C	-2.45	124.70	128.46
20	P	1268	PGV	C02-O01-C1	-2.45	111.77	117.79
20	A	524	PGV	C3-C2-C1	-2.45	104.72	113.62
20	Z	1524	PGV	C02-O01-C1	2.44	123.80	117.79
19	A	521	TGL	CA8-CA7-CA6	-2.44	102.03	114.42
25	C	264	PEK	O01-C1-C2	-2.42	106.29	111.50
19	N	1521	TGL	CA3-CA2-CA1	-2.41	104.85	113.62
20	Z	1524	PGV	C3-C2-C1	-2.41	104.85	113.62
26	C	270	CDL	C52-C51-CB5	-2.41	104.86	113.62
19	N	1521	TGL	CB7-CB6-CB5	-2.40	102.23	114.42
18	A	516	HEA	CBD-CAD-C3D	2.40	116.91	112.49
25	C	265	PEK	C2-C3-C4	2.39	117.49	113.23
24	M	526	DMU	C10-O1-C9	2.39	118.37	113.69
20	N	1266	PGV	C01-O03-C19	-2.38	108.30	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	60	CHD	C19-C10-C9	-2.38	107.90	111.18
20	N	1266	PGV	O03-C01-C02	2.37	115.33	108.43
19	L	522	TGL	OG1-CG1-CG2	2.36	115.31	108.43
25	C	264	PEK	O03-C21-O04	2.36	129.55	123.59
25	P	1265	PEK	C24-C23-C22	2.36	121.68	113.19
19	A	521	TGL	CB7-CB6-CB5	-2.36	102.44	114.42
23	W	1060	CHD	C19-C10-C1	-2.36	104.46	108.26
25	P	1265	PEK	C2-C3-C4	2.36	117.43	113.23
23	J	60	CHD	C18-C13-C12	-2.35	106.67	109.07
23	P	1271	CHD	C9-C11-C12	2.35	117.40	114.30
25	P	1264	PEK	O03-C21-O04	2.34	129.50	123.59
18	A	515	HEA	C17-C18-C19	-2.34	122.03	127.66
18	N	515	HEA	C16-C15-C14	2.32	125.82	121.12
23	C	271	CHD	C9-C11-C12	2.32	117.36	114.30
19	A	521	TGL	OG2-CG2-CG3	2.32	116.79	108.40
26	T	1269	CDL	C19-C18-C17	2.31	126.16	114.42
23	B	1086	CHD	C14-C13-C12	-2.31	105.25	107.40
25	C	265	PEK	O03-C01-C02	2.31	115.14	108.43
26	T	1269	CDL	C83-C82-C81	2.30	126.11	114.42
25	P	1264	PEK	O03-C21-C22	-2.30	104.69	111.91
19	L	522	TGL	CC4-CC3-CC2	2.30	121.45	113.19
19	N	1521	TGL	CA8-CA7-CA6	-2.30	102.75	114.42
18	N	515	HEA	CMC-C2C-C3C	2.30	128.98	124.68
19	Q	1523	TGL	CA3-CA2-CA1	-2.29	105.31	113.62
18	N	516	HEA	CMD-C2D-C3D	2.28	129.24	124.94
24	P	1272	DMU	C2-C3-C4	-2.27	105.71	110.93
23	P	1525	CHD	C14-C8-C9	-2.27	106.60	109.71
26	G	269	CDL	C19-C18-C17	2.26	125.91	114.42
18	A	515	HEA	C27-C19-C20	2.26	119.07	115.27
23	J	60	CHD	C19-C10-C1	-2.26	104.62	108.26
26	T	1269	CDL	OB8-CB7-C71	-2.25	104.84	111.91
19	A	521	TGL	CA6-CA5-CA4	-2.25	102.99	114.42
26	T	1269	CDL	C20-C19-C18	2.25	125.85	114.42
19	N	1521	TGL	CA6-CA5-CA4	-2.25	103.03	114.42
19	D	523	TGL	CC3-CC2-CC1	-2.24	105.48	113.62
18	A	515	HEA	C16-C15-C14	2.24	125.64	121.12
19	N	1521	TGL	OG2-CG2-CG3	2.24	116.50	108.40
23	P	1525	CHD	C6-C5-C10	2.23	115.03	112.66
19	L	522	TGL	CC7-CC6-CC5	2.22	125.71	114.42
18	N	515	HEA	C21-C20-C19	-2.22	105.69	112.98
23	J	60	CHD	C9-C11-C12	2.20	117.21	114.30
23	P	1525	CHD	C5-C4-C3	2.20	115.99	112.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	N	1521	TGL	OG1-CG1-CG2	2.20	114.83	108.43
25	T	263	PEK	C2-C3-C4	2.19	117.13	113.23
23	P	1271	CHD	C9-C10-C5	2.19	111.65	108.58
19	N	1522	TGL	C10-CB9-CB8	2.19	125.53	114.42
26	C	270	CDL	OB6-CB5-OB7	2.18	128.97	123.70
23	B	1086	CHD	O3-C3-C4	-2.17	105.52	109.85
23	W	1060	CHD	C19-C10-C5	-2.17	106.69	110.36
19	Q	1523	TGL	CC3-CC2-CC1	-2.16	105.76	113.62
26	G	269	CDL	C83-C82-C81	2.15	125.36	114.42
26	P	1270	CDL	C52-C51-CB5	-2.15	105.79	113.62
18	N	515	HEA	C13-C14-C15	-2.15	122.48	127.66
23	O	229	CHD	C14-C8-C9	-2.15	106.76	109.71
26	G	269	CDL	C80-C79-C78	2.14	125.31	114.42
23	C	525	CHD	C9-C10-C5	-2.14	105.57	108.58
18	A	516	HEA	CMD-C2D-C3D	2.14	128.97	124.94
25	P	1264	PEK	O01-C1-C2	-2.14	106.89	111.50
20	A	604	PGV	O01-C1-C2	-2.14	106.90	111.50
18	A	515	HEA	C21-C20-C19	-2.14	105.95	112.98
23	C	271	CHD	C18-C13-C14	-2.13	107.87	111.21
22	B	230	PSC	P-O12-C04	2.13	132.08	121.59
25	P	1265	PEK	O03-C01-C02	2.13	114.64	108.43
19	A	521	TGL	CB9-CB8-CB7	-2.13	103.62	114.42
23	J	60	CHD	C19-C10-C5	-2.13	106.76	110.36
18	A	515	HEA	CMD-C2D-C3D	2.12	128.94	124.94
20	P	1267	PGV	O01-C1-C2	-2.12	106.94	111.50
18	N	515	HEA	C27-C19-C20	2.11	118.82	115.27
19	L	522	TGL	C10-CB9-CB8	2.11	125.12	114.42
20	P	1268	PGV	O03-C01-C02	2.10	114.55	108.43
23	P	1525	CHD	C21-C20-C22	-2.09	107.08	110.36
18	N	516	HEA	CMC-C2C-C3C	2.09	128.59	124.68
20	C	267	PGV	C3-C2-C1	-2.09	106.03	113.62
23	C	525	CHD	C18-C13-C12	2.09	111.19	109.07
19	N	1522	TGL	OG2-CB1-OB1	2.09	128.74	123.70
23	W	1060	CHD	C17-C13-C12	-2.08	115.76	117.67
23	B	1086	CHD	C2-C1-C10	2.08	116.34	112.78
23	C	525	CHD	C6-C5-C10	2.08	114.86	112.66
25	P	1264	PEK	C01-O03-C21	-2.07	109.44	117.12
20	A	524	PGV	O01-C1-C2	-2.07	107.04	111.50
26	G	269	CDL	OB8-CB7-C71	-2.07	105.42	111.91
19	N	1521	TGL	C12-C11-C10	-2.07	103.93	114.42
20	A	604	PGV	O03-C01-C02	2.07	114.45	108.43
22	O	1230	PSC	O01-C1-C2	-2.07	107.05	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	1269	CDL	OB8-CB6-CB4	2.06	114.44	108.43
25	T	263	PEK	C03-C02-C01	2.06	116.67	111.79
23	C	271	CHD	C18-C13-C12	-2.06	106.97	109.07
23	P	1271	CHD	C18-C13-C14	-2.05	108.00	111.21
19	A	521	TGL	C12-C11-C10	-2.05	104.02	114.42
19	N	1522	TGL	CC7-CC6-CC5	2.04	124.80	114.42
18	A	516	HEA	C3C-C4C-NC	2.04	111.85	109.21
25	C	264	PEK	C23-C22-C21	-2.04	106.20	113.62
23	O	229	CHD	C4-C5-C10	-2.04	110.49	112.66
18	A	515	HEA	C20-C19-C18	2.03	125.23	121.12
19	N	1522	TGL	CA8-CA7-CA6	-2.03	104.11	114.42
19	N	1521	TGL	C10-CB9-CB8	2.03	124.74	114.42
18	N	515	HEA	C3C-C4C-NC	2.02	111.82	109.21
26	T	1269	CDL	C80-C79-C78	2.02	124.66	114.42
24	C	272	DMU	C10-O7-C3	2.01	122.94	117.96
24	P	1272	DMU	O5-C6-O16	2.01	114.73	109.97
19	A	521	TGL	CB6-CB5-CB4	2.01	124.62	114.42
19	A	521	TGL	C10-CB9-CB8	2.01	124.62	114.42
20	C	267	PGV	O01-C1-O02	2.00	128.54	123.70
19	Q	1523	TGL	CA5-CA4-CA3	-2.00	104.27	114.42

All (54) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	J	60	CHD	C12
23	J	60	CHD	C8
23	J	60	CHD	C9
23	J	60	CHD	C14
23	J	60	CHD	C17
18	A	515	HEA	ND
18	A	515	HEA	NA
18	A	515	HEA	NB
24	C	272	DMU	C5
24	C	272	DMU	C6
24	C	272	DMU	C9
24	C	272	DMU	C4
24	C	272	DMU	C2
24	C	272	DMU	C10
18	N	516	HEA	ND
18	N	516	HEA	NA
18	N	516	HEA	NB
23	P	1271	CHD	C12

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Mol	Chain	Res	Type	Atom
23	P	1271	CHD	C8
23	P	1271	CHD	C3
23	P	1271	CHD	C9
23	P	1271	CHD	C14
18	N	515	HEA	ND
18	N	515	HEA	NA
18	N	515	HEA	NB
23	C	271	CHD	C12
23	C	271	CHD	C8
23	C	271	CHD	C3
23	C	271	CHD	C9
23	C	271	CHD	C14
24	M	526	DMU	C2
24	M	526	DMU	C4
24	M	526	DMU	C6
24	M	526	DMU	C9
24	M	526	DMU	C5
23	W	1060	CHD	C12
23	W	1060	CHD	C8
23	W	1060	CHD	C9
23	W	1060	CHD	C14
23	W	1060	CHD	C17
24	P	1272	DMU	C5
24	P	1272	DMU	C6
24	P	1272	DMU	C9
24	P	1272	DMU	C4
24	P	1272	DMU	C2
24	P	1272	DMU	C10
24	Z	1526	DMU	C2
24	Z	1526	DMU	C4
24	Z	1526	DMU	C6
24	Z	1526	DMU	C9
24	Z	1526	DMU	C5
18	A	516	HEA	ND
18	A	516	HEA	NA
18	A	516	HEA	NB

All (846) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	G	269	CDL	C1-CB2-OB2-PB2
26	G	269	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
26	G	269	CDL	CB3-OB5-PB2-OB4
26	G	269	CDL	OB6-CB4-CB6-OB8
23	J	60	CHD	C16-C17-C20-C21
23	J	60	CHD	C16-C17-C20-C22
22	B	230	PSC	C03-O11-P-O14
22	B	230	PSC	C04-O12-P-O14
25	P	1265	PEK	C03-O11-P-O13
25	P	1265	PEK	C04-O12-P-O11
25	P	1265	PEK	C04-O12-P-O13
25	P	1265	PEK	C04-O12-P-O14
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	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
25	C	265	PEK	C04-O12-P-O11
25	C	265	PEK	C04-O12-P-O13
25	C	265	PEK	C04-O12-P-O14
26	T	1269	CDL	C1-CB2-OB2-PB2
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	C	268	PGV	C04-O12-P-O11
20	C	268	PGV	C04-O12-P-O13
20	C	268	PGV	C04-O12-P-O14
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	O04-C19-O03-C01
20	A	524	PGV	C20-C19-O03-C01
24	M	526	DMU	O5-C6-O16-C18
23	W	1060	CHD	C16-C17-C20-C21
23	W	1060	CHD	C16-C17-C20-C22
25	T	263	PEK	C03-O11-P-O14
25	T	263	PEK	O12-C04-C05-N
20	Z	1524	PGV	C04-O12-P-O11

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Mol	Chain	Res	Type	Atoms
20	Z	1524	PGV	C04-O12-P-O13
20	Z	1524	PGV	C04-O12-P-O14
20	Z	1524	PGV	C02-C03-O11-P
20	Z	1524	PGV	C05-C04-O12-P
20	Z	1524	PGV	C04-C05-C06-O06
20	Z	1524	PGV	O02-C1-O01-C02
20	Z	1524	PGV	O04-C19-O03-C01
20	Z	1524	PGV	C20-C19-O03-C01
22	O	1230	PSC	C03-O11-P-O14
22	O	1230	PSC	C04-O12-P-O14
24	Z	1526	DMU	O5-C6-O16-C18
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	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
25	G	1263	PEK	C03-O11-P-O14
25	G	1263	PEK	O12-C04-C05-N
20	P	1268	PGV	C04-O12-P-O11
20	P	1268	PGV	C04-O12-P-O13
20	P	1268	PGV	C04-O12-P-O14
19	D	523	TGL	OC1-CC1-OG3-CG3
19	Q	1523	TGL	OC1-CC1-OG3-CG3
22	B	230	PSC	O02-C1-O01-C02
19	A	521	TGL	OB1-CB1-OG2-CG2
22	O	1230	PSC	O02-C1-O01-C02
19	N	1521	TGL	OB1-CB1-OG2-CG2
20	A	524	PGV	C2-C1-O01-C02
20	Z	1524	PGV	C2-C1-O01-C02
19	A	521	TGL	OA1-CA1-OG1-CG1
19	N	1521	TGL	OA1-CA1-OG1-CG1
26	G	269	CDL	C17-C18-C19-C20
26	G	269	CDL	C77-C78-C79-C80
26	P	1270	CDL	C40-C41-C42-C43
26	P	1270	CDL	C57-C58-C59-C60
26	P	1270	CDL	C60-C61-C62-C63
26	T	1269	CDL	C17-C18-C19-C20
26	T	1269	CDL	C20-C21-C22-C23
26	T	1269	CDL	C40-C41-C42-C43
26	T	1269	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
26	C	270	CDL	C40-C41-C42-C43
26	C	270	CDL	C57-C58-C59-C60
26	C	270	CDL	C80-C81-C82-C83
26	G	269	CDL	C31-CA7-OA8-CA6
19	D	523	TGL	CC2-CC1-OG3-CG3
26	T	1269	CDL	C31-CA7-OA8-CA6
19	Q	1523	TGL	CC2-CC1-OG3-CG3
26	G	269	CDL	C20-C21-C22-C23
26	G	269	CDL	C40-C41-C42-C43
26	G	269	CDL	C80-C81-C82-C83
26	P	1270	CDL	C20-C21-C22-C23
26	P	1270	CDL	C77-C78-C79-C80
26	P	1270	CDL	C80-C81-C82-C83
19	A	521	TGL	C16-C15-CC9-CC8
26	T	1269	CDL	C60-C61-C62-C63
19	N	1521	TGL	C16-C15-CC9-CC8
26	C	270	CDL	C20-C21-C22-C23
26	C	270	CDL	C60-C61-C62-C63
26	C	270	CDL	C77-C78-C79-C80
26	G	269	CDL	C37-C38-C39-C40
26	G	269	CDL	C57-C58-C59-C60
26	G	269	CDL	C60-C61-C62-C63
26	P	1270	CDL	C17-C18-C19-C20
26	T	1269	CDL	C37-C38-C39-C40
26	T	1269	CDL	C57-C58-C59-C60
26	T	1269	CDL	C80-C81-C82-C83
26	P	1270	CDL	OA7-CA5-OA6-CA4
26	C	270	CDL	OA7-CA5-OA6-CA4
26	G	269	CDL	OA9-CA7-OA8-CA6
26	T	1269	CDL	OA9-CA7-OA8-CA6
19	N	1522	TGL	OA1-CA1-OG1-CG1
19	L	522	TGL	C21-C20-CA9-CA8
19	N	1522	TGL	C21-C20-CA9-CA8
26	C	270	CDL	C17-C18-C19-C20
26	C	270	CDL	C37-C38-C39-C40
26	P	1270	CDL	C37-C38-C39-C40
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	Q	1523	TGL	C21-C20-CA9-CA8
19	L	522	TGL	OA1-CA1-OG1-CG1

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Mol	Chain	Res	Type	Atoms
24	P	1272	DMU	O6-C11-C9-O1
19	A	521	TGL	CB2-CB1-OG2-CG2
19	N	1521	TGL	CB2-CB1-OG2-CG2
19	D	523	TGL	C21-C20-CA9-CA8
24	C	272	DMU	O6-C11-C9-O1
19	L	522	TGL	C11-C10-CB9-CB8
19	N	1522	TGL	C11-C10-CB9-CB8
19	D	523	TGL	C11-C10-CB9-CB8
19	D	523	TGL	C16-C15-CC9-CC8
19	A	521	TGL	C21-C20-CA9-CA8
19	A	521	TGL	C11-C10-CB9-CB8
19	N	1521	TGL	C21-C20-CA9-CA8
19	N	1521	TGL	C11-C10-CB9-CB8
19	Q	1523	TGL	C11-C10-CB9-CB8
19	Q	1523	TGL	C16-C15-CC9-CC8
19	L	522	TGL	C16-C15-CC9-CC8
19	N	1522	TGL	C16-C15-CC9-CC8
23	J	60	CHD	C17-C20-C22-C23
23	W	1060	CHD	C17-C20-C22-C23
18	A	515	HEA	C21-C22-C23-C25
19	N	1522	TGL	CA2-CA1-OG1-CG1
22	B	230	PSC	C2-C1-O01-C02
26	G	269	CDL	CB2-C1-CA2-OA2
26	T	1269	CDL	CB2-C1-CA2-OA2
20	A	524	PGV	O12-C04-C05-C06
20	Z	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
24	M	526	DMU	O6-C11-C9-C8
24	C	272	DMU	C3-C4-C57-O61
26	G	269	CDL	O1-C1-CB2-OB2
26	P	1270	CDL	O1-C1-CB2-OB2
26	T	1269	CDL	O1-C1-CB2-OB2
20	A	524	PGV	O12-C04-C05-O05
20	Z	1524	PGV	O12-C04-C05-O05
26	C	270	CDL	O1-C1-CB2-OB2
23	J	60	CHD	C21-C20-C22-C23
23	W	1060	CHD	C21-C20-C22-C23
24	C	272	DMU	C1-C6-O16-C18
24	P	1272	DMU	C1-C6-O16-C18
25	T	263	PEK	O03-C01-C02-O01

