



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:36 pm BST

PDB ID : 2EIJ
Title : Bovine heart cytochrome C oxidase in the fully reduced state
Authors : Muramoto, K.; Hirata, K.; Shinzawa-Itoh, K.; Yoko-o, S.; Yamashita, E.;
Aoyama, H.; Tsukihara, T.; Yoshikawa, S.
Deposited on : 2007-03-13
Resolution : 1.90 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

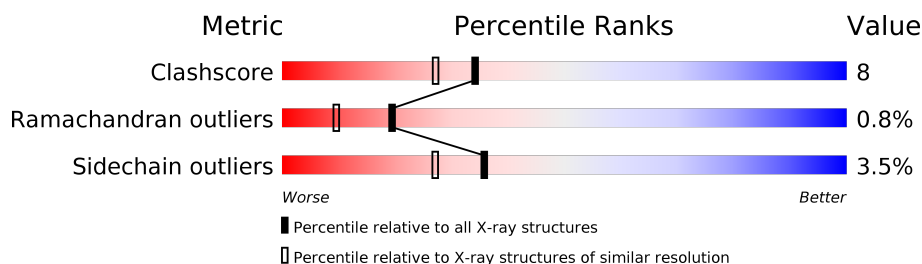
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)



















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	88% 11% .
1	N	514	82% 17% .
2	B	227	84% 15% .
2	O	227	73% 25% .
3	C	261	89% 11% .
3	P	261	87% 11% ..
4	D	147	89% 9% .
4	Q	147	76% 21% ..

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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
17	HEA	A	515	X	-	-	-
17	HEA	A	516	X	-	-	-
17	HEA	N	515	X	-	-	-
17	HEA	N	516	X	-	-	-
22	CHD	C	271	X	-	-	-
22	CHD	J	60	X	-	-	-
22	CHD	P	1271	X	-	-	-

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

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 32488 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		

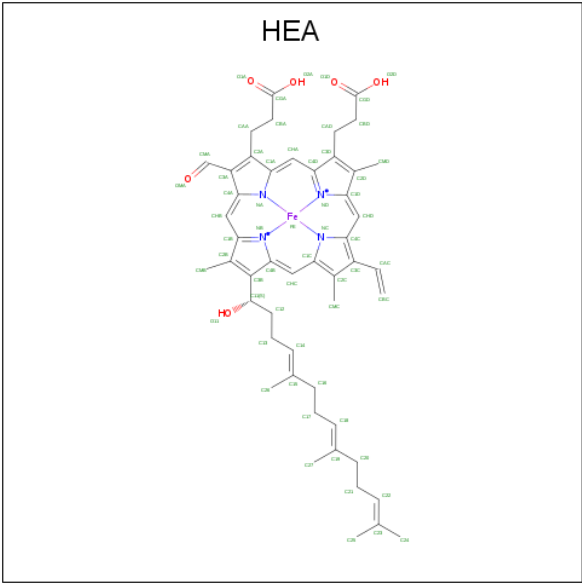
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

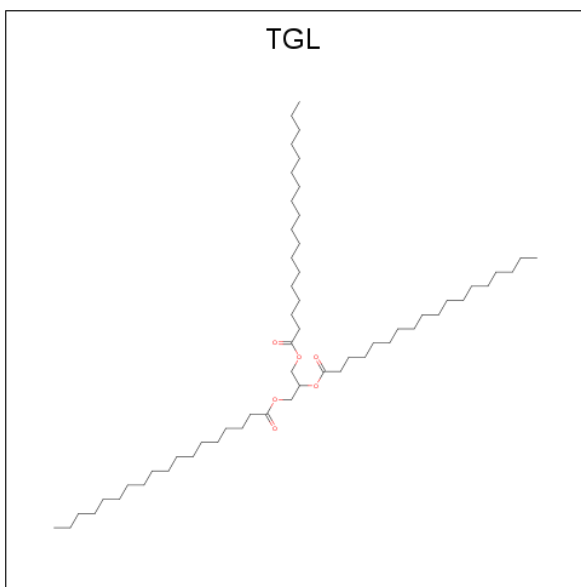
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

- Molecule 17 is HEME-A (three-letter code: HEA) (formula: C₄₉H₅₆FeN₄O₆).



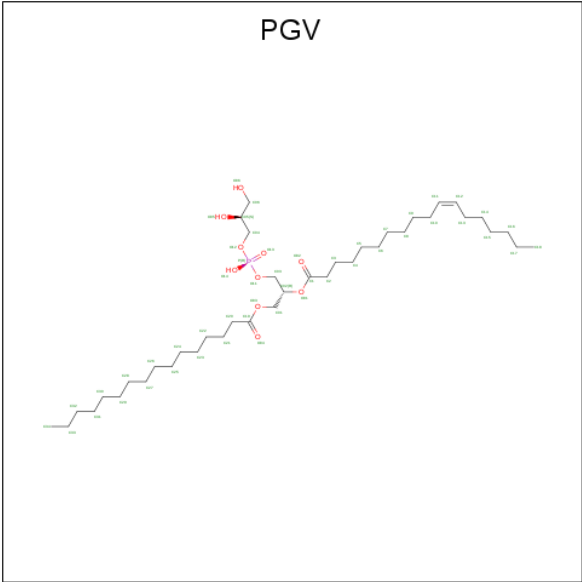
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 18 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



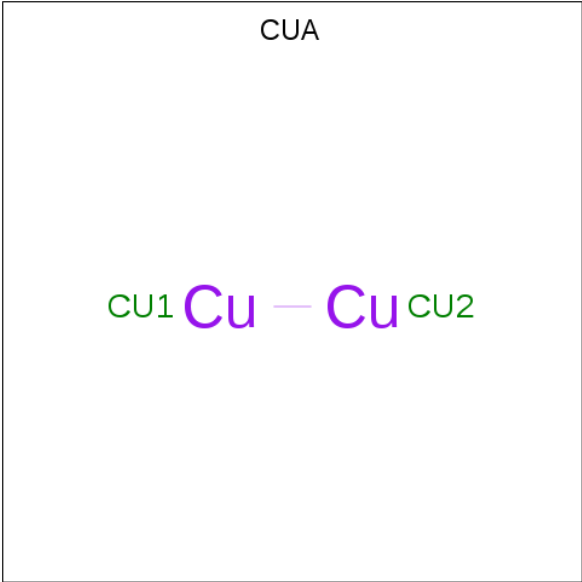
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			63	57	6		
18	B	1	Total	C	O	0	0
			63	57	6		
18	L	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		

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



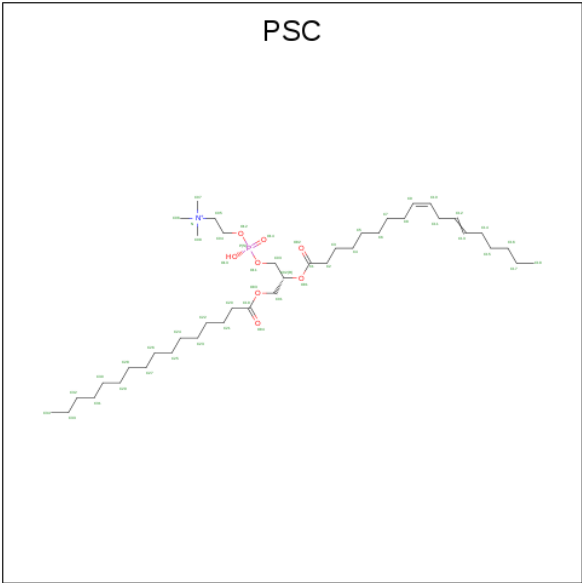
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

- Molecule 20 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu₂).



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

- Molecule 21 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).



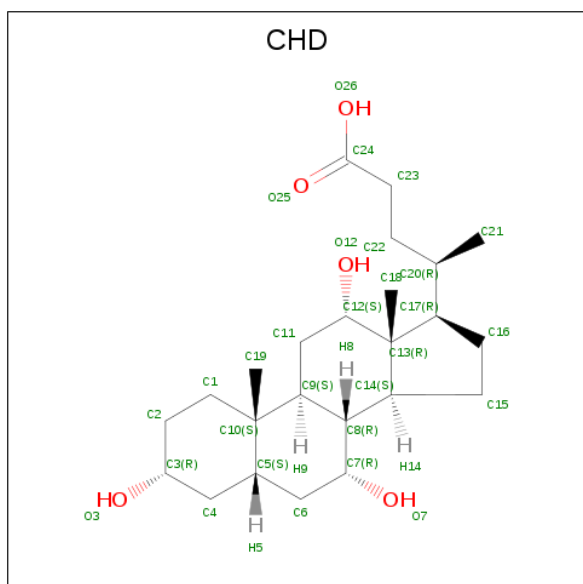
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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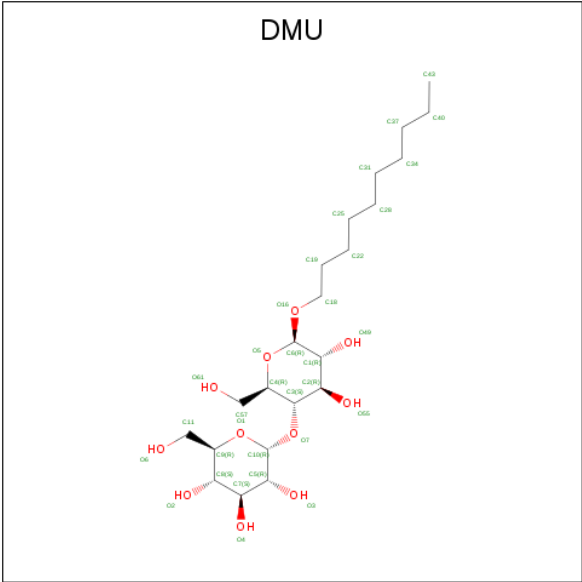
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



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

- Molecule 23 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: $C_{22}H_{42}O_{11}$).

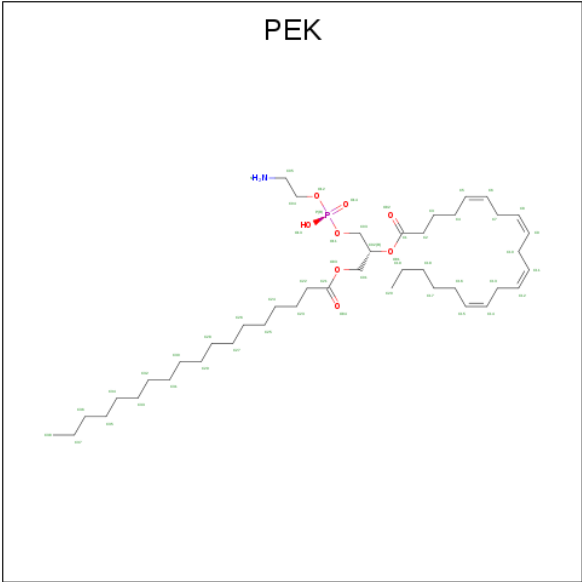


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total	C	O	0	0
			33	22	11		
23	M	1	Total	C	O	0	0
			33	22	11		
23	P	1	Total	C	O	0	0
			33	22	11		
23	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 24 is ZINC ION (three-letter code: ZN) (formula: Zn).

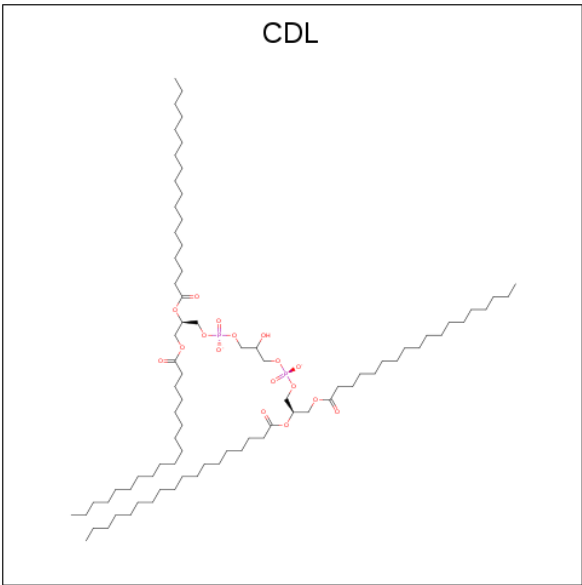
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	P	1	Total	Zn	0	0
			1	1		
24	C	1	Total	Zn	0	0
			1	1		
24	F	1	Total	Zn	0	0
			1	1		
24	S	1	Total	Zn	0	0
			1	1		

- Molecule 25 is (1S)-2-[[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYL)OXY]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: C₈₁H₁₅₆O₁₇P₂).



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

- Molecule 27 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	A	237	Total	O	0	0
			237	237		
27	B	145	Total	O	0	0
			145	145		
27	C	110	Total	O	0	0
			110	110		
27	D	94	Total	O	0	0
			94	94		
27	E	60	Total	O	0	0
			60	60		
27	F	72	Total	O	0	0
			72	72		
27	G	44	Total	O	0	0
			44	44		
27	H	50	Total	O	0	0
			50	50		

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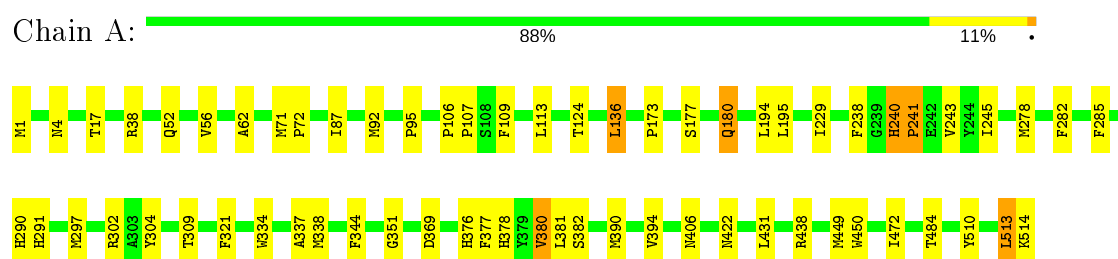
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	I	38	Total 38	O 38	0	0
27	J	23	Total 23	O 23	0	0
27	K	22	Total 22	O 22	0	0
27	L	27	Total 27	O 27	0	0
27	M	24	Total 24	O 24	0	0
27	N	218	Total 218	O 218	0	0
27	O	122	Total 122	O 122	0	0
27	P	112	Total 112	O 112	0	0
27	Q	53	Total 53	O 53	0	0
27	R	45	Total 45	O 45	0	0
27	S	76	Total 76	O 76	0	0
27	T	42	Total 42	O 42	0	0
27	U	46	Total 46	O 46	0	0
27	V	25	Total 25	O 25	0	0
27	W	18	Total 18	O 18	0	0
27	X	21	Total 21	O 21	0	0
27	Y	17	Total 17	O 17	0	0
27	Z	15	Total 15	O 15	0	0

3 Residue-property plots [i](#)

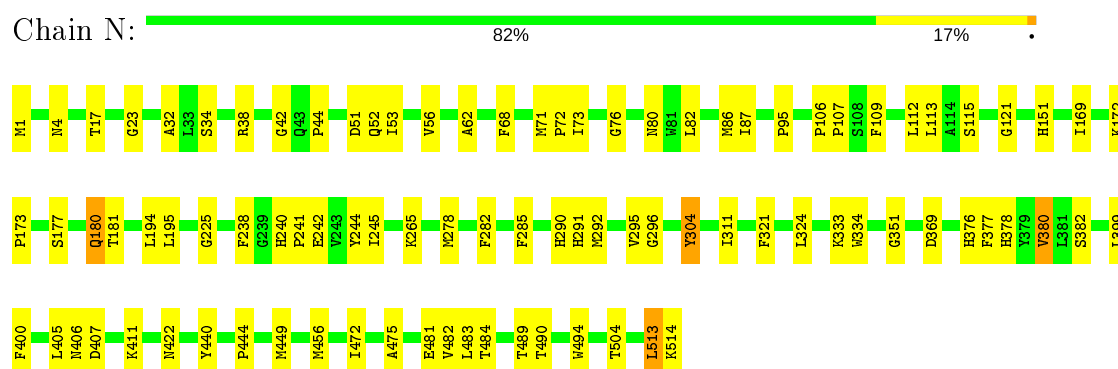
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

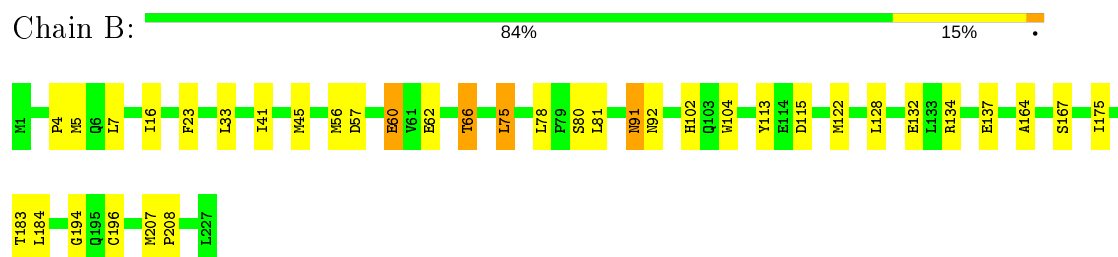
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 1: Cytochrome c oxidase subunit 1

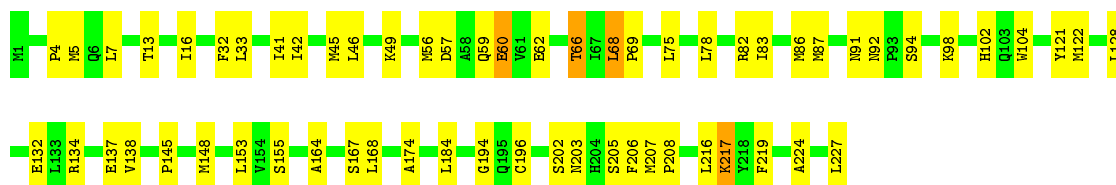


• Molecule 2: Cytochrome c oxidase subunit 2



• Molecule 2: Cytochrome c oxidase subunit 2





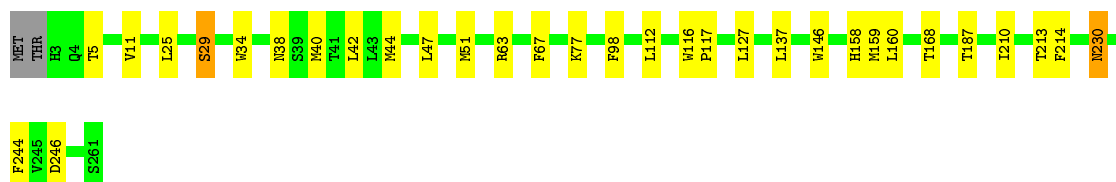
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 89% 11% .



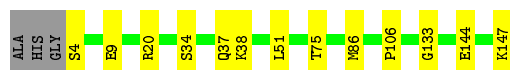
• Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 87% 11% ..



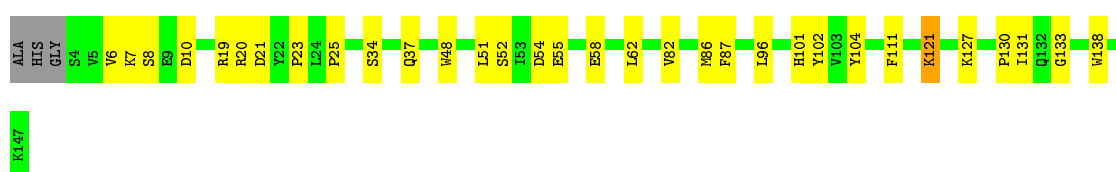
• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D: 89% 9% .



• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q: 76% 21% ..




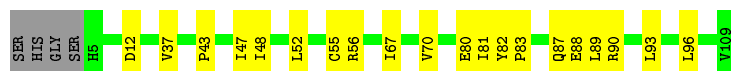
• Molecule 5: Cytochrome c oxidase polypeptide Va

Chain E: 85% 11% .




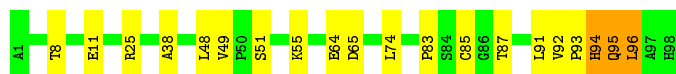
• Molecule 5: Cytochrome c oxidase polypeptide Va

Chain R:  78% 18% •



- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F:  80% 17% •



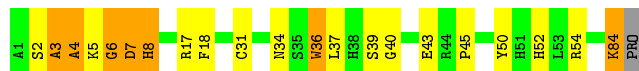
- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S:  74% 18% 5% •



- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G:  74% 16% 8% •



- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T:  74% 20% 5% •



- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain H:  80% 12% 7% •




- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain U:  75% 15% 7% •




- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I:  90% 8%



- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V:  86% 14%



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain J:  90% 7%



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain W:  90% 8%



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K:  77% 11% 13%




- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X:  73% 13% 13%




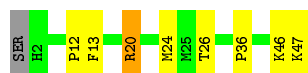
- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:  81% 17%



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y:  81% 15% . .



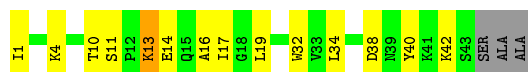
- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M:  74% 17% • 7%



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain Z:  63% 28% • 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	183.06Å 206.58Å 178.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.206 , 0.234	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32488	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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, 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	0.52	0/4156	0.69	2/5678 (0.0%)
1	N	0.52	0/4156	0.66	0/5678
2	B	0.51	0/1860	0.77	1/2534 (0.0%)
2	O	0.52	0/1860	0.79	1/2534 (0.0%)
3	C	0.53	0/2197	0.59	0/3005
3	P	0.51	0/2197	0.62	1/3005 (0.0%)
4	D	0.51	0/1229	0.67	1/1658 (0.1%)
4	Q	0.54	0/1229	0.67	1/1658 (0.1%)
5	E	0.53	0/871	0.67	0/1182
5	R	0.54	0/871	0.70	0/1182
6	F	0.50	0/765	0.82	2/1038 (0.2%)
6	S	0.49	0/765	0.81	2/1038 (0.2%)
7	G	0.51	0/690	0.71	1/937 (0.1%)
7	T	0.55	0/690	0.72	1/937 (0.1%)
8	H	0.49	0/682	0.68	0/921
8	U	0.48	0/682	0.69	0/921
9	I	0.52	0/605	0.61	0/802
9	V	0.49	0/605	0.60	0/802
10	J	0.46	0/471	0.63	0/636
10	W	0.48	0/471	0.65	0/636
11	K	0.53	0/398	0.68	0/546
11	X	0.50	0/398	0.66	0/546
12	L	0.51	0/393	0.59	0/526
12	Y	0.54	0/393	0.60	0/526
13	M	0.50	0/345	0.65	0/470
13	Z	0.47	0/345	0.60	0/470
All	All	0.52	0/29324	0.68	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	3
8	U	0	1
All	All	0	5

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	33	LEU	CA-CB-CG	6.53	130.31	115.30
6	S	94	HIS	N-CA-C	6.39	128.27	111.00
4	D	133	GLY	N-CA-C	6.33	128.93	113.10
6	F	94	HIS	N-CA-C	6.21	127.75	111.00
4	Q	133	GLY	N-CA-C	5.94	127.94	113.10
6	F	93	PRO	N-CA-C	5.58	126.60	112.10
3	P	127	LEU	CA-CB-CG	5.20	127.25	115.30
6	S	93	PRO	N-CA-C	5.19	125.59	112.10
2	B	184	LEU	CA-CB-CG	5.15	127.14	115.30
1	A	136	LEU	CA-CB-CG	5.11	127.04	115.30
1	A	438	ARG	CB-CA-C	-5.06	100.28	110.40
2	O	184	LEU	CA-CB-CG	5.02	126.86	115.30
7	G	6	GLY	N-CA-C	5.00	125.60	113.10

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain
1	N	244	TYR	Sidechain
1	N	304	TYR	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	57	0
1	N	4027	0	4001	78	0
2	B	1824	0	1833	20	0
2	O	1824	0	1833	40	0
3	C	2110	0	2027	21	0
3	P	2110	0	2027	33	0
4	D	1195	0	1183	11	0
4	Q	1195	0	1183	23	0
5	E	852	0	845	7	0
5	R	852	0	845	12	0
6	F	748	0	728	12	0
6	S	748	0	728	21	0
7	G	675	0	644	26	0
7	T	675	0	644	20	0
8	H	662	0	623	6	0
8	U	662	0	623	9	0
9	I	601	0	613	4	0
9	V	601	0	613	7	0
10	J	460	0	459	5	0
10	W	460	0	459	5	0
11	K	384	0	366	3	0
11	X	384	0	366	10	0
12	L	380	0	380	12	0
12	Y	380	0	380	8	0
13	M	335	0	352	7	0
13	Z	335	0	352	8	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	120	0	108	6	0
17	N	120	0	108	5	0
18	A	63	0	110	4	0
18	B	63	0	110	7	0
18	L	63	0	110	20	0
18	N	189	0	330	27	0
19	A	51	0	76	7	0
19	C	153	0	228	6	0
19	N	102	0	152	8	0
19	P	102	0	152	6	0
20	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	O	2	0	0	0	0
21	B	52	0	80	11	0
21	O	52	0	80	15	0
22	B	29	0	39	1	0
22	C	58	0	78	3	0
22	J	29	0	39	2	0
22	O	29	0	39	1	0
22	P	58	0	78	1	0
22	W	29	0	39	4	0
23	C	33	0	36	3	0
23	M	33	0	36	0	0
23	P	33	0	36	8	0
23	Z	33	0	36	0	0
24	C	1	0	0	0	0
24	F	1	0	0	0	0
24	P	1	0	0	0	0
24	S	1	0	0	0	0
25	C	106	0	154	11	0
25	G	53	0	77	10	0
25	P	106	0	154	13	0
25	T	53	0	77	6	0
26	C	100	0	156	11	0
26	G	100	0	156	18	0
26	P	100	0	156	15	0
26	T	100	0	156	19	0
27	A	237	0	0	3	0
27	B	145	0	0	1	0
27	C	110	0	0	1	0
27	D	94	0	0	3	0
27	E	60	0	0	0	0
27	F	72	0	0	1	0
27	G	44	0	0	2	0
27	H	50	0	0	2	0
27	I	38	0	0	2	0
27	J	23	0	0	1	0
27	K	22	0	0	1	0
27	L	27	0	0	0	0
27	M	24	0	0	1	0
27	N	218	0	0	5	0
27	O	122	0	0	3	0
27	P	112	0	0	4	0
27	Q	53	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	R	45	0	0	0	0
27	S	76	0	0	6	0
27	T	42	0	0	1	0
27	U	46	0	0	2	0
27	V	25	0	0	1	0
27	W	18	0	0	0	0
27	X	21	0	0	2	0
27	Y	17	0	0	0	0
27	Z	15	0	0	1	0
All	All	32488	0	31294	523	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 8.