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Mol	Chain	Res	Type	Atoms
25	G	1263	PEK	O03-C01-C02-O01
24	P	1272	DMU	C3-C4-C57-O61
25	T	263	PEK	C28-C29-C30-C31
24	M	526	DMU	O5-C4-C57-O61
22	O	1230	PSC	C2-C1-O01-C02
23	J	60	CHD	C13-C17-C20-C22
23	W	1060	CHD	C13-C17-C20-C22
20	A	524	PGV	C19-C20-C21-C22
20	Z	1524	PGV	C19-C20-C21-C22
22	B	230	PSC	O04-C19-O03-C01
22	O	1230	PSC	O04-C19-O03-C01
25	G	1263	PEK	C28-C29-C30-C31
24	Z	1526	DMU	O6-C11-C9-C8
19	L	522	TGL	CC3-CC4-CC5-CC6
24	Z	1526	DMU	O5-C4-C57-O61
18	N	515	HEA	C21-C22-C23-C25
20	P	1268	PGV	O05-C05-C06-O06
18	A	515	HEA	C17-C18-C19-C27
18	N	515	HEA	C17-C18-C19-C27
22	B	230	PSC	C1-C2-C3-C4
19	D	523	TGL	CA2-CA1-OG1-CG1
19	Q	1523	TGL	CA2-CA1-OG1-CG1
22	B	230	PSC	C20-C21-C22-C23
26	T	1269	CDL	C73-C74-C75-C76
24	M	526	DMU	O16-C18-C19-C22
22	O	1230	PSC	C20-C21-C22-C23
24	Z	1526	DMU	O16-C18-C19-C22
22	O	1230	PSC	C1-C2-C3-C4
23	J	60	CHD	C13-C17-C20-C21
23	W	1060	CHD	C13-C17-C20-C21
19	N	1522	TGL	CC3-CC4-CC5-CC6
26	C	270	CDL	CB7-C71-C72-C73
26	G	269	CDL	C73-C74-C75-C76
20	C	268	PGV	O12-C04-C05-O05
20	P	1268	PGV	O12-C04-C05-O05
26	P	1270	CDL	CB7-C71-C72-C73
23	P	1271	CHD	C17-C20-C22-C23
23	C	271	CHD	C17-C20-C22-C23
24	Z	1526	DMU	C3-C4-C57-O61
26	G	269	CDL	C11-CA5-OA6-CA4
26	T	1269	CDL	C11-CA5-OA6-CA4
20	C	268	PGV	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
20	P	1268	PGV	C2-C1-O01-C02
26	G	269	CDL	CB3-OB5-PB2-OB2
26	P	1270	CDL	CA2-OA2-PA1-OA5
26	P	1270	CDL	CB2-OB2-PB2-OB5
26	T	1269	CDL	CB3-OB5-PB2-OB2
25	T	263	PEK	C03-O11-P-O12
26	C	270	CDL	CA2-OA2-PA1-OA5
26	C	270	CDL	CB2-OB2-PB2-OB5
25	G	1263	PEK	C03-O11-P-O12
25	C	265	PEK	C21-C22-C23-C24
26	G	269	CDL	CA2-C1-CB2-OB2
26	T	1269	CDL	CA2-C1-CB2-OB2
20	C	268	PGV	O12-C04-C05-C06
20	P	1268	PGV	O12-C04-C05-C06
26	G	269	CDL	OA7-CA5-OA6-CA4
26	T	1269	CDL	OA7-CA5-OA6-CA4
22	B	230	PSC	C29-C30-C31-C32
19	L	522	TGL	CB4-CB5-CB6-CB7
26	G	269	CDL	C13-C14-C15-C16
22	B	230	PSC	C2-C3-C4-C5
26	T	1269	CDL	C13-C14-C15-C16
20	C	268	PGV	C13-C14-C15-C16
20	Z	1524	PGV	C4-C5-C6-C7
22	O	1230	PSC	C29-C30-C31-C32
26	C	270	CDL	C51-C52-C53-C54
19	Q	1523	TGL	OA1-CA1-OG1-CG1
26	G	269	CDL	C58-C59-C60-C61
20	N	1266	PGV	C6-C7-C8-C9
25	P	1265	PEK	C25-C26-C27-C28
26	P	1270	CDL	C16-C17-C18-C19
26	P	1270	CDL	C59-C60-C61-C62
25	C	265	PEK	C25-C26-C27-C28
26	T	1269	CDL	C58-C59-C60-C61
20	A	604	PGV	C6-C7-C8-C9
20	C	268	PGV	C24-C25-C26-C27
24	M	526	DMU	C25-C28-C31-C34
22	O	1230	PSC	C2-C3-C4-C5
24	Z	1526	DMU	C25-C28-C31-C34
26	C	270	CDL	C16-C17-C18-C19
26	C	270	CDL	C59-C60-C61-C62
20	P	1268	PGV	C13-C14-C15-C16
20	P	1268	PGV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
20	C	268	PGV	O02-C1-O01-C02
20	P	1268	PGV	O02-C1-O01-C02
25	P	1265	PEK	C21-C22-C23-C24
25	T	263	PEK	C1-C2-C3-C4
22	B	230	PSC	C22-C23-C24-C25
26	P	1270	CDL	C51-C52-C53-C54
26	T	1269	CDL	C56-C57-C58-C59
20	A	524	PGV	C4-C5-C6-C7
19	N	1522	TGL	CB4-CB5-CB6-CB7
19	D	523	TGL	OA1-CA1-OG1-CG1
26	G	269	CDL	C56-C57-C58-C59
26	G	269	CDL	C72-C73-C74-C75
26	T	1269	CDL	C72-C73-C74-C75
20	P	1268	PGV	C22-C23-C24-C25
26	G	269	CDL	CA5-C11-C12-C13
20	C	268	PGV	C22-C23-C24-C25
25	T	263	PEK	C29-C30-C31-C32
24	P	1272	DMU	O5-C4-C57-O61
26	P	1270	CDL	C13-C14-C15-C16
20	A	604	PGV	C23-C24-C25-C26
25	T	263	PEK	C27-C28-C29-C30
25	G	1263	PEK	C29-C30-C31-C32
20	N	1266	PGV	C23-C24-C25-C26
25	P	1265	PEK	C16-C17-C18-C19
26	C	270	CDL	C13-C14-C15-C16
25	G	1263	PEK	C27-C28-C29-C30
20	C	268	PGV	C04-C05-C06-O06
20	P	1268	PGV	C04-C05-C06-O06
26	G	269	CDL	C15-C16-C17-C18
25	C	265	PEK	C16-C17-C18-C19
20	A	604	PGV	C29-C30-C31-C32
20	C	268	PGV	C3-C4-C5-C6
19	N	1522	TGL	CC2-CC3-CC4-CC5
25	C	264	PEK	C23-C24-C25-C26
20	C	267	PGV	C7-C8-C9-C10
25	C	264	PEK	C22-C21-O03-C01
26	P	1270	CDL	CA5-C11-C12-C13
26	T	1269	CDL	CA5-C11-C12-C13
20	C	268	PGV	C1-C2-C3-C4
26	C	270	CDL	CA5-C11-C12-C13
20	P	1268	PGV	C1-C2-C3-C4
20	N	1266	PGV	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	P	1267	PGV	C7-C8-C9-C10
20	P	1267	PGV	C22-C23-C24-C25
26	T	1269	CDL	C15-C16-C17-C18
20	Z	1524	PGV	C28-C29-C30-C31
26	C	270	CDL	C55-C56-C57-C58
20	P	1268	PGV	C3-C4-C5-C6
20	N	1266	PGV	C7-C8-C9-C10
20	N	1266	PGV	C29-C30-C31-C32
25	P	1264	PEK	C23-C24-C25-C26
25	P	1264	PEK	C31-C32-C33-C34
25	C	265	PEK	C31-C32-C33-C34
20	A	604	PGV	C5-C6-C7-C8
20	A	604	PGV	C7-C8-C9-C10
20	C	267	PGV	C22-C23-C24-C25
26	C	270	CDL	C73-C74-C75-C76
25	P	1265	PEK	C31-C32-C33-C34
26	P	1270	CDL	C55-C56-C57-C58
19	A	521	TGL	CB6-CB7-CB8-CB9
20	A	524	PGV	C28-C29-C30-C31
20	Z	1524	PGV	C22-C23-C24-C25
25	C	264	PEK	C31-C32-C33-C34
26	C	270	CDL	C74-C75-C76-C77
20	P	1268	PGV	C27-C28-C29-C30
19	A	521	TGL	OC1-CC1-OG3-CG3
19	L	522	TGL	CC2-CC3-CC4-CC5
20	C	268	PGV	C27-C28-C29-C30
24	P	1272	DMU	C25-C28-C31-C34
26	P	1270	CDL	C72-C73-C74-C75
26	P	1270	CDL	C73-C74-C75-C76
23	P	1271	CHD	C21-C20-C22-C23
23	C	271	CHD	C21-C20-C22-C23
26	G	269	CDL	C79-C80-C81-C82
26	P	1270	CDL	C74-C75-C76-C77
26	T	1269	CDL	C79-C80-C81-C82
20	A	524	PGV	C22-C23-C24-C25
26	P	1270	CDL	C75-C76-C77-C78
24	C	272	DMU	C25-C28-C31-C34
25	P	1264	PEK	C22-C21-O03-C01
25	P	1264	PEK	C16-C17-C18-C19
20	C	268	PGV	O05-C05-C06-O06
20	A	524	PGV	O05-C05-C06-O06
20	Z	1524	PGV	O05-C05-C06-O06

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Mol	Chain	Res	Type	Atoms
26	C	270	CDL	C75-C76-C77-C78
25	G	1263	PEK	C1-C2-C3-C4
26	C	270	CDL	C72-C73-C74-C75
19	N	1521	TGL	OC1-CC1-OG3-CG3
25	T	263	PEK	C25-C26-C27-C28
25	C	264	PEK	C16-C17-C18-C19
25	P	1264	PEK	O04-C21-O03-C01
25	P	1264	PEK	C22-C23-C24-C25
20	C	267	PGV	C25-C26-C27-C28
26	C	270	CDL	C71-C72-C73-C74
25	T	263	PEK	C26-C27-C28-C29
22	O	1230	PSC	C22-C23-C24-C25
19	N	1521	TGL	CB6-CB7-CB8-CB9
26	C	270	CDL	C18-C19-C20-C21
25	G	1263	PEK	C25-C26-C27-C28
26	G	269	CDL	C82-C83-C84-C85
26	P	1270	CDL	C18-C19-C20-C21
26	T	1269	CDL	C82-C83-C84-C85
25	G	1263	PEK	C26-C27-C28-C29
20	P	1267	PGV	C25-C26-C27-C28
26	P	1270	CDL	C63-C64-C65-C66
26	P	1270	CDL	C71-C72-C73-C74
25	C	265	PEK	C29-C30-C31-C32
20	C	268	PGV	C25-C26-C27-C28
20	P	1268	PGV	C25-C26-C27-C28
20	P	1268	PGV	C30-C31-C32-C33
20	C	268	PGV	C30-C31-C32-C33
25	C	264	PEK	O04-C21-O03-C01
25	C	264	PEK	C22-C23-C24-C25
23	P	1271	CHD	C13-C17-C20-C22
20	C	268	PGV	C11-C10-C9-C8
20	P	1268	PGV	C11-C10-C9-C8
26	C	270	CDL	OB7-CB5-OB6-CB4
26	T	1269	CDL	CB5-C51-C52-C53
26	T	1269	CDL	C43-C44-C45-C46
20	Z	1524	PGV	C24-C25-C26-C27
26	C	270	CDL	C63-C64-C65-C66
26	G	269	CDL	C21-C22-C23-C24
26	G	269	CDL	CB5-C51-C52-C53
25	P	1264	PEK	C1-C2-C3-C4
20	A	524	PGV	C24-C25-C26-C27
26	T	1269	CDL	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
20	C	268	PGV	C28-C29-C30-C31
24	P	1272	DMU	O5-C6-O16-C18
22	O	1230	PSC	C27-C28-C29-C30
26	P	1270	CDL	C51-CB5-OB6-CB4
26	C	270	CDL	C51-CB5-OB6-CB4
26	G	269	CDL	C43-C44-C45-C46
25	T	263	PEK	C34-C35-C36-C37
20	P	1268	PGV	C28-C29-C30-C31
26	P	1270	CDL	OB7-CB5-OB6-CB4
26	G	269	CDL	C41-C42-C43-C44
26	P	1270	CDL	C61-C62-C63-C64
25	P	1265	PEK	C29-C30-C31-C32
20	C	267	PGV	C23-C24-C25-C26
22	B	230	PSC	C04-C05-N-C08
22	O	1230	PSC	C04-C05-N-C08
22	B	230	PSC	C27-C28-C29-C30
26	C	270	CDL	C61-C62-C63-C64
23	C	271	CHD	C13-C17-C20-C22
22	O	1230	PSC	C13-C14-C15-C16
25	G	1263	PEK	C2-C3-C4-C5
26	P	1270	CDL	C36-C37-C38-C39
18	A	515	HEA	C21-C22-C23-C24
26	C	270	CDL	C36-C37-C38-C39
20	P	1267	PGV	C23-C24-C25-C26
26	C	270	CDL	C32-C33-C34-C35
26	T	1269	CDL	C41-C42-C43-C44
19	N	1522	TGL	OB1-CB1-OG2-CG2
26	G	269	CDL	C53-C54-C55-C56
25	C	264	PEK	C25-C26-C27-C28
25	G	1263	PEK	C34-C35-C36-C37
22	B	230	PSC	C04-O12-P-O11
26	G	269	CDL	C33-C34-C35-C36
26	T	1269	CDL	C33-C34-C35-C36
25	C	264	PEK	C1-C2-C3-C4
24	M	526	DMU	C3-C4-C57-O61
25	P	1264	PEK	C25-C26-C27-C28
26	P	1270	CDL	C32-C33-C34-C35
26	C	270	CDL	OB5-CB3-CB4-CB6
26	T	1269	CDL	C53-C54-C55-C56
20	A	524	PGV	C12-C13-C14-C15
20	Z	1524	PGV	C12-C13-C14-C15
19	L	522	TGL	OB1-CB1-OG2-CG2

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Mol	Chain	Res	Type	Atoms
20	P	1268	PGV	C4-C5-C6-C7
26	P	1270	CDL	C11-C12-C13-C14
22	B	230	PSC	C23-C24-C25-C26
26	P	1270	CDL	C64-C65-C66-C67
26	C	270	CDL	C64-C65-C66-C67
26	G	269	CDL	CB3-CB4-CB6-OB8
22	B	230	PSC	O03-C01-C02-C03
26	P	1270	CDL	CB3-CB4-CB6-OB8
26	T	1269	CDL	CB3-CB4-CB6-OB8
25	T	263	PEK	O03-C01-C02-C03
22	O	1230	PSC	O03-C01-C02-C03
26	C	270	CDL	C11-C12-C13-C14
26	C	270	CDL	CB3-CB4-CB6-OB8
25	G	1263	PEK	O03-C01-C02-C03
26	G	269	CDL	C31-C32-C33-C34
26	C	270	CDL	C84-C85-C86-C87
26	P	1270	CDL	C78-C79-C80-C81
20	C	268	PGV	C4-C5-C6-C7
20	A	524	PGV	C5-C6-C7-C8
26	P	1270	CDL	C44-C45-C46-C47
26	T	1269	CDL	C71-C72-C73-C74
20	C	268	PGV	C5-C6-C7-C8
20	P	1268	PGV	C5-C6-C7-C8
26	T	1269	CDL	C31-C32-C33-C34
26	C	270	CDL	C44-C45-C46-C47
26	P	1270	CDL	C42-C43-C44-C45
19	A	521	TGL	CG2-CG3-OG3-CC1
26	P	1270	CDL	C84-C85-C86-C87
22	O	1230	PSC	C14-C15-C16-C17
24	Z	1526	DMU	C22-C25-C28-C31
20	P	1267	PGV	C11-C10-C9-C8
22	B	230	PSC	C13-C14-C15-C16
20	C	268	PGV	C12-C13-C14-C15
25	T	263	PEK	C2-C3-C4-C5
20	C	267	PGV	C11-C10-C9-C8
20	P	1268	PGV	C12-C13-C14-C15
25	C	264	PEK	C24-C25-C26-C27
20	P	1267	PGV	C13-C14-C15-C16
20	C	267	PGV	C15-C16-C17-C18
20	P	1267	PGV	C15-C16-C17-C18
25	P	1264	PEK	C24-C25-C26-C27
19	A	521	TGL	CC2-CC1-OG3-CG3

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Mol	Chain	Res	Type	Atoms
22	O	1230	PSC	C23-C24-C25-C26
22	B	230	PSC	C14-C15-C16-C17
26	T	1269	CDL	C14-C15-C16-C17
20	A	524	PGV	C03-C02-O01-C1
20	Z	1524	PGV	C03-C02-O01-C1
24	M	526	DMU	C22-C25-C28-C31
26	G	269	CDL	C14-C15-C16-C17
22	B	230	PSC	C24-C25-C26-C27
20	C	268	PGV	C23-C24-C25-C26
20	C	268	PGV	C31-C32-C33-C34
26	C	270	CDL	C42-C43-C44-C45
19	N	1522	TGL	CC2-CC1-OG3-CG3
23	P	1271	CHD	C16-C17-C20-C21
23	P	1271	CHD	C13-C17-C20-C21
23	C	271	CHD	C13-C17-C20-C21
24	Z	1526	DMU	O6-C11-C9-O1
25	P	1264	PEK	C35-C36-C37-C38
20	P	1268	PGV	C31-C32-C33-C34
26	P	1270	CDL	C38-C39-C40-C41
20	C	268	PGV	C14-C15-C16-C17
20	C	267	PGV	C13-C14-C15-C16
26	G	269	CDL	C71-C72-C73-C74
20	N	1266	PGV	C30-C31-C32-C33
26	C	270	CDL	C78-C79-C80-C81
25	G	1263	PEK	C30-C31-C32-C33
23	C	271	CHD	C16-C17-C20-C21
20	Z	1524	PGV	C5-C6-C7-C8
26	C	270	CDL	C38-C39-C40-C41
20	P	1268	PGV	C14-C15-C16-C17
26	G	269	CDL	C35-C36-C37-C38
20	P	1268	PGV	C23-C24-C25-C26
24	Z	1526	DMU	C34-C37-C40-C43
19	N	1521	TGL	CC2-CC1-OG3-CG3
23	P	1271	CHD	C16-C17-C20-C22
26	T	1269	CDL	C35-C36-C37-C38
26	T	1269	CDL	C44-C45-C46-C47
26	G	269	CDL	C44-C45-C46-C47
26	G	269	CDL	OA5-CA3-CA4-CA6
26	P	1270	CDL	OB5-CB3-CB4-CB6
26	T	1269	CDL	OA5-CA3-CA4-CA6
20	A	524	PGV	C01-C02-C03-O11
25	G	1263	PEK	C01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
22	B	230	PSC	C3-C4-C5-C6
20	A	604	PGV	C30-C31-C32-C33
25	T	263	PEK	C30-C31-C32-C33
22	O	1230	PSC	C3-C4-C5-C6
19	L	522	TGL	CC2-CC1-OG3-CG3
26	T	1269	CDL	C19-C20-C21-C22
25	C	264	PEK	C35-C36-C37-C38
25	P	1265	PEK	C32-C33-C34-C35
26	P	1270	CDL	C39-C40-C41-C42
25	C	265	PEK	C32-C33-C34-C35
25	T	263	PEK	C22-C21-O03-C01
26	C	270	CDL	C39-C40-C41-C42
26	G	269	CDL	C19-C20-C21-C22
18	N	515	HEA	C21-C22-C23-C24
23	C	271	CHD	C16-C17-C20-C22
24	M	526	DMU	C34-C37-C40-C43
25	G	1263	PEK	C16-C17-C18-C19
25	P	1264	PEK	C26-C27-C28-C29
25	C	264	PEK	C17-C18-C19-C20
26	G	269	CDL	CA3-CA4-CA6-OA8
25	P	1264	PEK	O03-C01-C02-C03
26	T	1269	CDL	CA3-CA4-CA6-OA8
25	C	264	PEK	O03-C01-C02-C03
20	C	268	PGV	C15-C16-C17-C18
22	O	1230	PSC	C24-C25-C26-C27
19	N	1521	TGL	CG2-CG3-OG3-CC1
25	P	1264	PEK	C27-C28-C29-C30
25	P	1264	PEK	C17-C18-C19-C20
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	C	265	PEK	C11-C12-C13-C14
25	T	263	PEK	C6-C7-C8-C9
22	O	1230	PSC	C04-O12-P-O11
25	C	264	PEK	C5-C6-C7-C8
25	C	264	PEK	C9-C10-C11-C12
25	G	1263	PEK	C6-C7-C8-C9
19	N	1522	TGL	CC7-CC8-CC9-C15
26	P	1270	CDL	OA5-CA3-CA4-OA6
26	P	1270	CDL	OB5-CB3-CB4-OB6
26	C	270	CDL	OA5-CA3-CA4-OA6
26	C	270	CDL	OB5-CB3-CB4-OB6

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Mol	Chain	Res	Type	Atoms
25	G	1263	PEK	C22-C21-O03-C01
24	P	1272	DMU	C22-C25-C28-C31
20	P	1268	PGV	C15-C16-C17-C18
20	P	1267	PGV	C31-C32-C33-C34
22	B	230	PSC	O03-C01-C02-O01
26	P	1270	CDL	OB6-CB4-CB6-OB8
22	O	1230	PSC	O03-C01-C02-O01
26	C	270	CDL	OB6-CB4-CB6-OB8
25	C	264	PEK	C27-C28-C29-C30
22	O	1230	PSC	C11-C12-C13-C14
20	C	267	PGV	C31-C32-C33-C34
26	C	270	CDL	C34-C35-C36-C37
25	G	1263	PEK	C02-C03-O11-P
26	P	1270	CDL	C34-C35-C36-C37
20	Z	1524	PGV	C26-C27-C28-C29
19	L	522	TGL	CC7-CC8-CC9-C15
20	A	604	PGV	C25-C26-C27-C28
20	A	524	PGV	C26-C27-C28-C29
24	P	1272	DMU	C34-C37-C40-C43
25	C	264	PEK	C26-C27-C28-C29
25	T	263	PEK	O04-C21-O03-C01
26	C	270	CDL	C43-C44-C45-C46
25	G	1263	PEK	O04-C21-O03-C01
25	T	263	PEK	C01-C02-C03-O11
20	Z	1524	PGV	C01-C02-C03-O11
20	N	1266	PGV	C25-C26-C27-C28
25	C	264	PEK	C32-C33-C34-C35
22	B	230	PSC	C11-C12-C13-C14
26	T	1269	CDL	C24-C25-C26-C27
19	Q	1523	TGL	CA9-C20-C21-C22
20	C	268	PGV	C20-C19-O03-C01
26	G	269	CDL	CB7-C71-C72-C73
20	P	1267	PGV	C20-C21-C22-C23
26	P	1270	CDL	C43-C44-C45-C46
19	D	523	TGL	OB1-CB1-OG2-CG2
20	C	267	PGV	C20-C21-C22-C23
18	N	515	HEA	C15-C16-C17-C18
26	T	1269	CDL	CB7-C71-C72-C73
20	A	524	PGV	O03-C01-C02-C03
25	T	263	PEK	C02-C03-O11-P
20	Z	1524	PGV	O03-C01-C02-C03
20	P	1268	PGV	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
26	G	269	CDL	C24-C25-C26-C27
26	T	1269	CDL	C54-C55-C56-C57
20	C	268	PGV	O04-C19-O03-C01
19	D	523	TGL	OG2-CG2-CG3-OG3
20	A	524	PGV	O03-C01-C02-O01
19	A	521	TGL	C12-C13-C14-C29
19	D	523	TGL	CA9-C20-C21-C22
22	O	1230	PSC	C04-C05-N-C07
24	C	272	DMU	C34-C37-C40-C43
25	G	1263	PEK	C15-C16-C17-C18
22	B	230	PSC	C31-C32-C33-C34
26	P	1270	CDL	C24-C25-C26-C27
20	C	268	PGV	C26-C27-C28-C29
26	C	270	CDL	C24-C25-C26-C27
20	P	1267	PGV	C1-C2-C3-C4
20	Z	1524	PGV	C20-C21-C22-C23
22	O	1230	PSC	C31-C32-C33-C34
25	G	1263	PEK	C21-C22-C23-C24
26	T	1269	CDL	C12-C13-C14-C15
20	P	1268	PGV	C26-C27-C28-C29
20	P	1268	PGV	C20-C19-O03-C01
26	G	269	CDL	CB2-OB2-PB2-OB5
25	P	1265	PEK	C03-O11-P-O12
26	T	1269	CDL	CB2-OB2-PB2-OB5
22	O	1230	PSC	C03-O11-P-O12
26	G	269	CDL	C36-C37-C38-C39
25	P	1264	PEK	C32-C33-C34-C35
25	T	263	PEK	C21-C22-C23-C24
20	N	1266	PGV	C26-C27-C28-C29
26	G	269	CDL	CB4-CB3-OB5-PB2
20	P	1267	PGV	C02-C03-O11-P
26	T	1269	CDL	CB4-CB3-OB5-PB2
20	C	267	PGV	C02-C03-O11-P
22	B	230	PSC	C04-O12-P-O13
22	B	230	PSC	C04-C05-N-C07
25	P	1265	PEK	C03-O11-P-O14
25	C	265	PEK	C03-O11-P-O13
25	T	263	PEK	C03-O11-P-O13
22	O	1230	PSC	C03-O11-P-O13
22	O	1230	PSC	C04-O12-P-O13
22	O	1230	PSC	C04-C05-N-C06
25	G	1263	PEK	C03-O11-P-O13

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Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	C36-C37-C38-C39
20	P	1267	PGV	C24-C25-C26-C27
22	O	1230	PSC	C4-C5-C6-C7
19	N	1522	TGL	CC5-CC6-CC7-CC8
20	C	267	PGV	C24-C25-C26-C27
26	G	269	CDL	C54-C55-C56-C57
22	B	230	PSC	C4-C5-C6-C7
19	N	1521	TGL	C12-C13-C14-C29
26	G	269	CDL	C12-C13-C14-C15
26	G	269	CDL	CA7-C31-C32-C33
25	G	1263	PEK	O01-C02-C03-O11
26	G	269	CDL	C64-C65-C66-C67
25	T	263	PEK	C16-C17-C18-C19
22	B	230	PSC	C04-C05-N-C06
24	P	1272	DMU	O6-C11-C9-C8
25	C	265	PEK	C30-C31-C32-C33
26	G	269	CDL	OA6-CA4-CA6-OA8
25	P	1264	PEK	O03-C01-C02-O01
26	T	1269	CDL	OA6-CA4-CA6-OA8
20	Z	1524	PGV	O03-C01-C02-O01
25	C	264	PEK	O03-C01-C02-O01
19	Q	1523	TGL	OG2-CG2-CG3-OG3
25	P	1265	PEK	C30-C31-C32-C33
20	A	524	PGV	C20-C21-C22-C23
24	C	272	DMU	C22-C25-C28-C31
26	C	270	CDL	C23-C24-C25-C26
24	M	526	DMU	O6-C11-C9-O1
26	T	1269	CDL	C64-C65-C66-C67
25	G	1263	PEK	C31-C32-C33-C34
20	C	267	PGV	C1-C2-C3-C4
22	B	230	PSC	C01-C02-C03-O11
26	P	1270	CDL	OA5-CA3-CA4-CA6
26	C	270	CDL	OA5-CA3-CA4-CA6
26	C	270	CDL	C82-C83-C84-C85
26	T	1269	CDL	CA7-C31-C32-C33
26	C	270	CDL	C52-C53-C54-C55
20	C	267	PGV	C05-C04-O12-P
26	G	269	CDL	OA5-CA3-CA4-OA6
26	T	1269	CDL	OA5-CA3-CA4-OA6
25	T	263	PEK	O01-C02-C03-O11
20	A	604	PGV	C26-C27-C28-C29
26	P	1270	CDL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
22	B	230	PSC	C03-O11-P-O12
26	P	1270	CDL	CA3-OA5-PA1-OA2
20	A	524	PGV	C03-O11-P-O12
20	Z	1524	PGV	C03-O11-P-O12
26	C	270	CDL	CA3-OA5-PA1-OA2
19	L	522	TGL	CC5-CC6-CC7-CC8
26	P	1270	CDL	C56-C57-C58-C59
20	A	524	PGV	C25-C26-C27-C28
25	G	1263	PEK	C32-C33-C34-C35
26	P	1270	CDL	C1-CA2-OA2-PA1
26	C	270	CDL	C1-CA2-OA2-PA1
20	P	1268	PGV	C02-C03-O11-P
25	T	263	PEK	C32-C33-C34-C35
25	T	263	PEK	C31-C32-C33-C34
25	T	263	PEK	C15-C16-C17-C18
18	A	515	HEA	C15-C16-C17-C18
25	P	1264	PEK	O12-C04-C05-N
26	C	270	CDL	C76-C77-C78-C79
26	P	1270	CDL	C76-C77-C78-C79
26	P	1270	CDL	C22-C23-C24-C25
20	C	267	PGV	C29-C30-C31-C32
20	A	604	PGV	C9-C10-C11-C12
26	C	270	CDL	C56-C57-C58-C59
20	N	1266	PGV	C31-C32-C33-C34
20	Z	1524	PGV	C25-C26-C27-C28
26	C	270	CDL	C22-C23-C24-C25
20	C	267	PGV	C14-C15-C16-C17
20	P	1267	PGV	C29-C30-C31-C32
22	B	230	PSC	C03-C02-O01-C1
22	O	1230	PSC	C03-C02-O01-C1
24	C	272	DMU	O6-C11-C9-C8
20	N	1266	PGV	C9-C10-C11-C12
25	P	1265	PEK	C3-C4-C5-C6
25	C	265	PEK	C3-C4-C5-C6
22	B	230	PSC	C9-C10-C11-C12
25	P	1265	PEK	C12-C13-C14-C15
25	C	265	PEK	C12-C13-C14-C15
22	O	1230	PSC	C9-C10-C11-C12
26	P	1270	CDL	C52-C53-C54-C55
20	P	1267	PGV	C05-C04-O12-P
20	C	268	PGV	C02-C03-O11-P
25	P	1265	PEK	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
20	C	268	PGV	O01-C02-C03-O11
20	P	1268	PGV	O01-C02-C03-O11
26	P	1270	CDL	C82-C83-C84-C85
26	T	1269	CDL	C52-C53-C54-C55
25	T	263	PEK	C33-C34-C35-C36
22	O	1230	PSC	C01-C02-C03-O11
20	P	1267	PGV	C14-C15-C16-C17
25	C	265	PEK	C17-C18-C19-C20
20	A	604	PGV	C31-C32-C33-C34
26	G	269	CDL	C52-C53-C54-C55
19	N	1522	TGL	CB5-CB6-CB7-CB8
19	N	1521	TGL	C13-C14-C29-C30
19	Q	1523	TGL	OB1-CB1-OG2-CG2
25	P	1265	PEK	O03-C01-C02-O01
19	D	523	TGL	OG1-CG1-CG2-OG2
25	C	265	PEK	O03-C01-C02-O01
20	P	1268	PGV	O03-C01-C02-O01
19	Q	1523	TGL	OG1-CG1-CG2-OG2
25	P	1265	PEK	C17-C18-C19-C20
20	Z	1524	PGV	C21-C22-C23-C24
20	A	524	PGV	C11-C10-C9-C8
20	A	524	PGV	C21-C22-C23-C24
18	A	515	HEA	C17-C18-C19-C20
26	G	269	CDL	C11-C12-C13-C14
26	C	270	CDL	C41-C42-C43-C44
20	P	1267	PGV	C11-C12-C13-C14
19	L	522	TGL	OG2-CB1-CB2-CB3
19	L	522	TGL	CB5-CB6-CB7-CB8
19	A	521	TGL	C13-C14-C29-C30
25	C	265	PEK	C35-C36-C37-C38
19	N	1522	TGL	OG2-CB1-CB2-CB3
20	P	1268	PGV	C7-C8-C9-C10
25	T	263	PEK	C3-C4-C5-C6
20	A	604	PGV	O03-C19-C20-C21
24	C	272	DMU	O5-C6-O16-C18
20	C	268	PGV	C01-C02-C03-O11
20	P	1268	PGV	C01-C02-C03-O11
20	N	1266	PGV	O03-C19-C20-C21
26	T	1269	CDL	C11-C12-C13-C14
25	P	1264	PEK	C3-C4-C5-C6
26	T	1269	CDL	C39-C40-C41-C42
22	B	230	PSC	O03-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
19	N	1522	TGL	OG3-CC1-CC2-CC3
22	O	1230	PSC	O03-C19-C20-C21
20	C	268	PGV	O03-C01-C02-O01
25	P	1264	PEK	O01-C1-C2-C3
26	P	1270	CDL	C52-C51-CB5-OB6
25	C	264	PEK	O01-C1-C2-C3
25	T	263	PEK	C14-C15-C16-C17
25	G	1263	PEK	C33-C34-C35-C36
19	L	522	TGL	OG3-CC1-CC2-CC3
26	C	270	CDL	C52-C51-CB5-OB6
20	N	1266	PGV	C11-C12-C13-C14
20	Z	1524	PGV	C9-C10-C11-C12
20	C	267	PGV	C9-C10-C11-C12
20	C	267	PGV	C11-C12-C13-C14
25	G	1263	PEK	C3-C4-C5-C6
19	A	521	TGL	CG1-CG2-OG2-CB1
18	N	515	HEA	C17-C18-C19-C20
26	C	270	CDL	C32-C31-CA7-OA8
20	P	1267	PGV	C9-C10-C11-C12
22	B	230	PSC	C7-C8-C9-C10
20	A	604	PGV	C11-C12-C13-C14
25	C	264	PEK	C3-C4-C5-C6
25	G	1263	PEK	C14-C15-C16-C17
20	Z	1524	PGV	C11-C10-C9-C8
20	C	268	PGV	C7-C8-C9-C10
19	Q	1523	TGL	C21-C22-C23-C24
19	D	523	TGL	OG2-CB1-CB2-CB3
19	Q	1523	TGL	OG2-CB1-CB2-CB3
22	O	1230	PSC	C15-C16-C17-C18
22	B	230	PSC	C15-C16-C17-C18
20	A	524	PGV	C9-C10-C11-C12
26	P	1270	CDL	C32-C31-CA7-OA8
19	D	523	TGL	C21-C22-C23-C24
22	O	1230	PSC	C21-C22-C23-C24
22	B	230	PSC	C12-C13-C14-C15
22	O	1230	PSC	C7-C8-C9-C10
22	O	1230	PSC	C12-C13-C14-C15
26	P	1270	CDL	C12-C11-CA5-OA6
26	T	1269	CDL	C38-C39-C40-C41
22	B	230	PSC	O01-C1-C2-C3
20	A	524	PGV	O01-C1-C2-C3
26	C	270	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
26	C	270	CDL	C32-C31-CA7-OA9
26	G	269	CDL	C22-C23-C24-C25
20	Z	1524	PGV	O01-C1-C2-C3
26	P	1270	CDL	C32-C31-CA7-OA9
26	P	1270	CDL	C41-C42-C43-C44
22	B	230	PSC	O02-C1-C2-C3
19	D	523	TGL	OC1-CC1-CC2-CC3
20	A	524	PGV	O02-C1-C2-C3
22	O	1230	PSC	O02-C1-C2-C3
25	P	1264	PEK	O02-C1-C2-C3
26	G	269	CDL	C39-C40-C41-C42
19	Q	1523	TGL	CB2-CB3-CB4-CB5
20	Z	1524	PGV	O02-C1-C2-C3
22	B	230	PSC	O04-C19-C20-C21
22	O	1230	PSC	O04-C19-C20-C21
19	D	523	TGL	CB2-CB3-CB4-CB5
25	C	265	PEK	C03-O11-P-O12
22	O	1230	PSC	O01-C1-C2-C3
19	Q	1523	TGL	OC1-CC1-CC2-CC3
26	G	269	CDL	CA2-OA2-PA1-OA3
22	B	230	PSC	C03-O11-P-O13
25	C	265	PEK	C03-O11-P-O14
26	T	1269	CDL	CA2-OA2-PA1-OA3
20	A	524	PGV	C03-O11-P-O13
20	Z	1524	PGV	C03-O11-P-O13
25	C	264	PEK	O02-C1-C2-C3
19	A	521	TGL	OG1-CA1-CA2-CA3
26	G	269	CDL	C38-C39-C40-C41
22	B	230	PSC	C05-C04-O12-P
22	O	1230	PSC	C05-C04-O12-P
19	N	1521	TGL	CG1-CG2-OG2-CB1
25	P	1265	PEK	C34-C35-C36-C37
19	L	522	TGL	CA5-CA6-CA7-CA8
26	T	1269	CDL	C59-C60-C61-C62
19	N	1522	TGL	OC1-CC1-OG3-CG3
25	C	265	PEK	O03-C21-C22-C23
22	B	230	PSC	C21-C22-C23-C24
26	T	1269	CDL	C22-C23-C24-C25
19	D	523	TGL	OG3-CC1-CC2-CC3
26	P	1270	CDL	C15-C16-C17-C18
25	G	1263	PEK	C24-C25-C26-C27
26	P	1270	CDL	C52-C51-CB5-OB7

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Mol	Chain	Res	Type	Atoms
24	Z	1526	DMU	C28-C31-C34-C37
24	C	272	DMU	C5-C10-O7-C3
19	N	1521	TGL	OG1-CA1-CA2-CA3
25	P	1265	PEK	O03-C21-C22-C23

There are no ring outliers.

36 monomers are involved in 257 short contacts:

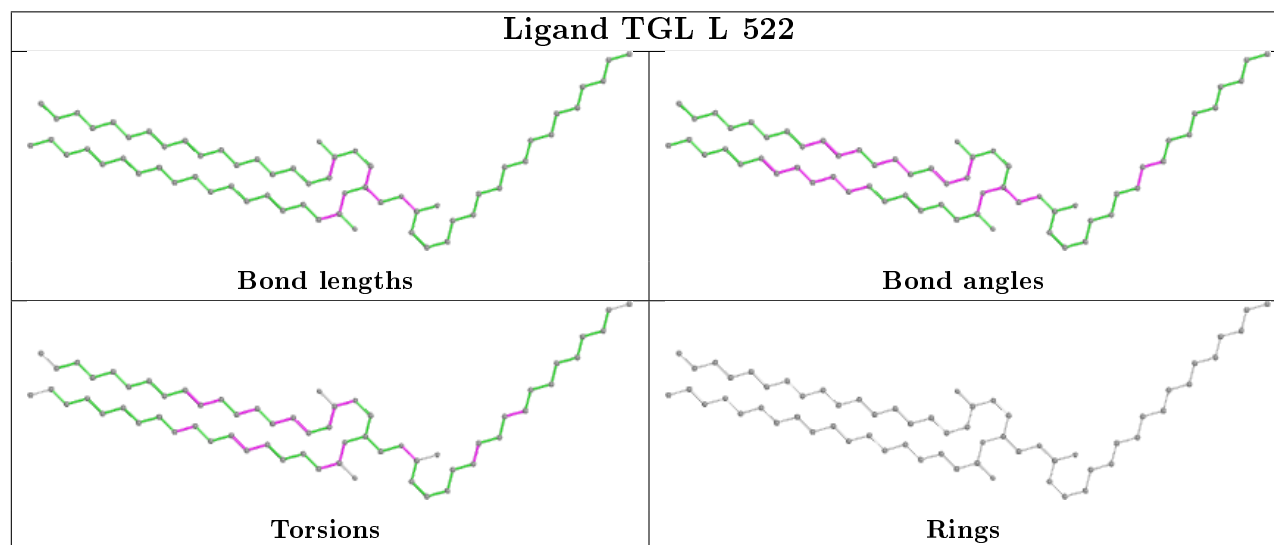
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	L	522	TGL	24	0
26	G	269	CDL	18	0
20	N	1266	PGV	1	0
20	P	1267	PGV	5	0
23	J	60	CHD	2	0
18	A	515	HEA	2	0
25	P	1264	PEK	7	0
22	B	230	PSC	15	0
25	P	1265	PEK	9	0
26	P	1270	CDL	16	0
19	D	523	TGL	4	0
19	A	521	TGL	9	0
26	T	1269	CDL	22	0
24	C	272	DMU	3	0
23	P	1271	CHD	2	0
20	A	604	PGV	1	0
24	P	1272	DMU	5	0
18	N	515	HEA	3	0
23	C	271	CHD	4	0
20	C	268	PGV	1	0
20	A	524	PGV	9	0
24	M	526	DMU	1	0
19	N	1522	TGL	16	0
25	C	265	PEK	8	0
25	T	263	PEK	9	0
20	Z	1524	PGV	6	0
22	O	1230	PSC	15	0
25	C	264	PEK	4	0
23	W	1060	CHD	3	0
20	C	267	PGV	6	0
19	N	1521	TGL	8	0
26	C	270	CDL	18	0
25	G	1263	PEK	7	0

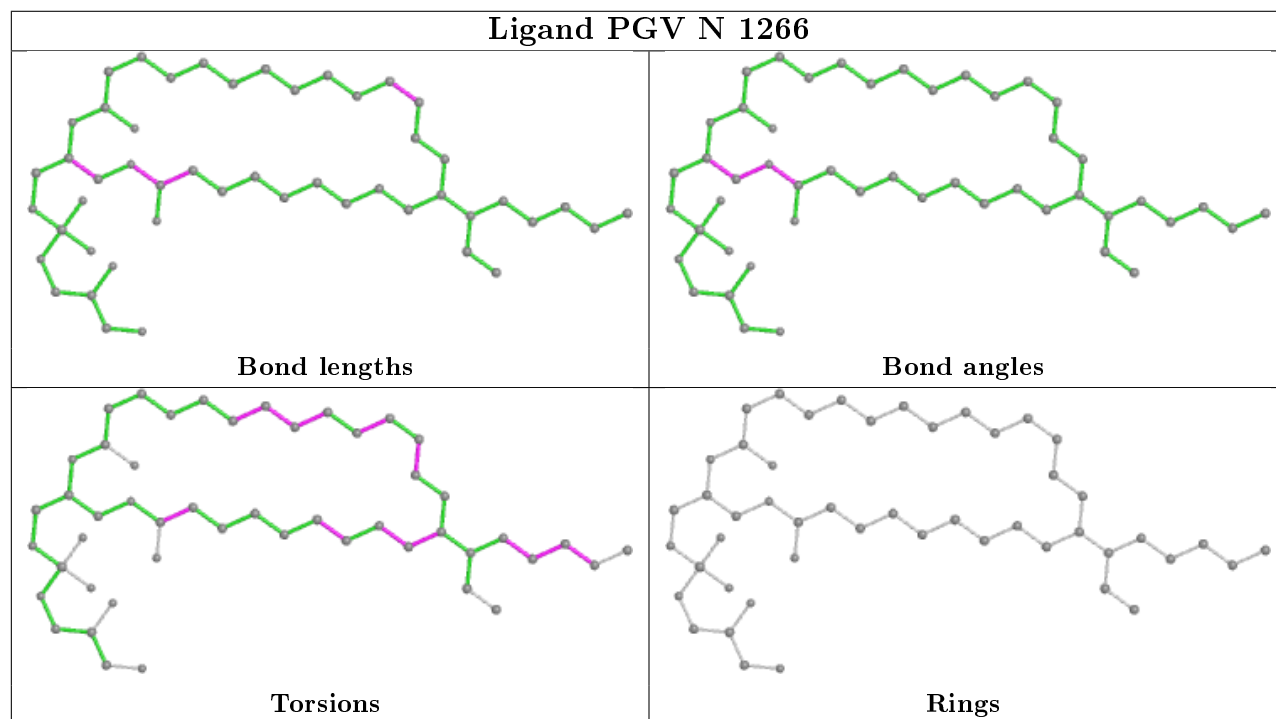
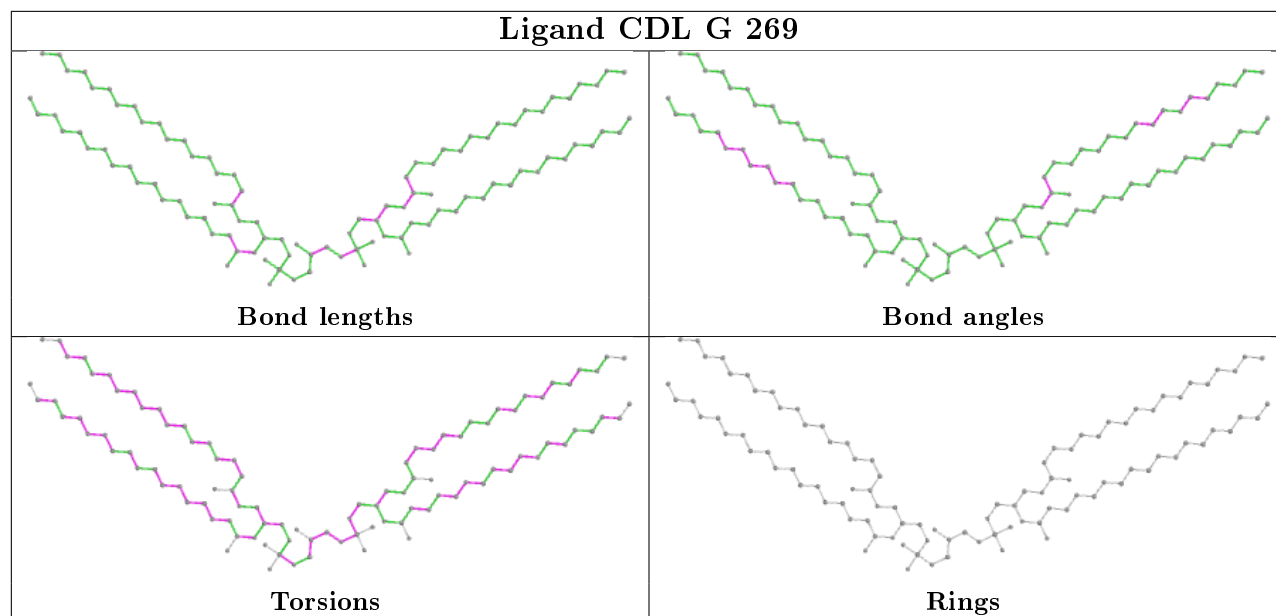
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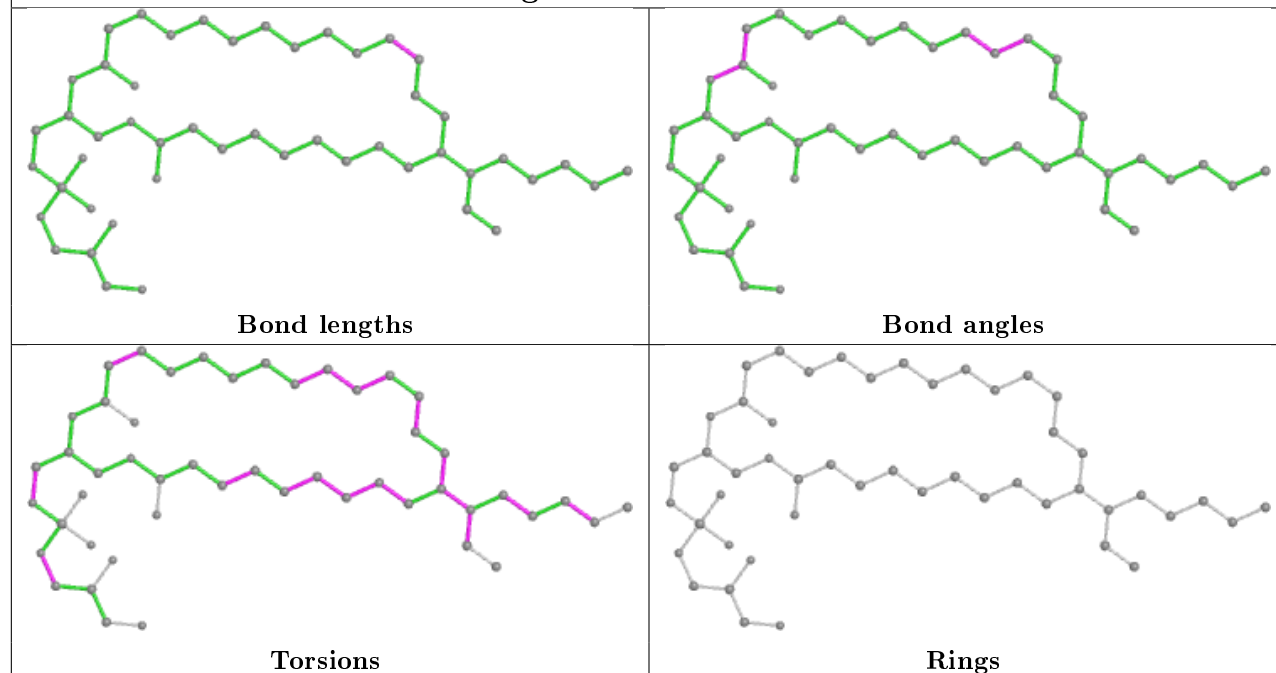
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	516	HEA	2	0
20	P	1268	PGV	1	0
19	Q	1523	TGL	5	0

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.