All (523) 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)
7:G:84:LYS:HD2	7:G:84:LYS:H	1.18	1.05
7:T:84:LYS:H	7:T:84:LYS:HD2	1.20	1.02
21:O:1230:PSC:H142	21:O:1230:PSC:H343	1.42	1.01
10:W:33:ARG:HG2	22:W:1060:CHD:H152	1.40	1.00
21:B:230:PSC:H343	21:B:230:PSC:H142	1.44	0.99
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.47	0.96
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.29	0.96
3:P:63:ARG:HE	26:P:1270:CDL:HA22	1.30	0.95
4:D:34:SER:H	4:D:37:GLN:HE21	1.10	0.94
26:C:270:CDL:H642	26:C:270:CDL:H191	1.50	0.93
18:N:1522:TGL:HC62	18:N:1522:TGL:HC22	1.52	0.92
25:C:264:PEK:H102	25:C:264:PEK:H161	1.51	0.91
26:P:1270:CDL:H642	26:P:1270:CDL:H191	1.50	0.91
18:L:522:TGL:HC62	18:L:522:TGL:HC22	1.53	0.91
25:P:1264:PEK:H102	25:P:1264:PEK:H161	1.54	0.88
6:S:85:CYS:SG	6:S:87:THR:HG23	2.12	0.87
26:G:269:CDL:H541	26:G:269:CDL:H231	1.55	0.87
6:S:94:HIS:CD2	6:S:95:GLN:H	1.94	0.86
26:T:1269:CDL:H541	26:T:1269:CDL:H231	1.57	0.85
7:G:5:LYS:HB2	25:G:1263:PEK:H362	1.60	0.84
7:T:31:CYS:SG	26:T:1269:CDL:H532	2.18	0.83
6:F:85:CYS:SG	6:F:87:THR:HG23	2.20	0.82
12:L:20:ARG:HH12	18:L:522:TGL:HC61	1.44	0.81
18:N:1522:TGL:HC31	12:Y:13:PHE:HA	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:13:PHE:HA	18:L:522:TGL:HC31	1.63	0.80
7:T:5:LYS:HG3	25:T:263:PEK:H383	1.61	0.79
26:G:269:CDL:H622	19:P:1268:PGV:H152	1.62	0.79
2:O:41:ILE:HD13	21:O:1230:PSC:H342	1.65	0.79
1:A:278:MET:SD	7:T:5:LYS:HB3	2.24	0.77
1:N:113:LEU:HB3	27:N:4646:HOH:O	1.82	0.77
18:L:522:TGL:H242	18:L:522:TGL:H202	1.68	0.76
18:B:521:TGL:H281	18:B:521:TGL:H102	1.67	0.76
6:S:75:HIS:H	6:S:80:GLN:HE22	1.35	0.74
18:N:1522:TGL:H202	18:N:1522:TGL:H242	1.68	0.74
18:N:1521:TGL:H281	18:N:1521:TGL:H102	1.68	0.74
2:O:224:ALA:O	2:O:227:LEU:HG	1.87	0.74
10:J:33:ARG:HG2	22:J:60:CHD:H152	1.68	0.73
1:N:1:FME:HCN	1:N:4:ASN:H	1.54	0.73
6:S:94:HIS:CG	6:S:95:GLN:H	2.04	0.73
13:M:42:LYS:HE3	13:M:42:LYS:HA	1.70	0.72
1:N:296:GLY:HA2	8:U:23:GLN:OE1	1.89	0.72
18:N:1521:TGL:C28	18:N:1521:TGL:H102	2.20	0.72
18:B:521:TGL:H102	18:B:521:TGL:C28	2.20	0.71
7:G:31:CYS:SG	26:G:269:CDL:H532	2.29	0.71
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.73	0.71
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.72	0.71
7:T:38:HIS:NE2	26:T:1269:CDL:H111	2.06	0.71
1:N:472:ILE:HG21	18:N:1522:TGL:HA92	1.71	0.70
3:P:67:PHE:HE1	26:P:1270:CDL:H1	1.55	0.70
18:B:521:TGL:H241	18:B:521:TGL:H201	1.74	0.70
3:C:160:LEU:HD13	22:C:271:CHD:H181	1.71	0.70
1:N:334:TRP:CZ3	18:N:1523:TGL:HA51	2.27	0.69
1:A:472:ILE:HG21	18:L:522:TGL:HA92	1.75	0.69
19:C:268:PGV:H152	26:T:1269:CDL:H622	1.74	0.69
3:P:246:ASP:HB2	27:P:4318:HOH:O	1.93	0.69
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.58	0.69
7:G:5:LYS:HB3	1:N:278:MET:SD	2.34	0.68
8:H:23:GLN:HG3	27:H:4369:HOH:O	1.92	0.68
18:N:1521:TGL:H201	18:N:1521:TGL:H241	1.74	0.68
26:G:269:CDL:C23	26:G:269:CDL:H541	2.23	0.68
21:B:230:PSC:H072	9:I:10:ARG:HH21	1.59	0.68
6:S:94:HIS:CD2	6:S:95:GLN:N	2.62	0.67
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.59	0.67
26:T:1269:CDL:H541	26:T:1269:CDL:C23	2.25	0.67
19:C:267:PGV:H172	26:C:270:CDL:H662	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:3:ALA:HB1	25:T:263:PEK:H382	1.77	0.67
7:T:84:LYS:N	7:T:84:LYS:HD2	2.04	0.66
2:B:41:ILE:HD13	21:B:230:PSC:H342	1.77	0.66
7:G:5:LYS:HG3	25:G:1263:PEK:H383	1.77	0.66
26:P:1270:CDL:H391	27:P:4876:HOH:O	1.95	0.66
5:R:89:LEU:O	5:R:93:LEU:HG	1.96	0.66
21:B:230:PSC:C07	9:I:10:ARG:HH21	2.08	0.66
11:X:54:ARG:NH2	11:X:54:ARG:HG3	2.09	0.66
4:D:34:SER:H	4:D:37:GLN:NE2	1.91	0.66
19:P:1267:PGV:H12	19:P:1267:PGV:H161	1.77	0.66
3:C:67:PHE:HE1	26:C:270:CDL:H1	1.60	0.66
12:L:20:ARG:HH22	18:L:522:TGL:HC32	1.61	0.65
1:A:334:TRP:CZ3	18:A:523:TGL:HA51	2.31	0.65
1:N:378:HIS:O	1:N:382:SER:HB2	1.96	0.65
18:N:1521:TGL:H161	2:O:7:LEU:HD11	1.78	0.65
7:G:84:LYS:N	7:G:84:LYS:HD2	2.02	0.65
18:N:1523:TGL:HC21	18:N:1523:TGL:HG11	1.77	0.65
19:C:267:PGV:H12	19:C:267:PGV:H161	1.77	0.64
12:Y:20:ARG:HB3	12:Y:20:ARG:HH11	1.63	0.64
18:A:523:TGL:HG11	18:A:523:TGL:HC21	1.80	0.64
3:P:160:LEU:HD13	22:P:1271:CHD:H181	1.80	0.64
2:O:217:LYS:HE2	2:O:217:LYS:HA	1.80	0.64
21:O:1230:PSC:H071	9:V:10:ARG:HE	1.62	0.63
26:T:1269:CDL:H172	26:T:1269:CDL:H511	1.81	0.63
7:G:84:LYS:H	7:G:84:LYS:CD	2.01	0.63
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.81	0.63
3:P:168:THR:HG22	25:P:1265:PEK:H14	1.81	0.62
3:P:51:MET:HB3	26:P:1270:CDL:H622	1.80	0.62
21:O:1230:PSC:H142	21:O:1230:PSC:C34	2.25	0.62
21:O:1230:PSC:C07	9:V:10:ARG:HE	2.12	0.62
12:L:24:MET:SD	18:L:522:TGL:H162	2.38	0.62
6:F:8:THR:OG1	6:F:11:GLU:HG3	2.00	0.62
1:A:484:THR:HB	13:M:2:THR:OG1	1.99	0.62
19:N:1524:PGV:H152	19:N:1524:PGV:H321	1.81	0.62
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.82	0.62
17:N:515:HEA:HMC1	17:N:515:HEA:HBC1	1.82	0.62
3:P:210:ILE:HG23	19:P:1267:PGV:H102	1.82	0.62
18:A:523:TGL:HC51	27:B:4817:HOH:O	2.00	0.62
6:F:92:VAL:O	6:F:92:VAL:HG23	1.99	0.61
1:N:449:MET:SD	2:O:5:MET:HG2	2.41	0.61
9:V:65:LYS:O	11:X:54:ARG:NH1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.81	0.61
21:O:1230:PSC:H222	21:O:1230:PSC:H21	1.81	0.61
26:G:269:CDL:H511	26:G:269:CDL:H172	1.82	0.61
4:Q:58:GLU:O	4:Q:62:LEU:HG	2.02	0.60
2:O:57:ASP:H	21:O:1230:PSC:H201	1.66	0.60
19:A:524:PGV:H302	13:M:19:LEU:HD23	1.82	0.59
1:A:282:PHE:HA	7:T:4:ALA:CB	2.32	0.59
3:C:51:MET:HB3	26:C:270:CDL:H622	1.84	0.59
21:B:230:PSC:C34	21:B:230:PSC:H142	2.27	0.59
21:B:230:PSC:H21	21:B:230:PSC:H222	1.84	0.59
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.37	0.59
19:A:524:PGV:H152	19:A:524:PGV:H321	1.84	0.59
2:B:62:GLU:O	2:B:66:THR:HB	2.03	0.59
10:J:7:GLU:HG3	27:J:4832:HOH:O	2.02	0.59
18:N:1521:TGL:HB91	2:O:32:PHE:HE2	1.68	0.59
19:P:1267:PGV:H172	26:P:1270:CDL:H662	1.84	0.58
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.86	0.58
18:B:521:TGL:HA82	18:B:521:TGL:H222	1.85	0.58
18:N:1521:TGL:H222	18:N:1521:TGL:HA82	1.85	0.58
1:N:51:ASP:OD1	2:O:206:PHE:HE1	1.85	0.58
3:P:34:TRP:CZ2	23:P:1272:DMU:H29	2.38	0.58
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.85	0.58
1:N:113:LEU:CD1	18:N:1522:TGL:H292	2.34	0.58
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.17	0.58
3:C:213:THR:HG23	26:C:270:CDL:H762	1.86	0.58
12:L:20:ARG:NH1	18:L:522:TGL:HC61	2.14	0.58
3:P:213:THR:HG23	26:P:1270:CDL:H762	1.85	0.57
18:B:521:TGL:HC22	27:I:2383:HOH:O	2.03	0.57
1:N:472:ILE:HG21	18:N:1522:TGL:CA9	2.34	0.57
26:G:269:CDL:H522	26:G:269:CDL:H202	1.87	0.57
26:T:1269:CDL:HA62	26:T:1269:CDL:H322	1.86	0.57
1:A:449:MET:SD	2:B:5:MET:HG2	2.45	0.57
25:C:264:PEK:H102	25:C:264:PEK:C16	2.31	0.57
1:A:377:PHE:O	1:A:381:LEU:HB3	2.05	0.57
26:G:269:CDL:HB32	1:N:304:TYR:HD1	1.68	0.57
7:T:5:LYS:HD2	25:T:263:PEK:H371	1.86	0.57
27:P:4928:HOH:O	10:W:1:PHE:HE2	1.88	0.56
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.20	0.56
1:N:472:ILE:HD13	18:N:1522:TGL:HA91	1.88	0.56
1:A:321:PHE:CD2	21:B:230:PSC:H341	2.40	0.56
3:C:34:TRP:HZ2	23:C:272:DMU:H29	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.54	0.56
1:A:17:THR:OG1	18:L:522:TGL:H281	2.05	0.56
4:D:20:ARG:HG3	27:D:4319:HOH:O	2.04	0.56
26:G:269:CDL:HA62	26:G:269:CDL:H322	1.86	0.56
1:N:333:LYS:HD2	27:N:4741:HOH:O	2.06	0.56
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.88	0.56
1:A:472:ILE:HG21	18:L:522:TGL:CA9	2.36	0.56
1:A:377:PHE:CD1	17:A:516:HEA:HAD1	2.41	0.55
12:L:20:ARG:NH2	18:L:522:TGL:HC32	2.21	0.55
7:G:2:SER:O	25:G:1263:PEK:H322	2.06	0.55
1:A:406:ASN:HD21	19:A:524:PGV:H21	1.72	0.55
4:D:34:SER:N	4:D:37:GLN:HE21	1.93	0.55
12:L:20:ARG:HH22	18:L:522:TGL:HC61	1.71	0.55
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.07	0.55
1:A:136:LEU:HB2	27:A:4400:HOH:O	2.06	0.55
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.42	0.54
19:A:524:PGV:H062	27:M:2160:HOH:O	2.06	0.54
5:R:48:ILE:O	5:R:52:LEU:HG	2.06	0.54
7:T:45:PRO:HD2	27:T:3152:HOH:O	2.06	0.54
6:F:64:GLU:O	6:F:65:ASP:HB2	2.08	0.54
26:C:270:CDL:H661	26:C:270:CDL:H242	1.90	0.54
25:P:1264:PEK:H102	25:P:1264:PEK:C16	2.33	0.54
26:T:1269:CDL:H522	26:T:1269:CDL:H202	1.89	0.54
8:U:23:GLN:HG3	27:U:4331:HOH:O	2.08	0.54
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.73	0.54
5:R:12:ASP:HA	5:R:47:ILE:HD11	1.90	0.54
4:D:34:SER:O	4:D:38:LYS:HG3	2.08	0.54
7:G:37:LEU:HD21	26:G:269:CDL:H361	1.89	0.54
10:J:40:LEU:HD12	22:J:60:CHD:H183	1.89	0.54
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.90	0.54
11:K:24:PHE:O	11:K:28:VAL:HG12	2.08	0.54
18:N:1521:TGL:HB91	2:O:32:PHE:CE2	2.42	0.54
1:N:406:ASN:HD21	19:N:1524:PGV:H21	1.73	0.54
1:N:52:GLN:O	1:N:56:VAL:HG23	2.08	0.54
1:A:1:FME:HCN	1:A:4:ASN:H	1.73	0.53
3:C:246:ASP:HB2	27:C:4168:HOH:O	2.07	0.53
1:A:177:SER:H	1:A:180:GLN:HE21	1.54	0.53
3:C:187:THR:HG22	25:C:264:PEK:H052	1.90	0.53
26:P:1270:CDL:H642	26:P:1270:CDL:C19	2.32	0.53
2:B:91:ASN:HD21	2:B:183:THR:HG21	1.73	0.53
25:C:265:PEK:H031	27:O:4672:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:HIS:O	1:A:382:SER:HB2	2.08	0.53
12:Y:20:ARG:HB3	12:Y:20:ARG:NH1	2.22	0.53
3:C:34:TRP:CZ2	23:C:272:DMU:H29	2.44	0.53
5:E:31:LYS:HE3	6:F:83:PRO:O	2.09	0.53
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.44	0.53
25:C:264:PEK:H32	25:C:264:PEK:H71	1.91	0.53
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.91	0.53
26:P:1270:CDL:H242	26:P:1270:CDL:H661	1.91	0.53
3:P:47:LEU:O	3:P:51:MET:HG2	2.09	0.53
26:C:270:CDL:C19	26:C:270:CDL:H642	2.33	0.53
10:J:56:PRO:HD3	12:L:46:LYS:HE3	1.91	0.53
25:P:1265:PEK:C38	26:T:1269:CDL:H273	2.38	0.53
25:C:265:PEK:C38	26:G:269:CDL:H273	2.39	0.53
1:N:482:VAL:HG13	13:Z:1:ILE:HD11	1.90	0.53
11:X:52:GLU:HB3	27:X:4935:HOH:O	2.08	0.52
4:D:86:MET:HE3	27:K:4869:HOH:O	2.09	0.52
7:G:3:ALA:HB1	25:G:1263:PEK:H382	1.91	0.52
13:M:42:LYS:CE	13:M:42:LYS:HA	2.38	0.52
1:N:87:ILE:O	1:N:173:PRO:HD3	2.08	0.52
2:B:56:MET:HG2	21:B:230:PSC:H211	1.91	0.52
19:C:267:PGV:H12	19:C:267:PGV:C16	2.40	0.52
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.91	0.52
8:U:7:LYS:O	8:U:8:ILE:HG22	2.10	0.52
1:N:514:LYS:HE3	27:N:3395:HOH:O	2.09	0.52
4:Q:86:MET:HE1	27:X:4838:HOH:O	2.08	0.52
7:T:3:ALA:O	7:T:4:ALA:HB2	2.09	0.52
3:P:168:THR:CG2	25:P:1265:PEK:H14	2.39	0.52
5:R:37:VAL:HG11	5:R:70:VAL:HG21	1.91	0.52
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.91	0.52
2:O:59:GLN:HG3	2:O:59:GLN:O	2.10	0.52
18:N:1521:TGL:HC22	27:Q:3383:HOH:O	2.09	0.52
1:N:406:ASN:HD21	19:N:1524:PGV:C2	2.23	0.52
1:N:407:ASP:O	1:N:411:LYS:HG3	2.10	0.52
17:N:516:HEA:HMD1	17:N:516:HEA:HBD2	1.92	0.52
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.41	0.52
1:A:297:MET:HE2	1:A:302:ARG:HG2	1.92	0.51
25:P:1264:PEK:H71	25:P:1264:PEK:H32	1.92	0.51
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.10	0.51
17:A:515:HEA:HMC1	17:A:515:HEA:HBC1	1.92	0.51
7:G:17:ARG:HD2	27:G:2309:HOH:O	2.10	0.51
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:290:HIS:CD2	1:N:291:HIS:CD2	2.99	0.51
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.92	0.51
25:C:265:PEK:H292	27:O:4536:HOH:O	2.11	0.51
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.93	0.50
1:N:481:GLU:HB2	13:Z:4:LYS:HE2	1.93	0.50
1:A:406:ASN:HD21	19:A:524:PGV:C2	2.24	0.50
2:B:128:LEU:HD11	2:B:134:ARG:HA	1.93	0.50
6:S:76:LYS:HE3	6:S:93:PRO:HG3	1.92	0.50
1:N:177:SER:H	1:N:180:GLN:NE2	2.10	0.50
6:S:19:GLU:HG2	27:S:4579:HOH:O	2.10	0.50
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.12	0.50
7:G:3:ALA:O	7:G:4:ALA:HB2	2.11	0.50
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.94	0.50
4:Q:82:VAL:O	4:Q:86:MET:HG3	2.12	0.50
3:C:168:THR:HG22	25:C:265:PEK:H14	1.92	0.49
25:C:265:PEK:H383	26:G:269:CDL:H273	1.92	0.49
11:K:42:PRO:HG2	11:K:47:ARG:HE	1.77	0.49
4:Q:52:SER:OG	4:Q:55:GLU:HG3	2.11	0.49
2:O:203:ASN:HD22	2:O:203:ASN:N	2.10	0.49
17:A:516:HEA:HMD1	17:A:516:HEA:HBD2	1.93	0.49
2:B:41:ILE:O	2:B:45:MET:HG2	2.13	0.49
18:L:522:TGL:C24	18:L:522:TGL:H202	2.41	0.49
2:O:41:ILE:CD1	21:O:1230:PSC:H342	2.39	0.49
18:N:1522:TGL:HG2	12:Y:12:PRO:HB2	1.93	0.49
2:B:7:LEU:HD11	18:B:521:TGL:H161	1.94	0.49
5:E:71:VAL:HG11	5:E:85:VAL:HG11	1.95	0.49
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.77	0.49
6:S:51:SER:O	6:S:94:HIS:N	2.46	0.49
19:N:1524:PGV:H311	13:Z:16:ALA:HA	1.95	0.49
1:A:113:LEU:HB3	27:A:4608:HOH:O	2.12	0.49
7:G:2:SER:OG	25:G:1263:PEK:H301	2.13	0.49
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.95	0.49
4:Q:127:LYS:O	4:Q:130:PRO:HD3	2.13	0.49
1:A:472:ILE:HD13	18:L:522:TGL:HA91	1.94	0.48
25:P:1265:PEK:H383	26:T:1269:CDL:H273	1.95	0.48
1:N:113:LEU:HD12	18:N:1522:TGL:H292	1.93	0.48
1:N:34:SER:HB2	17:N:515:HEA:C2B	2.44	0.48
2:O:62:GLU:O	2:O:66:THR:HB	2.13	0.48
1:A:1:FME:HA	1:A:1:FME:CE	2.43	0.48
6:S:22:LEU:HD12	27:S:4871:HOH:O	2.13	0.48
4:Q:138:TRP:CH2	11:X:50:PRO:HG2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.12	0.48
1:N:321:PHE:CD2	21:O:1230:PSC:H341	2.48	0.48
19:A:524:PGV:H311	13:M:16:ALA:HA	1.96	0.48
7:G:7:ASP:O	1:N:169:ILE:HD12	2.14	0.48
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.96	0.48
18:N:1523:TGL:H363	27:O:4849:HOH:O	2.13	0.47
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.96	0.47
2:O:56:MET:HG2	21:O:1230:PSC:H211	1.95	0.47
1:A:240:HIS:O	1:A:243:VAL:HG22	2.15	0.47
19:C:267:PGV:H182	26:C:270:CDL:H673	1.97	0.47
5:E:84:TYR:CZ	5:E:88:GLU:HG3	2.49	0.47
1:N:17:THR:OG1	18:N:1522:TGL:H281	2.14	0.47
1:N:76:GLY:O	1:N:80:ASN:HB2	2.14	0.47
10:W:40:LEU:HD12	22:W:1060:CHD:H183	1.97	0.47
1:A:177:SER:H	1:A:180:GLN:NE2	2.11	0.47
2:O:56:MET:HA	21:O:1230:PSC:H202	1.96	0.47
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.96	0.47
8:H:49:ASP:O	8:H:52:VAL:HG22	2.15	0.47
3:P:168:THR:HG21	25:P:1265:PEK:H12	1.97	0.47
8:U:49:ASP:O	8:U:52:VAL:HG22	2.15	0.47
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.97	0.47
23:C:272:DMU:H30	23:C:272:DMU:O1	2.15	0.47
7:G:5:LYS:HD3	1:N:278:MET:HB3	1.96	0.47
5:R:87:GLN:HG2	5:R:88:GLU:N	2.30	0.47
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.96	0.47
21:B:230:PSC:H12	21:B:230:PSC:H322	1.97	0.47
9:I:5:ALA:O	9:I:7:PRO:HD3	2.15	0.47
1:N:151:HIS:CD2	25:P:1264:PEK:H382	2.50	0.47
7:T:2:SER:O	7:T:3:ALA:HB3	2.15	0.47
22:W:1060:CHD:H161	22:W:1060:CHD:H212	1.75	0.47
3:C:244:PHE:HA	25:T:263:PEK:H9	1.98	0.46
18:L:522:TGL:H272	18:L:522:TGL:H231	1.97	0.46
21:O:1230:PSC:H322	21:O:1230:PSC:H12	1.98	0.46
4:Q:101:HIS:HD2	4:Q:102:TYR:CD2	2.34	0.46
2:B:164:ALA:O	2:B:194:GLY:HA3	2.15	0.46
26:P:1270:CDL:H532	26:P:1270:CDL:H561	1.63	0.46
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.50	0.46
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.14	0.46
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.44	0.46
2:O:68:LEU:CB	2:O:69:PRO:HD3	2.46	0.46
6:S:92:VAL:HG23	6:S:92:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:399:LEU:HB2	1:N:494:TRP:CZ3	2.51	0.46
2:O:202:SER:HB2	2:O:203:ASN:HD22	1.81	0.46
8:U:36:PHE:CD1	8:U:57:ARG:HB2	2.50	0.46
7:G:5:LYS:HD2	25:G:1263:PEK:H371	1.98	0.46
18:N:1522:TGL:H202	18:N:1522:TGL:C24	2.41	0.46
19:P:1267:PGV:H12	19:P:1267:PGV:C16	2.40	0.46
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.16	0.46
1:A:422:ASN:HB3	18:B:521:TGL:H242	1.97	0.46
2:B:102:HIS:O	2:B:104:TRP:HA	2.16	0.46
4:D:75:THR:HB	27:D:2332:HOH:O	2.16	0.46
1:N:422:ASN:HB3	18:N:1521:TGL:H242	1.98	0.46
6:F:25:ARG:HD2	27:F:4476:HOH:O	2.16	0.46
7:G:45:PRO:HD2	27:G:2152:HOH:O	2.15	0.46
19:N:1524:PGV:H062	27:Z:3160:HOH:O	2.15	0.46
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.51	0.46
1:A:513:LEU:HD22	1:A:513:LEU:HA	1.79	0.45
2:B:57:ASP:H	21:B:230:PSC:H201	1.81	0.45
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.46	0.45
1:A:113:LEU:HD12	18:L:522:TGL:H292	1.97	0.45
2:O:216:LEU:O	2:O:219:PHE:HB3	2.17	0.45
4:D:106:PRO:HA	27:D:4808:HOH:O	2.16	0.45
18:N:1523:TGL:HG11	18:N:1523:TGL:CC2	2.45	0.45
6:S:87:THR:HG21	27:S:3339:HOH:O	2.16	0.45
6:S:22:LEU:O	6:S:25:ARG:HB3	2.16	0.45
5:E:41:LEU:HA	27:I:2336:HOH:O	2.16	0.45
1:N:71:MET:HE3	1:N:195:LEU:HD21	1.99	0.45
1:N:377:PHE:CD1	17:N:516:HEA:HAD1	2.51	0.45
6:S:55:LYS:HA	6:S:74:LEU:O	2.17	0.45
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.16	0.45
2:O:121:TYR:O	2:O:138:VAL:HA	2.16	0.45
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.99	0.45
6:S:64:GLU:O	6:S:65:ASP:HB2	2.16	0.45
26:C:270:CDL:H532	26:C:270:CDL:H561	1.66	0.45
1:A:229:ILE:HD11	2:B:175:ILE:CD1	2.46	0.45
7:G:4:ALA:CB	1:N:282:PHE:HA	2.47	0.45
1:N:456:MET:HG2	4:Q:96:LEU:HD13	1.99	0.45
26:P:1270:CDL:H112	27:P:4853:HOH:O	2.16	0.45
3:P:187:THR:HG22	25:P:1264:PEK:H052	1.99	0.45
26:G:269:CDL:H601	26:G:269:CDL:H571	1.63	0.44
3:P:5:THR:HG22	6:S:96:LEU:HD13	1.99	0.44
6:F:92:VAL:O	6:F:92:VAL:CG2	2.63	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:62:ALA:HB2	17:N:515:HEA:HBD1	1.98	0.44
2:O:41:ILE:O	2:O:45:MET:HG2	2.16	0.44
26:P:1270:CDL:H602	26:P:1270:CDL:H632	1.59	0.44
1:N:82:LEU:O	1:N:86:MET:HG3	2.17	0.44
3:P:34:TRP:HE1	23:P:1272:DMU:H29	1.81	0.44
3:P:40:MET:O	3:P:44:MET:HG2	2.18	0.44
6:S:94:HIS:CG	6:S:95:GLN:N	2.80	0.44
1:A:52:GLN:O	1:A:56:VAL:HG23	2.18	0.44
5:R:52:LEU:O	5:R:55:CYS:HB2	2.16	0.44
10:J:50:LEU:HD22	10:J:50:LEU:O	2.18	0.44
18:L:522:TGL:CC2	18:L:522:TGL:HC62	2.29	0.44
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.80	0.44
19:P:1267:PGV:H182	26:P:1270:CDL:H673	1.99	0.44
25:C:265:PEK:H383	26:G:269:CDL:C27	2.48	0.44
1:N:292:MET:O	1:N:295:VAL:HG22	2.18	0.44
1:N:484:THR:HA	27:N:4470:HOH:O	2.18	0.44
26:P:1270:CDL:H171	26:P:1270:CDL:H202	1.79	0.44
6:S:18:ARG:HG2	27:S:4871:HOH:O	2.18	0.44
7:T:2:SER:O	25:T:263:PEK:H322	2.17	0.44
8:U:20:PHE:HE2	8:U:27:ARG:HG2	1.83	0.44
1:N:321:PHE:CZ	21:O:1230:PSC:H171	2.53	0.44
1:N:405:LEU:HD23	1:N:475:ALA:HB2	2.00	0.44
3:P:34:TRP:HZ2	23:P:1272:DMU:H29	1.80	0.44
18:A:523:TGL:HG11	18:A:523:TGL:CC2	2.45	0.44
7:G:50:TYR:HB3	7:G:52:HIS:CE1	2.52	0.44
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.75	0.44
18:N:1522:TGL:H272	18:N:1522:TGL:H231	1.99	0.44
26:G:269:CDL:H212	1:N:311:ILE:HD12	2.00	0.44
2:O:83:ILE:O	2:O:87:MET:HG3	2.18	0.44
3:P:34:TRP:HE1	23:P:1272:DMU:C57	2.30	0.44
7:T:84:LYS:H	7:T:84:LYS:CD	2.04	0.44
10:W:58:LYS:HE3	12:Y:47:LYS:HE3	2.00	0.44
11:X:24:PHE:O	11:X:28:VAL:HG12	2.18	0.44
1:A:297:MET:CE	1:A:302:ARG:HG2	2.48	0.43
1:A:390:MET:O	1:A:394:VAL:HG13	2.18	0.43
19:A:524:PGV:H152	19:A:524:PGV:H301	2.00	0.43
4:D:9:GLU:CD	4:D:9:GLU:H	2.21	0.43
1:N:95:PRO:HG2	3:P:11:VAL:CG2	2.48	0.43
6:S:75:HIS:H	6:S:80:GLN:NE2	2.10	0.43
6:F:55:LYS:HA	6:F:74:LEU:O	2.18	0.43
1:N:115:SER:O	1:N:121:GLY:HA2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:50:VAL:HG23	27:U:4689:HOH:O	2.19	0.43
7:G:36:TRP:HA	7:G:36:TRP:CE3	2.53	0.43
12:L:12:PRO:HB2	18:L:522:TGL:HG2	2.00	0.43
1:N:242:GLU:HA	1:N:245:ILE:HD12	2.00	0.43
19:N:1524:PGV:H12	4:Q:87:PHE:CD2	2.53	0.43
1:A:431:LEU:HD21	1:A:450:TRP:HB2	2.00	0.43
22:B:1086:CHD:H212	22:B:1086:CHD:H12	2.00	0.43
2:O:102:HIS:O	2:O:104:TRP:HA	2.18	0.43
3:P:158:HIS:NE2	25:P:1265:PEK:H051	2.34	0.43
3:P:34:TRP:NE1	23:P:1272:DMU:H29	2.34	0.43
5:R:81:ILE:HG12	9:V:7:PRO:HG2	2.00	0.43
3:C:47:LEU:O	3:C:51:MET:HG2	2.18	0.43
8:H:27:ARG:NH1	27:H:2303:HOH:O	2.51	0.43
12:L:20:ARG:NH2	18:L:522:TGL:HC61	2.33	0.43
1:A:282:PHE:HZ	26:T:1269:CDL:H761	1.84	0.43
9:V:35:TYR:C	9:V:37:PHE:H	2.22	0.43
25:G:1263:PEK:H182	3:P:98:PHE:CD2	2.54	0.43
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.54	0.43
1:A:304:TYR:HD1	26:T:1269:CDL:HB32	1.84	0.43
13:Z:11:SER:OG	13:Z:14:GLU:HG3	2.18	0.43
12:L:46:LYS:O	12:L:47:LYS:HB2	2.19	0.43
1:N:351:GLY:HA3	1:N:380:VAL:HG13	2.01	0.43
4:Q:48:TRP:HB2	5:R:96:LEU:O	2.19	0.43
26:T:1269:CDL:H571	26:T:1269:CDL:H601	1.63	0.43
7:T:38:HIS:CD2	26:T:1269:CDL:HA21	2.53	0.43
1:A:106:PRO:HB2	1:A:107:PRO:HD3	2.01	0.43
3:C:210:ILE:HG23	19:C:267:PGV:H102	2.00	0.43
7:G:2:SER:O	7:G:3:ALA:HB3	2.19	0.43
7:G:36:TRP:HA	7:G:36:TRP:HE3	1.84	0.43
8:H:43:MET:HE3	8:H:49:ASP:N	2.34	0.43
22:O:229:CHD:H212	22:O:229:CHD:H12	1.99	0.43
6:S:53:THR:HB	6:S:54:ASN:H	1.65	0.43
25:P:1265:PEK:H383	26:T:1269:CDL:C27	2.48	0.43
6:F:51:SER:HB2	6:F:91:LEU:HD11	2.00	0.42
9:I:35:TYR:C	9:I:37:PHE:H	2.22	0.42
4:Q:130:PRO:HG2	4:Q:131:ILE:HD12	2.01	0.42
1:A:87:ILE:O	1:A:173:PRO:HD3	2.19	0.42
1:A:92:MET:O	1:A:95:PRO:HD3	2.18	0.42
3:C:76:GLN:O	3:C:80:ARG:HG3	2.19	0.42
1:N:23:GLY:HA3	1:N:73:ILE:HG13	2.01	0.42
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:44:PRO:HG2	4:Q:111:PHE:CZ	2.54	0.42
1:N:225:GLY:HA3	3:P:112:LEU:HD21	2.01	0.42
23:P:1272:DMU:H25	25:P:1264:PEK:H341	2.01	0.42
3:C:158:HIS:CE1	25:C:265:PEK:H051	2.54	0.42
1:N:400:PHE:HB3	18:N:1522:TGL:C28	2.49	0.42
4:Q:48:TRP:CH2	5:R:56:ARG:HA	2.55	0.42
7:T:25:LEU:HA	7:T:25:LEU:HD23	1.88	0.42
22:C:271:CHD:H222	22:C:271:CHD:H162	1.76	0.42
5:E:84:TYR:O	5:E:88:GLU:HG2	2.19	0.42
26:G:269:CDL:HB32	1:N:304:TYR:CD1	2.50	0.42
2:O:56:MET:HA	21:O:1230:PSC:C20	2.50	0.42
2:O:145:PRO:HB2	2:O:148:MET:HG3	2.01	0.42
26:T:1269:CDL:H571	26:T:1269:CDL:H771	2.01	0.42
8:U:36:PHE:CE1	8:U:57:ARG:HB2	2.54	0.42
1:A:513:LEU:O	1:A:514:LYS:HB2	2.20	0.42
12:L:11:ILE:CG2	18:L:522:TGL:H271	2.49	0.42
1:N:42:GLY:HA3	4:Q:104:TYR:OH	2.19	0.42
1:N:53:ILE:HG12	27:N:3076:HOH:O	2.19	0.42
2:O:82:ARG:HG2	2:O:86:MET:HE3	2.01	0.42
4:D:144:GLU:OE1	4:D:147:LYS:HE3	2.19	0.42
25:G:1263:PEK:H9	3:P:244:PHE:HA	2.02	0.42
13:M:42:LYS:HE3	13:M:42:LYS:CA	2.45	0.42
1:N:483:LEU:HD23	1:N:483:LEU:HA	1.85	0.42
21:O:1230:PSC:H62	21:O:1230:PSC:H241	2.01	0.42
1:N:514:LYS:HA	6:S:38:ALA:HB3	2.02	0.42
9:V:15:ARG:HD2	27:V:4749:HOH:O	2.19	0.42
1:A:62:ALA:HB2	17:A:515:HEA:HBD1	2.02	0.42
3:C:164:PHE:CE1	22:C:271:CHD:H192	2.55	0.42
26:T:1269:CDL:H251	26:T:1269:CDL:H222	1.90	0.42
2:B:75:LEU:HA	2:B:75:LEU:HD12	1.89	0.42
26:C:270:CDL:H602	26:C:270:CDL:H632	1.59	0.42
1:N:400:PHE:HB3	18:N:1522:TGL:H283	2.02	0.42
2:O:98:LYS:HG2	2:O:153:LEU:HB2	2.01	0.42
1:A:376:HIS:O	1:A:380:VAL:HG22	2.19	0.42
2:B:4:PRO:HB2	11:K:43:SER:HA	2.02	0.42
10:W:33:ARG:CG	22:W:1060:CHD:H152	2.29	0.42
3:C:116:TRP:HA	3:C:117:PRO:C	2.39	0.41
2:O:164:ALA:O	2:O:194:GLY:HA3	2.19	0.41
2:O:42:ILE:O	2:O:46:LEU:HG	2.19	0.41
3:P:137:LEU:HA	3:P:137:LEU:HD23	1.88	0.41
1:A:195:LEU:HD23	1:A:245:ILE:HD13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:G:269:CDL:H152	26:G:269:CDL:H181	1.85	0.41
1:N:489:THR:HA	6:S:71:TRP:O	2.20	0.41
1:N:514:LYS:HE2	27:S:3339:HOH:O	2.19	0.41
4:Q:121:LYS:HG2	11:X:53:TRP:CD1	2.55	0.41
8:U:57:ARG:HA	8:U:60:TYR:CD2	2.55	0.41
1:A:351:GLY:HA3	1:A:380:VAL:HG13	2.02	0.41
2:O:13:THR:HB	2:O:168:LEU:HD23	2.01	0.41
26:T:1269:CDL:H181	26:T:1269:CDL:H152	1.87	0.41
1:A:240:HIS:HB3	1:A:241:PRO:HD3	2.03	0.41
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.08	0.41
21:B:230:PSC:H241	21:B:230:PSC:H62	2.01	0.41
1:N:376:HIS:O	1:N:380:VAL:HG22	2.21	0.41
1:N:351:GLY:C	1:N:380:VAL:HG13	2.41	0.41
1:N:71:MET:HB2	1:N:72:PRO:HD3	2.02	0.41
1:N:440:TYR:CZ	2:O:205:SER:HA	2.56	0.41
13:Z:13:LYS:O	13:Z:17:ILE:HG13	2.19	0.41
19:N:1524:PGV:H152	19:N:1524:PGV:H301	2.02	0.41
3:P:230:ASN:HB2	27:S:3287:HOH:O	2.20	0.41
19:N:1524:PGV:H322	13:Z:19:LEU:HD23	2.02	0.41
1:A:344:PHE:C	1:A:344:PHE:CD1	2.94	0.41
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.55	0.41
3:P:116:TRP:HA	3:P:117:PRO:C	2.40	0.41
23:P:1272:DMU:H30	23:P:1272:DMU:O1	2.21	0.41
25:G:1263:PEK:H042	3:P:77:LYS:NZ	2.36	0.41
1:A:378:HIS:CD2	1:A:382:SER:OG	2.74	0.41
7:G:34:ASN:ND2	26:G:269:CDL:H151	2.35	0.41
1:A:124:THR:HB	27:A:4100:HOH:O	2.20	0.41
1:A:510:TYR:CD2	6:F:49:VAL:HG13	2.56	0.41
26:P:1270:CDL:HB21	26:P:1270:CDL:CB3	2.51	0.41
2:B:81:LEU:HD13	26:T:1269:CDL:H122	2.03	0.41
1:A:1:FME:HE2	1:A:1:FME:HA	2.02	0.41
7:G:8:HIS:HD2	25:G:1263:PEK:H232	1.86	0.41
1:N:95:PRO:HG2	3:P:11:VAL:HG23	2.02	0.41
5:R:82:TYR:N	5:R:83:PRO:CD	2.84	0.41
13:Z:32:TRP:CZ3	13:Z:40:TYR:OH	2.72	0.41
1:A:309:THR:HG22	17:A:516:HEA:HMB2	2.04	0.40
2:O:4:PRO:HB2	11:X:43:SER:HA	2.04	0.40
4:D:20:ARG:HG3	4:D:20:ARG:H	1.69	0.40
26:G:269:CDL:H222	26:G:269:CDL:H251	1.91	0.40
2:O:155:SER:O	2:O:174:ALA:HB1	2.21	0.40
3:P:34:TRP:CE2	23:P:1272:DMU:H29	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:131:ILE:H	4:Q:131:ILE:HD12	1.87	0.40
2:B:23:PHE:CZ	2:B:80:SER:HB2	2.57	0.40
8:H:57:ARG:HA	8:H:60:TYR:CD2	2.56	0.40
4:Q:121:LYS:HG2	11:X:53:TRP:HD1	1.87	0.40
5:R:67:ILE:O	5:R:70:VAL:HG12	2.21	0.40
17:A:516:HEA:HMB1	17:A:516:HEA:H11	1.91	0.40
2:O:132:GLU:HB3	2:O:137:GLU:HG3	2.02	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%)	499 (98%)	13 (2%)	0	100	100
1	N	512/514 (100%)	501 (98%)	11 (2%)	0	100	100
2	B	225/227 (99%)	213 (95%)	10 (4%)	2 (1%)	17	7
2	O	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	17	7
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	34	24
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
5	E	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
6	F	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	4	0
6	S	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	4	0
7	G	81/85 (95%)	66 (82%)	8 (10%)	7 (9%)	1	0
7	T	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	1	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	H	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	5	1
8	U	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	5	1
9	I	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
9	V	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	56 (100%)	0	0	100	100
11	K	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3504/3614 (97%)	3359 (96%)	116 (3%)	29 (1%)	19	9