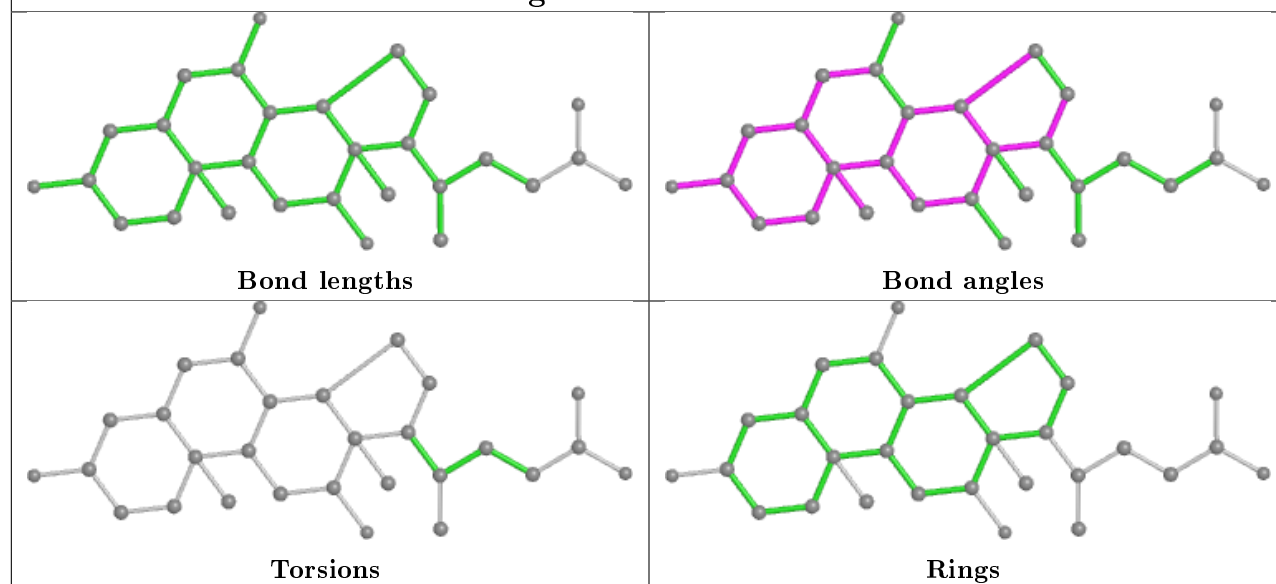




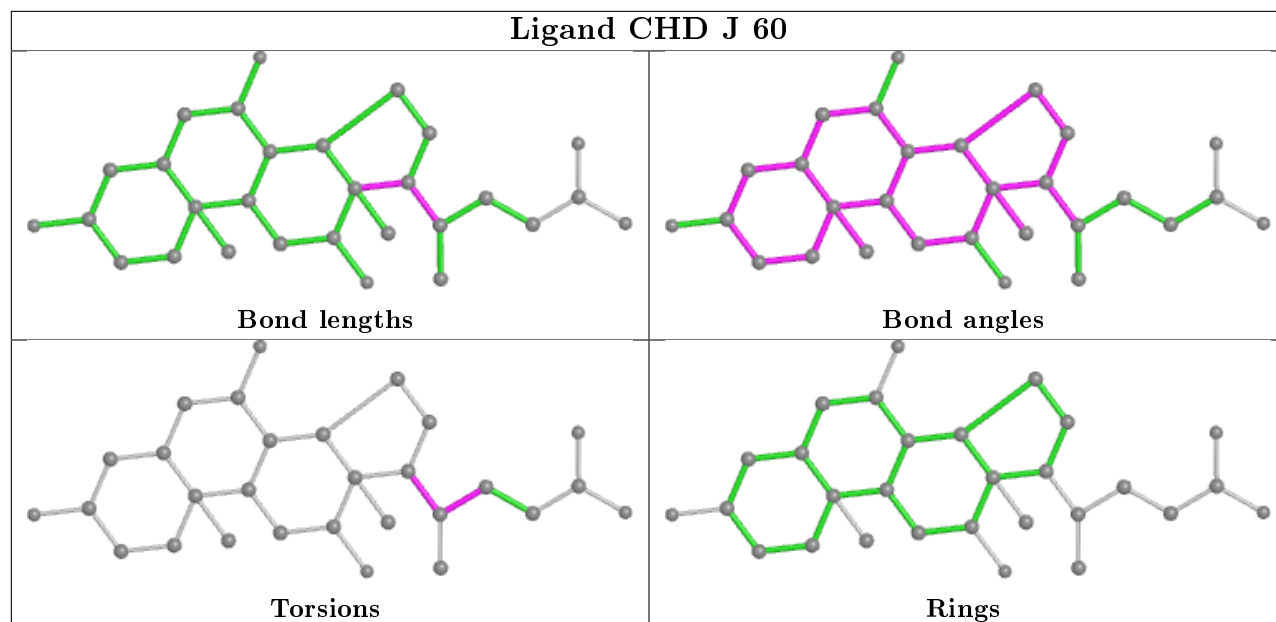
Ligand PGV P 1267



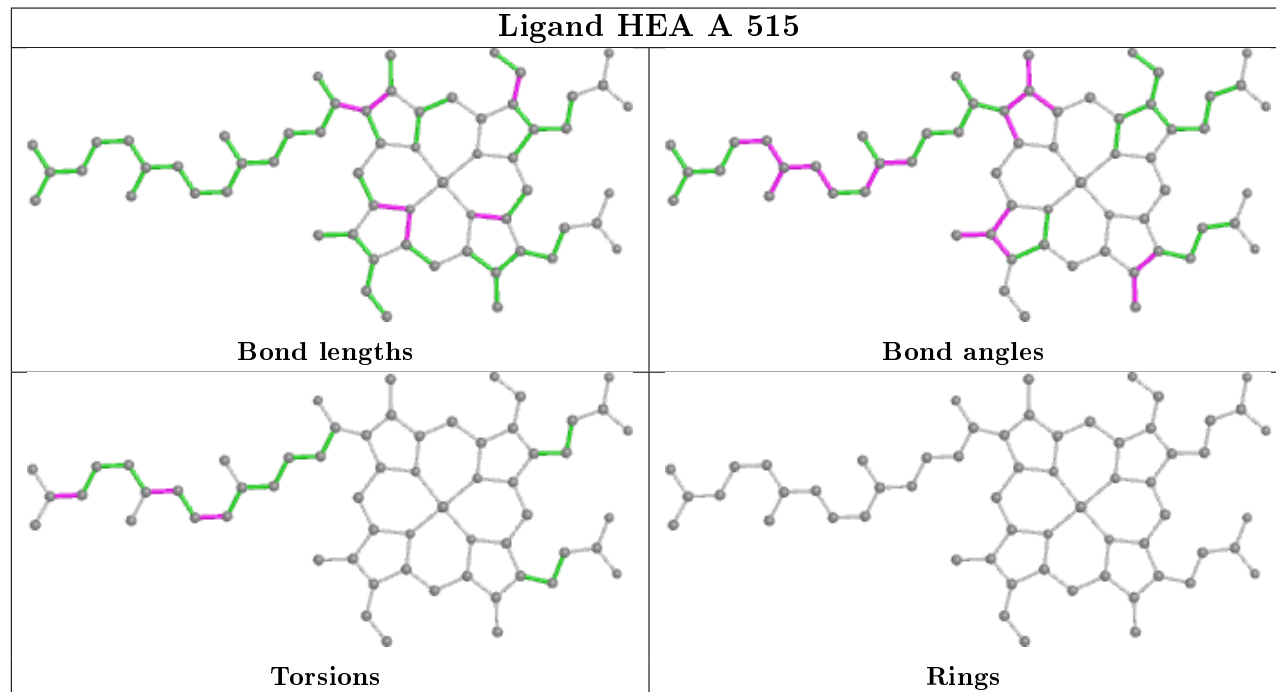
Ligand CHD O 229

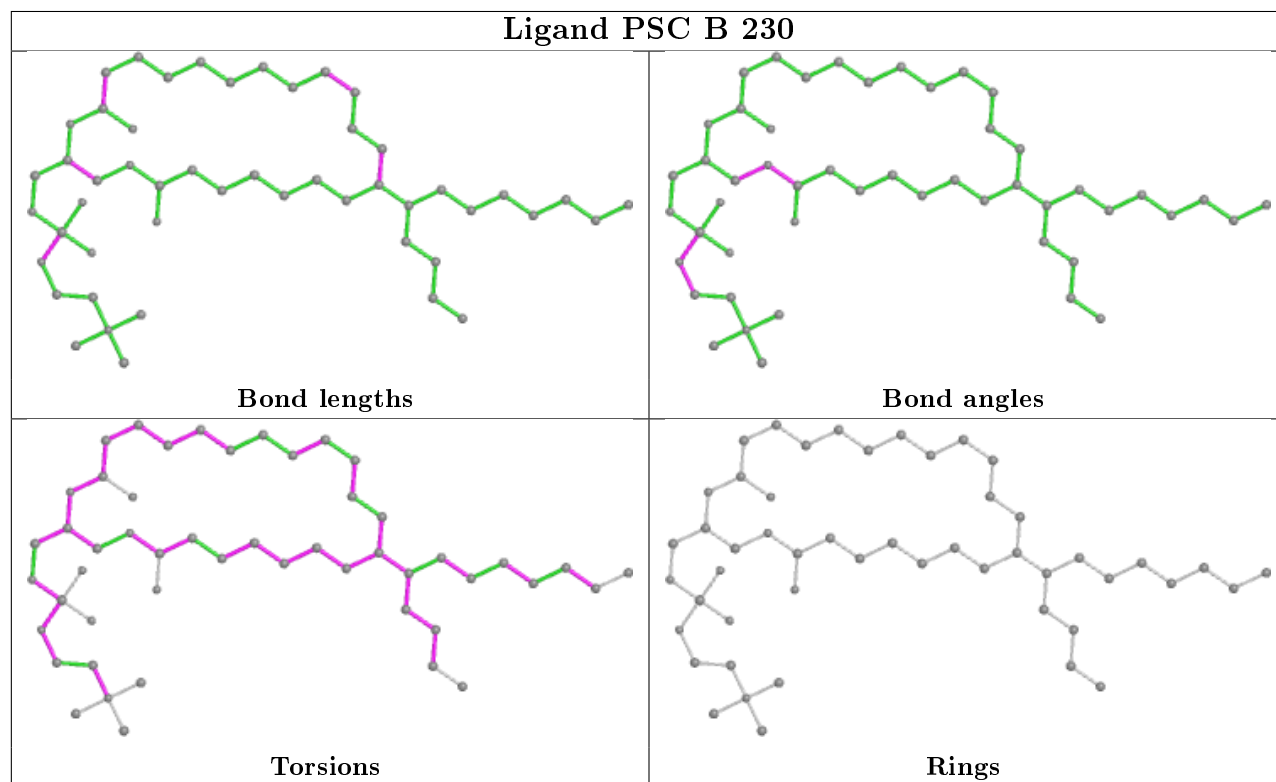
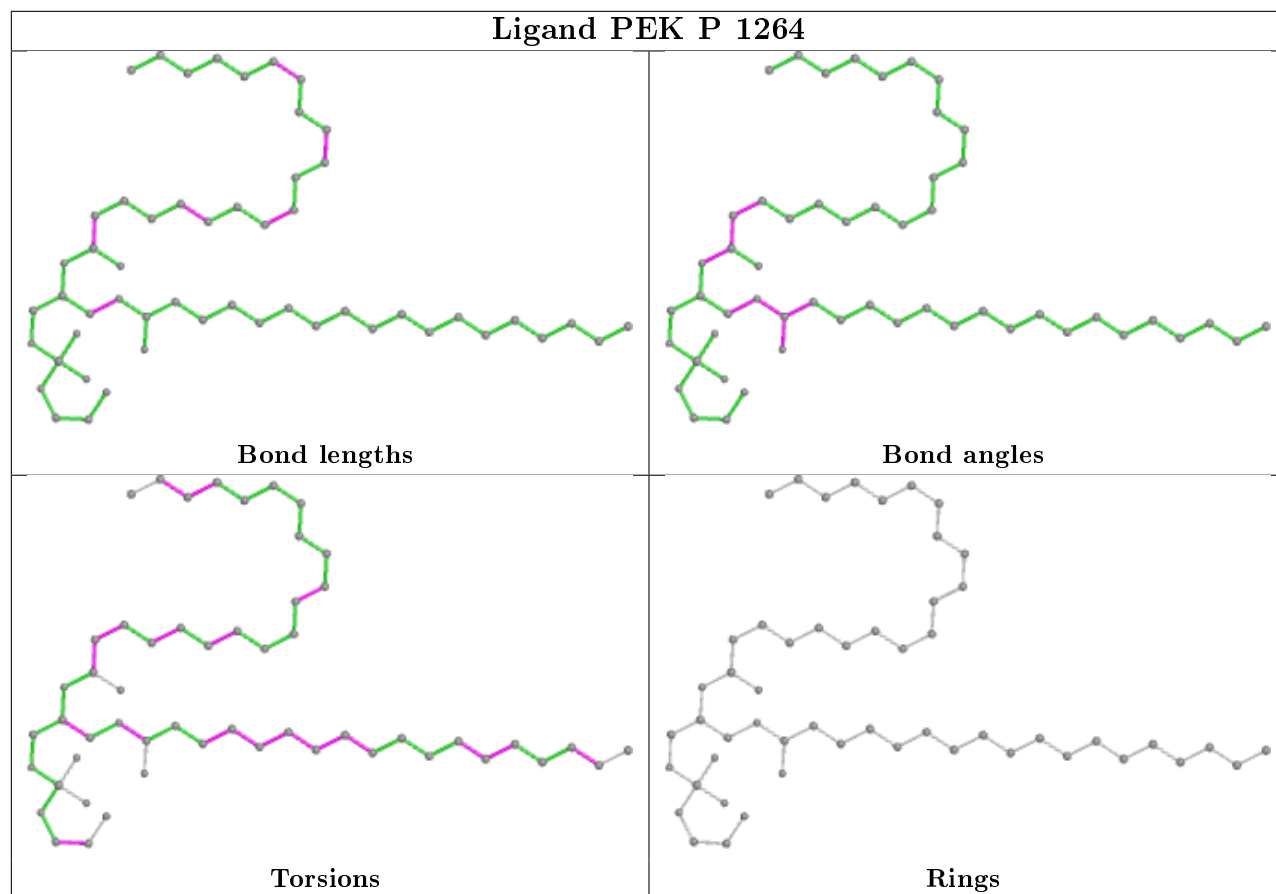


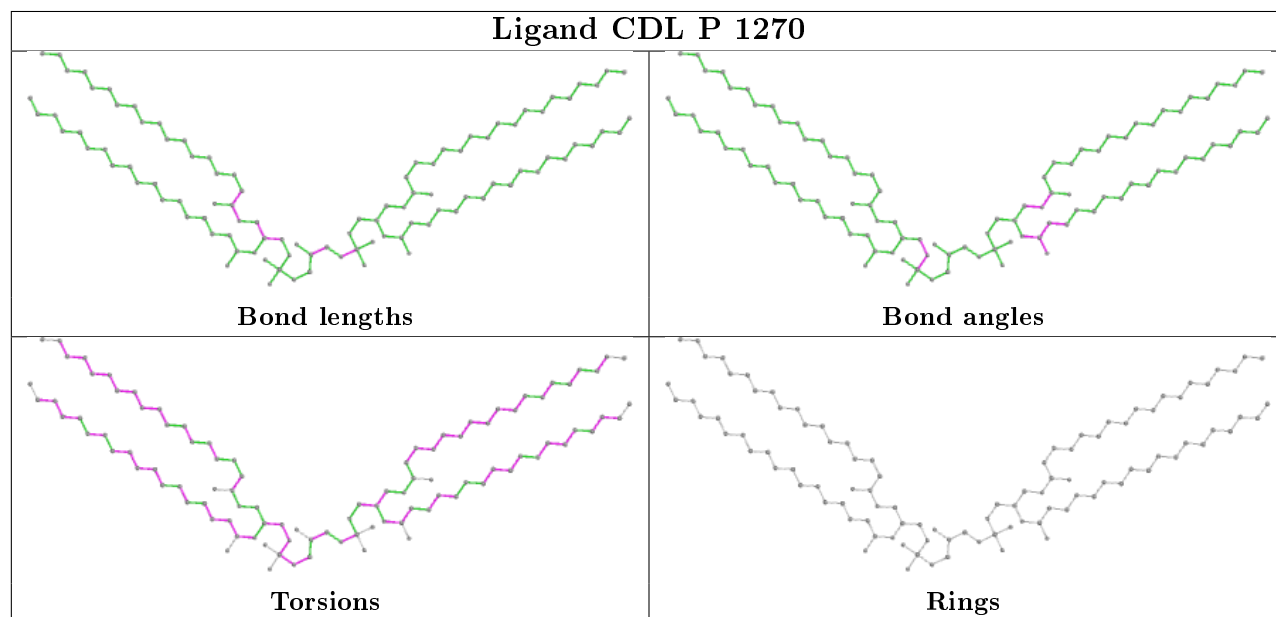
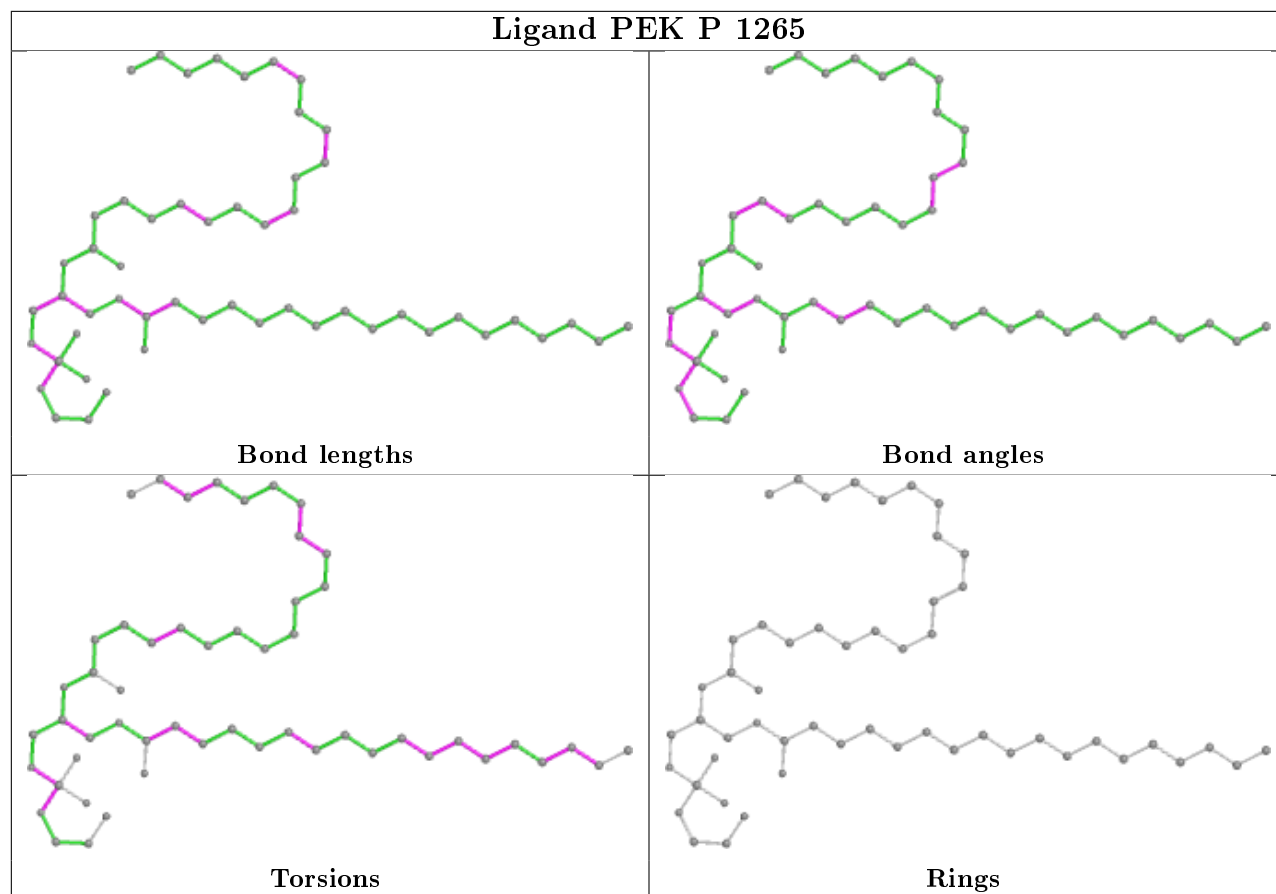
Ligand CHD J 60

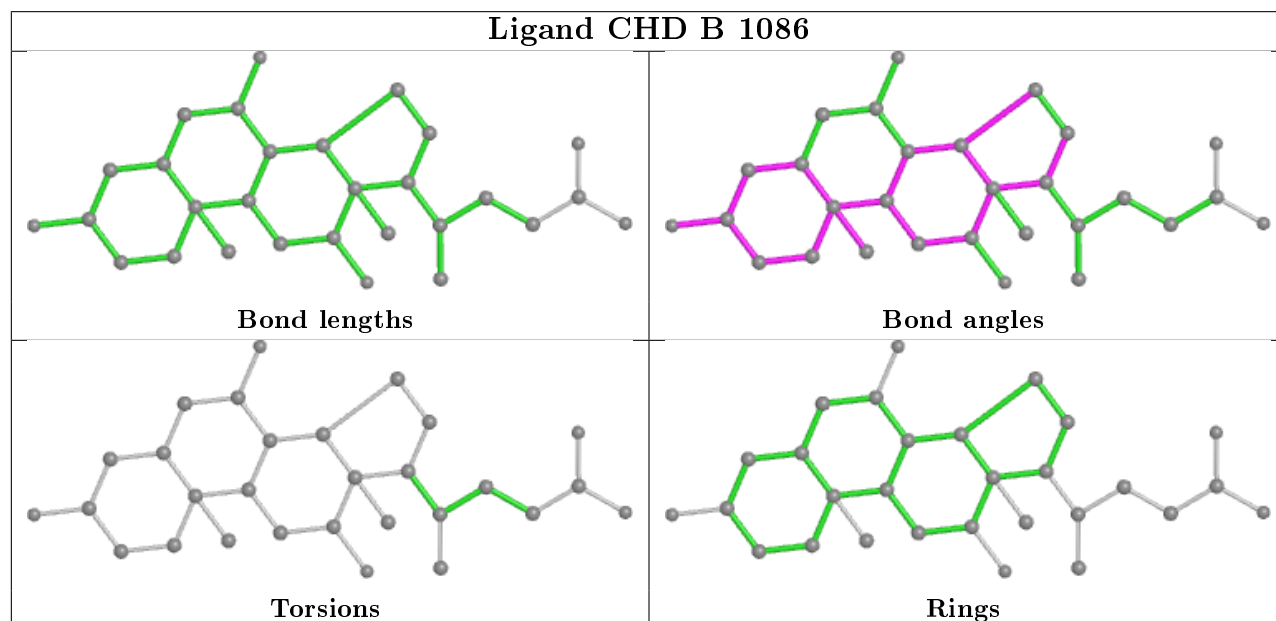
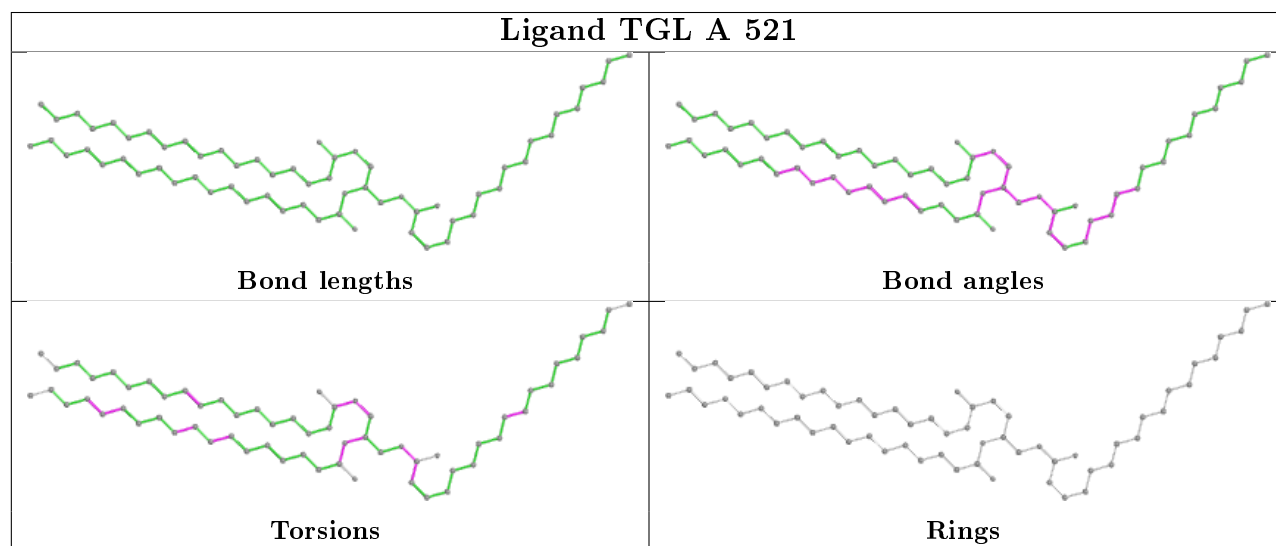
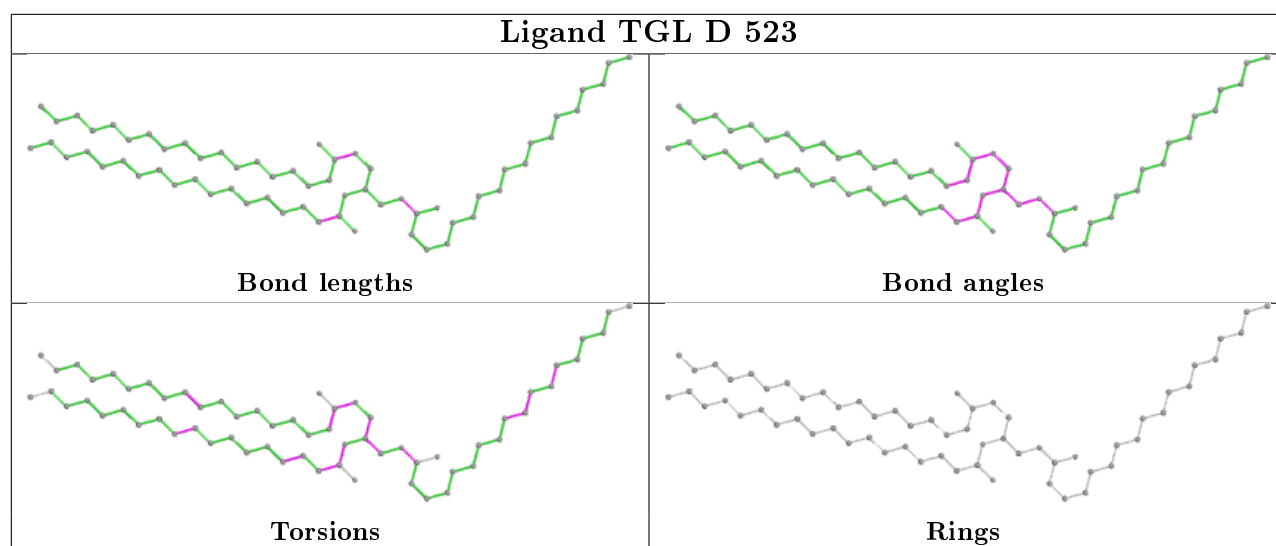


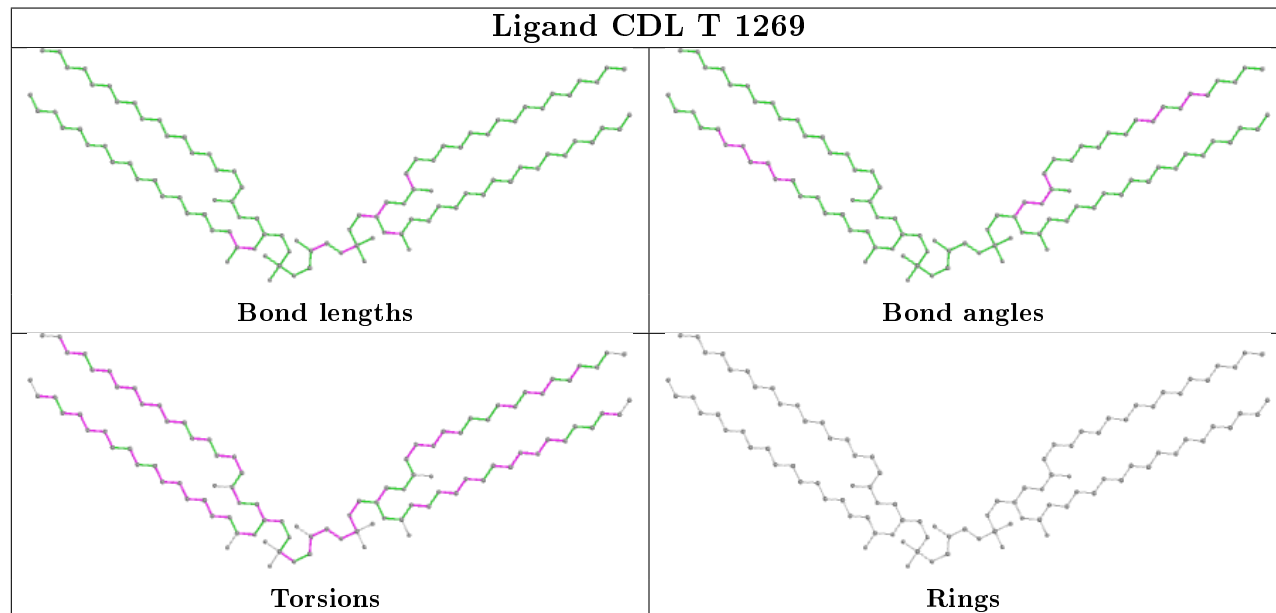
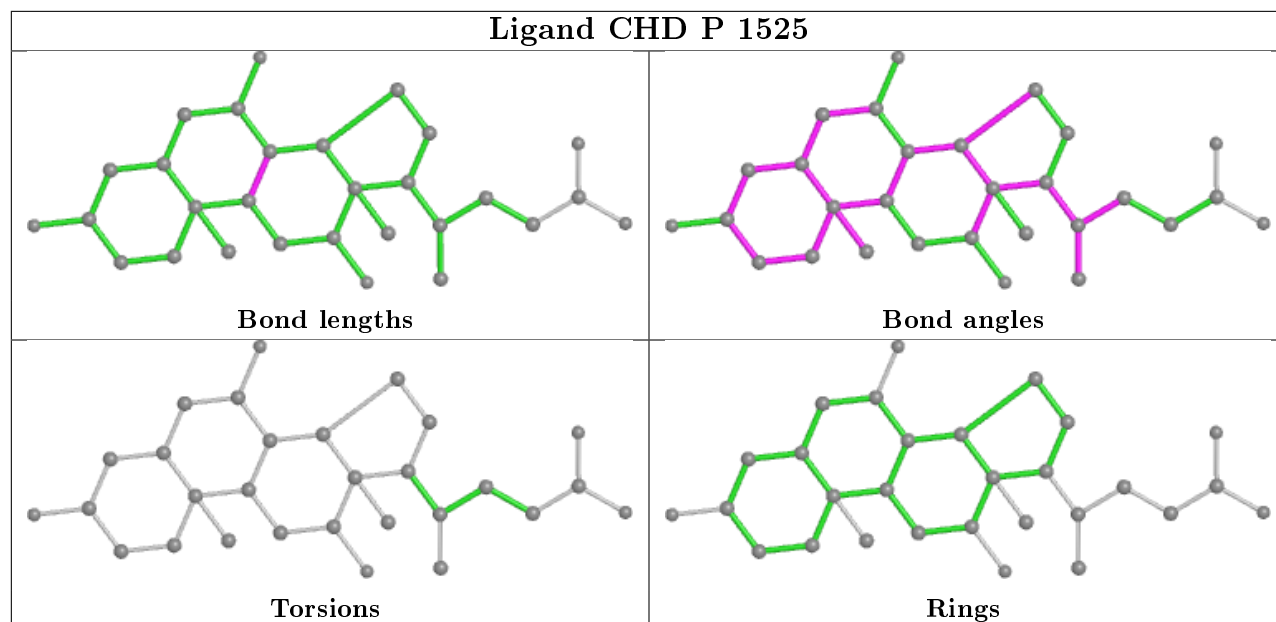
Ligand HEA A 515



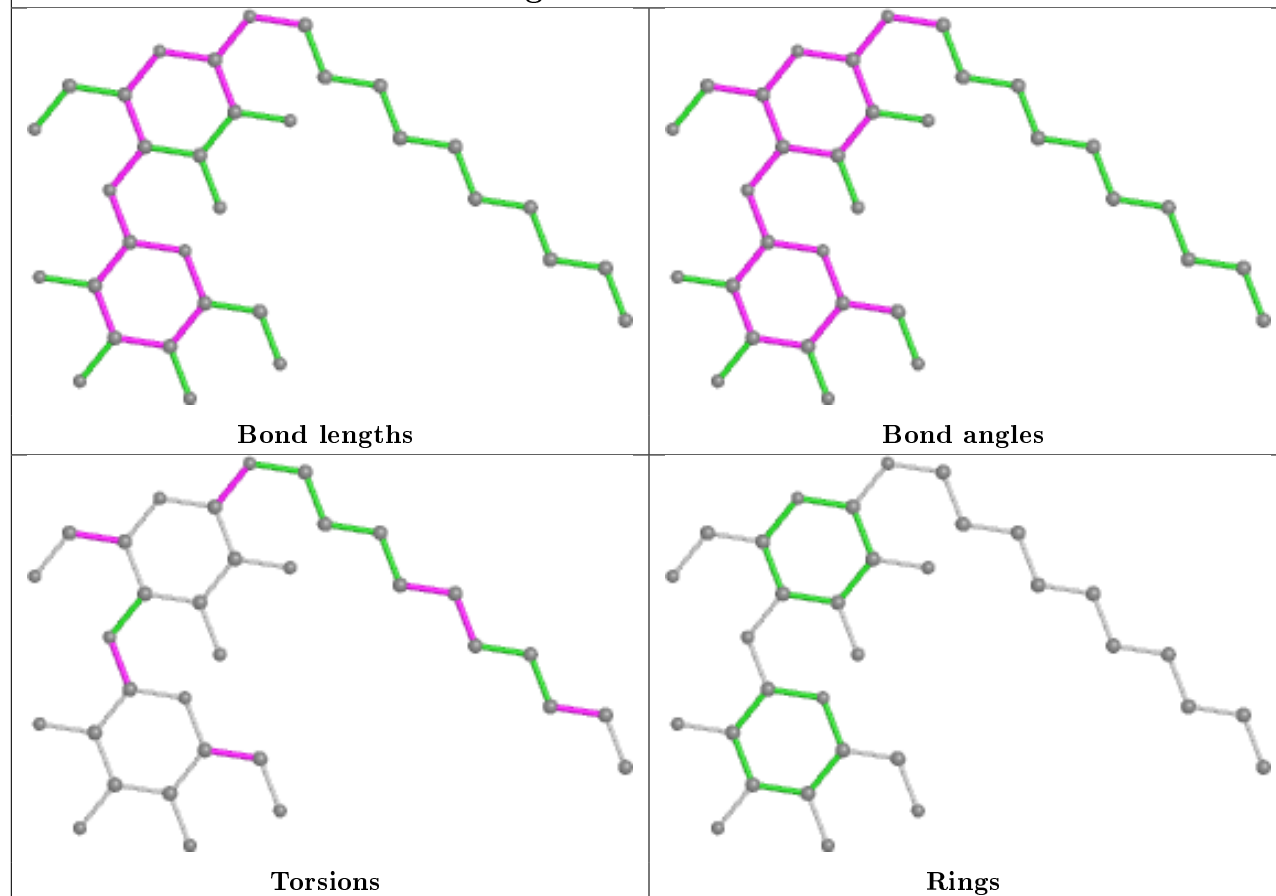




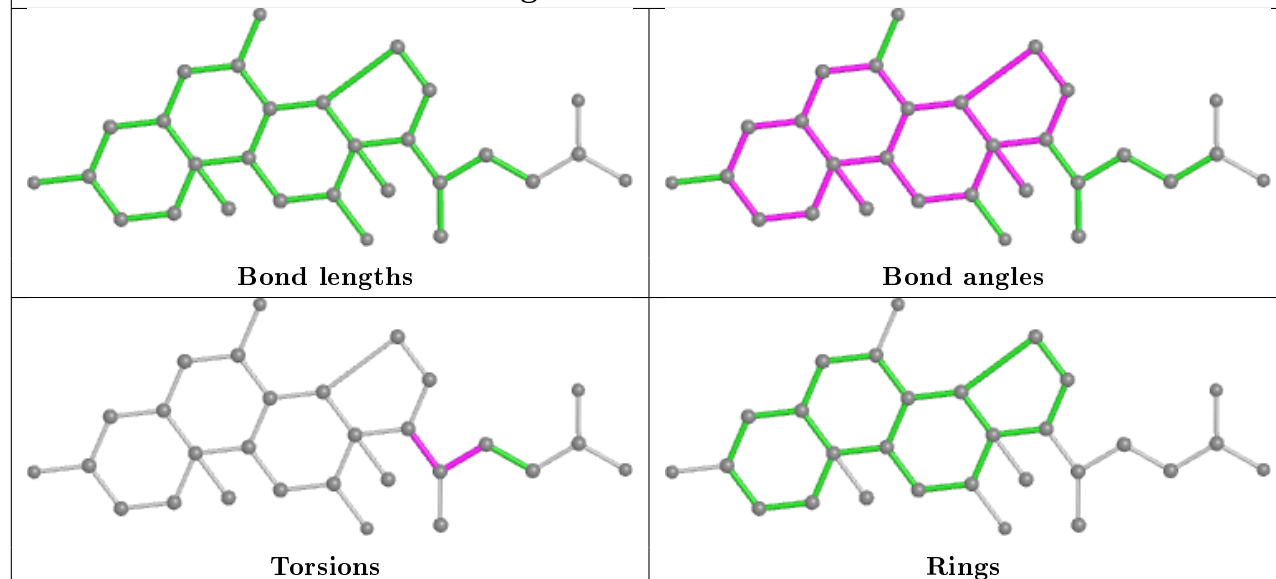


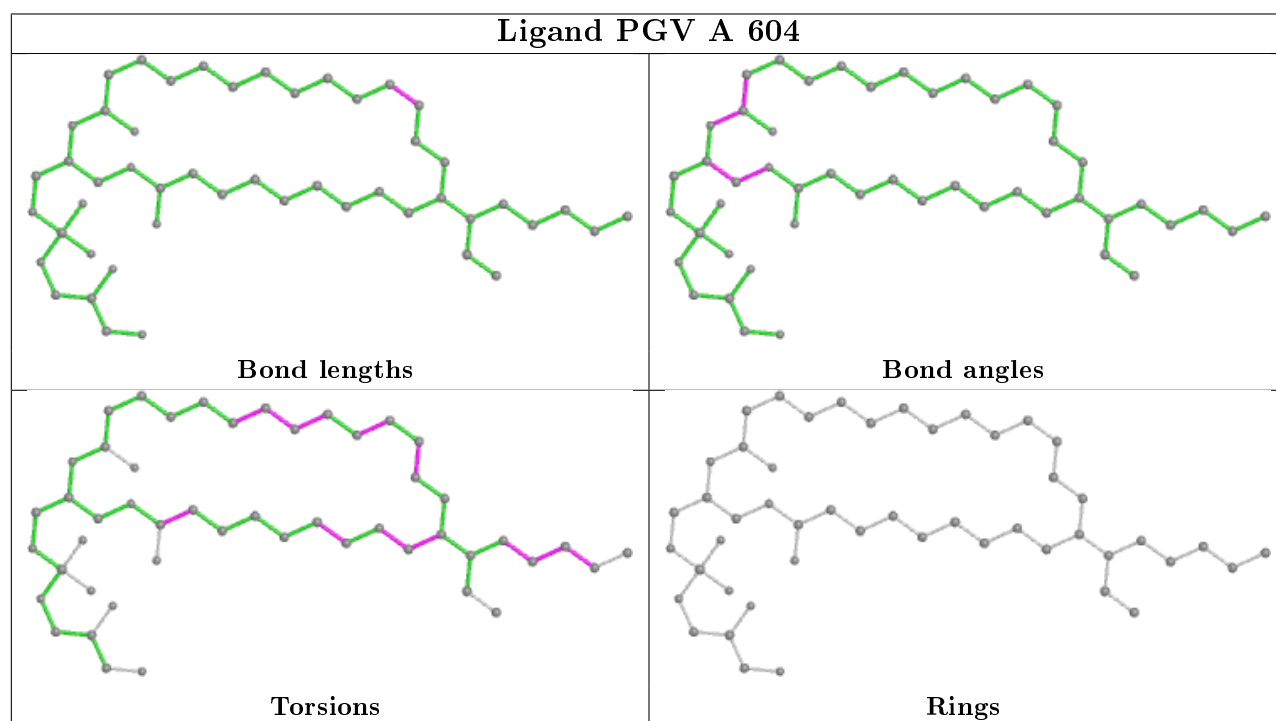
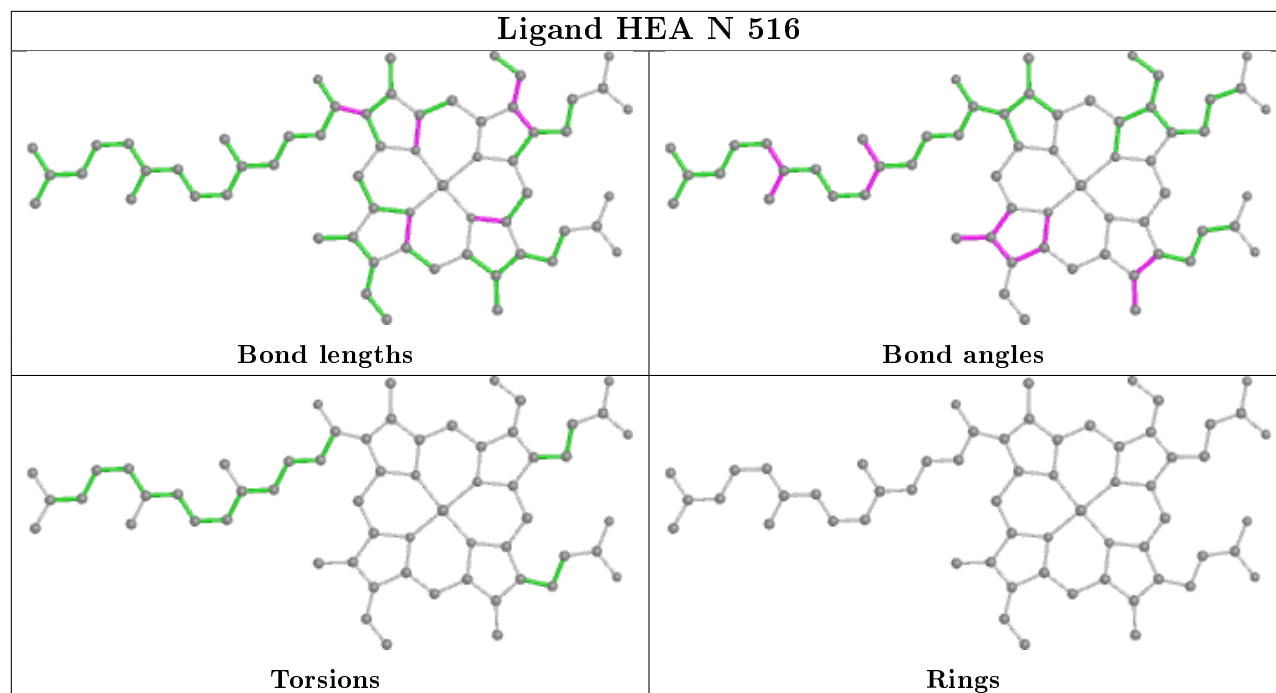