All (29) 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
6	F	94	HIS
6	F	95	GLN
7	G	3	ALA
7	G	40	GLY
8	H	8	ILE
8	H	46	LYS
7	T	3	ALA
7	T	40	GLY
8	U	8	ILE
8	U	46	LYS
2	B	60	GLU

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Mol	Chain	Res	Type
2	O	60	GLU
6	F	96	LEU
3	P	38	ASN
6	S	96	LEU
7	G	6	GLY
7	T	6	GLY
2	B	92	ASN
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%)	417 (98%)	9 (2%)	53	48
1	N	426/426 (100%)	416 (98%)	10 (2%)	50	45
2	B	210/210 (100%)	200 (95%)	10 (5%)	25	16
2	O	210/210 (100%)	199 (95%)	11 (5%)	23	14
3	C	224/226 (99%)	218 (97%)	6 (3%)	44	38
3	P	224/226 (99%)	220 (98%)	4 (2%)	59	55
4	D	128/129 (99%)	126 (98%)	2 (2%)	62	60
4	Q	128/129 (99%)	124 (97%)	4 (3%)	40	32
5	E	92/95 (97%)	90 (98%)	2 (2%)	52	47
5	R	92/95 (97%)	90 (98%)	2 (2%)	52	47
6	F	81/81 (100%)	79 (98%)	2 (2%)	47	41
6	S	81/81 (100%)	75 (93%)	6 (7%)	13	6
7	G	67/68 (98%)	62 (92%)	5 (8%)	13	5
7	T	67/68 (98%)	62 (92%)	5 (8%)	13	5
8	H	71/75 (95%)	69 (97%)	2 (3%)	43	36
8	U	71/75 (95%)	68 (96%)	3 (4%)	30	20
9	I	57/57 (100%)	54 (95%)	3 (5%)	22	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	V	57/57 (100%)	55 (96%)	2 (4%)	36	27
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	51
10	W	49/50 (98%)	48 (98%)	1 (2%)	55	51
11	K	39/46 (85%)	38 (97%)	1 (3%)	46	39
11	X	39/46 (85%)	37 (95%)	2 (5%)	24	14
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	39
12	Y	39/40 (98%)	37 (95%)	2 (5%)	24	14
13	M	37/38 (97%)	32 (86%)	5 (14%)	4	1
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	2
All	All	3040/3082 (99%)	2935 (96%)	105 (4%)	36	27

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	180	GLN
1	A	238	PHE
1	A	241	PRO
1	A	338	MET
1	A	369	ASP
1	A	380	VAL
1	A	513	LEU
2	B	16	ILE
2	B	33	LEU
2	B	60	GLU
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	113	TYR
2	B	115	ASP
2	B	167	SER
3	C	17	PRO
3	C	127	LEU
3	C	159	MET
3	C	179	SER
3	C	214	PHE
3	C	230	ASN

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Mol	Chain	Res	Type
4	D	4	SER
4	D	51	LEU
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
6	F	96	LEU
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
13	M	4	LYS
13	M	13	LYS
13	M	34	LEU
13	M	38	ASP
13	M	42	LYS
1	N	38	ARG
1	N	109	PHE
1	N	180	GLN
1	N	238	PHE
1	N	241	PRO
1	N	369	ASP
1	N	380	VAL
1	N	444	PRO
1	N	504	THR
1	N	513	LEU
2	O	16	ILE
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

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Mol	Chain	Res	Type
2	O	94	SER
2	O	167	SER
2	O	217	LYS
3	P	29	SER
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	8	SER
4	Q	51	LEU
4	Q	54	ASP
4	Q	121	LYS
5	R	80	GLU
5	R	90	ARG
6	S	37	LYS
6	S	48	LEU
6	S	53	THR
6	S	54	ASN
6	S	80	GLN
6	S	96	LEU
7	T	18	PHE
7	T	33	LEU
7	T	38	HIS
7	T	43	GLU
7	T	54	ARG
8	U	21	PRO
8	U	29	CYS
8	U	60	TYR
9	V	8	GLN
9	V	61	GLU
10	W	50	LEU
11	X	47	ARG
11	X	54	ARG
12	Y	20	ARG
12	Y	26	THR
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	98	ASN
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
4	D	37	GLN
4	D	109	HIS
5	E	94	ASN
9	I	8	GLN
9	I	53	ASN
10	J	29	ASN
11	K	35	GLN
1	N	80	ASN
1	N	98	ASN
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	91	ASN
2	O	181	GLN
2	O	195	GLN
2	O	203	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
9	V	8	GLN
10	W	57	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	FME	N	1	1	8,9,10	0.80	0	7,9,11	1.81	2 (28%)
1	FME	A	1	1	8,9,10	0.64	0	7,9,11	1.28	1 (14%)
7	TPO	T	11	7	8,10,11	1.24	1 (12%)	10,14,16	1.03	0
2	FME	O	1	2	8,9,10	0.72	0	7,9,11	2.13	2 (28%)
7	TPO	G	11	7	8,10,11	1.61	1 (12%)	10,14,16	0.99	0
9	SAC	V	1	9	7,8,9	2.75	2 (28%)	8,9,11	3.15	5 (62%)
2	FME	B	1	2	8,9,10	0.83	0	7,9,11	2.14	2 (28%)
9	SAC	I	1	9	7,8,9	2.41	2 (28%)	8,9,11	2.99	4 (50%)

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	-	3/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
7	TPO	T	11	7	-	4/9/11/13	-
2	FME	O	1	2	-	1/7/9/11	-
7	TPO	G	11	7	-	5/9/11/13	-
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	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	OAC-C1A	5.12	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	OAC-C1A	4.93	1.34	1.23
9	V	1	SAC	CA-N	4.76	1.53	1.46
9	I	1	SAC	CA-N	3.80	1.51	1.46
7	G	11	TPO	CB-CA	3.10	1.60	1.53
7	T	11	TPO	P-O1P	2.12	1.57	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	1	SAC	CA-N-C1A	-6.74	110.72	123.15
9	I	1	SAC	CA-N-C1A	-6.43	111.30	123.15
2	O	1	FME	C-CA-N	4.33	117.55	109.73
1	N	1	FME	CA-N-CN	-4.06	116.57	122.82
2	B	1	FME	C-CA-N	3.98	116.92	109.73
2	B	1	FME	CA-N-CN	-3.66	117.20	122.82
2	O	1	FME	CA-N-CN	-3.36	117.65	122.82
9	I	1	SAC	CB-CA-N	3.27	117.88	110.55
9	I	1	SAC	C-CA-N	-3.15	104.05	109.73
9	V	1	SAC	C-CA-N	-3.04	104.24	109.73
9	V	1	SAC	C2A-C1A-N	2.88	120.98	116.10
9	V	1	SAC	CB-CA-N	2.86	116.96	110.55
1	A	1	FME	CA-N-CN	-2.46	119.03	122.82
9	V	1	SAC	OAC-C1A-C2A	-2.20	117.98	122.06
9	I	1	SAC	C2A-C1A-N	2.14	119.72	116.10
1	N	1	FME	O-C-CA	-2.10	119.28	124.78

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
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
2	O	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2

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Mol	Chain	Res	Type	Atoms
7	G	11	TPO	CB-OG1-P-O3P
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
1	A	1	FME	C-CA-CB-CG
7	T	11	TPO	CB-OG1-P-O3P
7	G	11	TPO	CB-OG1-P-O2P

There are no ring outliers.

3 monomers are involved in 5 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 54 ligands modelled in this entry, 10 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
20	CUA	B	228	2	0,1,1	0.00	-	-		
19	PGV	N	1266	-	50,50,50	0.91	3 (6%)	53,56,56	0.81	2 (3%)
25	PEK	T	263	-	52,52,52	1.81	11 (21%)	55,57,57	1.19	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	PGV	C	268	-	50,50,50	1.15	3 (6%)	53,56,56	0.81	0
26	CDL	T	1269	-	99,99,99	0.95	6 (6%)	105,111,111	0.96	7 (6%)
17	HEA	N	516	1	44,67,67	1.38	6 (13%)	37,103,103	1.28	7 (18%)
18	TGL	B	521	-	62,62,62	0.69	0	65,65,65	1.45	9 (13%)
18	TGL	A	523	-	62,62,62	0.72	0	65,65,65	1.21	8 (12%)
19	PGV	C	266	-	50,50,50	0.87	2 (4%)	53,56,56	0.74	1 (1%)
22	CHD	B	1086	-	29,32,32	0.70	0	48,51,51	1.82	14 (29%)
17	HEA	A	516	1	44,67,67	1.27	5 (11%)	37,103,103	1.27	5 (13%)
25	PEK	G	1263	-	52,52,52	1.77	9 (17%)	55,57,57	1.18	5 (9%)
22	CHD	W	1060	-	29,32,32	1.18	3 (10%)	48,51,51	3.56	29 (60%)
18	TGL	N	1523	-	62,62,62	0.77	1 (1%)	65,65,65	1.20	5 (7%)
23	DMU	M	526	-	34,34,34	3.24	8 (23%)	45,45,45	4.30	20 (44%)
17	HEA	N	515	1	44,67,67	1.72	6 (13%)	37,103,103	1.42	7 (18%)
22	CHD	J	60	-	29,32,32	1.07	1 (3%)	48,51,51	3.55	30 (62%)
19	PGV	P	1267	-	50,50,50	0.85	2 (4%)	53,56,56	0.80	2 (3%)
25	PEK	P	1264	-	52,52,52	1.37	5 (9%)	55,57,57	0.98	3 (5%)
23	DMU	P	1272	-	34,34,34	2.86	11 (32%)	45,45,45	4.21	19 (42%)
20	CUA	O	228	2	0,1,1	0.00	-	-	-	-
18	TGL	L	522	-	62,62,62	1.09	5 (8%)	65,65,65	1.69	14 (21%)
26	CDL	G	269	-	99,99,99	0.97	6 (6%)	105,111,111	0.94	7 (6%)
19	PGV	N	1524	-	50,50,50	1.06	3 (6%)	53,56,56	0.93	5 (9%)
25	PEK	C	265	-	52,52,52	1.60	10 (19%)	55,57,57	1.13	7 (12%)
22	CHD	P	1271	-	29,32,32	0.81	0	48,51,51	3.73	24 (50%)
26	CDL	C	270	-	99,99,99	0.80	2 (2%)	105,111,111	0.93	6 (5%)
21	PSC	O	1230	-	51,51,51	1.19	3 (5%)	57,59,59	0.91	1 (1%)
22	CHD	P	1525	-	29,32,32	0.81	1 (3%)	48,51,51	1.56	9 (18%)
17	HEA	A	515	1	44,67,67	1.32	4 (9%)	37,103,103	1.25	3 (8%)
25	PEK	P	1265	-	52,52,52	1.61	11 (21%)	55,57,57	1.12	6 (10%)
21	PSC	B	230	-	51,51,51	1.20	3 (5%)	57,59,59	0.91	1 (1%)
22	CHD	C	525	-	29,32,32	0.78	0	48,51,51	1.60	8 (16%)
22	CHD	O	229	-	29,32,32	0.70	1 (3%)	48,51,51	1.87	14 (29%)
19	PGV	P	1268	-	50,50,50	1.15	3 (6%)	53,56,56	0.82	1 (1%)
19	PGV	C	267	-	50,50,50	0.80	1 (2%)	53,56,56	0.86	2 (3%)
25	PEK	C	264	-	52,52,52	1.37	4 (7%)	55,57,57	0.97	3 (5%)
23	DMU	C	272	-	34,34,34	2.74	13 (38%)	45,45,45	4.18	19 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	TGL	N	1521	-	62,62,62	0.75	1 (1%)	65,65,65	1.41	9 (13%)
26	CDL	P	1270	-	99,99,99	0.83	3 (3%)	105,111,111	0.91	5 (4%)
22	CHD	C	271	-	29,32,32	0.88	1 (3%)	48,51,51	3.74	23 (47%)
18	TGL	N	1522	-	62,62,62	1.14	4 (6%)	65,65,65	1.65	12 (18%)
23	DMU	Z	1526	-	34,34,34	3.16	8 (23%)	45,45,45	4.25	20 (44%)
19	PGV	A	524	-	50,50,50	1.07	3 (6%)	53,56,56	0.95	5 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	PGV	N	1266	-	-	13/55/55/55	-
25	PEK	T	263	-	-	29/56/56/56	-
19	PGV	C	268	-	-	33/55/55/55	-
26	CDL	T	1269	-	-	63/110/110/110	-
17	HEA	N	516	1	3/3/7/16	3/24/76/76	-
18	TGL	B	521	-	-	16/65/65/65	-
18	TGL	A	523	-	-	12/65/65/65	-
19	PGV	N	1524	-	-	33/55/55/55	-
22	CHD	B	1086	-	-	0/7/74/74	0/4/4/4
17	HEA	A	516	1	3/3/7/16	3/24/76/76	-
25	PEK	G	1263	-	-	29/56/56/56	-
22	CHD	W	1060	-	5/5/12/12	6/7/74/74	0/4/4/4
18	TGL	N	1523	-	-	13/65/65/65	-
23	DMU	M	526	-	5/5/10/10	12/19/59/59	0/2/2/2
17	HEA	N	515	1	3/3/7/16	2/24/76/76	-
22	CHD	J	60	-	5/5/12/12	6/7/74/74	0/4/4/4
19	PGV	P	1267	-	-	16/55/55/55	-
25	PEK	P	1264	-	-	23/56/56/56	-
23	DMU	P	1272	-	6/6/10/10	10/19/59/59	0/2/2/2
18	TGL	L	522	-	-	16/65/65/65	-
26	CDL	G	269	-	-	61/110/110/110	-
19	PGV	C	266	-	-	13/55/55/55	-
25	PEK	C	265	-	-	16/56/56/56	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	P	1271	-	5/5/12/12	6/7/74/74	0/4/4/4
26	CDL	C	270	-	-	70/110/110/110	-
21	PSC	O	1230	-	-	42/55/55/55	-
22	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
18	TGL	N	1522	-	-	18/65/65/65	-
25	PEK	P	1265	-	-	17/56/56/56	-
21	PSC	B	230	-	-	42/55/55/55	-
22	CHD	C	525	-	-	0/7/74/74	0/4/4/4
22	CHD	O	229	-	-	0/7/74/74	0/4/4/4
19	PGV	P	1268	-	-	33/55/55/55	-
19	PGV	C	267	-	-	17/55/55/55	-
25	PEK	C	264	-	-	23/56/56/56	-
23	DMU	C	272	-	6/6/10/10	9/19/59/59	0/2/2/2
18	TGL	N	1521	-	-	15/65/65/65	-
26	CDL	P	1270	-	-	71/110/110/110	-
22	CHD	C	271	-	5/5/12/12	6/7/74/74	0/4/4/4
17	HEA	A	515	1	3/3/7/16	2/24/76/76	-
23	DMU	Z	1526	-	5/5/10/10	11/19/59/59	0/2/2/2
19	PGV	A	524	-	-	33/55/55/55	-

All (172) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	M	526	DMU	O7-C3	-8.24	1.22	1.43
17	N	515	HEA	C3B-C11	-8.05	1.46	1.52
23	Z	1526	DMU	O7-C3	-7.75	1.23	1.43
23	M	526	DMU	O16-C6	-7.38	1.27	1.40
23	Z	1526	DMU	O16-C6	-7.25	1.27	1.40
23	M	526	DMU	O16-C18	-6.86	1.23	1.43
23	P	1272	DMU	O1-C9	-6.67	1.28	1.44
23	Z	1526	DMU	O16-C18	-6.62	1.24	1.43
23	M	526	DMU	O1-C9	-6.61	1.28	1.44
23	Z	1526	DMU	O1-C9	-6.49	1.28	1.44
23	M	526	DMU	O5-C4	-6.46	1.28	1.44
23	M	526	DMU	O7-C10	-6.30	1.24	1.41
23	C	272	DMU	O1-C9	-6.25	1.29	1.44
23	Z	1526	DMU	O7-C10	-6.25	1.24	1.41
23	P	1272	DMU	O16-C6	-6.21	1.29	1.40
23	P	1272	DMU	O7-C3	-6.11	1.28	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	1272	DMU	O16-C18	-6.04	1.26	1.43
23	Z	1526	DMU	O5-C4	-5.97	1.29	1.44
23	M	526	DMU	O1-C10	-5.72	1.27	1.41
23	Z	1526	DMU	O1-C10	-5.69	1.27	1.41
23	C	272	DMU	O16-C6	-5.68	1.30	1.40
23	C	272	DMU	O7-C3	-5.62	1.29	1.43
23	C	272	DMU	O16-C18	-5.59	1.27	1.43
17	A	515	HEA	C3B-C11	-4.94	1.49	1.52
18	N	1522	TGL	OG2-CB1	4.94	1.48	1.34
23	C	272	DMU	O5-C4	-4.90	1.32	1.44
23	P	1272	DMU	O5-C4	-4.88	1.32	1.44
25	G	1263	PEK	C12-C11	4.77	1.59	1.31
18	L	522	TGL	OG2-CB1	4.68	1.47	1.34
23	C	272	DMU	O1-C10	-4.66	1.30	1.41
23	M	526	DMU	O5-C6	-4.65	1.30	1.41
25	T	263	PEK	C12-C11	4.65	1.58	1.31
23	P	1272	DMU	O1-C10	-4.64	1.30	1.41
25	P	1264	PEK	C12-C11	4.62	1.58	1.31
25	C	264	PEK	C15-C14	4.61	1.58	1.31
23	P	1272	DMU	O7-C10	-4.59	1.28	1.41
25	P	1264	PEK	C15-C14	4.53	1.58	1.31
23	Z	1526	DMU	O5-C6	-4.50	1.30	1.41
25	C	264	PEK	C12-C11	4.49	1.57	1.31
19	C	268	PGV	C12-C11	4.41	1.57	1.31
19	P	1268	PGV	C12-C11	4.40	1.57	1.31
25	C	265	PEK	C9-C8	4.35	1.57	1.31
25	T	263	PEK	C6-C5	4.34	1.56	1.31
23	C	272	DMU	O7-C10	-4.32	1.29	1.41
25	C	265	PEK	C15-C14	4.28	1.56	1.31
21	O	1230	PSC	C10-C9	4.27	1.56	1.31
25	C	265	PEK	C12-C11	4.27	1.56	1.31
25	T	263	PEK	C9-C8	4.25	1.56	1.31
25	P	1265	PEK	C12-C11	4.25	1.56	1.31
25	G	1263	PEK	C6-C5	4.24	1.56	1.31
25	P	1265	PEK	C6-C5	4.22	1.56	1.31
25	T	263	PEK	C15-C14	4.21	1.56	1.31
21	B	230	PSC	C10-C9	4.21	1.56	1.31
25	G	1263	PEK	C9-C8	4.20	1.56	1.31
23	P	1272	DMU	O5-C6	-4.19	1.31	1.41
25	P	1265	PEK	C9-C8	4.14	1.55	1.31
25	P	1265	PEK	C15-C14	4.12	1.55	1.31
25	G	1263	PEK	C15-C14	4.12	1.55	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	O	1230	PSC	C13-C12	4.12	1.55	1.31
25	G	1263	PEK	C03-C02	4.09	1.63	1.50
25	P	1264	PEK	C6-C5	4.06	1.55	1.31
25	C	264	PEK	C6-C5	4.05	1.55	1.31
19	N	1524	PGV	C12-C11	4.01	1.55	1.31
25	C	265	PEK	C6-C5	4.01	1.55	1.31
25	T	263	PEK	C03-C02	4.00	1.63	1.50
25	C	264	PEK	C9-C8	3.94	1.54	1.31
25	P	1264	PEK	C9-C8	3.93	1.54	1.31
23	C	272	DMU	O5-C6	-3.90	1.31	1.41
21	B	230	PSC	C13-C12	3.89	1.54	1.31
19	A	524	PGV	C12-C11	3.86	1.54	1.31
19	N	1266	PGV	C12-C11	3.86	1.54	1.31
22	W	1060	CHD	C13-C17	3.82	1.62	1.55
19	C	266	PGV	C12-C11	3.74	1.53	1.31
18	N	1522	TGL	OG1-CA1	3.73	1.44	1.33
17	N	516	HEA	C4D-ND	3.72	1.43	1.36
25	T	263	PEK	O03-C21	3.71	1.44	1.33
25	G	1263	PEK	C01-C02	3.64	1.61	1.50
26	T	1269	CDL	CB6-CB4	3.64	1.61	1.50
25	G	1263	PEK	O03-C21	3.53	1.43	1.33
17	A	516	HEA	C4D-ND	3.47	1.43	1.36
25	T	263	PEK	C01-C02	3.44	1.61	1.50
19	A	524	PGV	O03-C19	3.36	1.43	1.33
17	N	516	HEA	C3B-C11	-3.33	1.50	1.52
17	N	515	HEA	C3A-CMA	-3.33	1.38	1.46
26	G	269	CDL	CB6-CB4	3.29	1.60	1.50
19	P	1267	PGV	C12-C11	3.27	1.50	1.31
19	C	267	PGV	C12-C11	3.20	1.50	1.31
17	N	516	HEA	C3A-CMA	-3.17	1.39	1.46
22	J	60	CHD	C13-C17	3.14	1.60	1.55
17	A	516	HEA	C3A-CMA	-3.12	1.39	1.46
19	P	1268	PGV	O01-C1	3.06	1.42	1.34
17	A	515	HEA	C3A-CMA	-3.05	1.39	1.46
17	A	516	HEA	C3A-C2A	-3.02	1.36	1.40
25	T	263	PEK	P-O11	2.96	1.71	1.59
19	N	1524	PGV	O03-C19	2.91	1.41	1.33
26	G	269	CDL	OA6-CA5	2.91	1.42	1.34
25	P	1265	PEK	O03-C21	2.86	1.41	1.33
17	N	516	HEA	C1B-NB	2.85	1.42	1.36
17	N	515	HEA	C1D-C2D	2.85	1.49	1.42
19	C	268	PGV	O01-C1	2.83	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	515	HEA	C1C-NC	2.83	1.42	1.36
18	L	522	TGL	OG1-CA1	2.80	1.41	1.33
18	L	522	TGL	CG1-CG2	2.79	1.59	1.50
26	T	1269	CDL	CB3-CB4	2.77	1.59	1.50
19	N	1266	PGV	C01-C02	2.77	1.59	1.50
25	G	1263	PEK	P-O11	2.74	1.70	1.59
18	N	1522	TGL	CG1-CG2	2.74	1.59	1.50
17	A	516	HEA	C3C-CAC	2.72	1.53	1.47
25	C	265	PEK	O03-C21	2.71	1.41	1.33
23	C	272	DMU	C3-C4	2.70	1.60	1.52
26	G	269	CDL	CB3-CB4	2.64	1.58	1.50
25	C	265	PEK	C03-C02	2.62	1.58	1.50
25	P	1265	PEK	C01-C02	2.59	1.58	1.50
25	T	263	PEK	O01-C1	2.58	1.41	1.34
21	O	1230	PSC	C2-C1	2.58	1.58	1.50
26	P	1270	CDL	CA6-CA4	2.58	1.58	1.50
19	C	266	PGV	C20-C19	2.53	1.58	1.50
26	G	269	CDL	C11-CA5	2.53	1.58	1.50
26	T	1269	CDL	C11-CA5	2.52	1.58	1.50
23	P	1272	DMU	C3-C4	2.52	1.59	1.52
21	B	230	PSC	C2-C1	2.51	1.58	1.50
25	C	265	PEK	C01-C02	2.50	1.58	1.50
25	P	1265	PEK	C22-C21	2.50	1.58	1.50
25	T	263	PEK	C2-C1	2.49	1.58	1.50
18	N	1521	TGL	OG2-CB1	2.47	1.41	1.34
19	N	1524	PGV	C20-C19	2.46	1.57	1.50
17	A	515	HEA	C4D-ND	2.45	1.41	1.36
17	N	516	HEA	C3C-CAC	2.42	1.52	1.47
25	C	265	PEK	C22-C21	2.42	1.57	1.50
26	C	270	CDL	CA6-CA4	2.41	1.58	1.50
25	P	1265	PEK	P-O11	2.39	1.69	1.59
17	N	516	HEA	C3A-C2A	-2.39	1.37	1.40
25	P	1265	PEK	C03-C02	2.39	1.58	1.50
22	P	1525	CHD	C8-C9	2.38	1.58	1.53
19	C	268	PGV	C04-C05	2.34	1.59	1.51
26	P	1270	CDL	CA3-CA4	2.34	1.57	1.50
22	W	1060	CHD	C20-C17	2.33	1.58	1.54
23	C	272	DMU	C7-C5	2.33	1.58	1.52
26	T	1269	CDL	OA6-CA5	2.33	1.40	1.34
23	C	272	DMU	C6-C1	2.32	1.59	1.52
25	C	265	PEK	P-O11	2.31	1.68	1.59
23	P	1272	DMU	C6-C1	2.30	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	A	516	HEA	C3C-C2C	-2.30	1.37	1.40
26	G	269	CDL	CA6-CA4	2.29	1.57	1.50
25	P	1265	PEK	P-O12	2.29	1.68	1.59
18	N	1523	TGL	OG2-CB1	2.28	1.40	1.34
19	A	524	PGV	C20-C19	2.27	1.57	1.50
19	P	1268	PGV	C04-C05	2.26	1.59	1.51
26	C	270	CDL	CA3-CA4	2.23	1.57	1.50
22	O	229	CHD	C8-C9	2.23	1.58	1.53
18	L	522	TGL	CC2-CC1	2.23	1.57	1.50
23	P	1272	DMU	C7-C5	2.23	1.58	1.52
17	N	515	HEA	C3A-C2A	-2.22	1.37	1.40
26	P	1270	CDL	C31-CA7	2.19	1.57	1.50
17	N	515	HEA	C4C-NC	2.18	1.40	1.36
19	N	1266	PGV	C20-C19	2.18	1.57	1.50
25	T	263	PEK	P-O12	2.18	1.68	1.59
22	W	1060	CHD	C8-C7	2.16	1.57	1.53
25	C	265	PEK	P-O12	2.16	1.68	1.59
25	G	1263	PEK	P-O12	2.15	1.68	1.59
26	T	1269	CDL	CA6-CA4	2.14	1.57	1.50
18	L	522	TGL	CG3-CG2	2.12	1.57	1.50
26	G	269	CDL	CB2-C1	2.10	1.58	1.51
25	P	1265	PEK	O01-C1	2.10	1.40	1.34
19	P	1267	PGV	C01-C02	2.09	1.57	1.50
18	N	1522	TGL	CG3-CG2	2.06	1.57	1.50
23	C	272	DMU	C8-C7	2.06	1.57	1.52
25	P	1264	PEK	C2-C1	2.03	1.56	1.50
26	T	1269	CDL	CB2-C1	2.02	1.58	1.51
17	A	515	HEA	C1B-NB	2.02	1.40	1.36
22	C	271	CHD	C19-C10	-2.02	1.50	1.54
23	C	272	DMU	C8-C9	2.00	1.57	1.53