Ligand DMU C 272

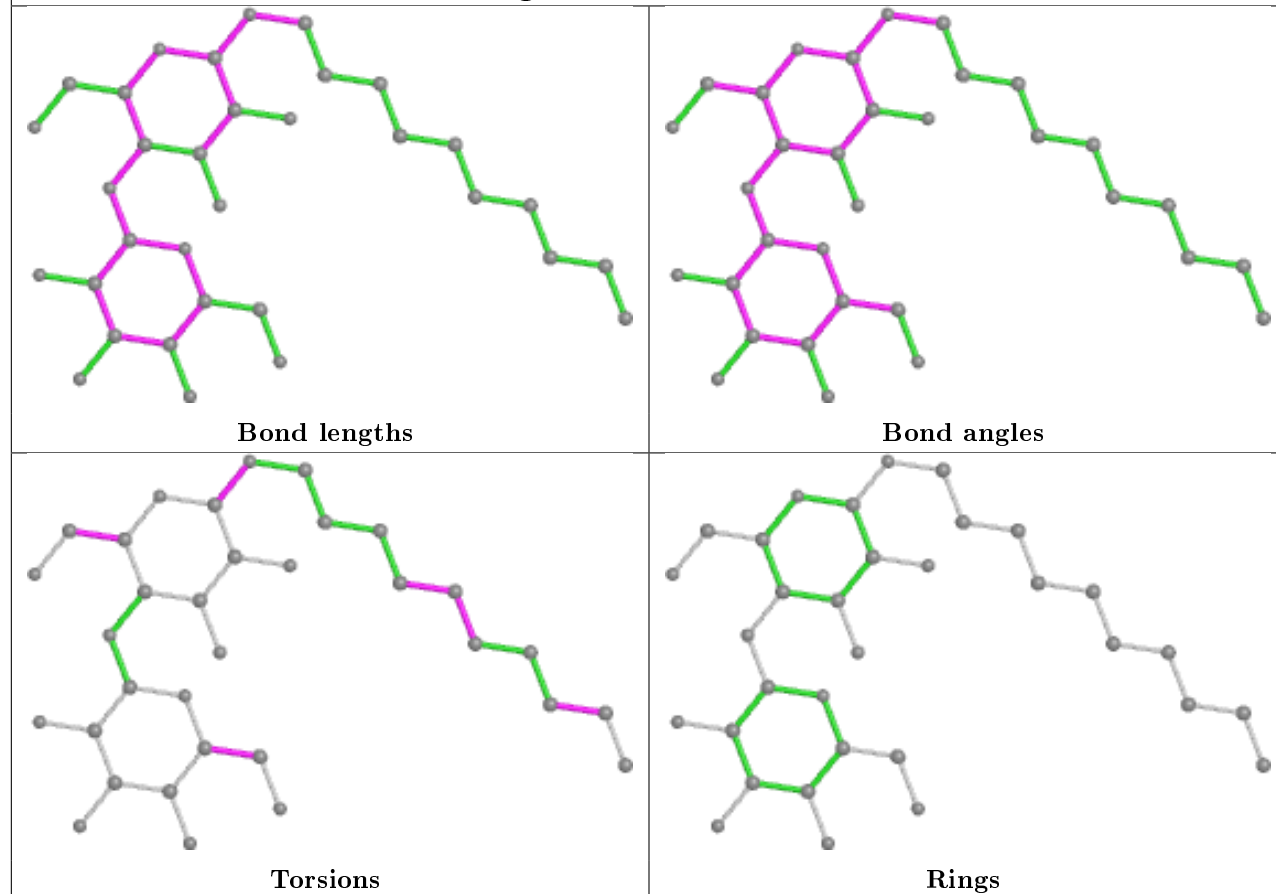


Ligand CHD P 1271

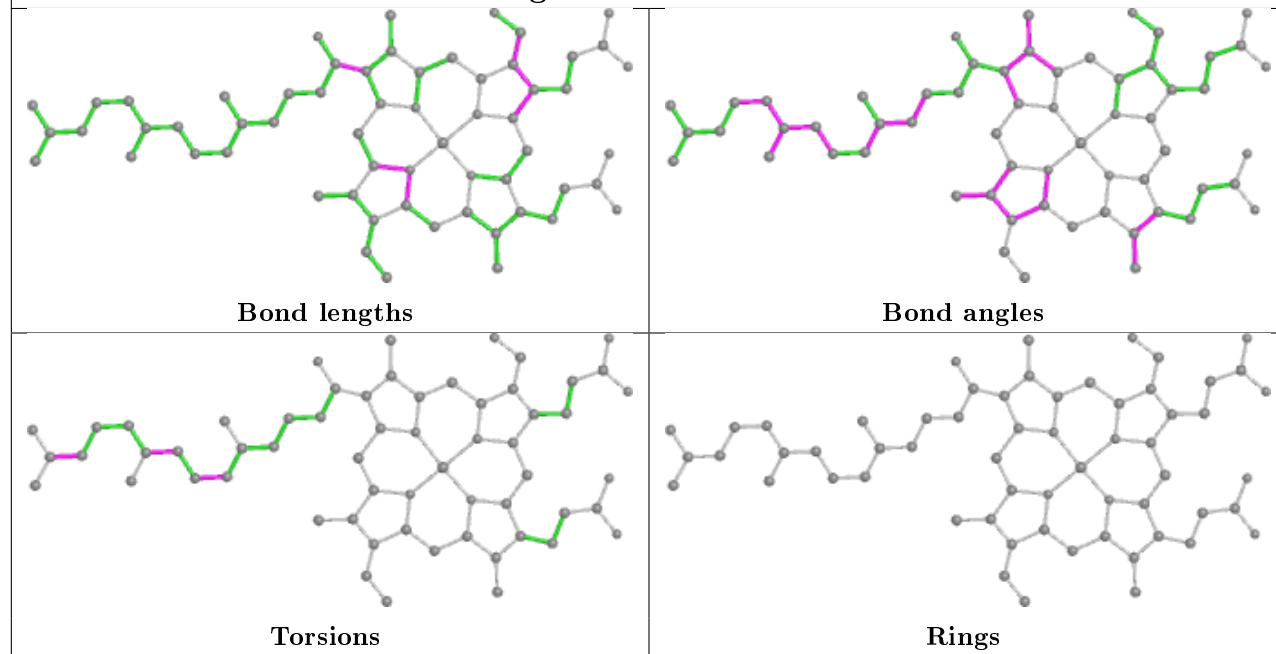


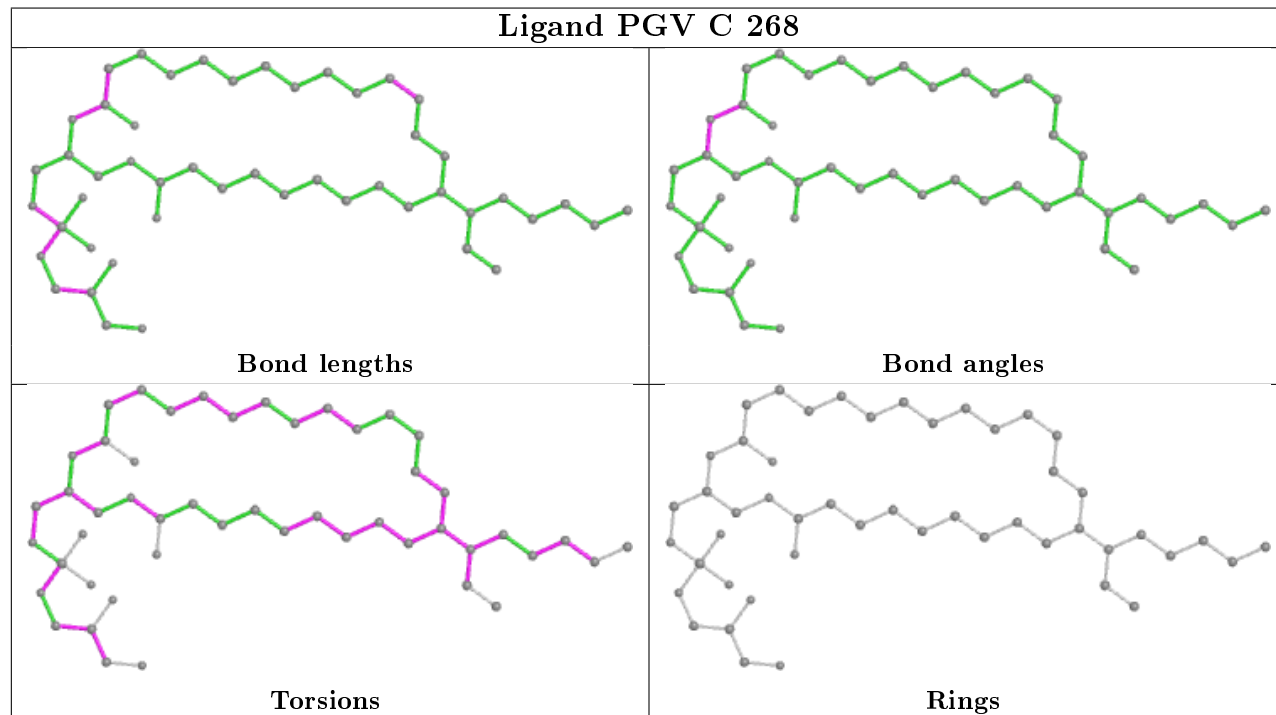
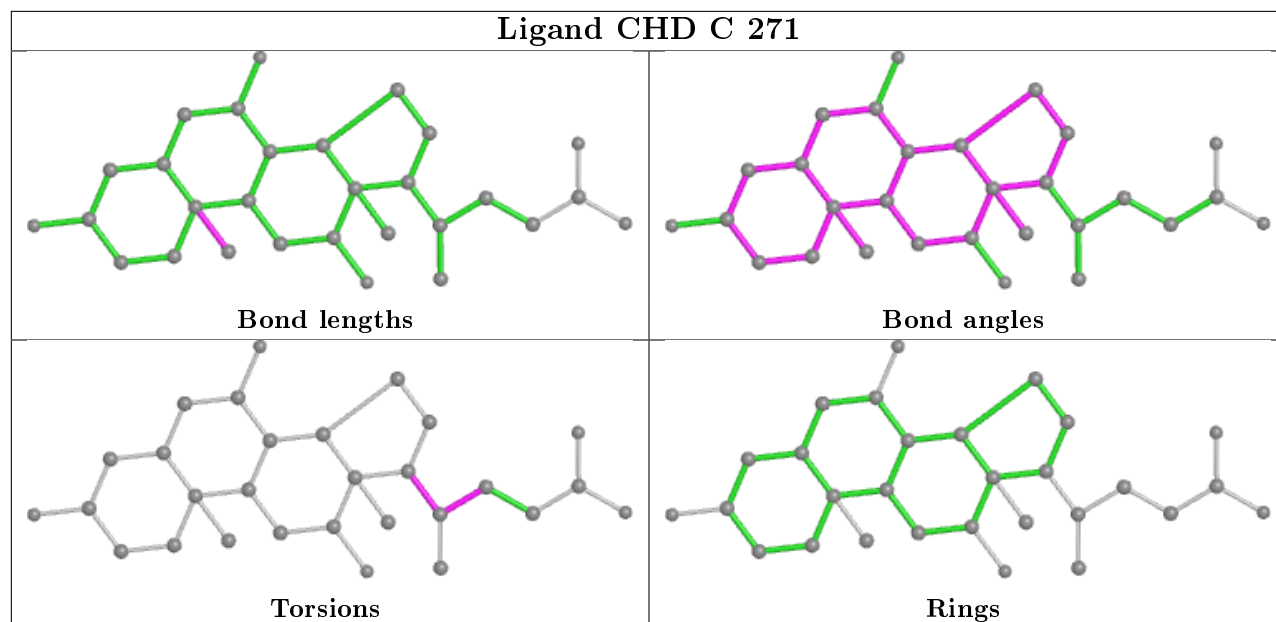


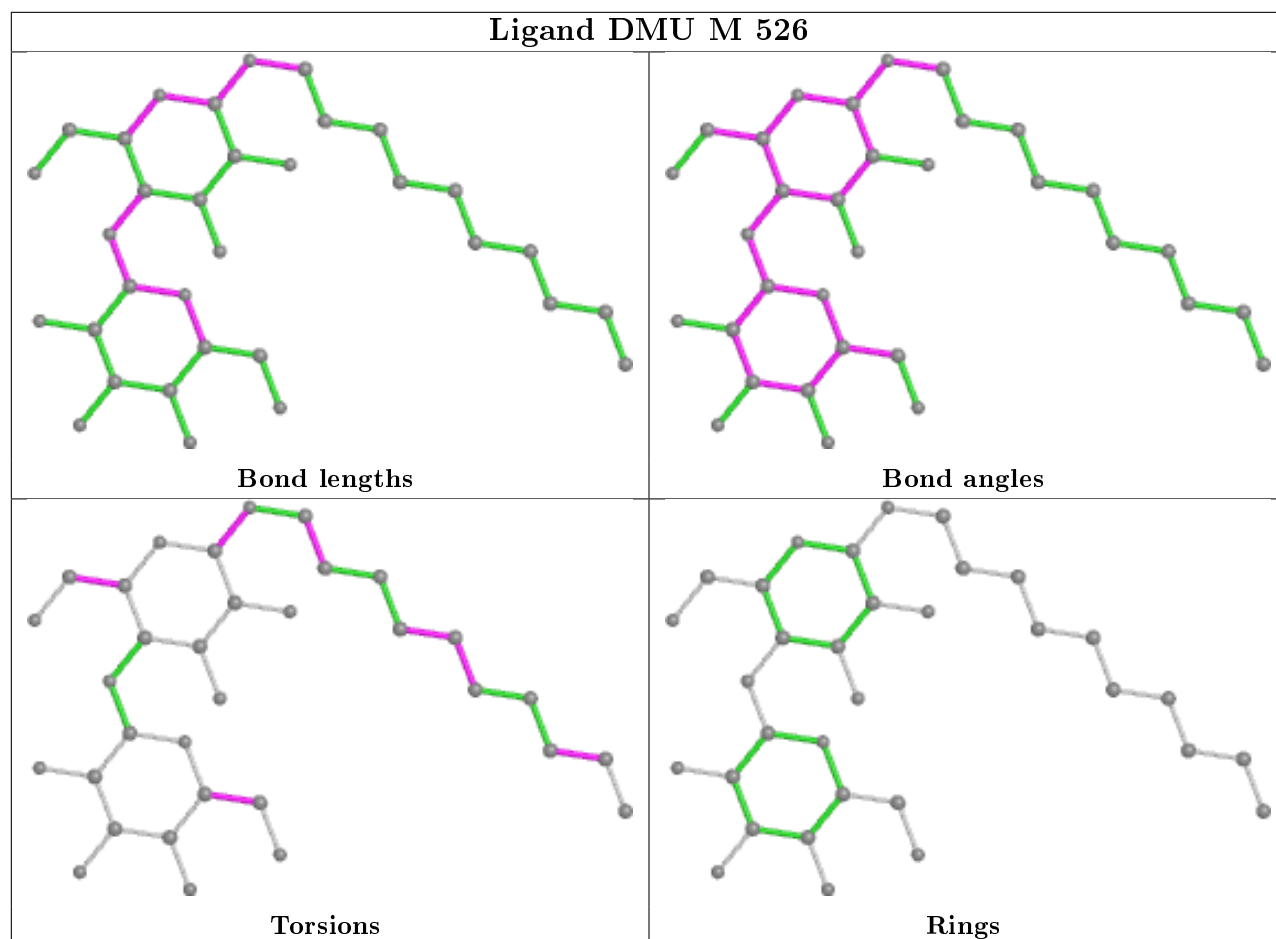
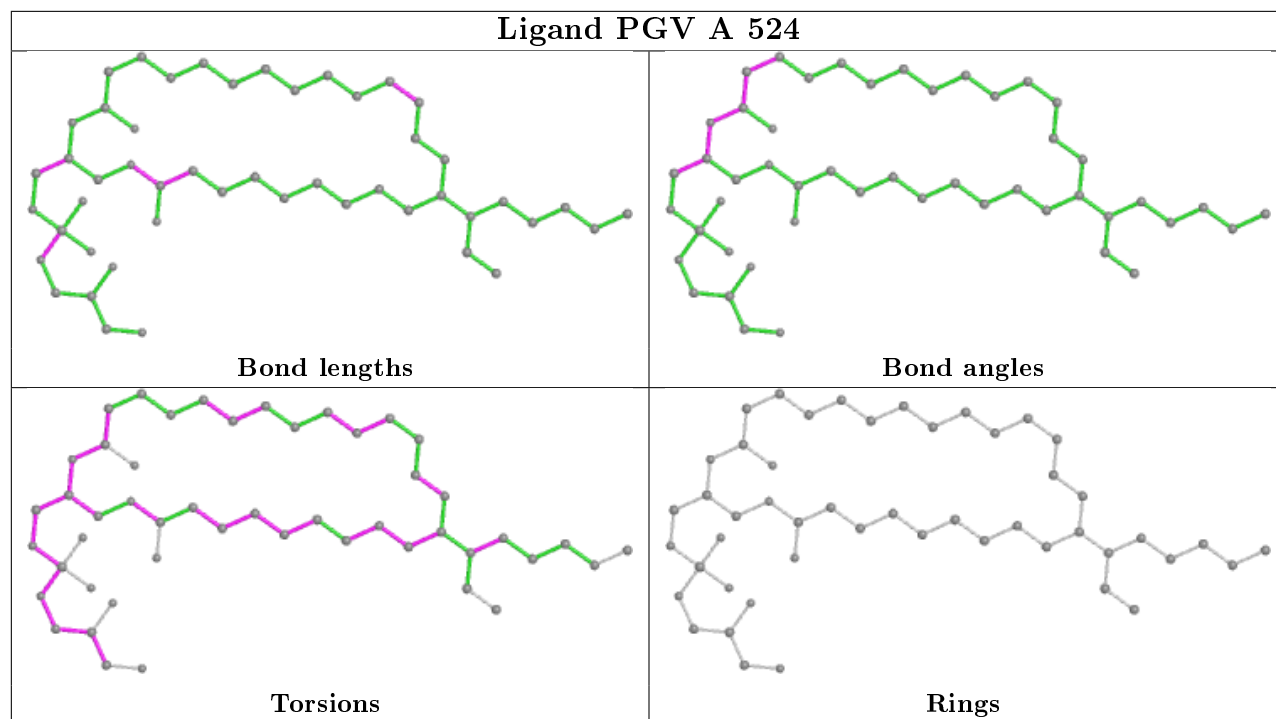
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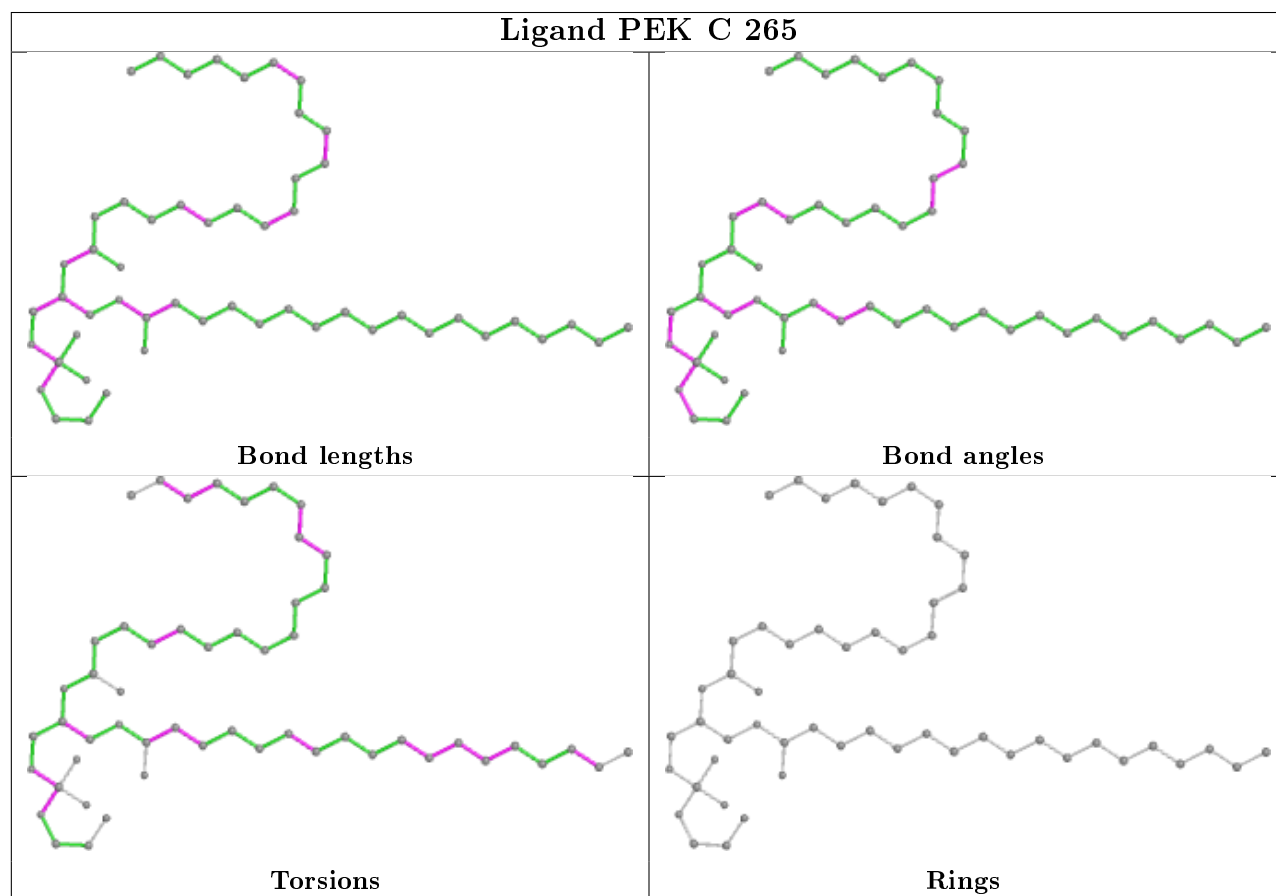
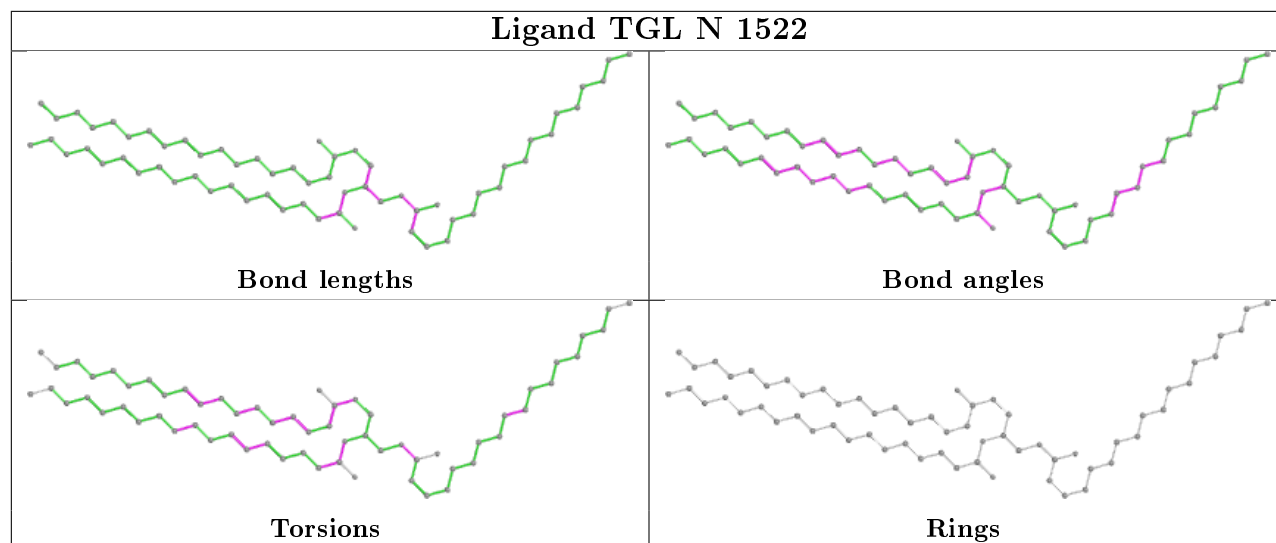


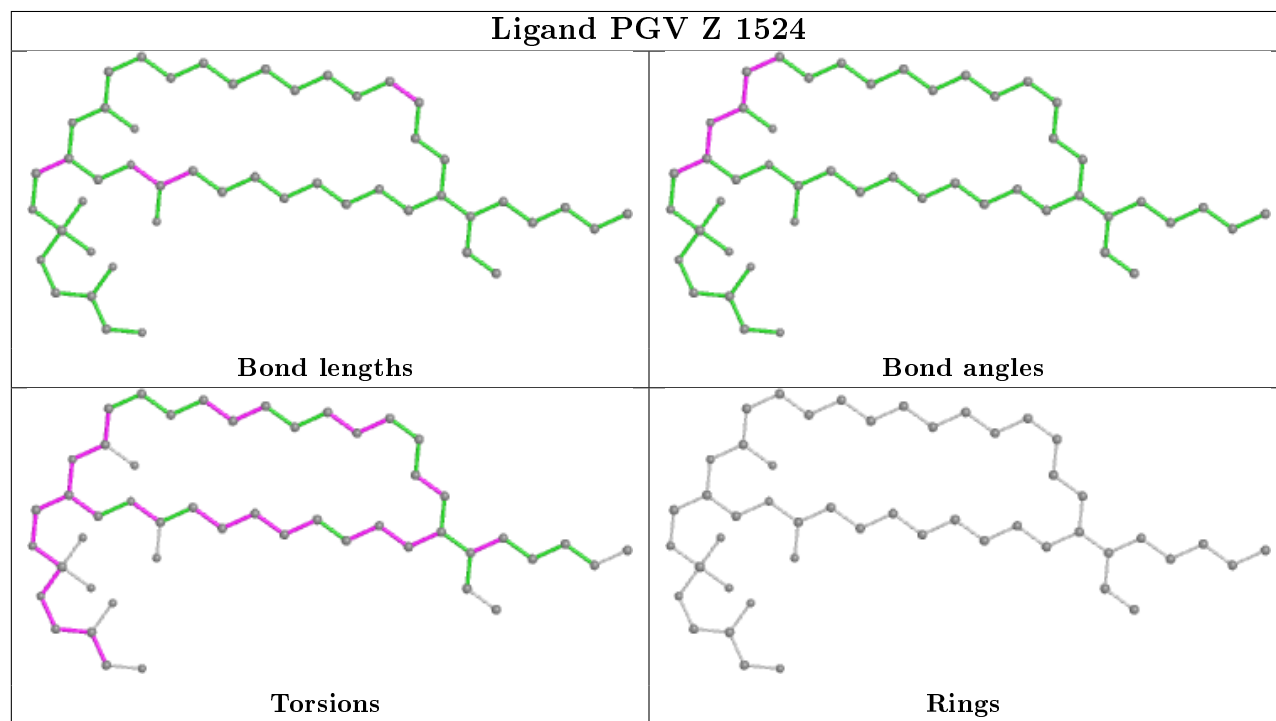
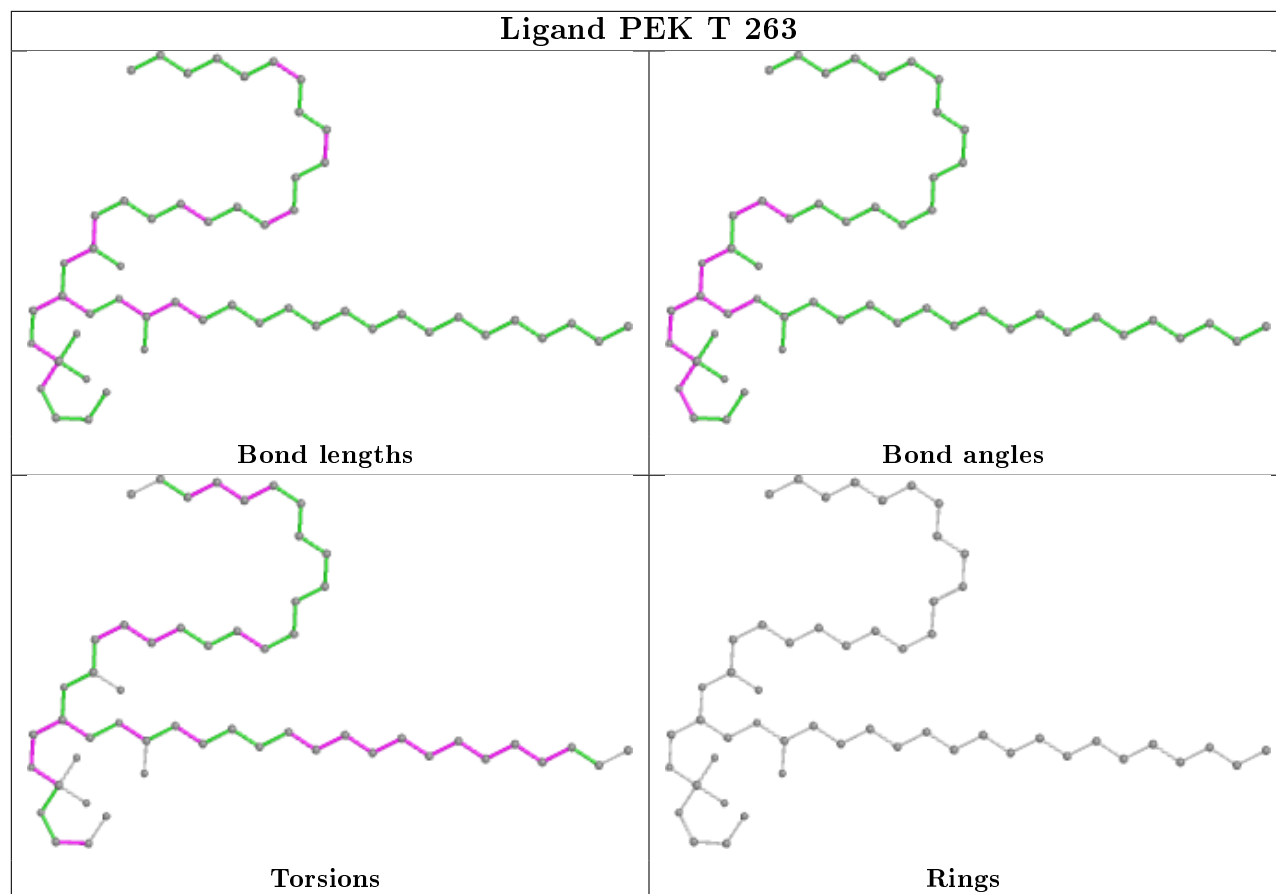
Ligand HEA N 515

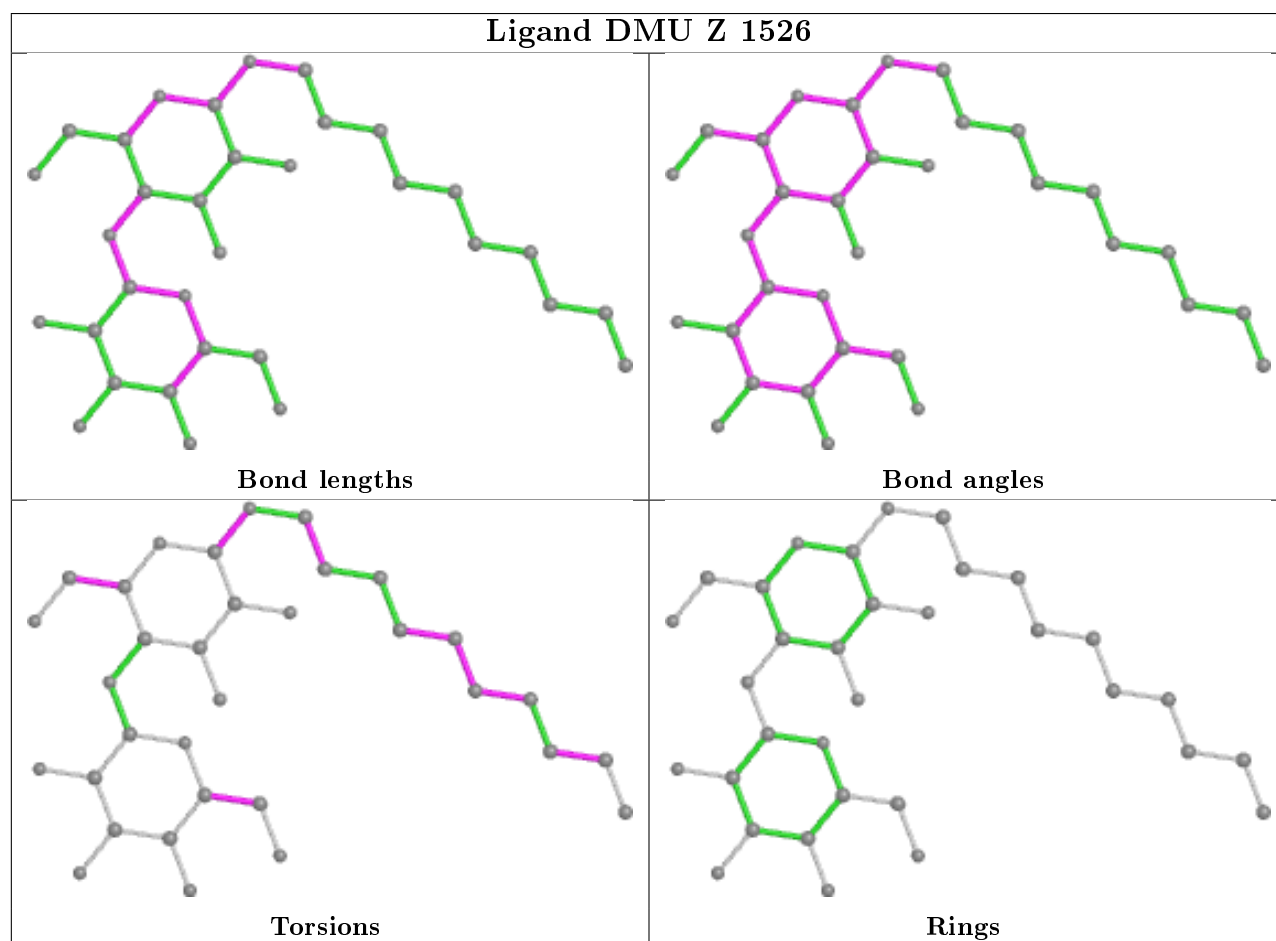
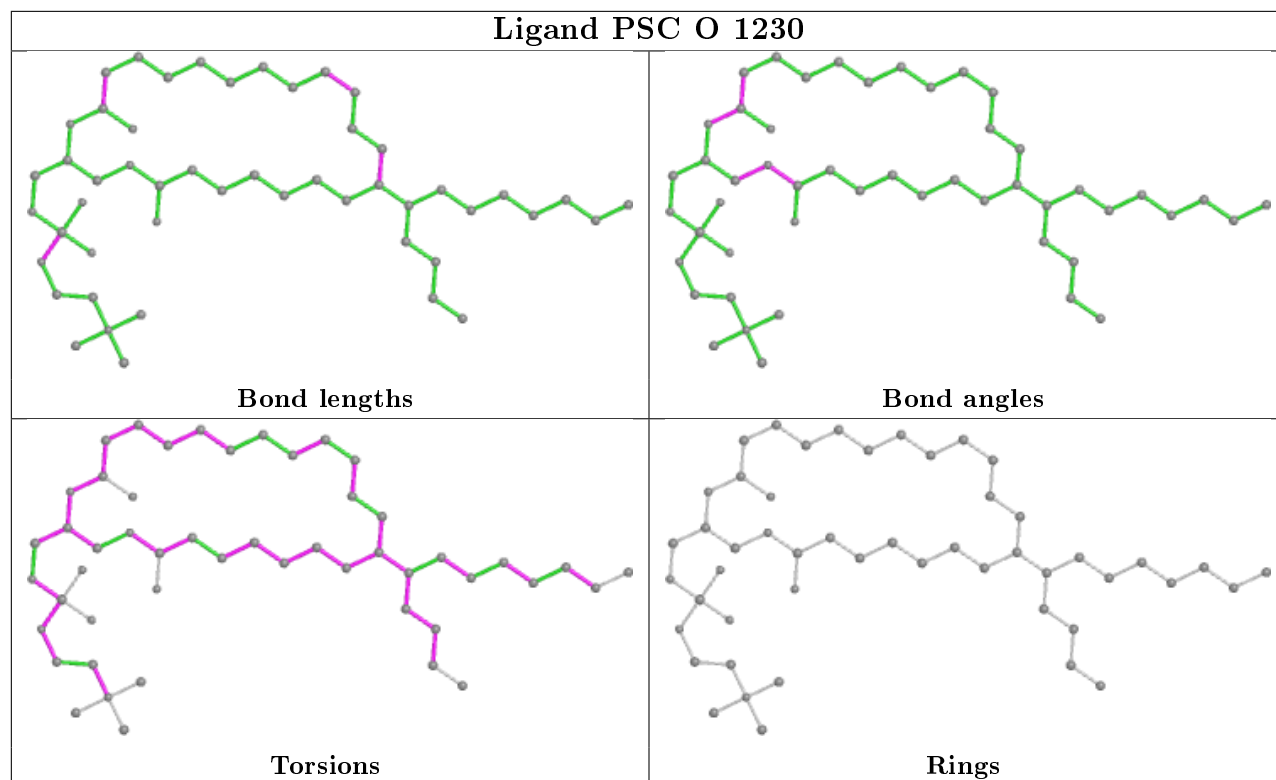


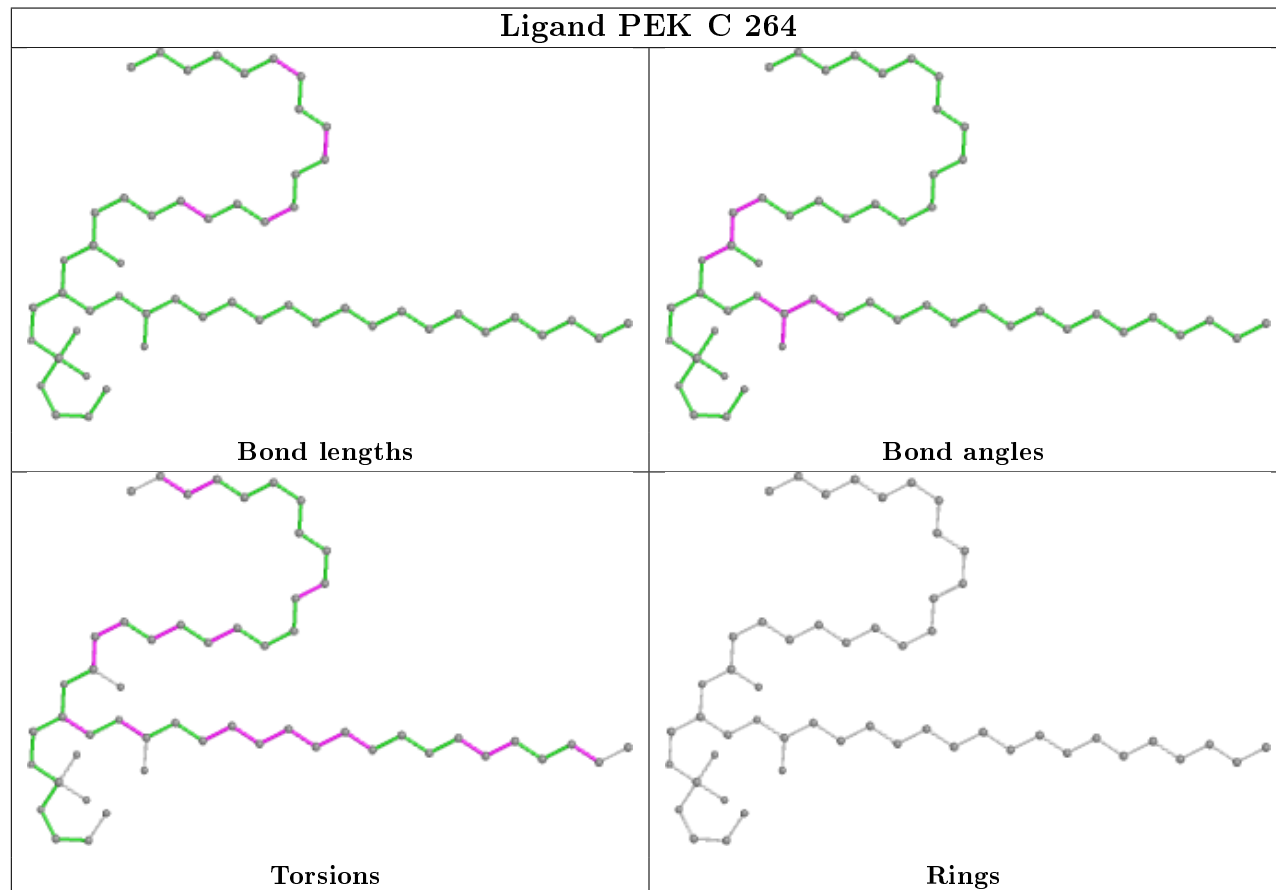
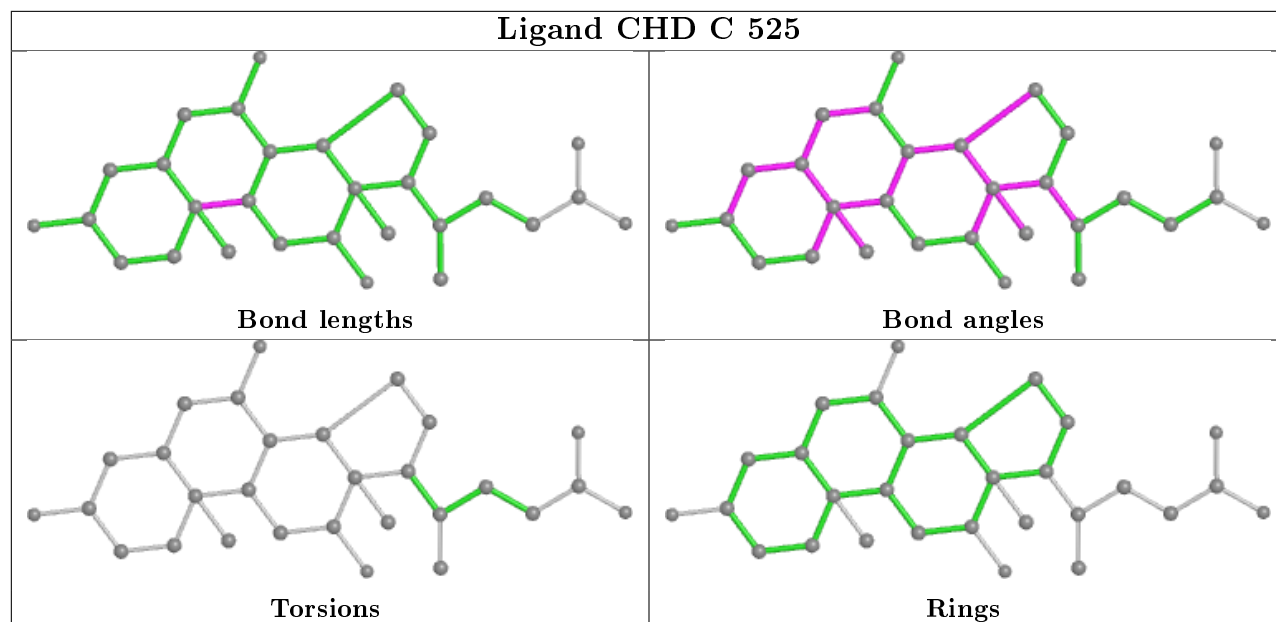