All (382) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	1271	CHD	C10-C9-C8	10.55	123.15	111.82
23	M	526	DMU	C10-C5-C7	10.55	131.97	110.00
22	P	1271	CHD	C17-C13-C14	10.51	110.69	100.09
22	C	271	CHD	C17-C13-C14	10.36	110.54	100.09
23	Z	1526	DMU	C10-C5-C7	10.35	131.55	110.00
22	C	271	CHD	C10-C9-C8	10.11	122.68	111.82
23	C	272	DMU	C1-C2-C3	9.63	131.66	109.68
23	P	1272	DMU	O16-C6-C1	9.47	123.09	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1272	DMU	C1-C2-C3	9.37	131.08	109.68
23	C	272	DMU	C6-O5-C4	9.35	132.04	113.69
22	J	60	CHD	C17-C13-C14	9.28	109.45	100.09
23	C	272	DMU	O16-C6-C1	8.95	122.28	108.30
23	C	272	DMU	C18-O16-C6	8.90	128.60	113.84
23	M	526	DMU	C1-C2-C3	8.88	129.95	109.68
22	P	1271	CHD	C17-C13-C12	-8.86	109.58	117.67
22	W	1060	CHD	C17-C13-C14	8.86	109.02	100.09
23	Z	1526	DMU	C1-C2-C3	8.78	129.73	109.68
23	P	1272	DMU	C6-O5-C4	8.71	130.79	113.69
22	C	271	CHD	C17-C13-C12	-8.59	109.82	117.67
22	C	271	CHD	C19-C10-C9	-8.27	99.79	111.18
23	C	272	DMU	O1-C9-C11	8.22	126.87	106.44
23	M	526	DMU	C6-O5-C4	8.17	129.73	113.69
23	Z	1526	DMU	C6-O5-C4	8.15	129.68	113.69
23	P	1272	DMU	O7-C3-C4	8.10	131.65	109.45
23	P	1272	DMU	C18-O16-C6	8.04	127.17	113.84
23	M	526	DMU	C8-C7-C5	-7.98	96.90	110.82
23	Z	1526	DMU	C8-C7-C5	-7.89	97.06	110.82
23	M	526	DMU	O5-C4-C3	7.77	126.14	109.75
22	P	1271	CHD	C19-C10-C9	-7.75	100.50	111.18
23	Z	1526	DMU	C7-C8-C9	7.73	124.03	110.24
23	M	526	DMU	C7-C8-C9	7.73	124.02	110.24
23	Z	1526	DMU	O5-C4-C3	7.62	125.83	109.75
23	Z	1526	DMU	O1-C9-C11	7.60	125.32	106.44
23	M	526	DMU	O1-C9-C11	7.45	124.96	106.44
23	P	1272	DMU	O1-C9-C11	7.44	124.94	106.44
23	P	1272	DMU	C8-C7-C5	7.37	123.69	110.82
23	C	272	DMU	O7-C3-C4	7.33	129.55	109.45
23	M	526	DMU	O1-C9-C8	7.32	122.98	109.69
23	P	1272	DMU	O5-C4-C3	7.31	125.16	109.75
23	Z	1526	DMU	O1-C9-C8	6.97	122.36	109.69
23	C	272	DMU	O5-C4-C3	6.95	124.41	109.75
23	Z	1526	DMU	O5-C6-O16	6.89	126.30	109.97
23	Z	1526	DMU	O5-C4-C57	6.72	123.15	106.44
22	W	1060	CHD	C13-C17-C20	6.64	127.42	119.50
23	P	1272	DMU	O1-C9-C8	6.62	121.72	109.69
22	W	1060	CHD	C10-C9-C8	6.62	118.93	111.82
22	J	60	CHD	C13-C17-C20	6.58	127.35	119.50
22	J	60	CHD	C10-C9-C8	6.55	118.85	111.82
23	M	526	DMU	O5-C6-O16	6.52	125.43	109.97
23	M	526	DMU	O5-C4-C57	6.46	122.49	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	60	CHD	C4-C3-C2	6.33	118.11	110.55
23	M	526	DMU	C18-O16-C6	6.30	124.29	113.84
23	C	272	DMU	O5-C4-C57	6.28	122.04	106.44
22	C	271	CHD	C1-C10-C5	6.11	116.80	107.77
22	W	1060	CHD	C4-C3-C2	6.07	117.80	110.55
22	C	271	CHD	C19-C10-C1	-6.05	98.52	108.26
23	Z	1526	DMU	C18-O16-C6	6.01	123.81	113.84
23	P	1272	DMU	O5-C4-C57	6.00	121.37	106.44
22	P	1271	CHD	C1-C10-C5	5.99	116.63	107.77
22	W	1060	CHD	C6-C5-C10	5.97	119.00	112.66
23	C	272	DMU	O7-C10-C5	5.96	123.54	108.10
23	P	1272	DMU	O7-C10-C5	5.87	123.32	108.10
23	M	526	DMU	O7-C3-C2	5.83	122.80	107.28
23	Z	1526	DMU	O7-C3-C2	5.79	122.67	107.28
22	P	1271	CHD	C19-C10-C1	-5.78	98.95	108.26
23	C	272	DMU	O7-C3-C2	5.77	122.63	107.28
22	J	60	CHD	C6-C5-C10	5.61	118.61	112.66
22	W	1060	CHD	C11-C12-C13	5.54	116.93	111.24
23	C	272	DMU	O1-C9-C8	5.51	119.70	109.69
22	W	1060	CHD	C15-C14-C8	-5.49	110.65	118.33
22	J	60	CHD	C5-C6-C7	5.44	120.46	114.46
23	C	272	DMU	C10-O1-C9	5.44	124.36	113.69
22	J	60	CHD	C11-C12-C13	5.43	116.81	111.24
22	O	229	CHD	C10-C9-C8	5.39	117.61	111.82
22	J	60	CHD	C15-C14-C8	-5.39	110.80	118.33
22	W	1060	CHD	C5-C6-C7	5.38	120.40	114.46
22	J	60	CHD	C11-C9-C10	5.34	119.23	113.73
23	P	1272	DMU	O7-C3-C2	5.32	121.44	107.28
18	B	521	TGL	CG2-OG2-CB1	5.24	130.68	117.79
23	P	1272	DMU	C10-O1-C9	5.19	123.88	113.69
22	W	1060	CHD	C11-C9-C10	5.18	119.07	113.73
22	C	271	CHD	C4-C5-C10	5.13	118.11	112.66
22	C	271	CHD	C4-C3-C2	5.12	116.66	110.55
22	P	1271	CHD	C15-C14-C8	-5.03	111.30	118.33
22	C	271	CHD	C15-C14-C8	-4.90	111.49	118.33
18	L	522	TGL	C12-C11-C10	-4.86	89.74	114.42
18	N	1521	TGL	CG2-OG2-CB1	4.86	129.75	117.79
22	C	271	CHD	C9-C8-C7	4.84	117.66	111.88
18	N	1522	TGL	C12-C11-C10	-4.78	90.17	114.42
22	P	1271	CHD	C4-C5-C10	4.77	117.73	112.66
22	C	271	CHD	C14-C13-C12	4.77	111.84	107.40
22	J	60	CHD	C9-C8-C7	4.76	117.57	111.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	1271	CHD	C9-C8-C7	4.76	117.56	111.88
22	W	1060	CHD	C9-C8-C7	4.73	117.53	111.88
22	J	60	CHD	C2-C1-C10	4.70	120.84	112.78
23	Z	1526	DMU	O5-C6-C1	4.66	120.22	110.35
22	J	60	CHD	C18-C13-C14	-4.65	103.93	111.21
22	W	1060	CHD	C18-C13-C14	-4.65	103.94	111.21
22	P	1271	CHD	C14-C13-C12	4.65	111.73	107.40
22	W	1060	CHD	C2-C1-C10	4.65	120.75	112.78
22	P	1271	CHD	C4-C3-C2	4.64	116.10	110.55
23	M	526	DMU	O5-C6-C1	4.56	120.00	110.35
22	J	60	CHD	C1-C10-C5	4.42	114.31	107.77
22	W	1060	CHD	C1-C10-C5	4.35	114.20	107.77
18	N	1522	TGL	CB9-CB8-CB7	-4.32	92.52	114.42
23	Z	1526	DMU	O7-C3-C4	4.29	121.21	109.45
23	P	1272	DMU	O5-C6-C1	4.25	119.35	110.35
23	C	272	DMU	C8-C7-C5	4.25	118.24	110.82
23	M	526	DMU	O7-C3-C4	4.23	121.05	109.45
23	C	272	DMU	O5-C6-C1	4.19	119.23	110.35
18	L	522	TGL	CB9-CB8-CB7	-4.11	93.57	114.42
22	B	1086	CHD	C10-C9-C8	4.11	116.23	111.82
22	P	1525	CHD	C1-C10-C5	4.08	113.80	107.77
23	M	526	DMU	O7-C10-C5	4.05	118.60	108.10
23	M	526	DMU	O16-C6-C1	4.00	114.55	108.30
22	W	1060	CHD	C18-C13-C12	-3.95	105.05	109.07
22	P	1271	CHD	C1-C10-C9	3.89	117.47	111.35
22	C	525	CHD	C14-C13-C12	-3.89	103.78	107.40
22	W	1060	CHD	C5-C4-C3	3.89	118.47	112.76
18	B	521	TGL	CG1-OG1-CA1	-3.87	102.77	117.12
25	T	263	PEK	O03-C01-C02	3.84	119.60	108.43
25	G	1263	PEK	O03-C01-C02	3.83	119.58	108.43
22	J	60	CHD	C5-C4-C3	3.79	118.33	112.76
18	L	522	TGL	C15-CC9-CC8	3.79	133.67	114.42
22	B	1086	CHD	C15-C14-C8	-3.78	113.05	118.33
22	P	1271	CHD	C5-C6-C7	3.76	118.61	114.46
18	N	1522	TGL	C15-CC9-CC8	3.75	133.49	114.42
22	C	271	CHD	C5-C6-C7	3.74	118.58	114.46
23	Z	1526	DMU	O7-C10-C5	3.72	117.74	108.10
22	B	1086	CHD	C16-C17-C13	-3.72	99.91	103.55
18	L	522	TGL	C16-C15-CC9	3.71	133.24	114.42
18	N	1522	TGL	C16-C15-CC9	3.69	133.16	114.42
22	C	271	CHD	C1-C10-C9	3.68	117.14	111.35
23	P	1272	DMU	O7-C10-O1	3.66	120.89	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	1521	TGL	CG1-OG1-CA1	-3.64	103.63	117.12
22	B	1086	CHD	C1-C10-C5	3.62	113.12	107.77
23	M	526	DMU	C10-O7-C3	3.61	126.90	117.96
22	J	60	CHD	C1-C2-C3	3.61	115.10	110.47
18	L	522	TGL	CG2-OG2-CB1	3.59	126.64	117.79
23	C	272	DMU	O7-C10-O1	3.58	120.66	110.67
22	W	1060	CHD	C1-C2-C3	3.54	115.01	110.47
18	L	522	TGL	C11-C10-CB9	3.52	132.32	114.42
25	G	1263	PEK	P-O11-C03	3.52	142.29	121.68
22	P	1525	CHD	C13-C17-C20	3.51	123.69	119.50
25	T	263	PEK	P-O11-C03	3.50	142.21	121.68
22	C	525	CHD	C1-C10-C5	3.50	112.94	107.77
23	C	272	DMU	O5-C6-O16	3.49	118.23	109.97
22	O	229	CHD	C15-C14-C8	-3.49	113.46	118.33
18	N	1522	TGL	C11-C10-CB9	3.47	132.05	114.42
23	C	272	DMU	C10-O7-C3	3.46	126.52	117.96
22	J	60	CHD	C6-C5-C4	3.45	115.16	111.19
22	P	1525	CHD	C15-C14-C8	-3.44	113.53	118.33
22	W	1060	CHD	C6-C5-C4	3.43	115.14	111.19
22	P	1271	CHD	C5-C4-C3	3.43	117.79	112.76
18	N	1522	TGL	CG2-OG2-CB1	3.42	126.22	117.79
22	C	271	CHD	C14-C8-C7	3.42	116.34	111.81
22	C	271	CHD	C18-C13-C12	-3.40	105.61	109.07
22	C	525	CHD	C15-C14-C8	-3.37	113.62	118.33
22	B	1086	CHD	C15-C14-C13	-3.36	100.26	103.55
22	C	525	CHD	C10-C9-C8	3.35	115.42	111.82
22	W	1060	CHD	C17-C13-C12	-3.34	114.62	117.67
22	J	60	CHD	C17-C13-C12	-3.33	114.63	117.67
23	Z	1526	DMU	O16-C6-C1	3.31	113.47	108.30
22	W	1060	CHD	C13-C14-C8	3.31	118.96	114.74
18	N	1521	TGL	CG3-OG3-CC1	3.29	129.31	117.12
17	A	516	HEA	C27-C19-C20	3.29	120.80	115.27
18	N	1522	TGL	CC3-CC2-CC1	3.28	125.55	113.62
18	L	522	TGL	CC3-CC2-CC1	3.28	125.53	113.62
22	J	60	CHD	C14-C8-C9	3.26	114.18	109.71
22	J	60	CHD	C13-C14-C8	3.26	118.89	114.74
22	J	60	CHD	C18-C13-C12	-3.25	105.75	109.07
22	P	1271	CHD	C14-C8-C7	3.25	116.12	111.81
22	W	1060	CHD	C14-C8-C9	3.24	114.16	109.71
22	O	229	CHD	C5-C6-C7	3.24	118.03	114.46
22	O	229	CHD	C16-C17-C13	-3.22	100.40	103.55
22	B	1086	CHD	C1-C2-C3	3.22	114.59	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	B	521	TGL	CG3-OG3-CC1	3.20	128.97	117.12
25	G	1263	PEK	C02-O01-C1	3.20	125.66	117.79
22	B	1086	CHD	C9-C11-C12	3.19	118.52	114.30
22	W	1060	CHD	C9-C11-C12	3.17	118.48	114.30
22	O	229	CHD	C9-C11-C12	3.16	118.47	114.30
18	A	523	TGL	CB3-CB2-CB1	3.16	125.11	113.62
17	N	516	HEA	C27-C19-C20	3.16	120.58	115.27
18	N	1523	TGL	CG3-OG3-CC1	3.16	128.81	117.12
18	N	1523	TGL	CG1-OG1-CA1	-3.15	105.45	117.12
22	W	1060	CHD	C16-C15-C14	3.13	111.34	105.13
22	O	229	CHD	C1-C10-C5	3.13	112.40	107.77
17	A	515	HEA	CMC-C2C-C3C	3.12	130.52	124.68
26	P	1270	CDL	PA1-OA5-CA3	3.12	139.99	121.68
25	C	265	PEK	P-O11-C03	3.10	139.85	121.68
22	J	60	CHD	C4-C5-C10	3.08	115.93	112.66
23	C	272	DMU	C2-C3-C4	-3.08	103.87	110.93
25	P	1265	PEK	P-O11-C03	3.08	139.72	121.68
25	T	263	PEK	C02-O01-C1	3.07	125.36	117.79
26	C	270	CDL	PA1-OA5-CA3	3.06	139.64	121.68
18	A	523	TGL	CG3-OG3-CC1	3.05	128.43	117.12
26	C	270	CDL	OB6-CB5-C51	-3.05	104.92	111.50
23	P	1272	DMU	O5-C6-O16	3.04	117.18	109.97
17	N	515	HEA	CMB-C2B-C3B	3.01	130.58	124.69
22	C	525	CHD	C13-C17-C20	3.01	123.08	119.50
23	Z	1526	DMU	C10-O7-C3	3.00	125.38	117.96
21	B	230	PSC	C01-O03-C19	-2.99	106.05	117.12
23	P	1272	DMU	C2-C3-C4	-2.99	104.08	110.93
25	C	264	PEK	O03-C21-C22	-2.97	102.58	111.91
22	J	60	CHD	C9-C11-C12	2.96	118.21	114.30
23	Z	1526	DMU	O7-C10-O1	2.95	118.92	110.67
22	J	60	CHD	C16-C15-C14	2.95	110.98	105.13
23	M	526	DMU	C2-C3-C4	-2.94	104.18	110.93
18	A	523	TGL	CG1-OG1-CA1	-2.94	106.23	117.12
18	N	1523	TGL	OG2-CG2-CG3	2.93	119.02	108.40
26	T	1269	CDL	C23-C22-C21	2.91	129.21	114.42
21	O	1230	PSC	C01-O03-C19	-2.91	106.36	117.12
17	N	515	HEA	CMB-C2B-C1B	-2.90	124.00	128.46
25	P	1264	PEK	C3-C2-C1	-2.90	103.06	113.62
22	W	1060	CHD	C4-C5-C10	2.90	115.74	112.66
22	C	525	CHD	C14-C8-C9	-2.89	105.75	109.71
26	T	1269	CDL	C22-C21-C20	2.89	129.08	114.42
25	C	265	PEK	C24-C23-C22	2.89	123.56	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	271	CHD	C5-C4-C3	2.87	116.97	112.76
22	P	1271	CHD	C6-C5-C10	2.87	115.70	112.66
26	G	269	CDL	C22-C21-C20	2.86	128.96	114.42
26	G	269	CDL	C23-C22-C21	2.85	128.91	114.42
22	P	1271	CHD	C15-C16-C17	2.85	110.79	105.13
22	B	1086	CHD	C17-C13-C14	2.85	102.96	100.09
23	Z	1526	DMU	C2-C3-C4	-2.84	104.40	110.93
22	P	1525	CHD	C14-C8-C9	-2.84	105.81	109.71
22	C	271	CHD	C15-C16-C17	2.83	110.74	105.13
18	N	1522	TGL	C13-C12-C11	2.82	128.73	114.42
25	P	1264	PEK	O03-C21-C22	-2.82	103.07	111.91
22	J	60	CHD	C15-C16-C17	2.80	110.68	105.13
22	O	229	CHD	C1-C2-C3	2.79	114.05	110.47
22	B	1086	CHD	C18-C13-C12	-2.78	106.23	109.07
18	L	522	TGL	C20-CA9-CA8	2.77	128.48	114.42
22	C	271	CHD	C16-C15-C14	2.76	110.60	105.13
22	O	229	CHD	C14-C13-C12	-2.76	104.84	107.40
18	L	522	TGL	CC4-CC3-CC2	2.75	123.06	113.19
25	C	264	PEK	C3-C2-C1	-2.75	103.64	113.62
22	P	1271	CHD	C16-C15-C14	2.74	110.56	105.13
22	P	1271	CHD	C18-C13-C12	-2.74	106.28	109.07
18	B	521	TGL	CG3-CG2-CG1	2.74	118.26	111.79
22	O	229	CHD	C15-C14-C13	-2.72	100.88	103.55
22	C	271	CHD	C6-C5-C10	2.72	115.54	112.66
17	A	515	HEA	CMC-C2C-C1C	-2.72	124.29	128.46
18	N	1523	TGL	CB3-CB2-CB1	2.71	123.47	113.62
18	L	522	TGL	OG1-CG1-CG2	2.71	116.31	108.43
22	P	1525	CHD	C5-C6-C7	2.70	117.44	114.46
22	P	1271	CHD	C1-C2-C3	2.69	113.92	110.47
22	J	60	CHD	C19-C10-C5	-2.68	105.82	110.36
25	P	1265	PEK	C24-C23-C22	2.66	122.76	113.19
22	W	1060	CHD	C15-C16-C17	2.66	110.41	105.13
22	C	271	CHD	C1-C2-C3	2.66	113.88	110.47
17	N	516	HEA	C3C-C4C-NC	2.66	112.65	109.21
26	P	1270	CDL	OB6-CB5-C51	-2.66	105.77	111.50
22	W	1060	CHD	C19-C10-C5	-2.66	105.86	110.36
22	C	271	CHD	C9-C11-C12	2.65	117.80	114.30
22	J	60	CHD	C19-C10-C9	-2.64	107.54	111.18
22	O	229	CHD	C5-C4-C3	2.64	116.63	112.76
23	M	526	DMU	C10-O1-C9	2.63	118.86	113.69
26	P	1270	CDL	CB6-OB8-CB7	-2.63	107.37	117.12
22	P	1525	CHD	C1-C2-C3	2.63	113.84	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	1522	TGL	OG1-CG1-CG2	2.62	116.07	108.43
23	M	526	DMU	O7-C10-O1	2.62	118.00	110.67
18	N	1522	TGL	C20-CA9-CA8	2.62	127.71	114.42
18	L	522	TGL	C13-C12-C11	2.62	127.70	114.42
22	W	1060	CHD	C14-C13-C12	2.61	109.83	107.40
25	P	1265	PEK	C11-C10-C9	2.61	124.87	112.02
25	T	263	PEK	C03-C02-C01	2.60	117.95	111.79
18	A	523	TGL	OG2-CG2-CG3	2.60	117.80	108.40
25	C	265	PEK	C11-C10-C9	2.58	124.73	112.02
18	N	1521	TGL	CG3-CG2-CG1	2.58	117.89	111.79
25	P	1265	PEK	P-O12-C04	2.58	134.27	121.59
19	C	267	PGV	O01-C1-C2	-2.57	105.95	111.50
17	A	515	HEA	C26-C15-C16	2.55	119.56	115.27
26	C	270	CDL	CB6-OB8-CB7	-2.54	107.71	117.12
22	P	1271	CHD	C9-C11-C12	2.53	117.64	114.30
19	N	1524	PGV	C3-C2-C1	-2.50	104.53	113.62
25	C	265	PEK	C2-C3-C4	2.49	117.66	113.23
25	G	1263	PEK	C03-C02-C01	2.49	117.67	111.79
17	N	516	HEA	C17-C18-C19	2.48	133.64	127.66
19	N	1266	PGV	O01-C1-C2	-2.48	106.15	111.50
18	A	523	TGL	OG1-CG1-CG2	2.48	115.65	108.43
18	N	1522	TGL	CC4-CC3-CC2	2.48	122.09	113.19
17	N	515	HEA	CMC-C2C-C3C	2.47	129.30	124.68
17	A	516	HEA	CMC-C2C-C3C	2.46	129.28	124.68
23	P	1272	DMU	C10-O7-C3	2.46	124.04	117.96
19	A	524	PGV	C02-O01-C1	2.45	123.83	117.79
18	N	1521	TGL	C10-CB9-CB8	2.45	126.85	114.42
18	N	1521	TGL	OG2-CG2-CG3	2.45	117.26	108.40
26	C	270	CDL	OB6-CB5-OB7	2.44	129.61	123.70
19	N	1524	PGV	C02-O01-C1	2.44	123.80	117.79
17	A	516	HEA	C20-C19-C18	-2.43	116.19	121.12
22	P	1525	CHD	C14-C13-C12	-2.43	105.14	107.40
22	O	229	CHD	C19-C10-C1	-2.42	104.36	108.26
22	P	1271	CHD	C18-C13-C14	-2.42	107.43	111.21
25	C	265	PEK	P-O12-C04	2.41	133.44	121.59
25	P	1264	PEK	O03-C21-O04	2.39	129.62	123.59
17	N	515	HEA	C4B-C3B-C2B	2.38	108.53	106.87
17	N	515	HEA	CMD-C2D-C3D	2.38	129.42	124.94
25	C	264	PEK	O03-C21-O04	2.37	129.58	123.59
25	P	1265	PEK	C2-C3-C4	2.36	117.44	113.23
23	Z	1526	DMU	C10-O1-C9	2.36	118.33	113.69
17	N	515	HEA	C26-C15-C16	2.36	119.25	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	525	CHD	C5-C6-C7	2.36	117.07	114.46
22	W	1060	CHD	C19-C10-C1	-2.36	104.46	108.26
19	N	1266	PGV	O03-C01-C02	2.35	115.29	108.43
19	C	266	PGV	O01-C1-C2	-2.35	106.44	111.50
18	B	521	TGL	CA8-CA7-CA6	-2.35	102.52	114.42
25	C	265	PEK	O03-C01-C02	2.33	115.23	108.43
18	B	521	TGL	OG2-CG2-CG3	2.33	116.84	108.40
22	B	1086	CHD	C14-C8-C9	-2.33	106.52	109.71
18	B	521	TGL	C10-CB9-CB8	2.32	126.22	114.42
17	N	516	HEA	C26-C15-C16	2.32	119.18	115.27
22	O	229	CHD	C18-C13-C12	-2.32	106.70	109.07
22	P	1525	CHD	C10-C9-C8	2.32	114.31	111.82
22	O	229	CHD	C17-C13-C14	2.31	102.43	100.09
26	G	269	CDL	C19-C18-C17	2.30	126.11	114.42
25	P	1265	PEK	O03-C01-C02	2.29	115.11	108.43
22	W	1060	CHD	C14-C8-C7	2.29	114.84	111.81
22	B	1086	CHD	C14-C13-C12	-2.29	105.27	107.40
17	N	516	HEA	C20-C19-C18	-2.28	116.50	121.12
26	T	1269	CDL	C19-C18-C17	2.28	126.00	114.42
26	T	1269	CDL	OB8-CB6-CB4	2.28	115.07	108.43
17	N	515	HEA	C1B-C2B-C3B	-2.28	105.41	107.00
22	J	60	CHD	C14-C8-C7	2.27	114.82	111.81
18	N	1521	TGL	CA8-CA7-CA6	-2.27	102.91	114.42
19	A	524	PGV	C3-C2-C1	-2.27	105.38	113.62
19	C	267	PGV	C9-C10-C11	-2.27	99.45	112.43
26	T	1269	CDL	OB8-CB7-C71	-2.26	104.80	111.91
26	G	269	CDL	C20-C19-C18	2.26	125.90	114.42
22	B	1086	CHD	C19-C10-C1	-2.24	104.65	108.26
22	C	271	CHD	C18-C13-C14	-2.24	107.71	111.21
19	P	1267	PGV	C9-C10-C11	-2.22	99.68	112.43
26	P	1270	CDL	OB6-CB5-OB7	2.22	129.08	123.70
19	A	524	PGV	C04-C05-C06	2.22	119.56	111.67
22	J	60	CHD	C14-C13-C12	2.22	109.47	107.40
22	P	1525	CHD	C9-C11-C12	2.22	117.23	114.30
19	N	1524	PGV	C04-C05-C06	2.21	119.54	111.67
26	C	270	CDL	OA8-CA6-CA4	2.21	114.88	108.43
22	B	1086	CHD	C5-C4-C3	2.21	116.00	112.76
19	N	1524	PGV	O01-C02-C03	2.20	116.37	108.40
19	N	1524	PGV	C03-C02-C01	2.20	116.98	111.79
22	W	1060	CHD	C19-C10-C9	-2.19	108.16	111.18
23	P	1272	DMU	O1-C10-C5	2.18	114.97	110.35
17	A	516	HEA	C26-C15-C16	2.18	118.94	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	516	HEA	CMC-C2C-C1C	-2.18	125.12	128.46
22	J	60	CHD	C19-C10-C1	-2.18	104.76	108.26
25	T	263	PEK	P-O12-C04	2.17	132.26	121.59
23	C	272	DMU	O1-C10-C5	2.16	114.93	110.35
26	C	270	CDL	C52-C51-CB5	-2.14	105.82	113.62
22	C	525	CHD	C19-C10-C9	-2.14	108.24	111.18
18	N	1523	TGL	OG1-CG1-CG2	2.13	114.65	108.43
22	C	271	CHD	C9-C10-C5	2.13	111.58	108.58
18	L	522	TGL	OG2-CB1-OB1	2.13	128.85	123.70
22	O	229	CHD	C13-C17-C20	-2.13	116.95	119.50
26	T	1269	CDL	C20-C19-C18	2.12	125.20	114.42
25	G	1263	PEK	P-O12-C04	2.11	131.98	121.59
26	G	269	CDL	C79-C78-C77	2.10	125.11	114.42
18	B	521	TGL	OG1-CG1-CG2	2.10	114.55	108.43
26	T	1269	CDL	C79-C78-C77	2.10	125.07	114.42
18	N	1521	TGL	CA6-CA5-CA4	-2.10	103.78	114.42
19	A	524	PGV	C03-C02-C01	2.09	116.74	111.79
19	A	524	PGV	O01-C02-C03	2.09	115.98	108.40
26	G	269	CDL	OB8-CB6-CB4	2.09	114.52	108.43
22	B	1086	CHD	C5-C6-C7	2.08	116.76	114.46
17	N	516	HEA	CMC-C2C-C1C	-2.08	125.27	128.46
22	J	60	CHD	O7-C7-C6	2.07	115.08	109.94
26	P	1270	CDL	OA8-CA6-CA4	2.07	114.44	108.43
22	P	1271	CHD	C2-C1-C10	2.06	116.32	112.78
18	L	522	TGL	C10-CB9-CB8	2.06	124.87	114.42
18	N	1522	TGL	C10-CB9-CB8	2.06	124.86	114.42
18	A	523	TGL	CB4-CB3-CB2	2.05	120.57	113.19
25	C	265	PEK	C03-C02-C01	2.05	116.64	111.79
18	A	523	TGL	OG2-CG2-CG1	2.05	115.82	108.40
19	P	1267	PGV	O01-C1-C2	-2.05	107.08	111.50
18	B	521	TGL	CA6-CA5-CA4	-2.05	104.02	114.42
18	A	523	TGL	CA3-CA2-CA1	-2.05	106.17	113.62
19	P	1268	PGV	C02-O01-C1	-2.03	112.80	117.79
26	G	269	CDL	OB8-CB7-C71	-2.03	105.55	111.91
17	N	516	HEA	C16-C15-C14	-2.02	117.03	121.12
22	P	1271	CHD	O12-C12-C13	2.02	114.44	111.03
18	N	1521	TGL	OG1-CG1-CG2	2.02	114.30	108.43
18	L	522	TGL	CC7-CC6-CC5	2.01	124.63	114.42

All (54) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
17	N	516	HEA	ND
17	N	516	HEA	NA
17	N	516	HEA	NB
17	A	516	HEA	ND
17	A	516	HEA	NA
17	A	516	HEA	NB
22	W	1060	CHD	C12
22	W	1060	CHD	C8
22	W	1060	CHD	C9
22	W	1060	CHD	C14
22	W	1060	CHD	C17
23	M	526	DMU	C2
23	M	526	DMU	C4
23	M	526	DMU	C6
23	M	526	DMU	C5
23	M	526	DMU	C9
17	N	515	HEA	ND
17	N	515	HEA	NA
17	N	515	HEA	NB
22	J	60	CHD	C12
22	J	60	CHD	C8
22	J	60	CHD	C9
22	J	60	CHD	C14
22	J	60	CHD	C17
23	P	1272	DMU	C5
23	P	1272	DMU	C6
23	P	1272	DMU	C9
23	P	1272	DMU	C4
23	P	1272	DMU	C2
23	P	1272	DMU	C10
22	P	1271	CHD	C12
22	P	1271	CHD	C8
22	P	1271	CHD	C3
22	P	1271	CHD	C9
22	P	1271	CHD	C14
17	A	515	HEA	ND
17	A	515	HEA	NA
17	A	515	HEA	NB
23	C	272	DMU	C5
23	C	272	DMU	C6
23	C	272	DMU	C9

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Mol	Chain	Res	Type	Atom
23	C	272	DMU	C4
23	C	272	DMU	C2
23	C	272	DMU	C10
22	C	271	CHD	C12
22	C	271	CHD	C8
22	C	271	CHD	C3
22	C	271	CHD	C9
22	C	271	CHD	C14
23	Z	1526	DMU	C2
23	Z	1526	DMU	C4
23	Z	1526	DMU	C6
23	Z	1526	DMU	C5
23	Z	1526	DMU	C9

All (843) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	T	263	PEK	C03-O11-P-O14
25	T	263	PEK	O12-C04-C05-N
19	C	268	PGV	C04-O12-P-O11
19	C	268	PGV	C04-O12-P-O13
19	C	268	PGV	C04-O12-P-O14
19	C	268	PGV	C04-C05-C06-O06
26	T	1269	CDL	CB2-C1-CA2-OA2
26	T	1269	CDL	CA2-OA2-PA1-OA3
26	T	1269	CDL	C1-CB2-OB2-PB2
26	T	1269	CDL	CB3-OB5-PB2-OB3
26	T	1269	CDL	CB3-OB5-PB2-OB4
26	T	1269	CDL	OB6-CB4-CB6-OB8
17	N	516	HEA	C2D-C3D-CAD-CBD
17	N	516	HEA	C4D-C3D-CAD-CBD
17	A	516	HEA	C4D-C3D-CAD-CBD
25	G	1263	PEK	C03-O11-P-O14
25	G	1263	PEK	O12-C04-C05-N
22	W	1060	CHD	C16-C17-C20-C21
22	W	1060	CHD	C16-C17-C20-C22
23	M	526	DMU	O5-C6-O16-C18
22	J	60	CHD	C16-C17-C20-C21
22	J	60	CHD	C16-C17-C20-C22
25	C	264	PEK	O12-C04-C05-N
19	N	1524	PGV	C04-O12-P-O11
19	N	1524	PGV	C04-O12-P-O13

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Mol	Chain	Res	Type	Atoms
19	N	1524	PGV	C04-O12-P-O14
19	N	1524	PGV	C02-C03-O11-P
19	N	1524	PGV	C05-C04-O12-P
19	N	1524	PGV	C04-C05-C06-O06
19	N	1524	PGV	O05-C05-C06-O06
19	N	1524	PGV	O02-C1-O01-C02
19	N	1524	PGV	C20-C19-O03-C01
25	C	265	PEK	C04-O12-P-O13
25	C	265	PEK	C04-O12-P-O14
25	C	265	PEK	C11-C12-C13-C14
26	C	270	CDL	CA2-C1-CB2-OB2
26	C	270	CDL	CA2-OA2-PA1-OA3
26	C	270	CDL	CA2-OA2-PA1-OA4
26	C	270	CDL	CA2-OA2-PA1-OA5
26	C	270	CDL	CA4-CA3-OA5-PA1
26	C	270	CDL	C11-CA5-OA6-CA4
26	C	270	CDL	CB2-OB2-PB2-OB3
26	C	270	CDL	CB2-OB2-PB2-OB4
21	O	1230	PSC	C03-O11-P-O14
21	O	1230	PSC	C04-O12-P-O14
21	O	1230	PSC	O02-C1-O01-C02
25	P	1265	PEK	C04-O12-P-O13
25	P	1265	PEK	C04-O12-P-O14
25	P	1265	PEK	C11-C12-C13-C14
21	B	230	PSC	C03-O11-P-O14
21	B	230	PSC	C04-O12-P-O14
21	B	230	PSC	O02-C1-O01-C02
19	P	1268	PGV	C04-O12-P-O11
19	P	1268	PGV	C04-O12-P-O13
19	P	1268	PGV	C04-O12-P-O14
26	G	269	CDL	CB2-C1-CA2-OA2
26	G	269	CDL	CA2-OA2-PA1-OA3
26	G	269	CDL	C1-CB2-OB2-PB2
26	G	269	CDL	CB3-OB5-PB2-OB3
26	G	269	CDL	CB3-OB5-PB2-OB4
26	G	269	CDL	OB6-CB4-CB6-OB8
26	P	1270	CDL	CA2-C1-CB2-OB2
26	P	1270	CDL	CA2-OA2-PA1-OA3
26	P	1270	CDL	CA2-OA2-PA1-OA4
26	P	1270	CDL	CA4-CA3-OA5-PA1
26	P	1270	CDL	C11-CA5-OA6-CA4
26	P	1270	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	CB2-OB2-PB2-OB4
25	P	1264	PEK	O12-C04-C05-N
23	Z	1526	DMU	O5-C6-O16-C18
19	A	524	PGV	C04-O12-P-O11
19	A	524	PGV	C04-O12-P-O13
19	A	524	PGV	C04-O12-P-O14
19	A	524	PGV	C02-C03-O11-P
19	A	524	PGV	C05-C04-O12-P
19	A	524	PGV	C04-C05-C06-O06
19	A	524	PGV	O05-C05-C06-O06
19	A	524	PGV	O02-C1-O01-C02
19	A	524	PGV	C20-C19-O03-C01
19	N	1524	PGV	O04-C19-O03-C01
19	A	524	PGV	O04-C19-O03-C01
18	A	523	TGL	OC1-CC1-OG3-CG3
18	N	1523	TGL	OC1-CC1-OG3-CG3
18	B	521	TGL	OB1-CB1-OG2-CG2
26	C	270	CDL	OA7-CA5-OA6-CA4
18	N	1521	TGL	OB1-CB1-OG2-CG2
26	T	1269	CDL	C31-CA7-OA8-CA6
26	G	269	CDL	C31-CA7-OA8-CA6
19	N	1524	PGV	C2-C1-O01-C02
18	N	1521	TGL	CB2-CB1-OG2-CG2
19	A	524	PGV	C2-C1-O01-C02
23	C	272	DMU	O6-C11-C9-O1
18	N	1521	TGL	OA1-CA1-OG1-CG1
26	T	1269	CDL	C20-C21-C22-C23
26	T	1269	CDL	C77-C78-C79-C80
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	C20-C21-C22-C23
26	P	1270	CDL	C40-C41-C42-C43
26	P	1270	CDL	C57-C58-C59-C60
26	P	1270	CDL	C80-C81-C82-C83
18	B	521	TGL	CA2-CA1-OG1-CG1
18	A	523	TGL	CC2-CC1-OG3-CG3
18	N	1523	TGL	CC2-CC1-OG3-CG3
18	N	1521	TGL	CA2-CA1-OG1-CG1
26	T	1269	CDL	C17-C18-C19-C20
26	T	1269	CDL	C57-C58-C59-C60
26	T	1269	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
26	C	270	CDL	C20-C21-C22-C23
26	G	269	CDL	C17-C18-C19-C20
26	G	269	CDL	C57-C58-C59-C60
26	G	269	CDL	C77-C78-C79-C80
26	P	1270	CDL	C20-C21-C22-C23
26	P	1270	CDL	C37-C38-C39-C40
26	P	1270	CDL	C60-C61-C62-C63
26	T	1269	CDL	C37-C38-C39-C40
26	T	1269	CDL	C80-C81-C82-C83
26	C	270	CDL	C37-C38-C39-C40
26	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	C40-C41-C42-C43
26	G	269	CDL	C60-C61-C62-C63
26	G	269	CDL	C80-C81-C82-C83
26	P	1270	CDL	OA7-CA5-OA6-CA4
26	T	1269	CDL	OA9-CA7-OA8-CA6
18	B	521	TGL	OA1-CA1-OG1-CG1
26	G	269	CDL	OA9-CA7-OA8-CA6
26	T	1269	CDL	C40-C41-C42-C43
18	B	521	TGL	C16-C15-CC9-CC8
26	C	270	CDL	C17-C18-C19-C20
18	N	1521	TGL	C16-C15-CC9-CC8
26	P	1270	CDL	C17-C18-C19-C20
26	P	1270	CDL	C77-C78-C79-C80
18	A	523	TGL	C21-C20-CA9-CA8
18	N	1523	TGL	C21-C20-CA9-CA8
18	N	1522	TGL	C21-C20-CA9-CA8
26	T	1269	CDL	O1-C1-CA2-OA2
26	G	269	CDL	O1-C1-CA2-OA2
18	L	522	TGL	C21-C20-CA9-CA8
18	B	521	TGL	CB2-CB1-OG2-CG2
18	B	521	TGL	C21-C20-CA9-CA8
18	L	522	TGL	C11-C10-CB9-CB8
18	N	1522	TGL	C11-C10-CB9-CB8
18	B	521	TGL	C11-C10-CB9-CB8
18	A	523	TGL	C11-C10-CB9-CB8
18	N	1523	TGL	C11-C10-CB9-CB8
18	N	1521	TGL	C21-C20-CA9-CA8
18	N	1521	TGL	C11-C10-CB9-CB8
18	A	523	TGL	C16-C15-CC9-CC8

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Mol	Chain	Res	Type	Atoms
18	N	1523	TGL	C16-C15-CC9-CC8
18	L	522	TGL	C16-C15-CC9-CC8
18	N	1522	TGL	C16-C15-CC9-CC8
18	N	1522	TGL	OA1-CA1-OG1-CG1
18	L	522	TGL	OA1-CA1-OG1-CG1
22	J	60	CHD	C13-C17-C20-C22
19	N	1524	PGV	O12-C04-C05-C06
19	A	524	PGV	O12-C04-C05-C06
18	L	522	TGL	CA2-CA1-OG1-CG1
21	O	1230	PSC	C20-C19-O03-C01
21	B	230	PSC	C20-C19-O03-C01
18	N	1522	TGL	CA2-CA1-OG1-CG1
22	W	1060	CHD	C13-C17-C20-C22
23	M	526	DMU	O5-C4-C57-O61
23	C	272	DMU	C3-C4-C57-O61
26	T	1269	CDL	O1-C1-CB2-OB2
19	N	1524	PGV	O12-C04-C05-O05
26	C	270	CDL	O1-C1-CB2-OB2
26	G	269	CDL	O1-C1-CB2-OB2
26	P	1270	CDL	O1-C1-CB2-OB2
19	A	524	PGV	O12-C04-C05-O05
23	P	1272	DMU	C1-C6-O16-C18
23	C	272	DMU	C1-C6-O16-C18
23	Z	1526	DMU	O5-C4-C57-O61
23	P	1272	DMU	O6-C11-C9-O1
18	L	522	TGL	CC3-CC4-CC5-CC6
23	M	526	DMU	O6-C11-C9-C8
19	N	1524	PGV	C19-C20-C21-C22
21	O	1230	PSC	C1-C2-C3-C4
21	B	230	PSC	C1-C2-C3-C4
19	A	524	PGV	C19-C20-C21-C22
23	Z	1526	DMU	O6-C11-C9-C8
18	N	1522	TGL	CC3-CC4-CC5-CC6
25	T	263	PEK	C28-C29-C30-C31
25	G	1263	PEK	C28-C29-C30-C31
21	B	230	PSC	C2-C1-O01-C02
21	B	230	PSC	C20-C21-C22-C23
22	J	60	CHD	C13-C17-C20-C21
23	P	1272	DMU	C3-C4-C57-O61
21	B	230	PSC	O04-C19-O03-C01
21	B	230	PSC	C22-C23-C24-C25
21	O	1230	PSC	O04-C19-O03-C01

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Mol	Chain	Res	Type	Atoms
21	O	1230	PSC	C20-C21-C22-C23
26	C	270	CDL	CB7-C71-C72-C73
26	G	269	CDL	CA5-C11-C12-C13
26	P	1270	CDL	CB7-C71-C72-C73
19	C	268	PGV	O12-C04-C05-O05
19	P	1268	PGV	O12-C04-C05-O05
22	W	1060	CHD	C13-C17-C20-C21
18	N	1521	TGL	OC1-CC1-OG3-CG3
26	T	1269	CDL	CA5-C11-C12-C13
22	P	1271	CHD	C17-C20-C22-C23
22	C	271	CHD	C17-C20-C22-C23
18	B	521	TGL	OC1-CC1-OG3-CG3
21	O	1230	PSC	C2-C1-O01-C02
19	P	1268	PGV	C2-C1-O01-C02
21	O	1230	PSC	C22-C23-C24-C25
25	T	263	PEK	C03-O11-P-O12
26	T	1269	CDL	CB3-OB5-PB2-OB2
25	G	1263	PEK	C03-O11-P-O12
25	C	265	PEK	C04-O12-P-O11
26	C	270	CDL	CB2-OB2-PB2-OB5
25	P	1265	PEK	C04-O12-P-O11
26	G	269	CDL	CB3-OB5-PB2-OB2
26	P	1270	CDL	CA2-OA2-PA1-OA5
26	P	1270	CDL	CB2-OB2-PB2-OB5
18	A	523	TGL	CA2-CA1-OG1-CG1
18	N	1523	TGL	CA2-CA1-OG1-CG1
19	C	268	PGV	O12-C04-C05-C06
26	T	1269	CDL	CA2-C1-CB2-OB2
23	P	1272	DMU	O5-C4-C57-O61
19	P	1268	PGV	O12-C04-C05-C06
26	G	269	CDL	CA2-C1-CB2-OB2
26	T	1269	CDL	OA7-CA5-OA6-CA4
26	G	269	CDL	OA7-CA5-OA6-CA4
26	G	269	CDL	C15-C16-C17-C18
26	C	270	CDL	CA5-C11-C12-C13
19	C	268	PGV	C2-C1-O01-C02
26	T	1269	CDL	C11-CA5-OA6-CA4
26	G	269	CDL	C11-CA5-OA6-CA4
23	Z	1526	DMU	O6-C11-C9-O1
22	W	1060	CHD	C17-C20-C22-C23
26	T	1269	CDL	C72-C73-C74-C75
19	C	266	PGV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
23	M	526	DMU	C25-C28-C31-C34
21	O	1230	PSC	C2-C3-C4-C5
21	B	230	PSC	C2-C3-C4-C5
26	G	269	CDL	C72-C73-C74-C75
18	N	1522	TGL	CB4-CB5-CB6-CB7
23	Z	1526	DMU	C25-C28-C31-C34
19	C	268	PGV	C24-C25-C26-C27
26	T	1269	CDL	C58-C59-C60-C61
18	L	522	TGL	CB4-CB5-CB6-CB7
26	C	270	CDL	C16-C17-C18-C19
19	P	1268	PGV	C24-C25-C26-C27
26	G	269	CDL	C13-C14-C15-C16
26	G	269	CDL	C58-C59-C60-C61
26	P	1270	CDL	C16-C17-C18-C19
19	C	268	PGV	O02-C1-O01-C02
19	P	1268	PGV	O02-C1-O01-C02
26	T	1269	CDL	C13-C14-C15-C16
25	G	1263	PEK	C27-C28-C29-C30
18	L	522	TGL	CC2-CC3-CC4-CC5
18	N	1522	TGL	CC2-CC3-CC4-CC5
19	N	1266	PGV	C23-C24-C25-C26
25	T	263	PEK	C27-C28-C29-C30
21	O	1230	PSC	C29-C30-C31-C32
21	B	230	PSC	C29-C30-C31-C32
26	G	269	CDL	C56-C57-C58-C59
26	P	1270	CDL	C59-C60-C61-C62
19	A	524	PGV	C24-C25-C26-C27
19	C	268	PGV	C13-C14-C15-C16
26	C	270	CDL	C59-C60-C61-C62
19	P	1268	PGV	C13-C14-C15-C16
25	C	264	PEK	C1-C2-C3-C4
26	P	1270	CDL	CA5-C11-C12-C13
25	T	263	PEK	O03-C01-C02-O01
25	G	1263	PEK	O03-C01-C02-O01
25	C	264	PEK	C22-C21-O03-C01
19	N	1266	PGV	C6-C7-C8-C9
26	T	1269	CDL	C56-C57-C58-C59
19	C	266	PGV	C6-C7-C8-C9
19	N	1524	PGV	C4-C5-C6-C7
25	C	265	PEK	C16-C17-C18-C19
26	C	270	CDL	C51-C52-C53-C54
26	T	1269	CDL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
19	N	1524	PGV	C24-C25-C26-C27
26	C	270	CDL	C73-C74-C75-C76
25	P	1265	PEK	C16-C17-C18-C19
19	P	1268	PGV	C22-C23-C24-C25
25	P	1264	PEK	C1-C2-C3-C4
25	C	265	PEK	C25-C26-C27-C28
25	P	1265	PEK	C25-C26-C27-C28
26	P	1270	CDL	C51-C52-C53-C54
19	N	1524	PGV	C22-C23-C24-C25
26	P	1270	CDL	C73-C74-C75-C76
19	A	524	PGV	C4-C5-C6-C7
19	A	524	PGV	C22-C23-C24-C25
19	P	1268	PGV	C04-C05-C06-O06
19	C	268	PGV	C22-C23-C24-C25
26	P	1270	CDL	C55-C56-C57-C58
25	P	1264	PEK	C31-C32-C33-C34
19	C	268	PGV	C30-C31-C32-C33
25	G	1263	PEK	C29-C30-C31-C32
19	P	1267	PGV	C22-C23-C24-C25
25	C	264	PEK	C31-C32-C33-C34
23	P	1272	DMU	C25-C28-C31-C34
19	N	1524	PGV	C28-C29-C30-C31
26	C	270	CDL	C55-C56-C57-C58
19	P	1268	PGV	C30-C31-C32-C33
19	C	267	PGV	C22-C23-C24-C25
19	A	524	PGV	C28-C29-C30-C31
23	P	1272	DMU	O5-C6-O16-C18
25	T	263	PEK	C29-C30-C31-C32
25	T	263	PEK	C25-C26-C27-C28
26	T	1269	CDL	C79-C80-C81-C82
19	C	266	PGV	C29-C30-C31-C32
25	G	1263	PEK	C25-C26-C27-C28
26	G	269	CDL	C79-C80-C81-C82
26	P	1270	CDL	C75-C76-C77-C78
25	P	1264	PEK	C25-C26-C27-C28
25	T	263	PEK	C1-C2-C3-C4
18	A	523	TGL	OA1-CA1-OG1-CG1
18	N	1523	TGL	OA1-CA1-OG1-CG1
19	N	1266	PGV	C29-C30-C31-C32
19	C	268	PGV	C27-C28-C29-C30
25	C	264	PEK	C25-C26-C27-C28
19	P	1268	PGV	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
25	P	1264	PEK	C22-C21-O03-C01
25	C	265	PEK	C29-C30-C31-C32
22	W	1060	CHD	C21-C20-C22-C23
22	J	60	CHD	C21-C20-C22-C23
22	P	1271	CHD	C21-C20-C22-C23
22	C	271	CHD	C21-C20-C22-C23
23	M	526	DMU	C19-C18-O16-C6
23	Z	1526	DMU	C19-C18-O16-C6
26	C	270	CDL	C75-C76-C77-C78
19	C	267	PGV	C7-C8-C9-C10
23	C	272	DMU	C25-C28-C31-C34
19	P	1267	PGV	C7-C8-C9-C10
26	C	270	CDL	C72-C73-C74-C75
25	P	1265	PEK	C29-C30-C31-C32
26	P	1270	CDL	C72-C73-C74-C75
25	P	1264	PEK	C16-C17-C18-C19
25	C	264	PEK	O03-C01-C02-C03
25	P	1264	PEK	O03-C01-C02-C03
22	J	60	CHD	C17-C20-C22-C23
26	T	1269	CDL	C43-C44-C45-C46
25	C	264	PEK	C16-C17-C18-C19
25	C	265	PEK	C31-C32-C33-C34
26	P	1270	CDL	C61-C62-C63-C64
19	C	268	PGV	O05-C05-C06-O06
19	P	1268	PGV	O05-C05-C06-O06
19	C	268	PGV	C3-C4-C5-C6
26	C	270	CDL	C61-C62-C63-C64
26	G	269	CDL	C43-C44-C45-C46
25	P	1265	PEK	C31-C32-C33-C34
19	N	1266	PGV	C5-C6-C7-C8
19	P	1268	PGV	C3-C4-C5-C6
25	G	1263	PEK	C1-C2-C3-C4
26	T	1269	CDL	C54-C55-C56-C57
26	C	270	CDL	OB7-CB5-OB6-CB4
25	C	264	PEK	C23-C24-C25-C26
25	T	263	PEK	C34-C35-C36-C37
19	C	268	PGV	C25-C26-C27-C28
26	C	270	CDL	C74-C75-C76-C77
25	C	264	PEK	C22-C23-C24-C25
25	G	1263	PEK	C34-C35-C36-C37
19	C	266	PGV	C5-C6-C7-C8
25	P	1264	PEK	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
25	G	1263	PEK	C30-C31-C32-C33
26	C	270	CDL	C32-C33-C34-C35
25	C	264	PEK	O04-C21-O03-C01
25	P	1264	PEK	O04-C21-O03-C01
26	P	1270	CDL	C71-C72-C73-C74
25	P	1264	PEK	C23-C24-C25-C26
19	C	268	PGV	C11-C10-C9-C8
19	P	1268	PGV	C11-C10-C9-C8
26	P	1270	CDL	OB7-CB5-OB6-CB4
18	B	521	TGL	CC2-CC1-OG3-CG3
18	N	1521	TGL	CC2-CC1-OG3-CG3
26	C	270	CDL	C71-C72-C73-C74
19	N	1266	PGV	C7-C8-C9-C10
25	T	263	PEK	C30-C31-C32-C33
18	B	521	TGL	CB6-CB7-CB8-CB9
19	P	1268	PGV	C25-C26-C27-C28
26	G	269	CDL	C54-C55-C56-C57
26	P	1270	CDL	C74-C75-C76-C77
26	P	1270	CDL	C13-C14-C15-C16
26	P	1270	CDL	C32-C33-C34-C35
19	C	268	PGV	C1-C2-C3-C4
25	C	265	PEK	C21-C22-C23-C24
19	P	1268	PGV	C1-C2-C3-C4
19	C	266	PGV	C7-C8-C9-C10
26	C	270	CDL	C13-C14-C15-C16
26	T	1269	CDL	C41-C42-C43-C44
26	C	270	CDL	C18-C19-C20-C21
19	C	267	PGV	C25-C26-C27-C28
26	P	1270	CDL	C18-C19-C20-C21
26	C	270	CDL	C51-CB5-OB6-CB4
26	P	1270	CDL	C51-CB5-OB6-CB4
19	P	1267	PGV	C25-C26-C27-C28
26	G	269	CDL	C33-C34-C35-C36
26	G	269	CDL	C41-C42-C43-C44
25	P	1264	PEK	C27-C28-C29-C30
18	L	522	TGL	OB1-CB1-OG2-CG2
23	P	1272	DMU	O6-C11-C9-C8
25	P	1265	PEK	C21-C22-C23-C24
25	G	1263	PEK	C26-C27-C28-C29
25	C	264	PEK	C27-C28-C29-C30
26	G	269	CDL	C73-C74-C75-C76
18	N	1521	TGL	CB6-CB7-CB8-CB9

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Mol	Chain	Res	Type	Atoms
25	P	1264	PEK	C24-C25-C26-C27
25	T	263	PEK	C26-C27-C28-C29
26	G	269	CDL	C21-C22-C23-C24
21	O	1230	PSC	C04-C05-N-C08
26	T	1269	CDL	C33-C34-C35-C36
26	G	269	CDL	C82-C83-C84-C85
25	G	1263	PEK	C2-C3-C4-C5
25	G	1263	PEK	C15-C16-C17-C18
19	P	1268	PGV	C12-C13-C14-C15
26	T	1269	CDL	C21-C22-C23-C24
26	T	1269	CDL	C73-C74-C75-C76
26	T	1269	CDL	C82-C83-C84-C85
21	O	1230	PSC	C11-C12-C13-C14
25	C	264	PEK	C24-C25-C26-C27
26	C	270	CDL	C42-C43-C44-C45
26	P	1270	CDL	C63-C64-C65-C66
18	N	1522	TGL	OB1-CB1-OG2-CG2
26	P	1270	CDL	C42-C43-C44-C45
21	O	1230	PSC	C04-O12-P-O11
21	B	230	PSC	C04-O12-P-O11
25	T	263	PEK	C01-C02-C03-O11
25	G	1263	PEK	C01-C02-C03-O11
26	C	270	CDL	OB5-CB3-CB4-CB6
26	P	1270	CDL	OB5-CB3-CB4-CB6
26	C	270	CDL	C63-C64-C65-C66
25	T	263	PEK	C2-C3-C4-C5
19	C	268	PGV	C12-C13-C14-C15
19	N	1524	PGV	C11-C10-C9-C8
21	O	1230	PSC	C13-C14-C15-C16
26	P	1270	CDL	C78-C79-C80-C81
19	C	267	PGV	C13-C14-C15-C16
19	P	1267	PGV	C13-C14-C15-C16
25	T	263	PEK	O03-C01-C02-C03
26	T	1269	CDL	CB3-CB4-CB6-OB8
25	G	1263	PEK	O03-C01-C02-C03
18	N	1523	TGL	CA9-C20-C21-C22
26	C	270	CDL	CB3-CB4-CB6-OB8
26	G	269	CDL	CB3-CB4-CB6-OB8
26	P	1270	CDL	CB3-CB4-CB6-OB8
19	C	268	PGV	C28-C29-C30-C31
26	C	270	CDL	C44-C45-C46-C47
26	C	270	CDL	C78-C79-C80-C81

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Mol	Chain	Res	Type	Atoms
18	A	523	TGL	CA9-C20-C21-C22
21	O	1230	PSC	C27-C28-C29-C30
26	P	1270	CDL	C44-C45-C46-C47
21	B	230	PSC	C27-C28-C29-C30
25	C	264	PEK	C32-C33-C34-C35
19	P	1267	PGV	C11-C10-C9-C8
19	N	1524	PGV	C12-C13-C14-C15
21	B	230	PSC	C13-C14-C15-C16
19	C	267	PGV	C11-C10-C9-C8
19	A	524	PGV	C11-C10-C9-C8
19	A	524	PGV	C12-C13-C14-C15
26	C	270	CDL	C84-C85-C86-C87
23	M	526	DMU	O6-C11-C9-O1
23	P	1272	DMU	C34-C37-C40-C43
19	P	1268	PGV	C28-C29-C30-C31
26	P	1270	CDL	C84-C85-C86-C87
26	T	1269	CDL	C44-C45-C46-C47
19	N	1524	PGV	C20-C21-C22-C23
19	P	1268	PGV	C5-C6-C7-C8
19	N	1524	PGV	C03-C02-O01-C1
19	A	524	PGV	C03-C02-O01-C1
19	P	1267	PGV	C15-C16-C17-C18
19	C	267	PGV	C15-C16-C17-C18
26	G	269	CDL	C44-C45-C46-C47
23	Z	1526	DMU	C34-C37-C40-C43
19	C	268	PGV	C5-C6-C7-C8
26	P	1270	CDL	C23-C24-C25-C26
26	C	270	CDL	C23-C24-C25-C26
26	G	269	CDL	C53-C54-C55-C56
21	B	230	PSC	C3-C4-C5-C6
19	P	1268	PGV	C14-C15-C16-C17
18	N	1522	TGL	CC7-CC8-CC9-C15
21	O	1230	PSC	O03-C01-C02-O01
26	G	269	CDL	OA6-CA4-CA6-OA8
25	P	1264	PEK	C32-C33-C34-C35
19	A	524	PGV	C5-C6-C7-C8
23	M	526	DMU	C34-C37-C40-C43
21	B	230	PSC	C23-C24-C25-C26
19	P	1268	PGV	C4-C5-C6-C7
19	A	524	PGV	C20-C21-C22-C23
19	N	1266	PGV	C30-C31-C32-C33
19	C	268	PGV	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	C53-C54-C55-C56
26	C	270	CDL	C36-C37-C38-C39
21	O	1230	PSC	C3-C4-C5-C6
26	P	1270	CDL	C36-C37-C38-C39
19	C	268	PGV	C4-C5-C6-C7
19	C	268	PGV	C31-C32-C33-C34
23	Z	1526	DMU	C22-C25-C28-C31
23	M	526	DMU	C22-C25-C28-C31
21	B	230	PSC	C24-C25-C26-C27
19	P	1268	PGV	C31-C32-C33-C34
22	C	271	CHD	C13-C17-C20-C22
18	L	522	TGL	CC7-CC8-CC9-C15
21	B	230	PSC	C11-C12-C13-C14
19	C	266	PGV	C30-C31-C32-C33
19	N	1524	PGV	C5-C6-C7-C8
25	P	1264	PEK	C26-C27-C28-C29
26	T	1269	CDL	OA5-CA3-CA4-CA6
19	N	1524	PGV	C01-C02-C03-O11
26	C	270	CDL	OA5-CA3-CA4-CA6
26	G	269	CDL	OA5-CA3-CA4-CA6
19	A	524	PGV	C01-C02-C03-O11
23	Z	1526	DMU	O16-C18-C19-C22
21	O	1230	PSC	C23-C24-C25-C26
18	N	1522	TGL	CC2-CC1-OG3-CG3
22	P	1271	CHD	C13-C17-C20-C22
25	C	264	PEK	C26-C27-C28-C29
26	C	270	CDL	C64-C65-C66-C67
23	C	272	DMU	C34-C37-C40-C43
19	C	268	PGV	C23-C24-C25-C26
21	O	1230	PSC	C24-C25-C26-C27
19	A	524	PGV	C26-C27-C28-C29
19	P	1267	PGV	C20-C21-C22-C23
19	C	267	PGV	C20-C21-C22-C23
26	T	1269	CDL	C19-C20-C21-C22
26	P	1270	CDL	C64-C65-C66-C67
19	C	267	PGV	C23-C24-C25-C26
26	G	269	CDL	C19-C20-C21-C22
21	B	230	PSC	C04-C05-N-C08
26	P	1270	CDL	C39-C40-C41-C42
25	T	263	PEK	C6-C7-C8-C9
26	T	1269	CDL	CB2-OB2-PB2-OB5
25	G	1263	PEK	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	C	264	PEK	C5-C6-C7-C8
25	C	264	PEK	C9-C10-C11-C12
21	O	1230	PSC	C9-C10-C11-C12
21	B	230	PSC	C9-C10-C11-C12
26	G	269	CDL	CB2-OB2-PB2-OB5
25	P	1264	PEK	C5-C6-C7-C8
25	P	1264	PEK	C9-C10-C11-C12
26	T	1269	CDL	CB5-C51-C52-C53
26	G	269	CDL	CB5-C51-C52-C53
22	P	1271	CHD	C13-C17-C20-C21
22	C	271	CHD	C13-C17-C20-C21
19	N	1266	PGV	C26-C27-C28-C29
26	P	1270	CDL	OB5-CB3-CB4-OB6
26	C	270	CDL	C34-C35-C36-C37
25	P	1264	PEK	C17-C18-C19-C20
19	C	268	PGV	C15-C16-C17-C18
19	P	1267	PGV	C23-C24-C25-C26
25	C	264	PEK	C17-C18-C19-C20
19	N	1524	PGV	C26-C27-C28-C29
26	G	269	CDL	C14-C15-C16-C17
19	P	1267	PGV	C24-C25-C26-C27
19	P	1268	PGV	C23-C24-C25-C26
26	T	1269	CDL	OA6-CA4-CA6-OA8
26	C	270	CDL	OB6-CB4-CB6-OB8
21	B	230	PSC	O03-C01-C02-O01
26	P	1270	CDL	OB6-CB4-CB6-OB8
19	C	268	PGV	C20-C19-O03-C01
26	C	270	CDL	C39-C40-C41-C42
26	P	1270	CDL	C34-C35-C36-C37
23	C	272	DMU	O5-C6-O16-C18
21	B	230	PSC	C31-C32-C33-C34
26	G	269	CDL	C35-C36-C37-C38
26	T	1269	CDL	C14-C15-C16-C17
25	P	1265	PEK	C32-C33-C34-C35
21	O	1230	PSC	C4-C5-C6-C7
21	O	1230	PSC	C31-C32-C33-C34
19	C	267	PGV	C24-C25-C26-C27
26	P	1270	CDL	C24-C25-C26-C27
25	T	263	PEK	C02-C03-O11-P
25	G	1263	PEK	C02-C03-O11-P
23	Z	1526	DMU	C3-C4-C57-O61
25	T	263	PEK	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	C71-C72-C73-C74
23	P	1272	DMU	C22-C25-C28-C31
26	C	270	CDL	C24-C25-C26-C27
21	B	230	PSC	C4-C5-C6-C7
21	O	1230	PSC	C04-C05-N-C07
18	B	521	TGL	C12-C13-C14-C29
18	N	1521	TGL	C12-C13-C14-C29
19	P	1268	PGV	C15-C16-C17-C18
18	L	522	TGL	CC2-CC1-OG3-CG3
26	T	1269	CDL	C35-C36-C37-C38
19	N	1266	PGV	C4-C5-C6-C7
19	C	266	PGV	C4-C5-C6-C7
26	P	1270	CDL	OA5-CA3-CA4-CA6
25	G	1263	PEK	C16-C17-C18-C19
26	G	269	CDL	C64-C65-C66-C67
23	M	526	DMU	O16-C18-C19-C22
26	G	269	CDL	C71-C72-C73-C74
26	T	1269	CDL	C39-C40-C41-C42
26	T	1269	CDL	C64-C65-C66-C67
21	B	230	PSC	C14-C15-C16-C17
26	C	270	CDL	C38-C39-C40-C41
19	N	1266	PGV	C31-C32-C33-C34
26	G	269	CDL	C24-C25-C26-C27
25	T	263	PEK	C22-C21-O03-C01
19	P	1268	PGV	C20-C19-O03-C01
25	C	265	PEK	C32-C33-C34-C35
22	C	271	CHD	C16-C17-C20-C22
19	C	266	PGV	C31-C32-C33-C34
26	T	1269	CDL	CB4-CB3-OB5-PB2
21	O	1230	PSC	O03-C01-C02-C03
21	B	230	PSC	O03-C01-C02-C03
21	O	1230	PSC	C14-C15-C16-C17
26	C	270	CDL	OA5-CA3-CA4-OA6
26	C	270	CDL	OB5-CB3-CB4-OB6
26	P	1270	CDL	OA5-CA3-CA4-OA6
19	C	268	PGV	O04-C19-O03-C01
18	N	1523	TGL	OG2-CG2-CG3-OG3
19	N	1524	PGV	O03-C01-C02-O01
26	T	1269	CDL	C24-C25-C26-C27
25	G	1263	PEK	C31-C32-C33-C34
25	T	263	PEK	O04-C21-O03-C01
26	P	1270	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
22	P	1271	CHD	C16-C17-C20-C22
23	C	272	DMU	C22-C25-C28-C31
25	G	1263	PEK	O04-C21-O03-C01
19	P	1268	PGV	O04-C19-O03-C01
19	C	268	PGV	C26-C27-C28-C29
25	T	263	PEK	C31-C32-C33-C34
26	P	1270	CDL	C56-C57-C58-C59
26	P	1270	CDL	C11-C12-C13-C14
26	C	270	CDL	C11-C12-C13-C14
19	P	1268	PGV	C26-C27-C28-C29
25	G	1263	PEK	C22-C21-O03-C01
26	P	1270	CDL	C76-C77-C78-C79
21	O	1230	PSC	C03-O11-P-O12
21	B	230	PSC	C03-O11-P-O12
25	T	263	PEK	C16-C17-C18-C19
26	C	270	CDL	C56-C57-C58-C59
26	T	1269	CDL	C31-C32-C33-C34
19	P	1267	PGV	C02-C03-O11-P
19	C	267	PGV	C02-C03-O11-P
26	G	269	CDL	CB4-CB3-OB5-PB2
25	T	263	PEK	C03-O11-P-O13
25	G	1263	PEK	C03-O11-P-O13
21	O	1230	PSC	C03-O11-P-O13
21	O	1230	PSC	C04-O12-P-O13
21	B	230	PSC	C03-O11-P-O13
21	B	230	PSC	C04-O12-P-O13
21	B	230	PSC	C04-C05-N-C07
19	P	1268	PGV	C01-C02-C03-O11
26	C	270	CDL	C76-C77-C78-C79
23	Z	1526	DMU	C28-C31-C34-C37
19	C	266	PGV	C26-C27-C28-C29
26	T	1269	CDL	C12-C13-C14-C15
25	P	1264	PEK	C29-C30-C31-C32
26	G	269	CDL	C31-C32-C33-C34
25	G	1263	PEK	C21-C22-C23-C24
26	G	269	CDL	C39-C40-C41-C42
26	G	269	CDL	CB7-C71-C72-C73
18	N	1521	TGL	CG2-CG3-OG3-CC1
25	T	263	PEK	O01-C02-C03-O11
19	P	1267	PGV	C31-C32-C33-C34
25	P	1265	PEK	C30-C31-C32-C33
18	N	1522	TGL	CC5-CC6-CC7-CC8