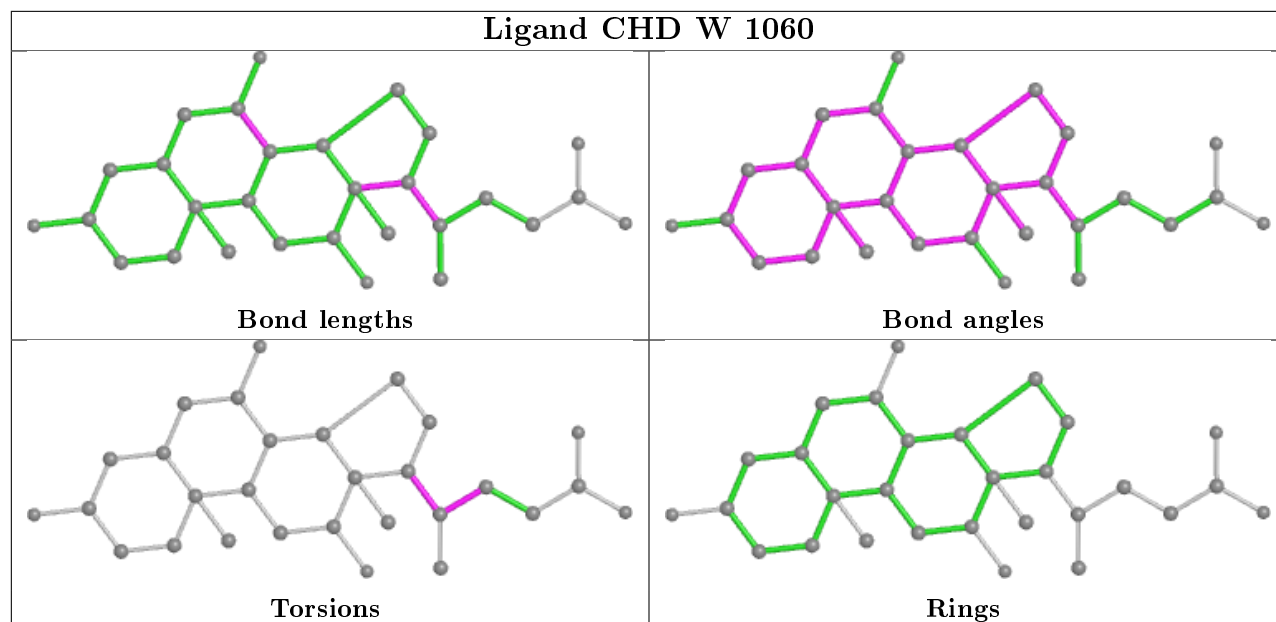




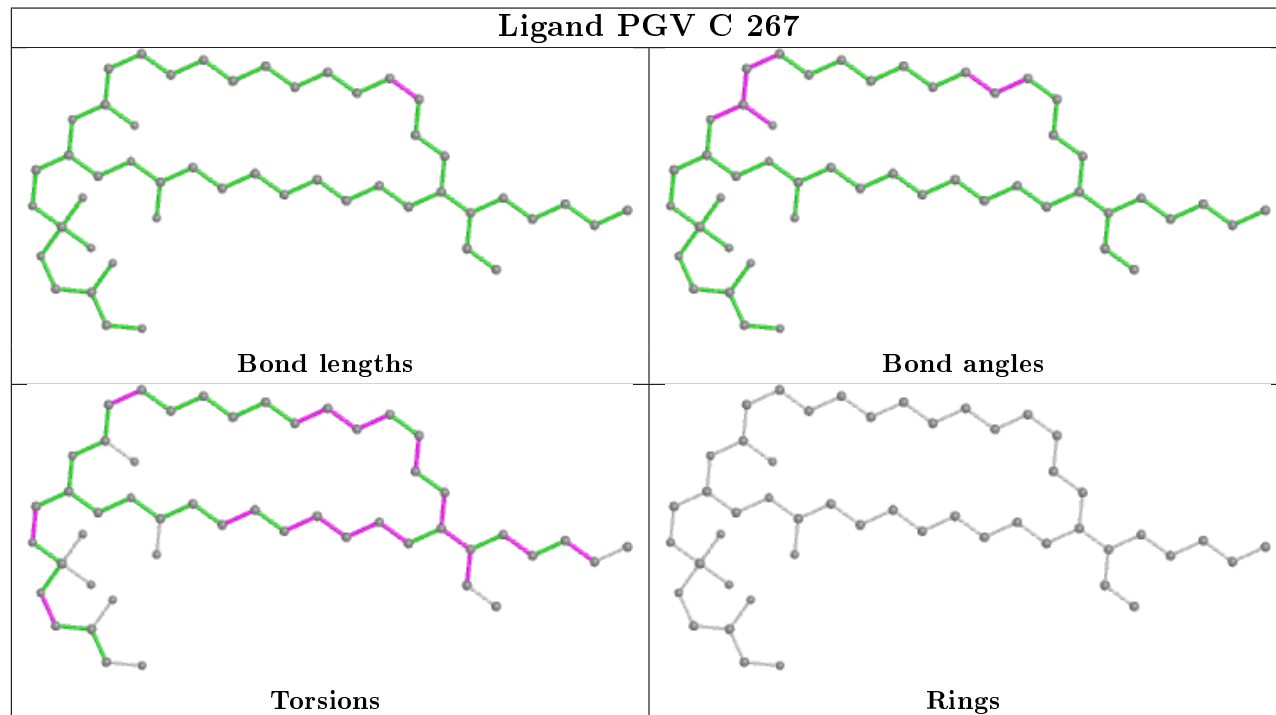


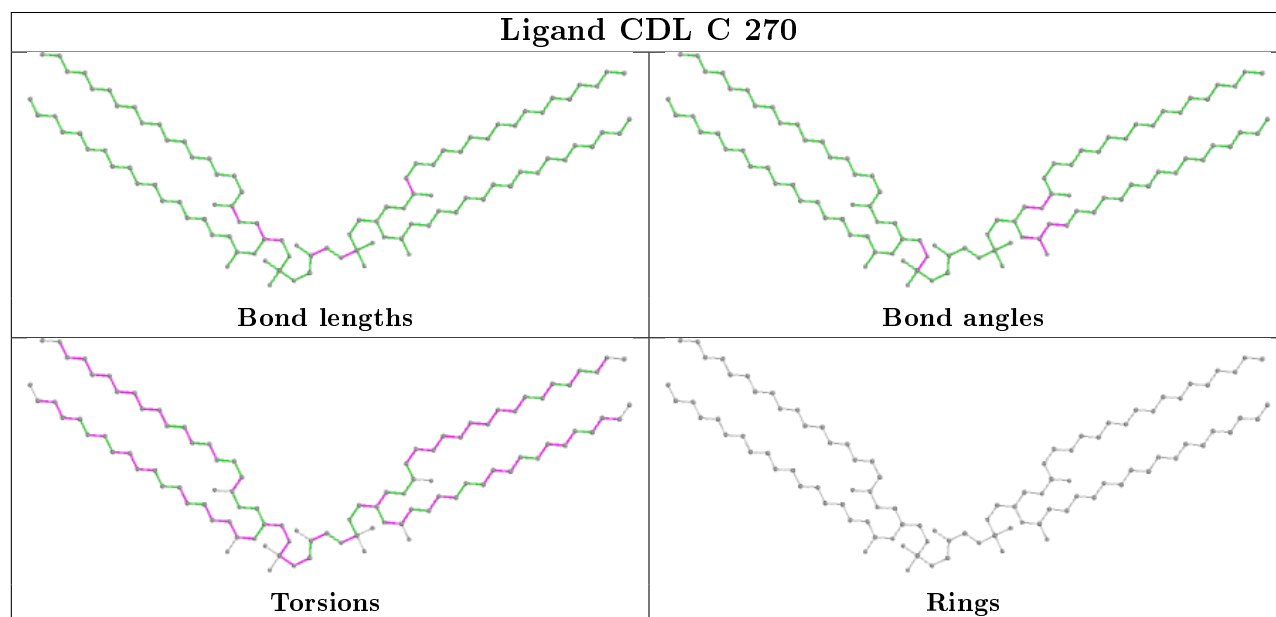
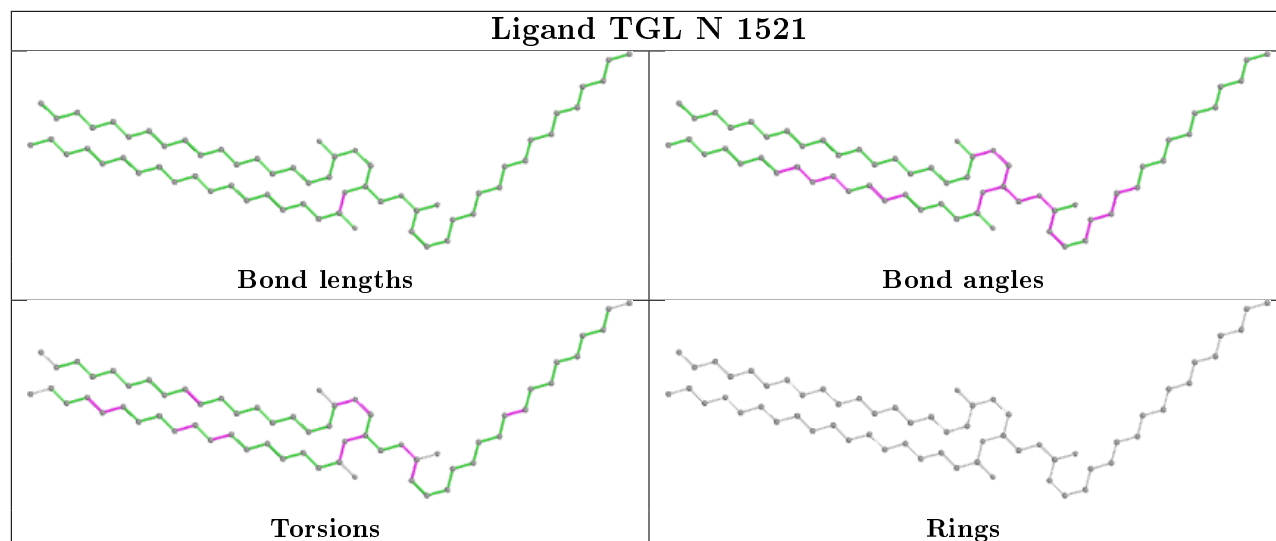


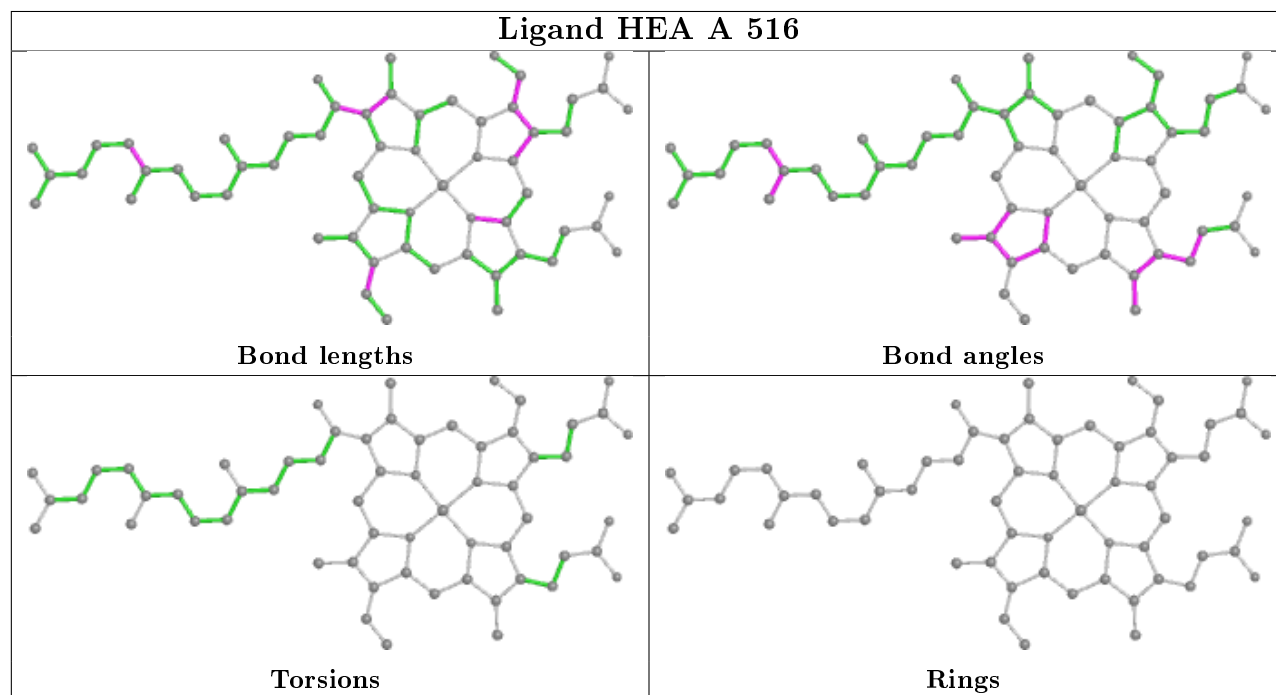
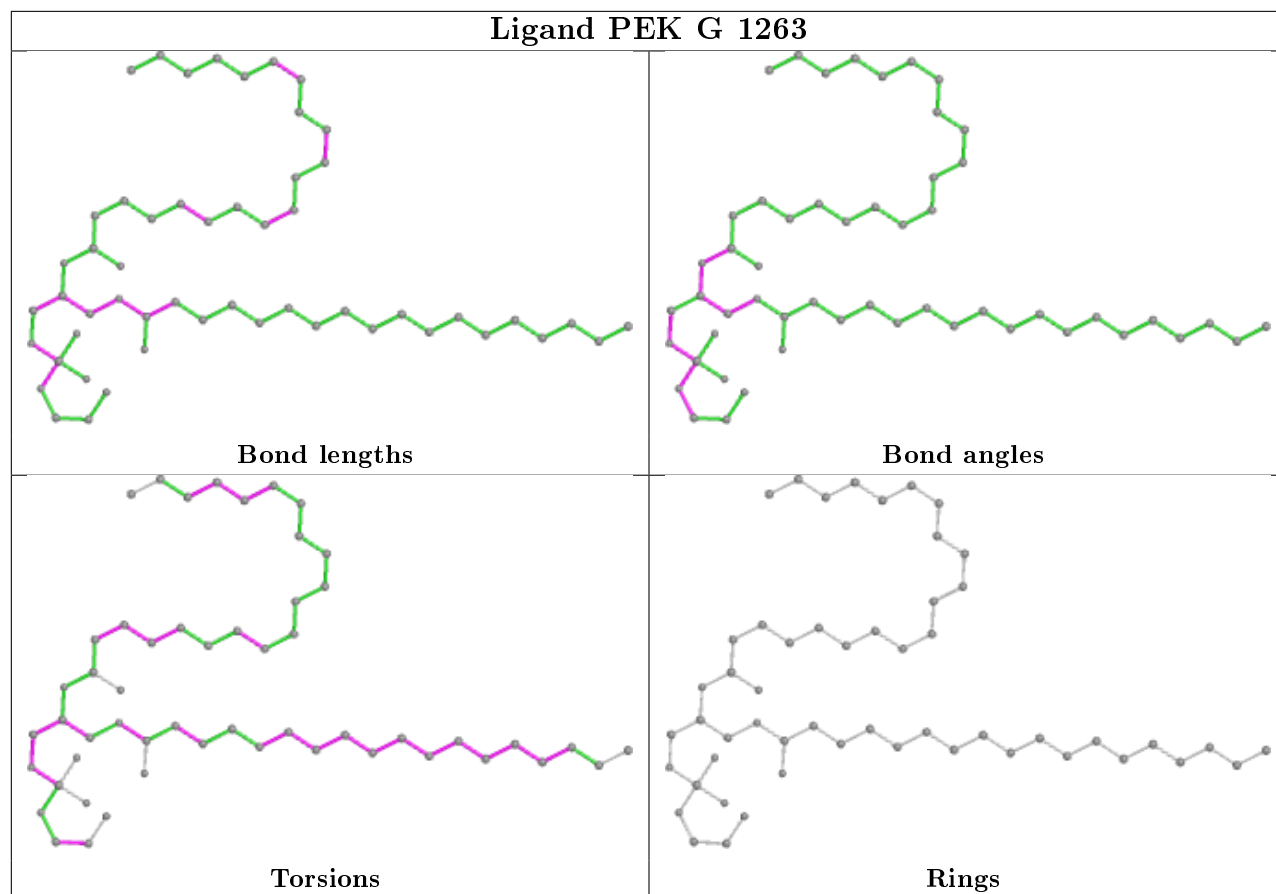
Ligand CHD W 1060

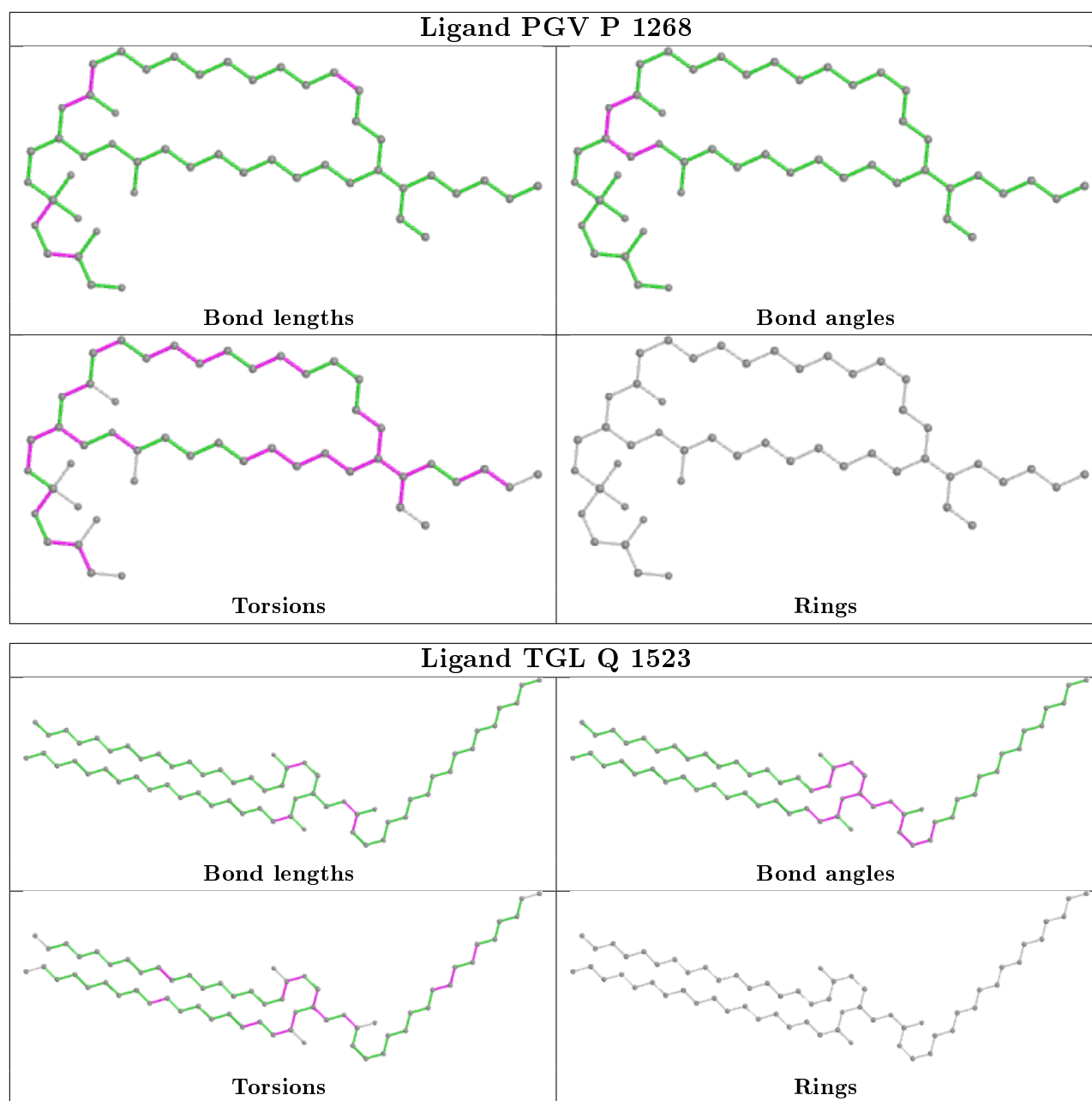


Ligand PGV C 267









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.