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Mol	Chain	Res	Type	Atoms
21	O	1230	PSC	C04-C05-N-C06
21	B	230	PSC	C04-C05-N-C06
26	T	1269	CDL	CA3-CA4-CA6-OA8
17	A	516	HEA	C2D-C3D-CAD-CBD
19	N	1524	PGV	O03-C01-C02-C03
26	G	269	CDL	CA3-CA4-CA6-OA8
19	A	524	PGV	O03-C01-C02-C03
18	A	523	TGL	OG2-CG2-CG3-OG3
25	C	264	PEK	O03-C01-C02-O01
25	P	1264	PEK	O03-C01-C02-O01
19	A	524	PGV	O03-C01-C02-O01
25	C	265	PEK	C30-C31-C32-C33
26	G	269	CDL	C12-C13-C14-C15
26	T	1269	CDL	CB7-C71-C72-C73
19	C	267	PGV	C31-C32-C33-C34
25	T	263	PEK	C21-C22-C23-C24
18	B	521	TGL	CG2-CG3-OG3-CC1
21	O	1230	PSC	C21-C22-C23-C24
21	O	1230	PSC	C03-C02-O01-C1
21	B	230	PSC	C03-C02-O01-C1
19	C	268	PGV	C01-C02-C03-O11
22	P	1271	CHD	C16-C17-C20-C21
22	C	271	CHD	C16-C17-C20-C21
26	C	270	CDL	C43-C44-C45-C46
26	P	1270	CDL	C43-C44-C45-C46
25	C	264	PEK	C29-C30-C31-C32
19	C	268	PGV	O01-C02-C03-O11
25	G	1263	PEK	O01-C02-C03-O11
19	P	1268	PGV	O01-C02-C03-O11
19	C	268	PGV	O03-C01-C02-O01
19	P	1268	PGV	O03-C01-C02-O01
19	N	1524	PGV	C03-O11-P-O12
26	C	270	CDL	CA3-OA5-PA1-OA2
26	P	1270	CDL	CA3-OA5-PA1-OA2
19	A	524	PGV	C03-O11-P-O12
18	L	522	TGL	CC5-CC6-CC7-CC8
19	C	267	PGV	C11-C12-C13-C14
21	B	230	PSC	C21-C22-C23-C24
19	C	268	PGV	C02-C03-O11-P
26	C	270	CDL	C1-CA2-OA2-PA1
26	P	1270	CDL	C1-CA2-OA2-PA1
26	P	1270	CDL	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
19	C	267	PGV	C14-C15-C16-C17
23	P	1272	DMU	C4-C3-O7-C10
23	M	526	DMU	C28-C31-C34-C37
26	G	269	CDL	C38-C39-C40-C41
19	P	1267	PGV	C14-C15-C16-C17
25	G	1263	PEK	C32-C33-C34-C35
26	C	270	CDL	C22-C23-C24-C25
19	P	1268	PGV	C02-C03-O11-P
25	T	263	PEK	C32-C33-C34-C35
19	P	1267	PGV	C11-C12-C13-C14
25	C	265	PEK	C3-C4-C5-C6
25	P	1265	PEK	C3-C4-C5-C6
25	P	1264	PEK	C3-C4-C5-C6
25	C	265	PEK	C35-C36-C37-C38
26	T	1269	CDL	C38-C39-C40-C41
25	C	264	PEK	C35-C36-C37-C38
25	C	264	PEK	C3-C4-C5-C6
25	P	1265	PEK	C17-C18-C19-C20
26	C	270	CDL	C15-C16-C17-C18
25	P	1265	PEK	C35-C36-C37-C38
26	P	1270	CDL	C15-C16-C17-C18
23	M	526	DMU	C3-C4-C57-O61
18	B	521	TGL	C10-C11-C12-C13
19	N	1266	PGV	C25-C26-C27-C28
25	C	265	PEK	C17-C18-C19-C20
26	C	270	CDL	C52-C53-C54-C55
25	C	265	PEK	C26-C27-C28-C29
25	C	265	PEK	O03-C01-C02-O01
18	N	1522	TGL	OC1-CC1-OG3-CG3
18	N	1522	TGL	CC6-CC7-CC8-CC9
18	N	1521	TGL	C10-C11-C12-C13
23	C	272	DMU	C18-C19-C22-C25
19	C	267	PGV	C29-C30-C31-C32
25	G	1263	PEK	C14-C15-C16-C17
19	C	267	PGV	C1-C2-C3-C4
25	P	1265	PEK	C26-C27-C28-C29
19	C	266	PGV	O03-C19-C20-C21
18	L	522	TGL	OG2-CB1-CB2-CB3
19	A	524	PGV	C25-C26-C27-C28
19	P	1267	PGV	C29-C30-C31-C32
26	G	269	CDL	CA7-C31-C32-C33
26	P	1270	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
19	C	267	PGV	C05-C04-O12-P
25	P	1265	PEK	O03-C01-C02-O01
18	L	522	TGL	CC6-CC7-CC8-CC9
18	N	1522	TGL	OG2-CB1-CB2-CB3
19	N	1266	PGV	C11-C12-C13-C14
25	T	263	PEK	C3-C4-C5-C6
25	G	1263	PEK	C3-C4-C5-C6
21	O	1230	PSC	C7-C8-C9-C10
21	B	230	PSC	C7-C8-C9-C10
25	P	1264	PEK	C35-C36-C37-C38
18	L	522	TGL	OG3-CC1-CC2-CC3
17	N	515	HEA	C26-C15-C16-C17
26	T	1269	CDL	CA2-OA2-PA1-OA5
26	G	269	CDL	CA2-OA2-PA1-OA5
18	N	1522	TGL	OG3-CC1-CC2-CC3
25	C	264	PEK	O01-C1-C2-C3
26	C	270	CDL	C12-C11-CA5-OA6
25	T	263	PEK	C14-C15-C16-C17
19	P	1267	PGV	C9-C10-C11-C12
21	B	230	PSC	C15-C16-C17-C18
18	A	523	TGL	CG1-CG2-OG2-CB1
18	N	1523	TGL	CG1-CG2-OG2-CB1
26	P	1270	CDL	C52-C53-C54-C55
18	A	523	TGL	OG2-CB1-CB2-CB3
19	N	1524	PGV	O01-C1-C2-C3
21	O	1230	PSC	O03-C19-C20-C21
26	P	1270	CDL	C32-C31-CA7-OA8
26	C	270	CDL	C82-C83-C84-C85
21	B	230	PSC	O03-C19-C20-C21
19	C	266	PGV	C9-C10-C11-C12
19	C	266	PGV	C11-C12-C13-C14
26	G	269	CDL	C78-C79-C80-C81
18	N	1523	TGL	OG2-CB1-CB2-CB3
26	C	270	CDL	C32-C31-CA7-OA8
25	P	1264	PEK	O01-C1-C2-C3
19	A	524	PGV	O01-C1-C2-C3
19	P	1267	PGV	C1-C2-C3-C4
19	N	1266	PGV	C9-C10-C11-C12
19	N	1524	PGV	C9-C10-C11-C12
19	C	267	PGV	C9-C10-C11-C12
19	N	1266	PGV	O03-C19-C20-C21
19	C	266	PGV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
23	C	272	DMU	C4-C3-O7-C10
21	O	1230	PSC	C15-C16-C17-C18
21	O	1230	PSC	C01-C02-C03-O11
21	B	230	PSC	C01-C02-C03-O11
18	N	1523	TGL	OG1-CG1-CG2-OG2
26	T	1269	CDL	C36-C37-C38-C39
19	A	524	PGV	C9-C10-C11-C12
21	O	1230	PSC	O01-C1-C2-C3
21	B	230	PSC	O01-C1-C2-C3
19	N	1524	PGV	C25-C26-C27-C28
26	C	270	CDL	C52-C51-CB5-OB6
26	T	1269	CDL	CA7-C31-C32-C33
26	T	1269	CDL	C78-C79-C80-C81
26	P	1270	CDL	C52-C51-CB5-OB6
25	C	264	PEK	O02-C1-C2-C3
18	N	1521	TGL	OG1-CA1-CA2-CA3
26	P	1270	CDL	C82-C83-C84-C85
19	A	524	PGV	C2-C3-C4-C5
21	B	230	PSC	O04-C19-C20-C21
17	N	516	HEA	C26-C15-C16-C17
17	N	515	HEA	C14-C15-C16-C17
26	G	269	CDL	C36-C37-C38-C39
23	M	526	DMU	C19-C22-C25-C28
26	C	270	CDL	CB2-C1-CA2-OA2
18	N	1523	TGL	OC1-CC1-CC2-CC3
26	C	270	CDL	C32-C31-CA7-OA9
26	P	1270	CDL	C32-C31-CA7-OA9
25	T	263	PEK	C33-C34-C35-C36
18	A	523	TGL	OC1-CC1-CC2-CC3
21	O	1230	PSC	O02-C1-C2-C3
21	B	230	PSC	O02-C1-C2-C3
25	P	1264	PEK	O02-C1-C2-C3
26	P	1270	CDL	C14-C15-C16-C17
21	B	230	PSC	C26-C27-C28-C29
18	B	521	TGL	OG1-CA1-CA2-CA3
21	O	1230	PSC	O04-C19-C20-C21
17	A	515	HEA	C14-C15-C16-C17
26	G	269	CDL	C11-C12-C13-C14
25	P	1265	PEK	C03-O11-P-O14
26	P	1270	CDL	CA3-OA5-PA1-OA3
19	N	1524	PGV	O02-C1-C2-C3
21	O	1230	PSC	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
19	A	524	PGV	O02-C1-C2-C3
19	N	1524	PGV	C2-C3-C4-C5
26	C	270	CDL	C14-C15-C16-C17
18	N	1521	TGL	C13-C14-C29-C30
18	B	521	TGL	CG1-CG2-OG2-CB1
21	O	1230	PSC	C05-C04-O12-P
21	B	230	PSC	C05-C04-O12-P
26	T	1269	CDL	C11-C12-C13-C14
25	G	1263	PEK	C33-C34-C35-C36
26	T	1269	CDL	OB9-CB7-OB8-CB6
26	P	1270	CDL	CB2-C1-CA2-OA2
18	B	521	TGL	C13-C14-C29-C30
17	A	516	HEA	C26-C15-C16-C17
17	A	515	HEA	C26-C15-C16-C17
21	O	1230	PSC	C12-C13-C14-C15
21	B	230	PSC	C12-C13-C14-C15
18	L	522	TGL	OC1-CC1-CC2-CC3
18	N	1522	TGL	CB5-CB6-CB7-CB8
18	N	1522	TGL	OC1-CC1-CC2-CC3
26	T	1269	CDL	C22-C23-C24-C25

There are no ring outliers.

36 monomers are involved in 235 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	T	263	PEK	6	0
19	C	268	PGV	1	0
26	T	1269	CDL	19	0
17	N	516	HEA	2	0
18	B	521	TGL	7	0
18	A	523	TGL	4	0
22	B	1086	CHD	1	0
17	A	516	HEA	4	0
25	G	1263	PEK	10	0
22	W	1060	CHD	4	0
18	N	1523	TGL	4	0
17	N	515	HEA	3	0
22	J	60	CHD	2	0
19	P	1267	PGV	5	0
25	P	1264	PEK	6	0
23	P	1272	DMU	8	0
18	L	522	TGL	20	0

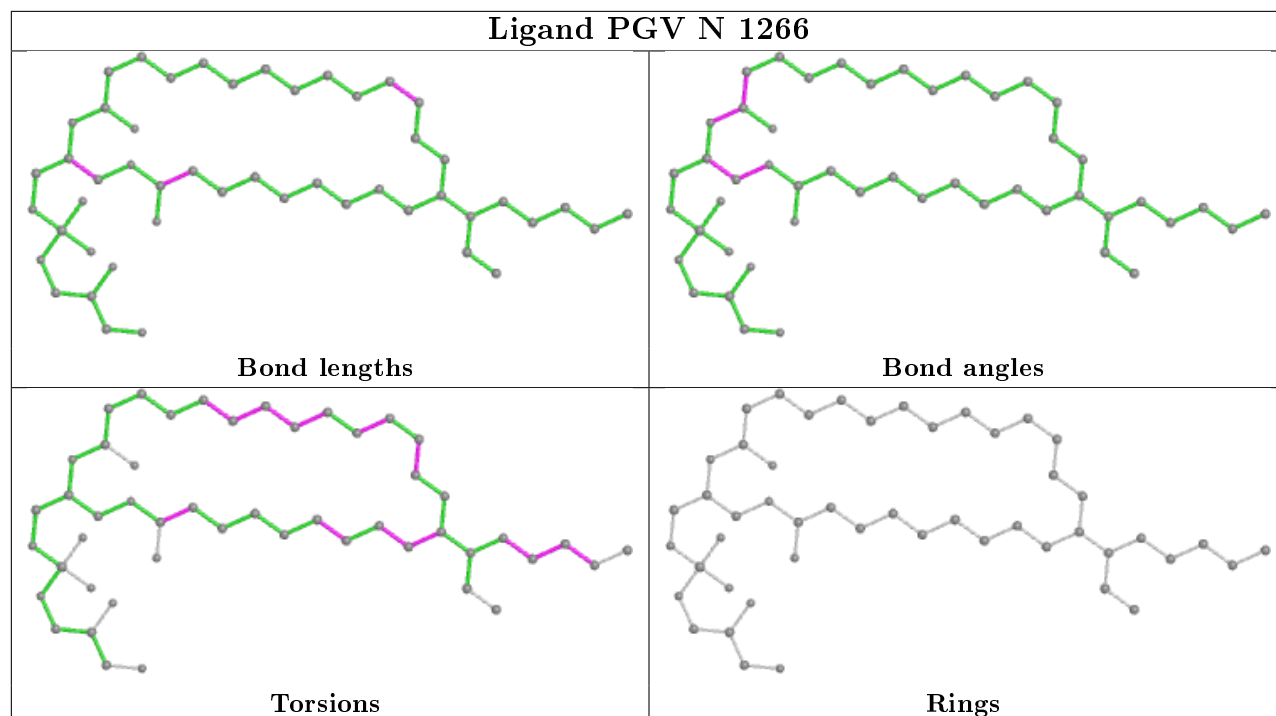
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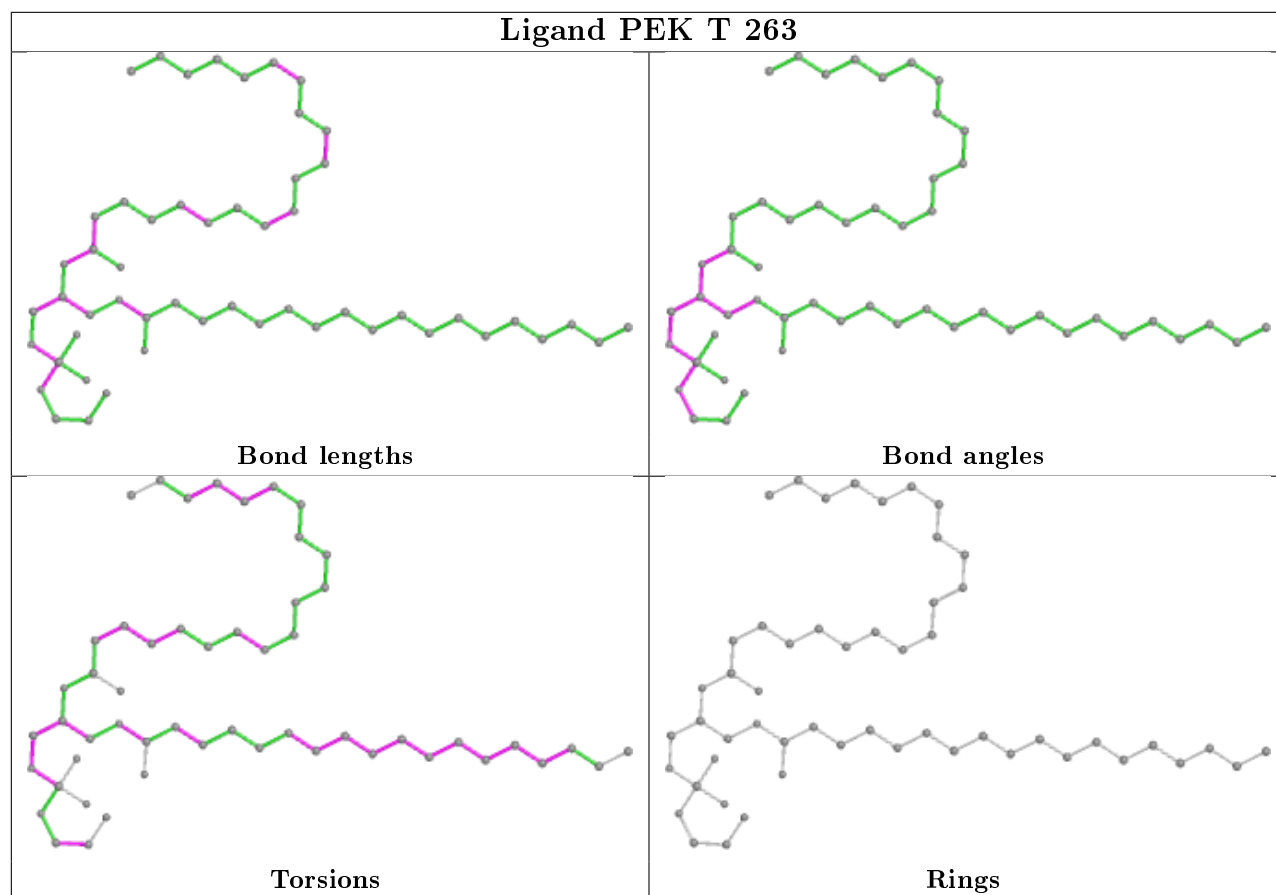
Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	G	269	CDL	18	0
19	N	1524	PGV	8	0
25	C	265	PEK	7	0
22	P	1271	CHD	1	0
26	C	270	CDL	11	0
21	O	1230	PSC	15	0
17	A	515	HEA	2	0
25	P	1265	PEK	7	0
21	B	230	PSC	11	0
22	O	229	CHD	1	0
19	P	1268	PGV	1	0
19	C	267	PGV	5	0
25	C	264	PEK	4	0
23	C	272	DMU	3	0
18	N	1521	TGL	9	0
26	P	1270	CDL	15	0
22	C	271	CHD	3	0
18	N	1522	TGL	14	0
19	A	524	PGV	7	0

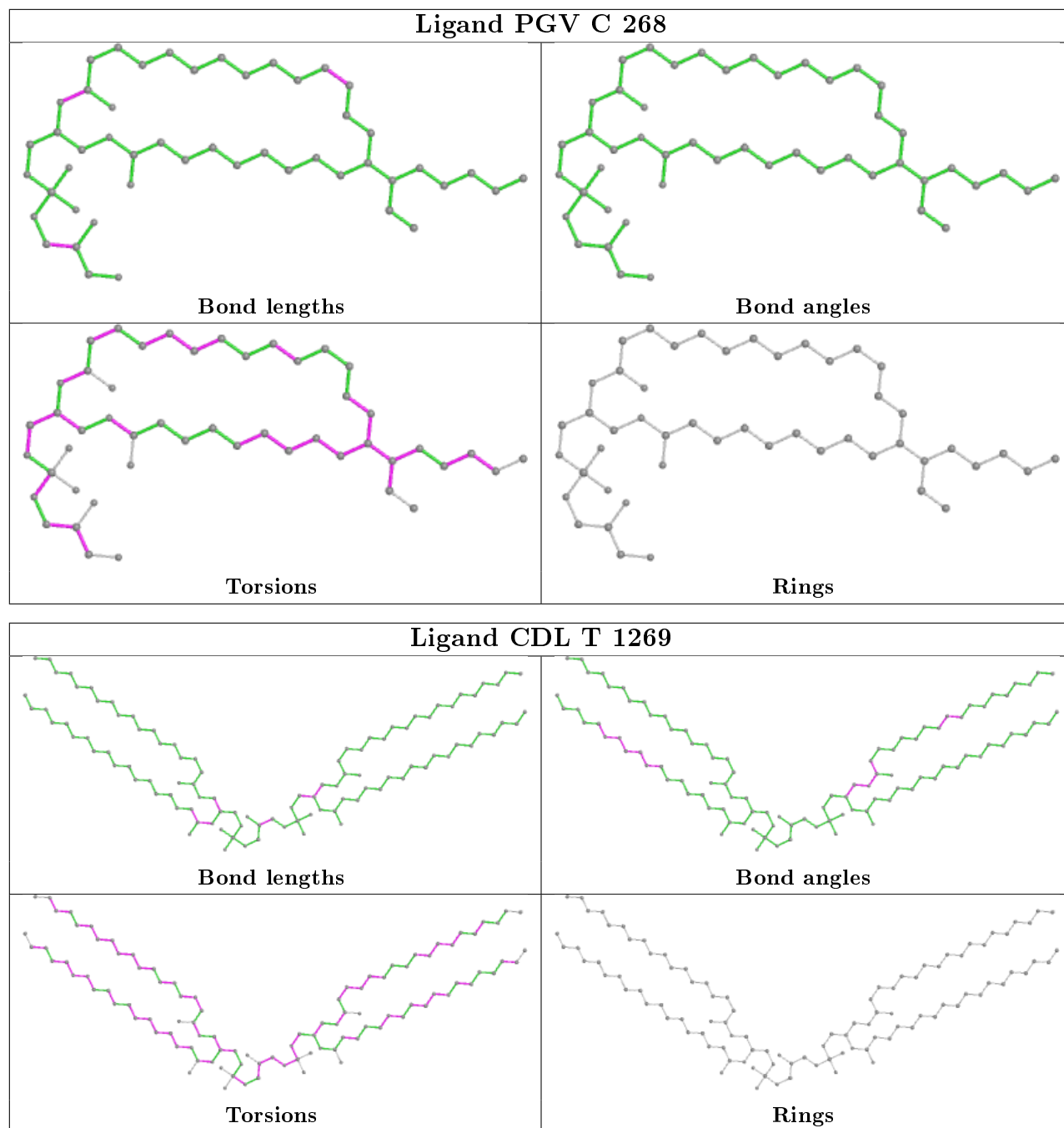
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

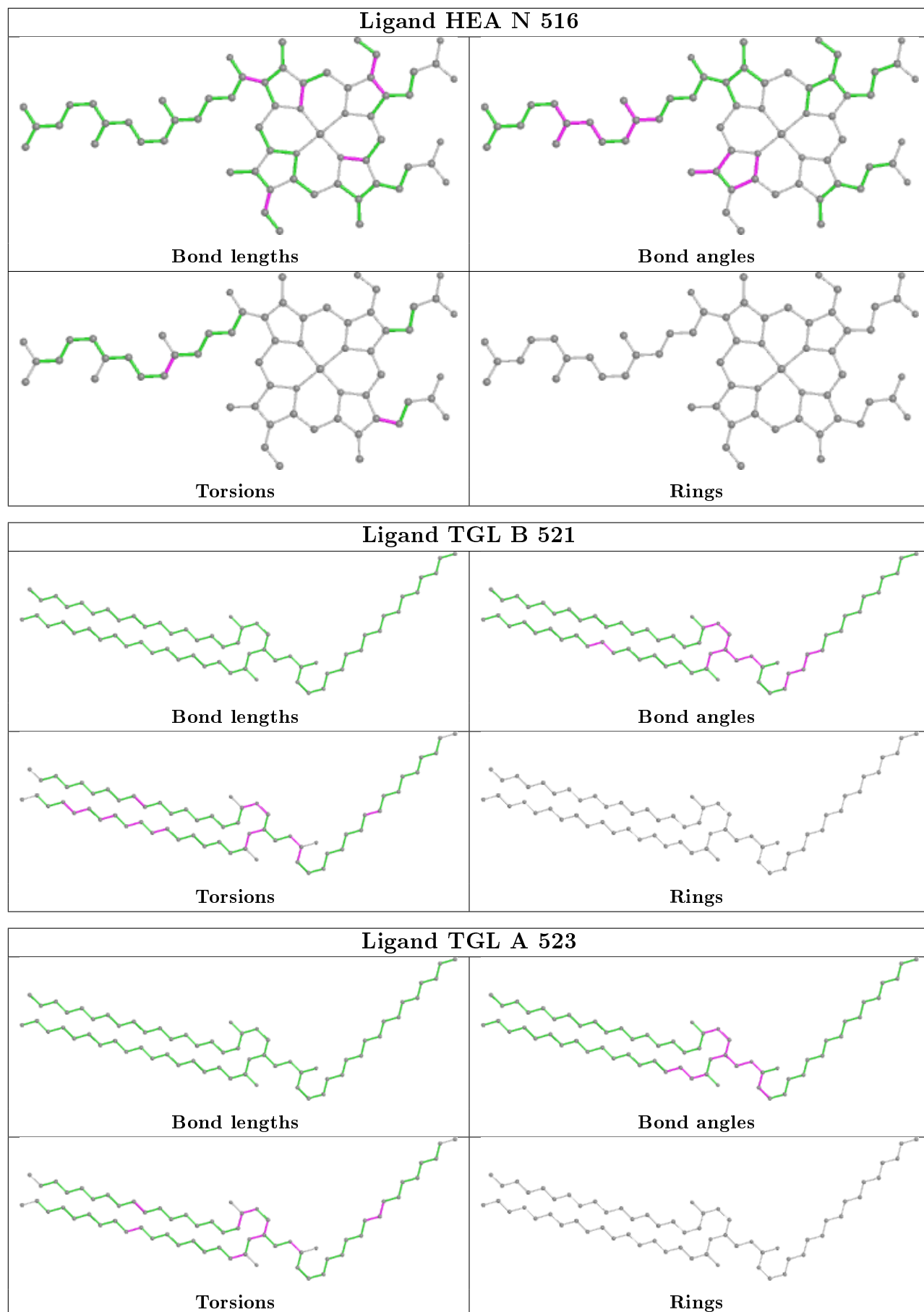
Ligand PGV N 1266

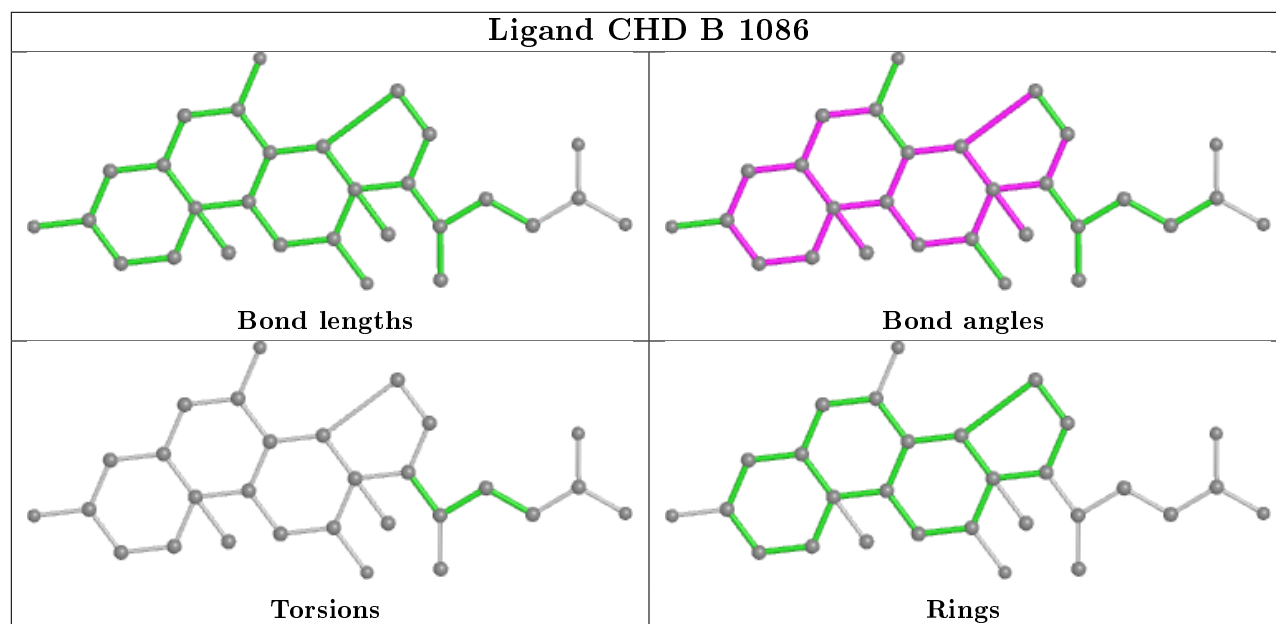
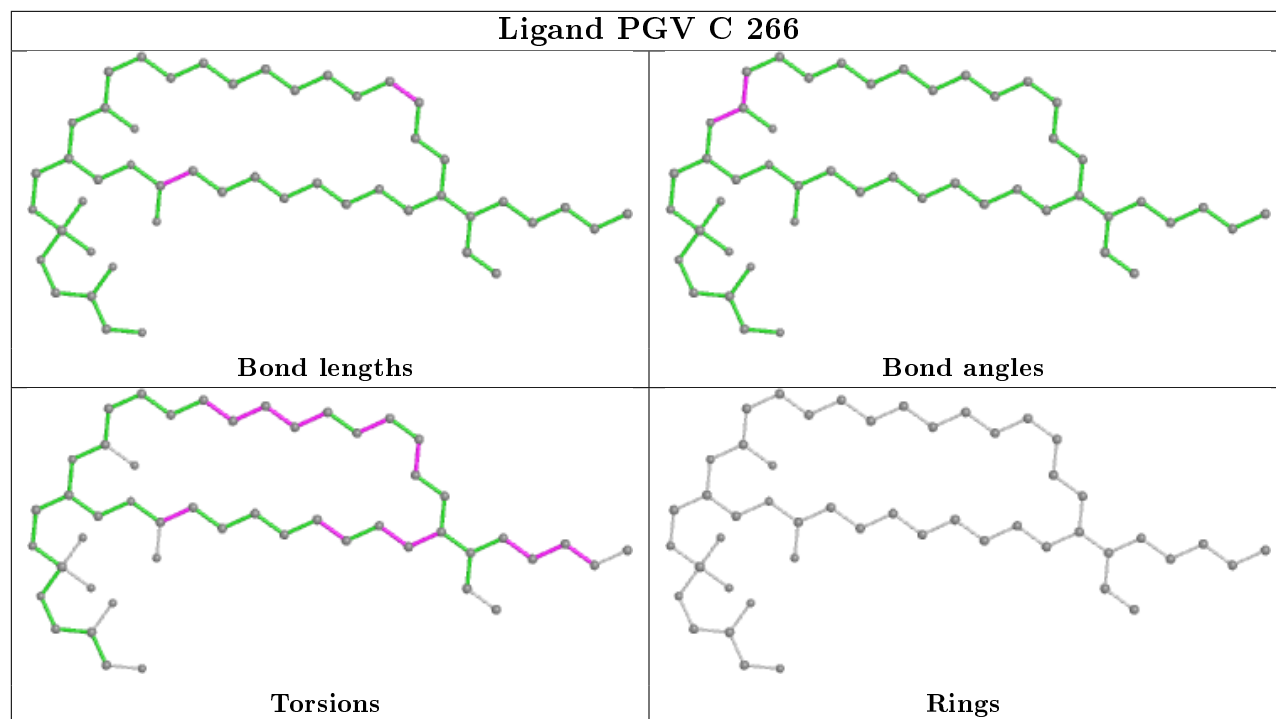


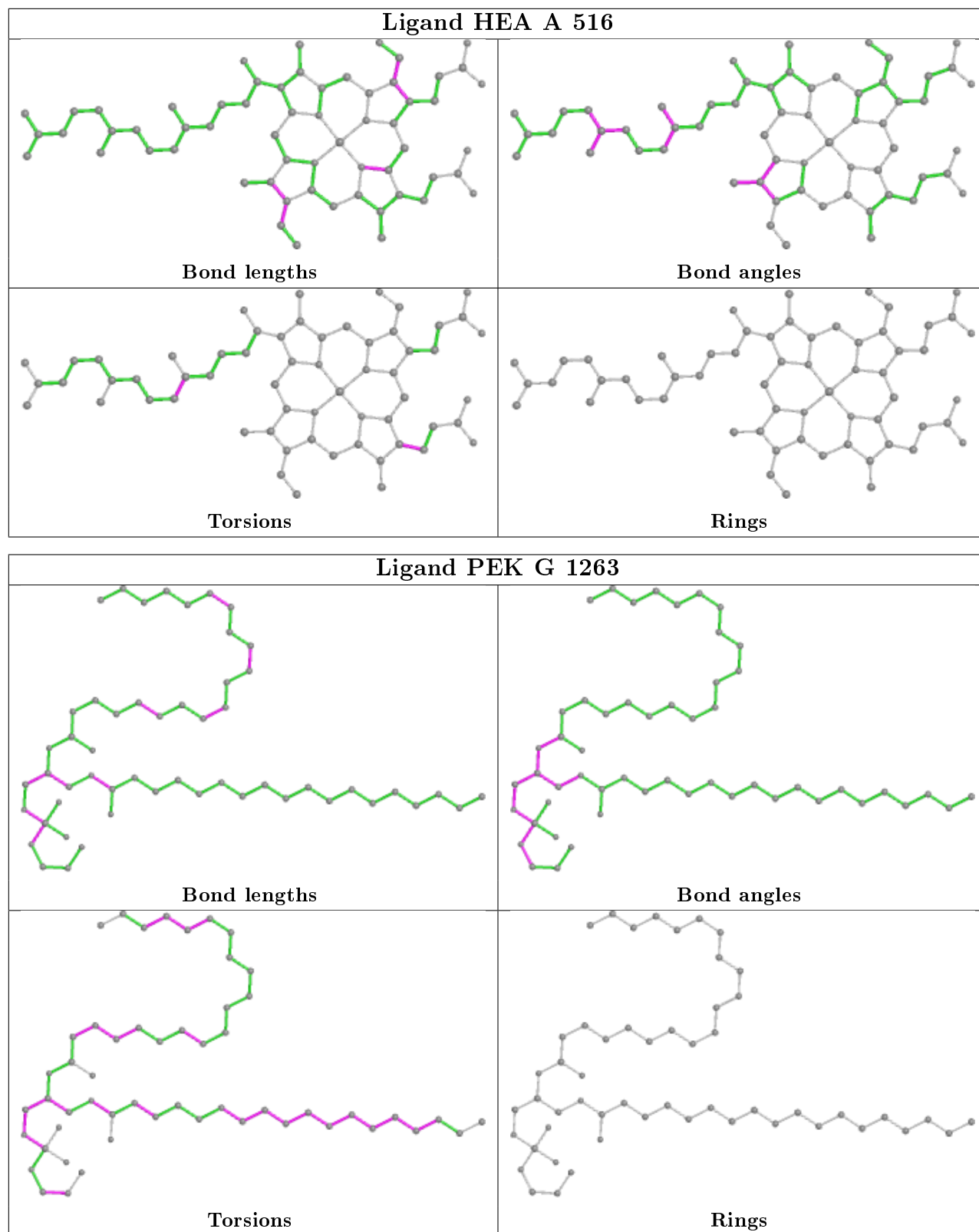
Ligand PEK T 263



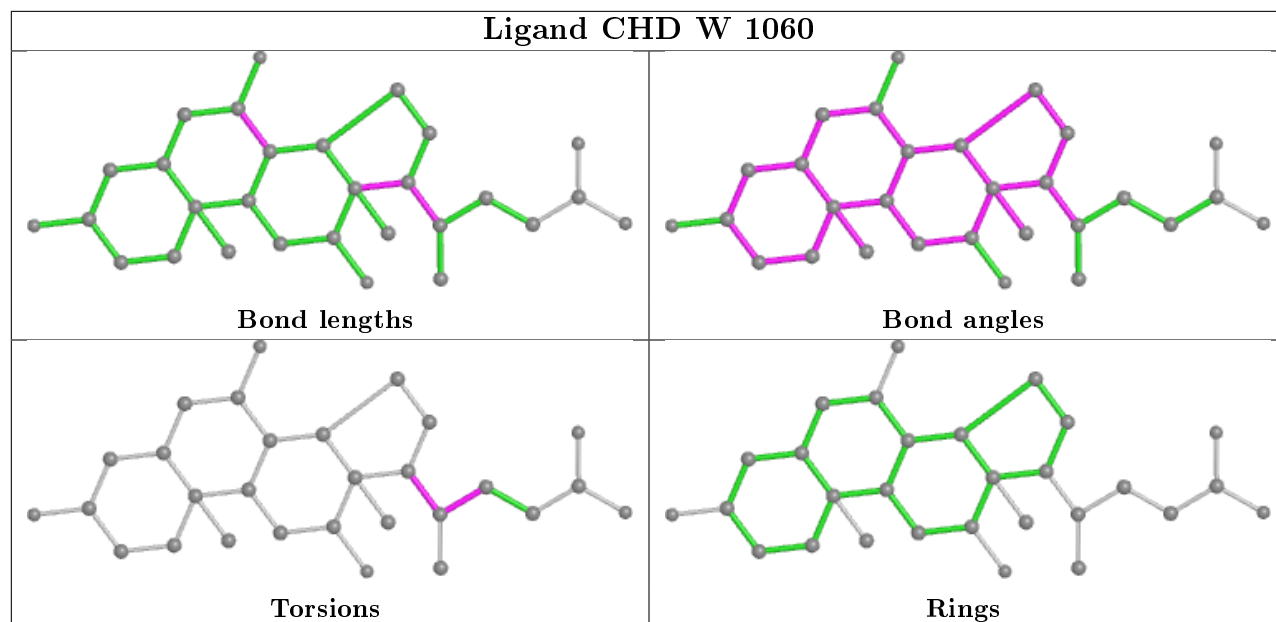




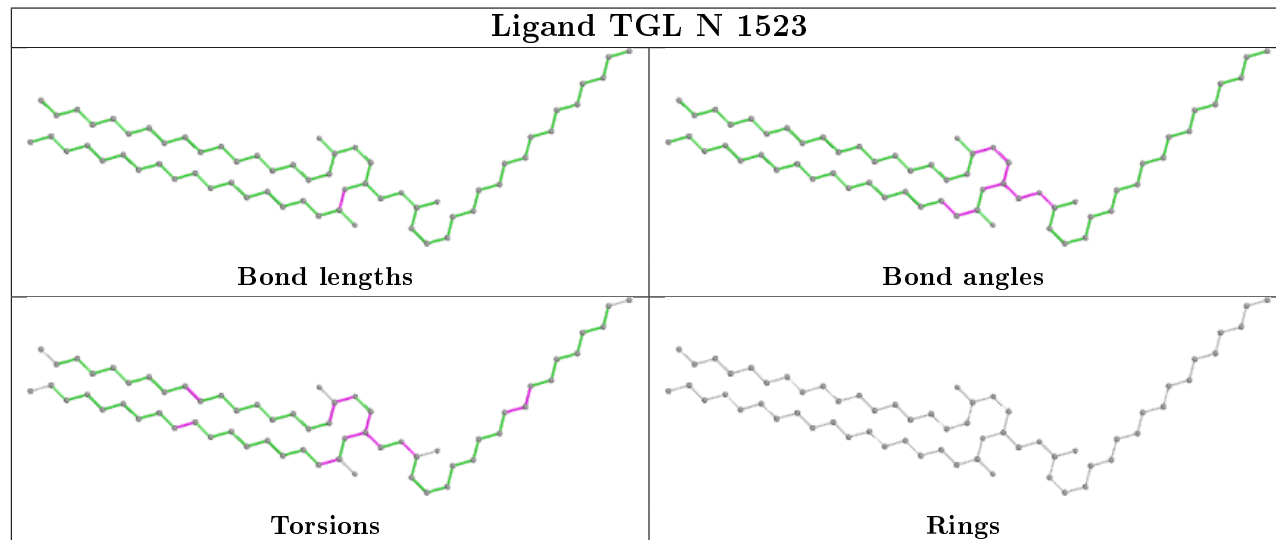




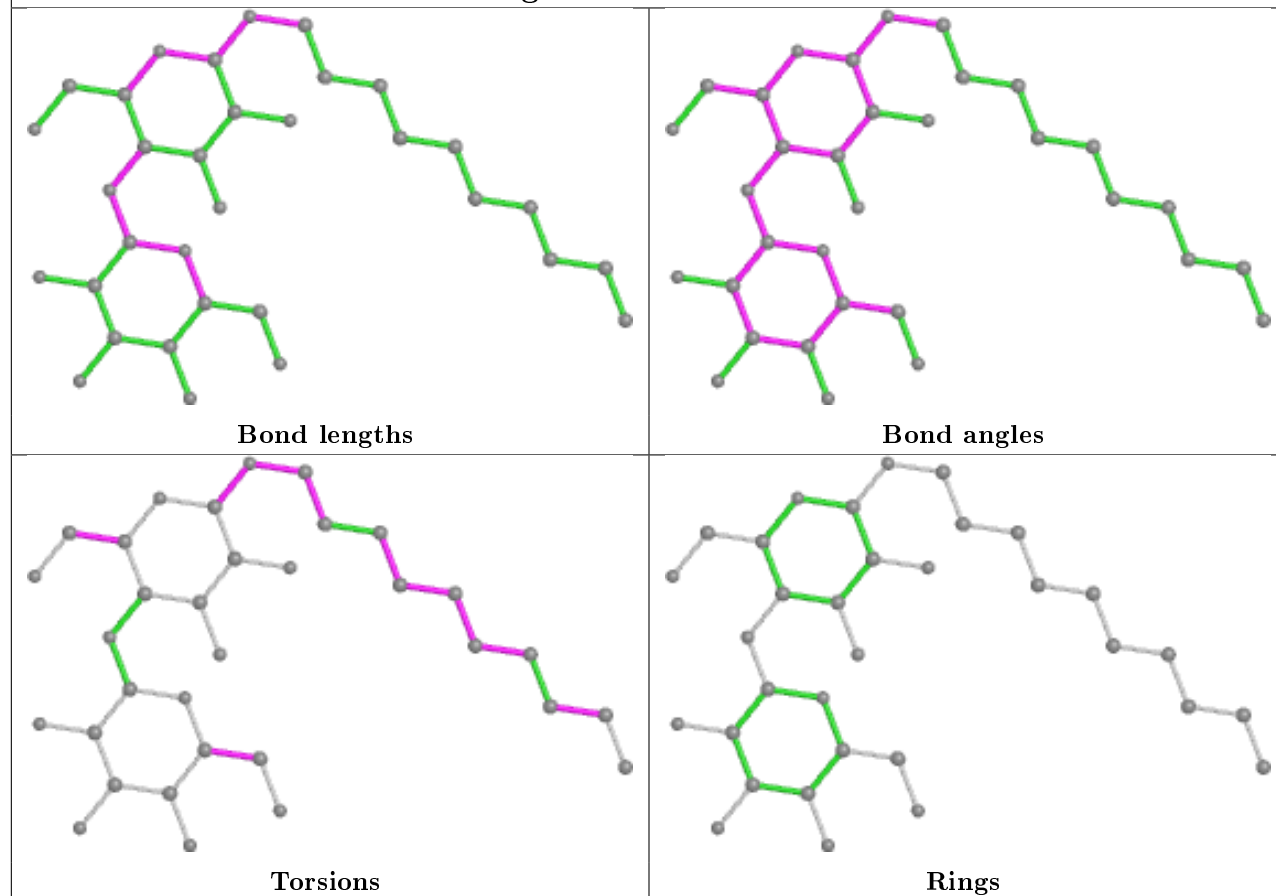
Ligand CHD W 1060



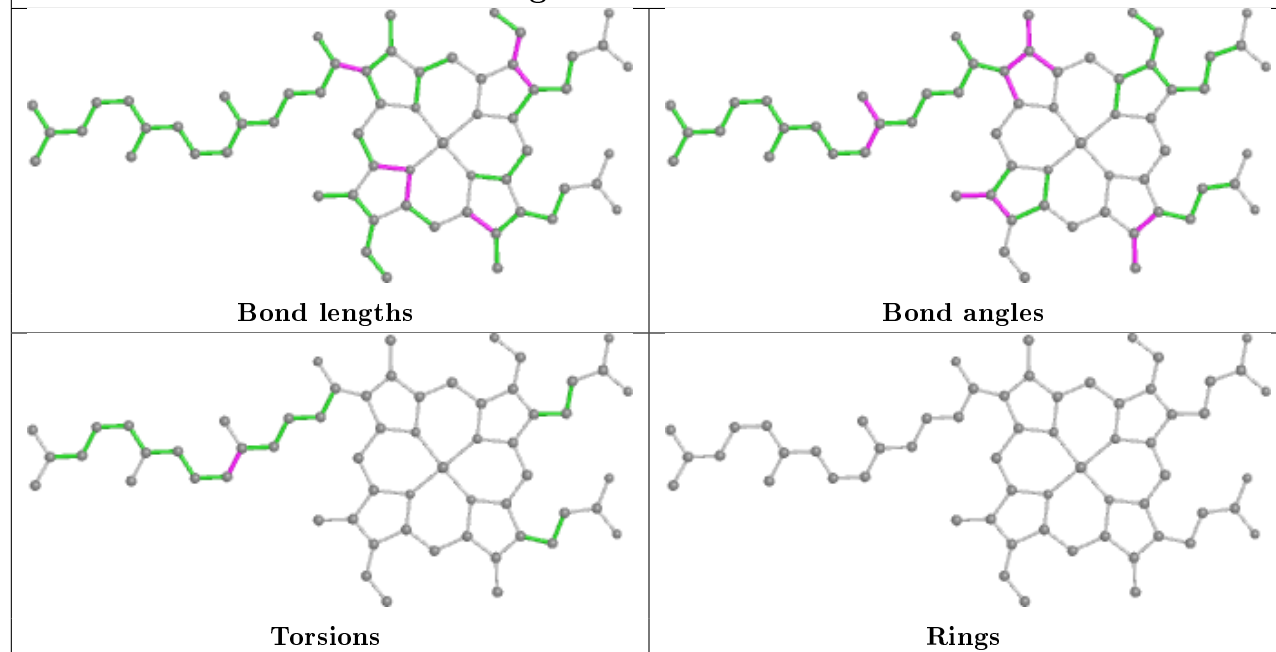
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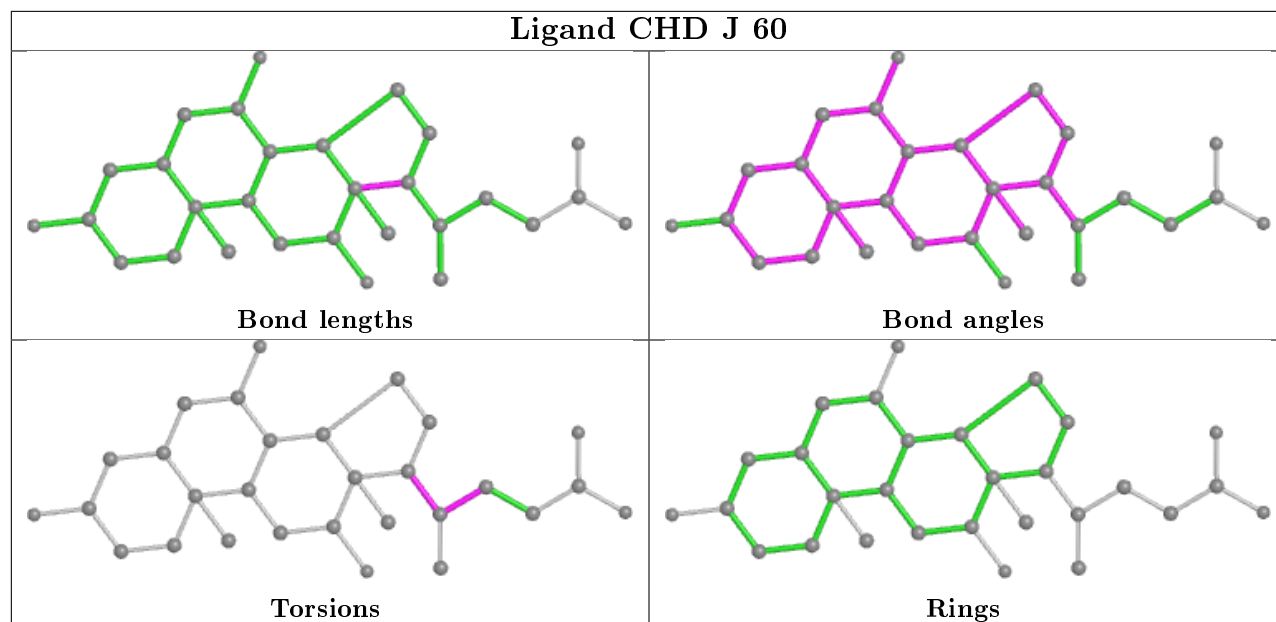
Ligand DMU M 526



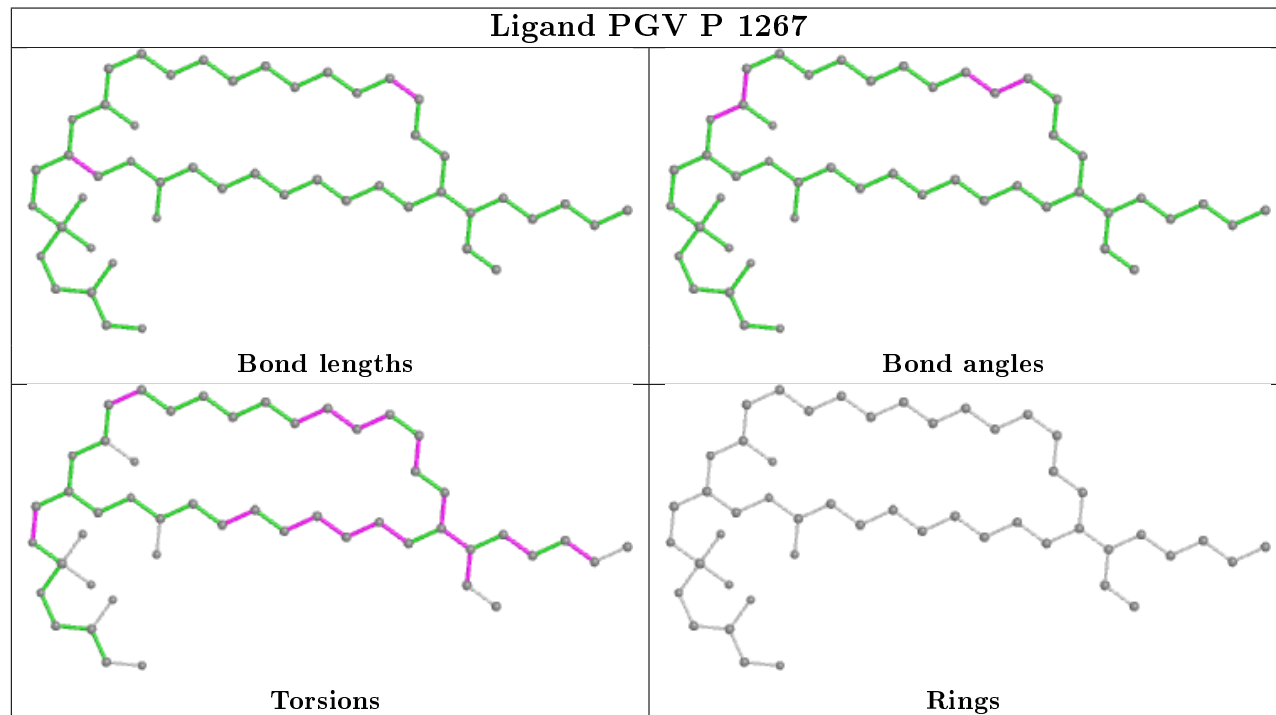
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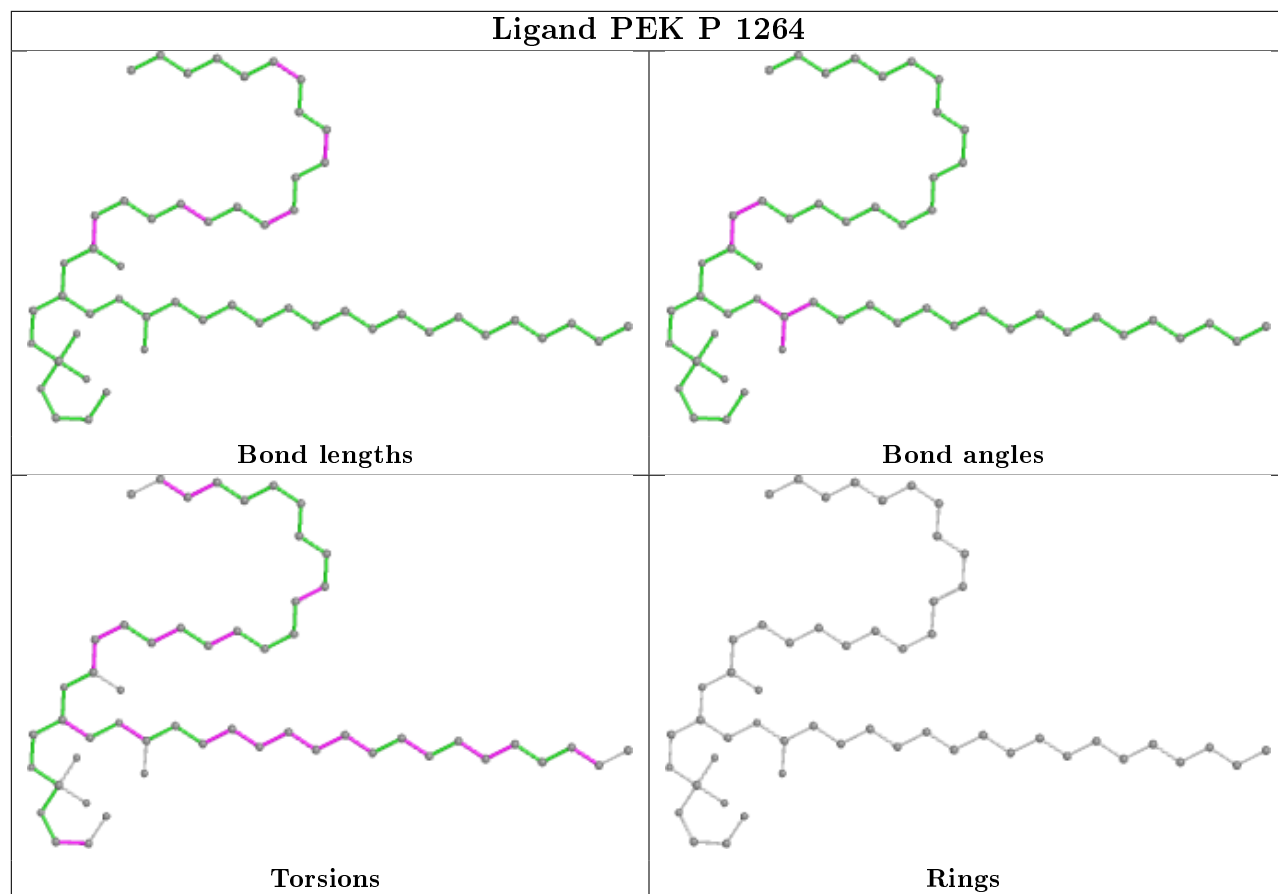


Ligand CHD J 60

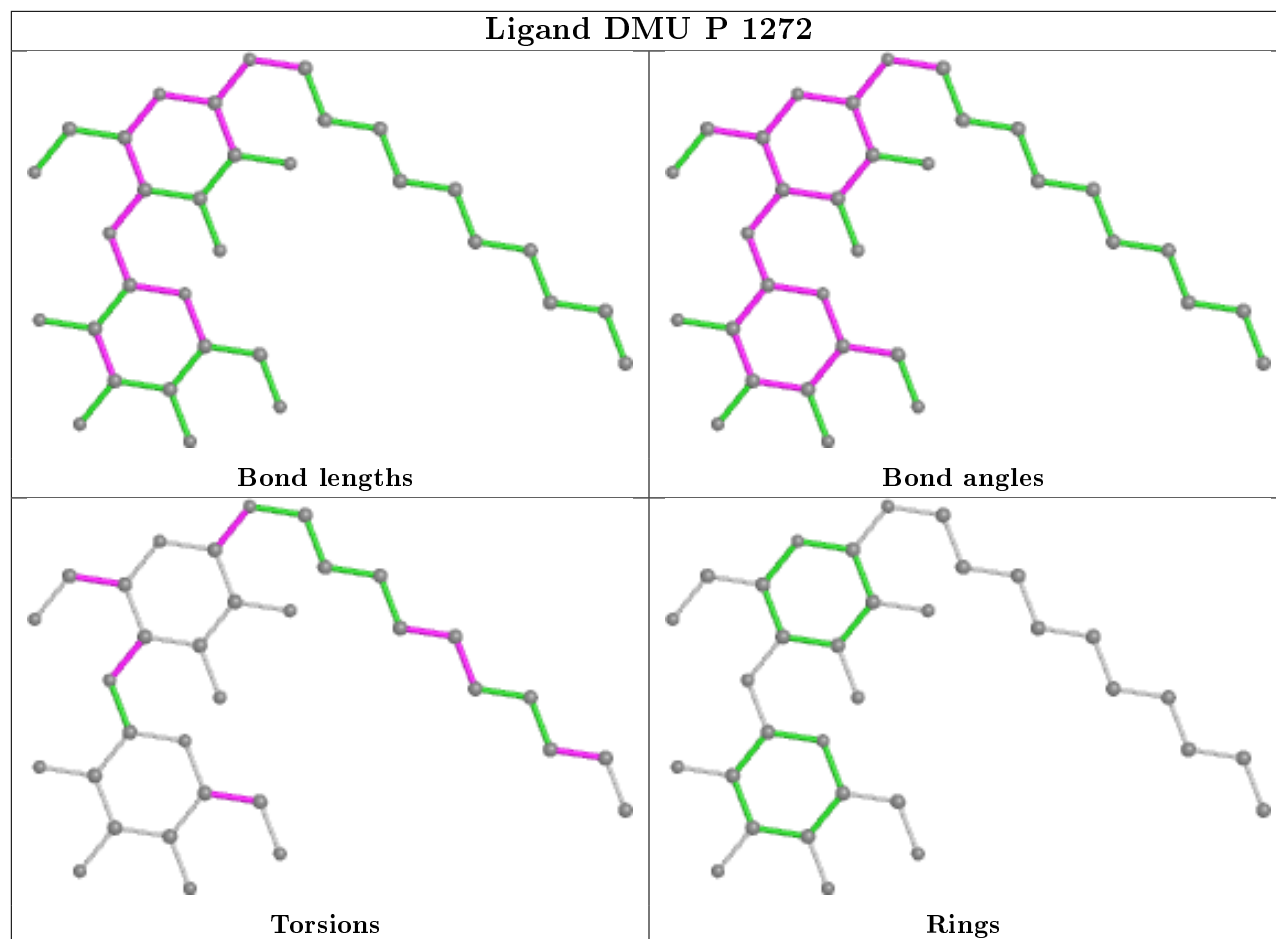


Ligand PGV P 1267

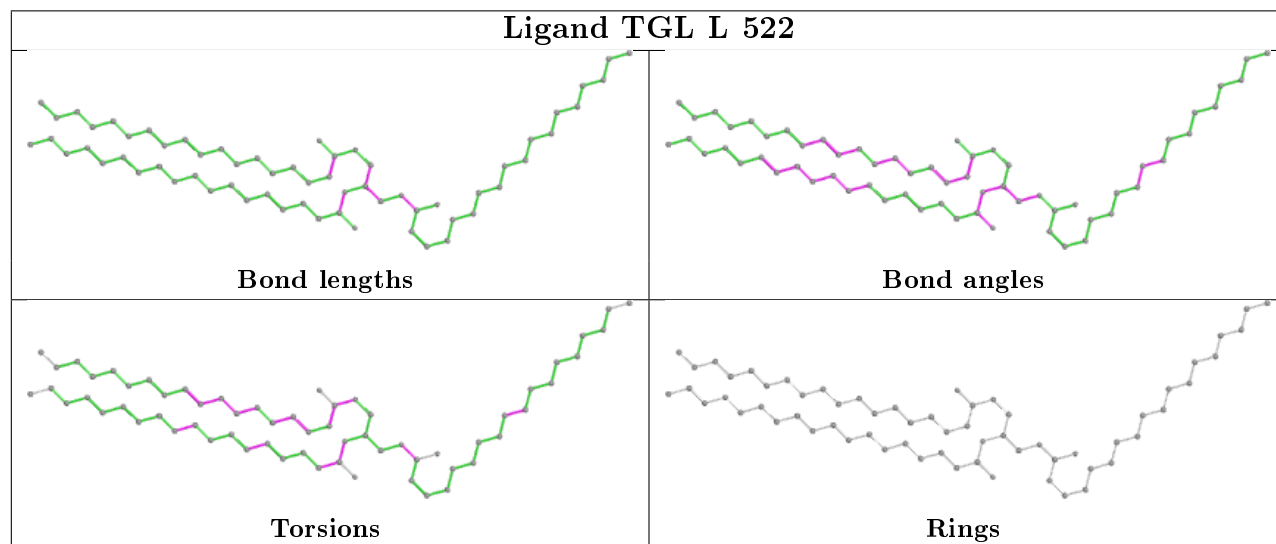


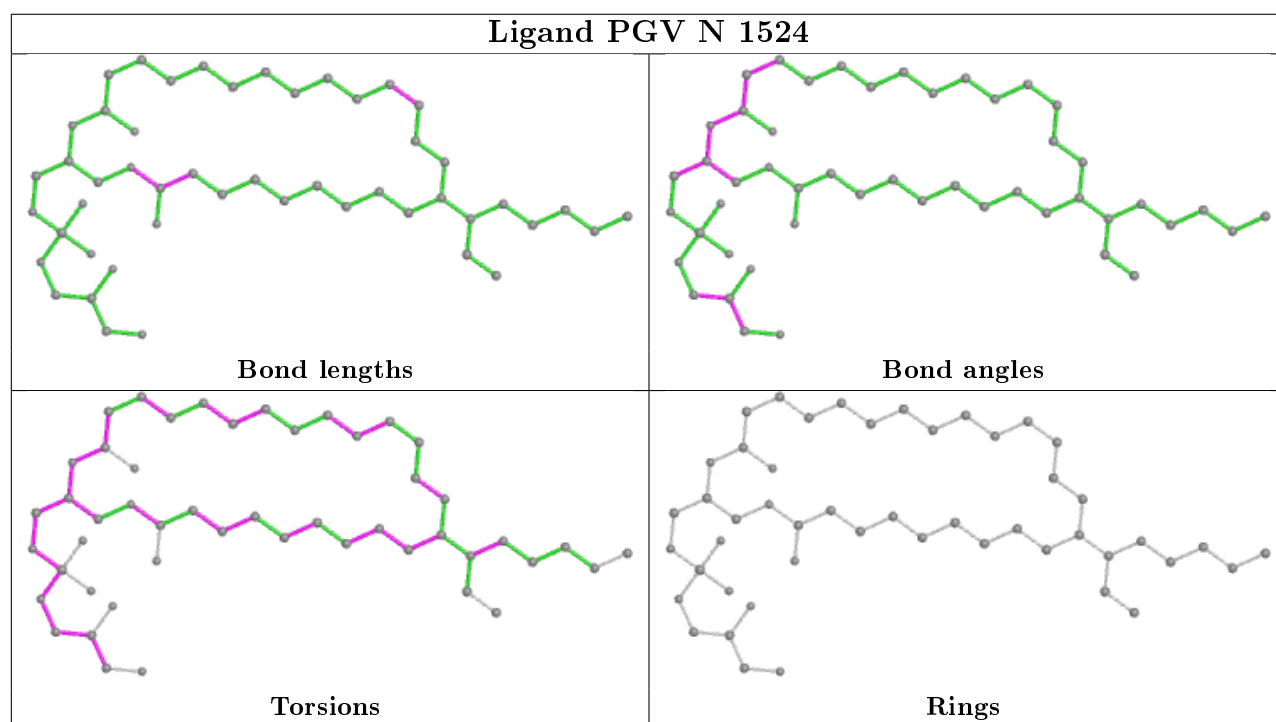
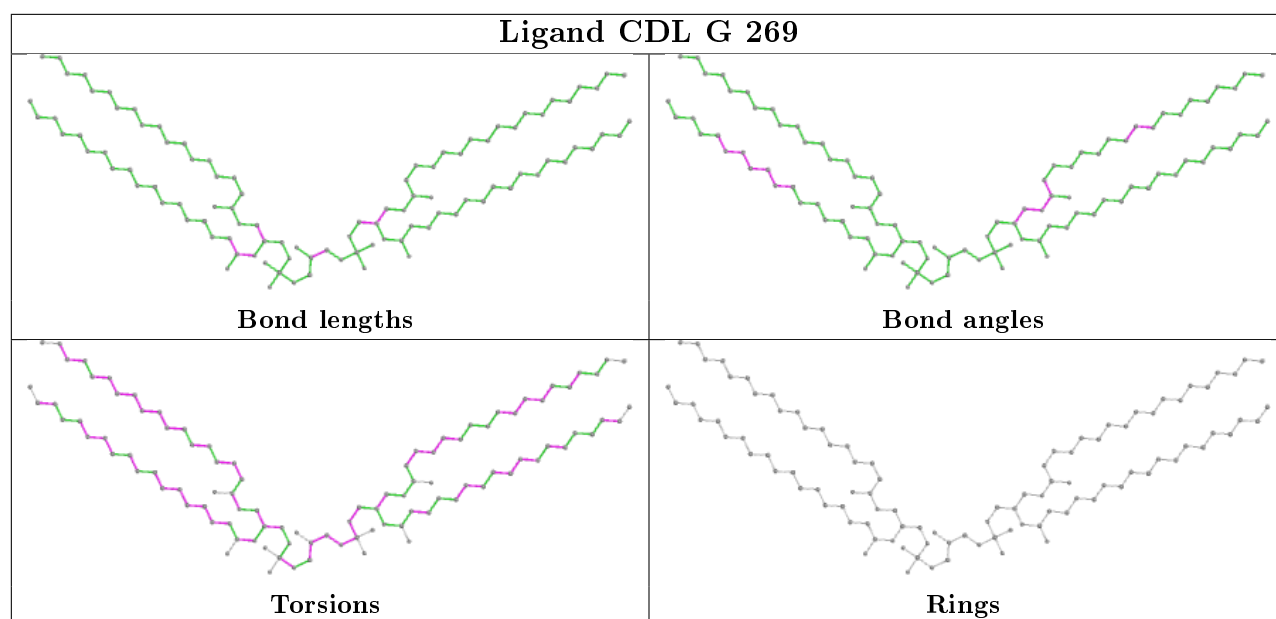


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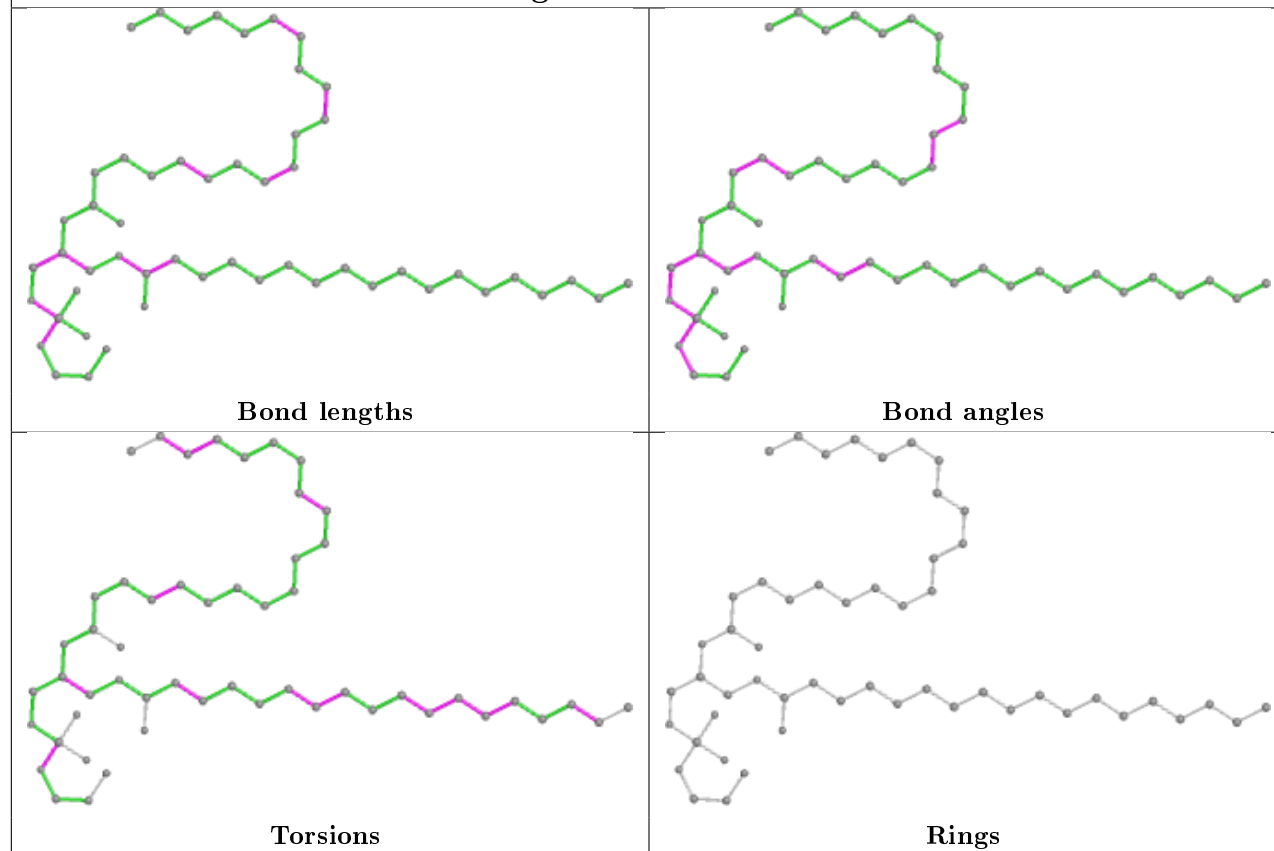


Ligand TGL L 522

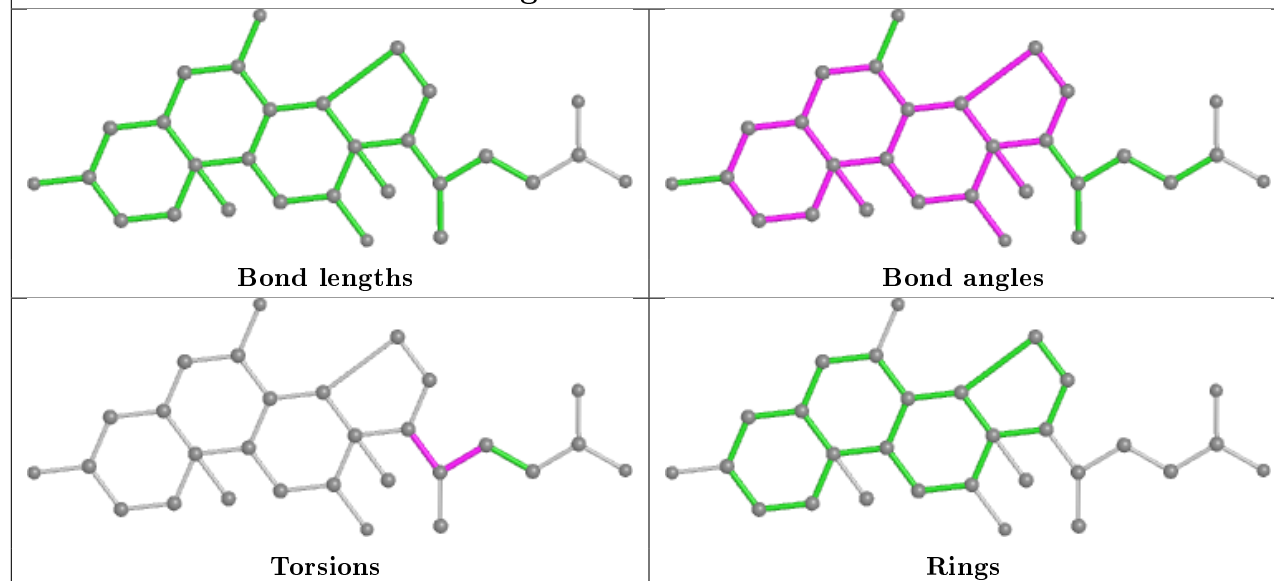


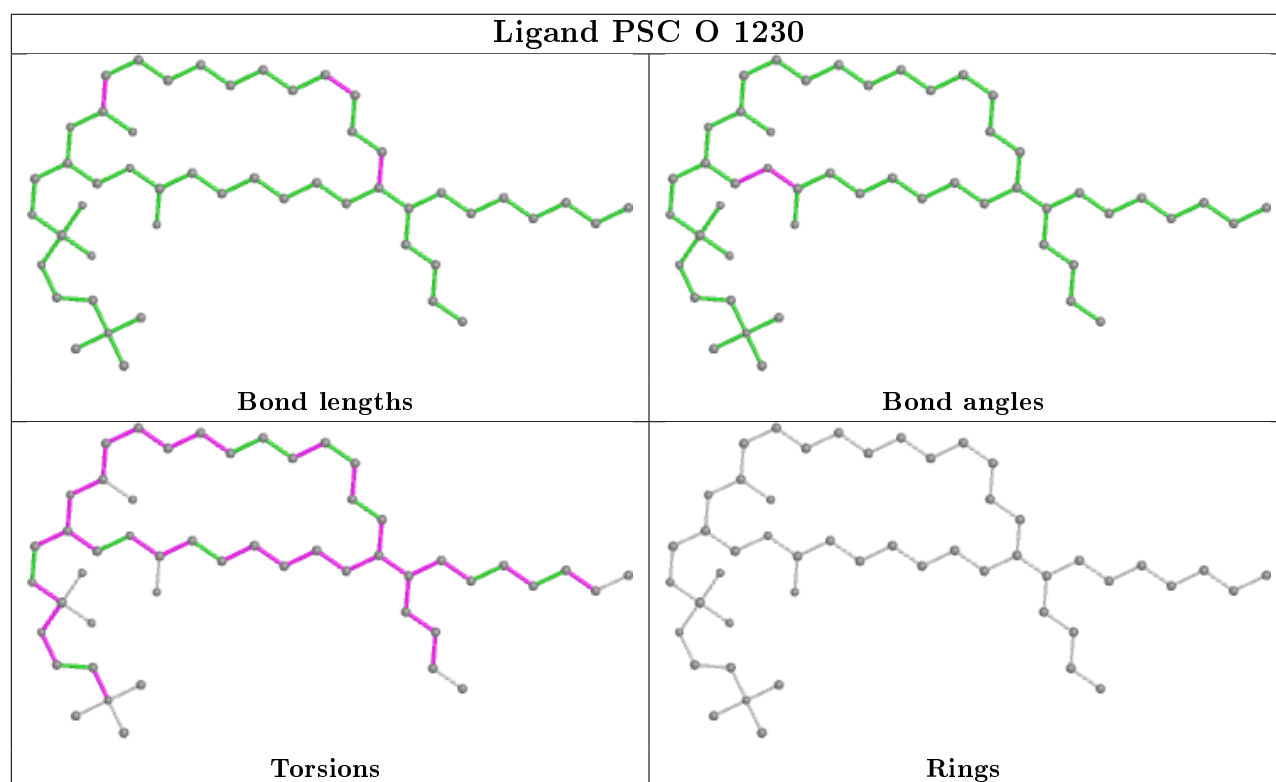
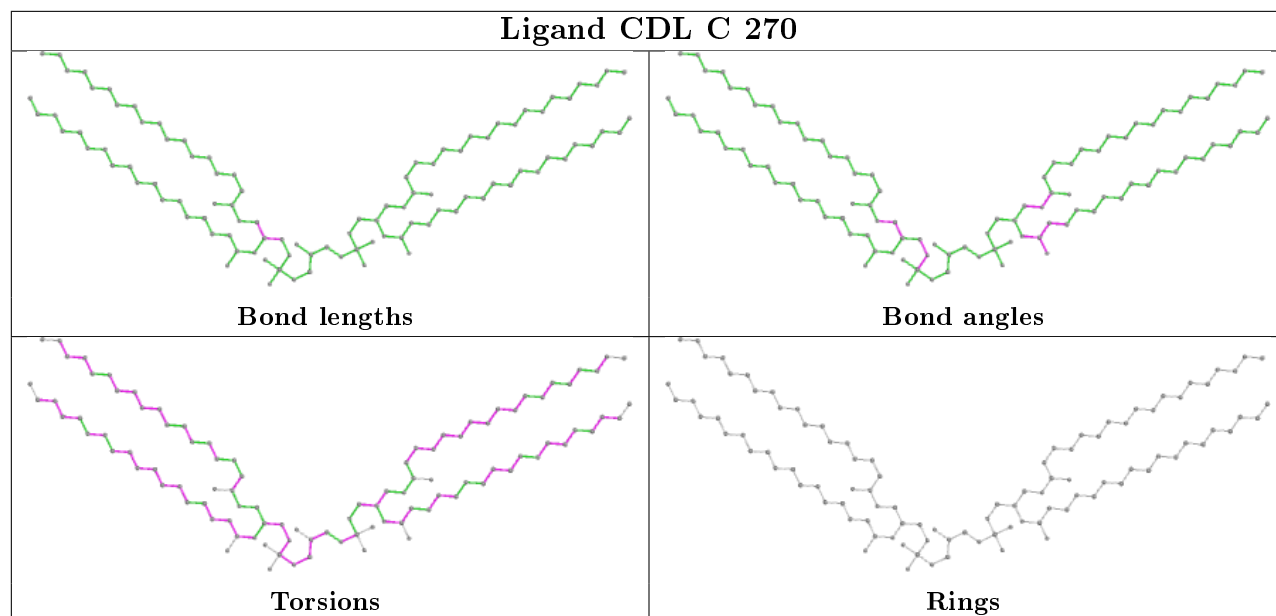


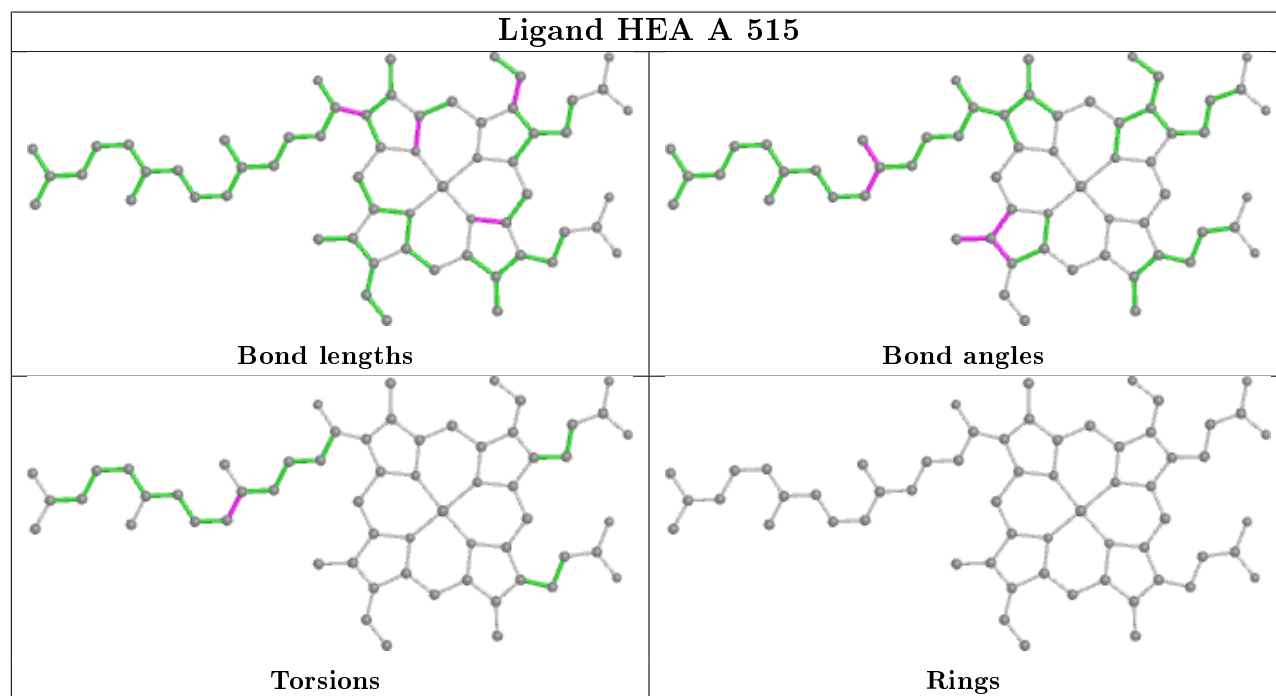
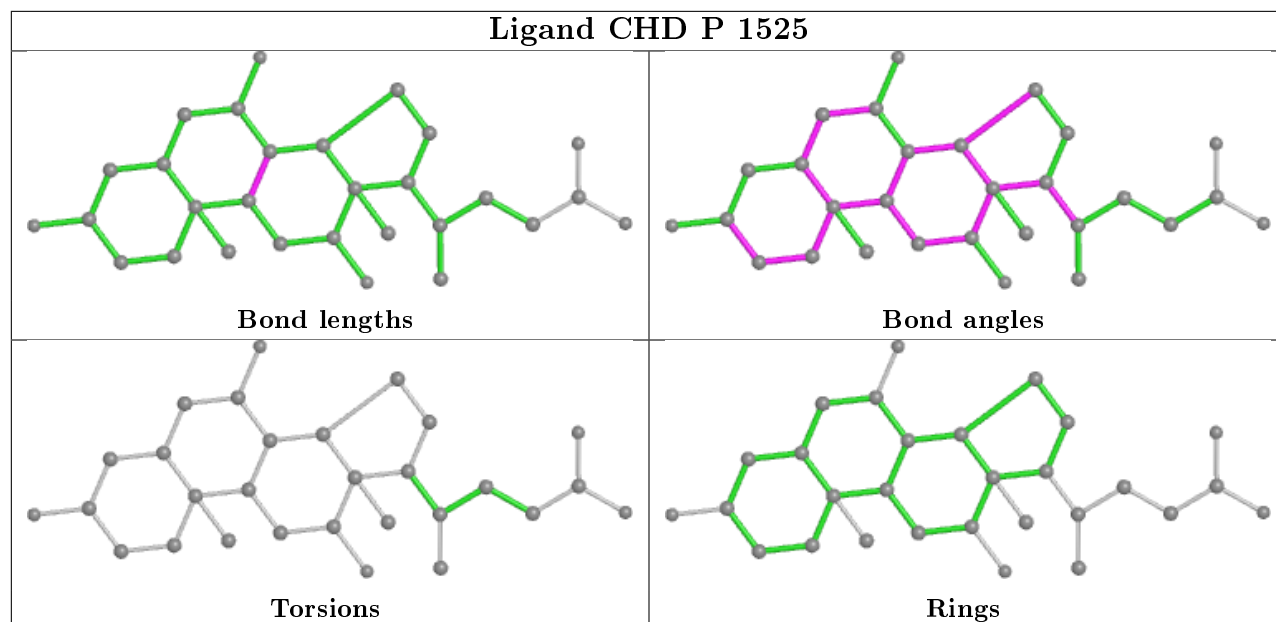
Ligand PEK C 265

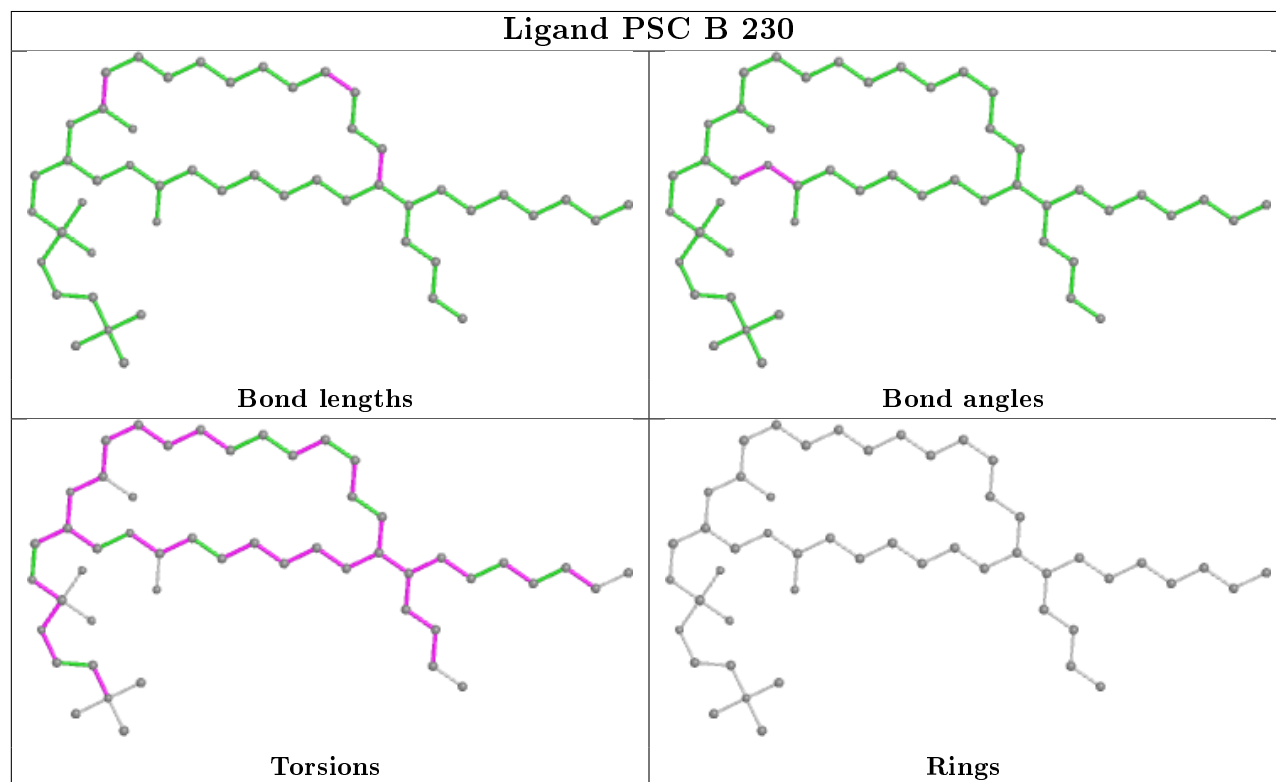
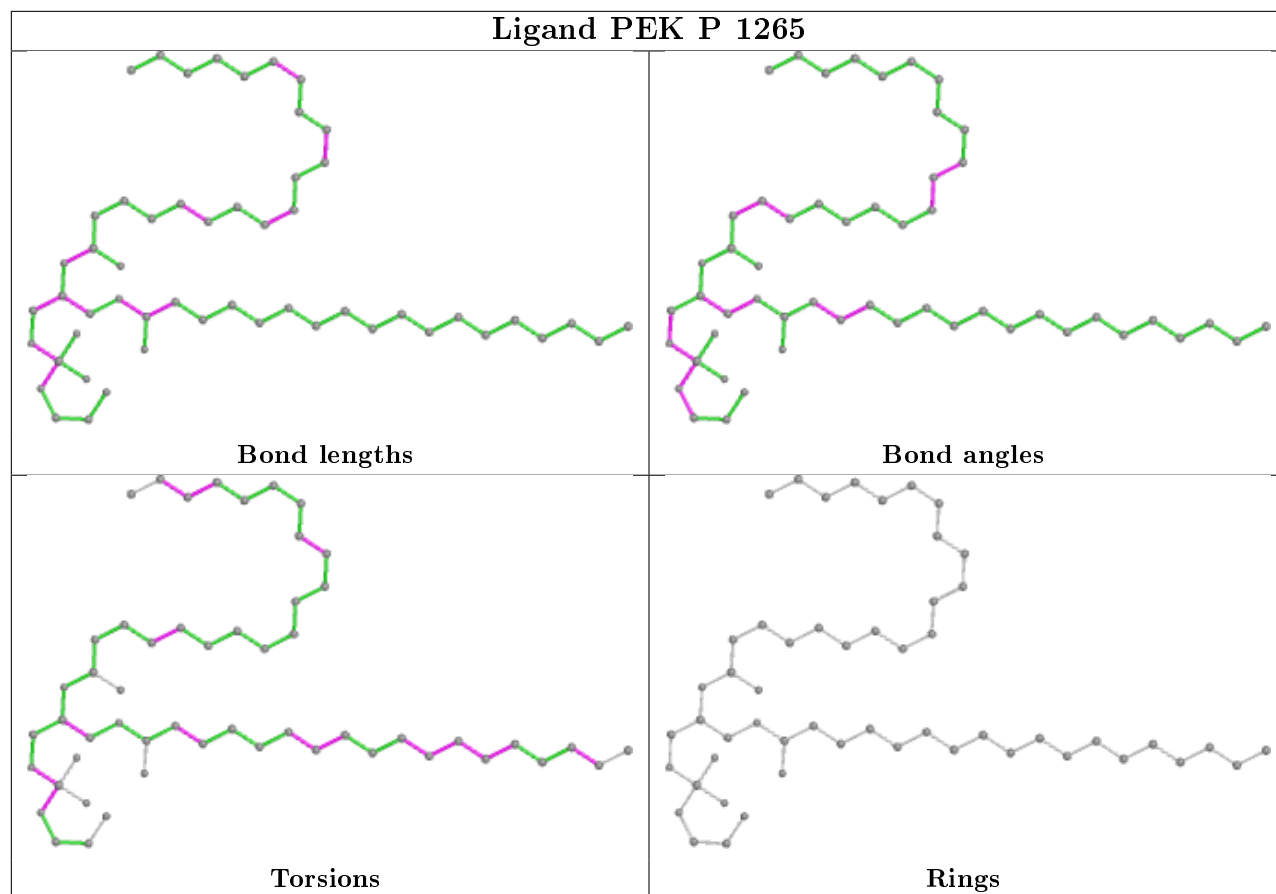


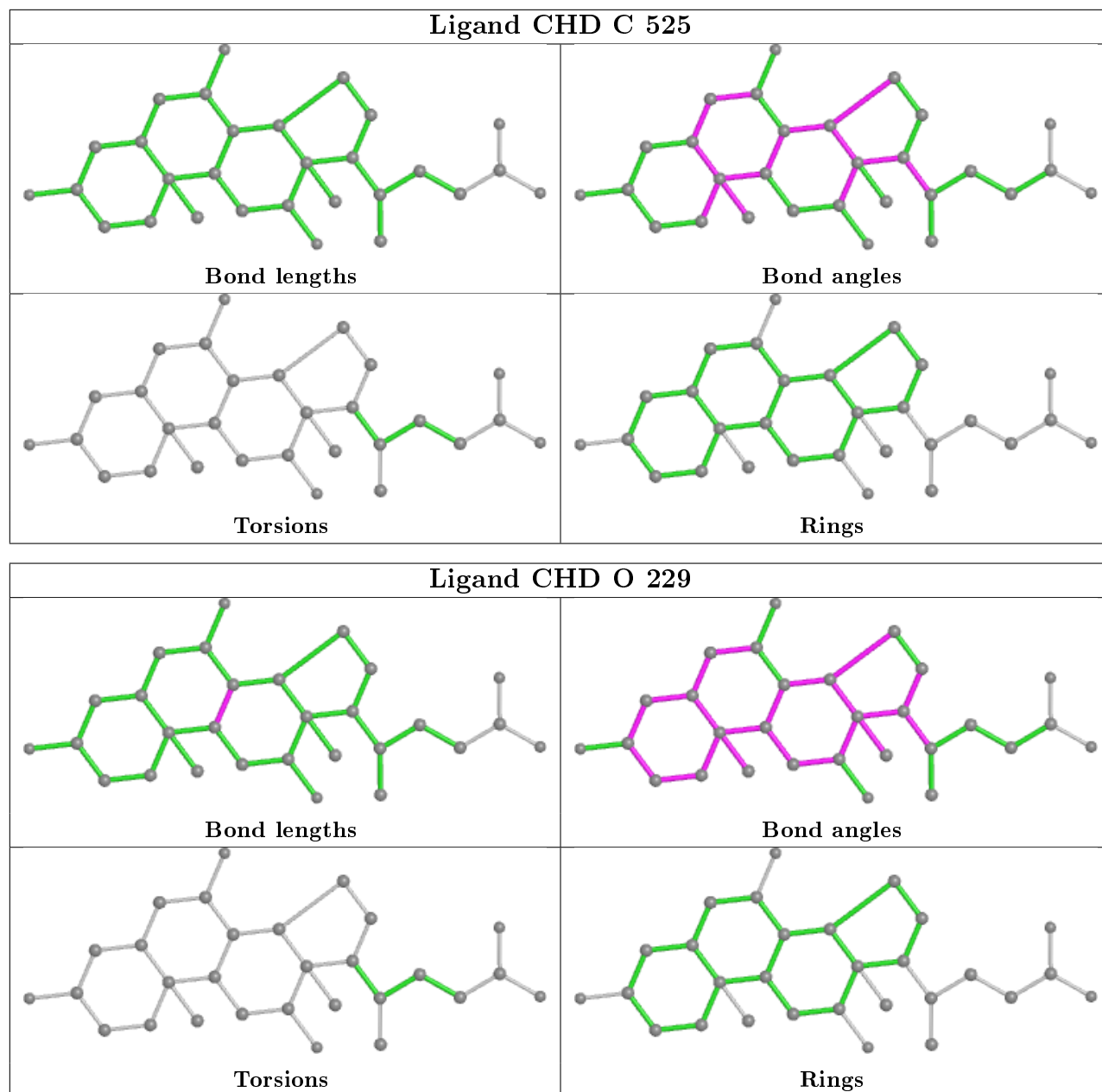
Ligand CHD P 1271



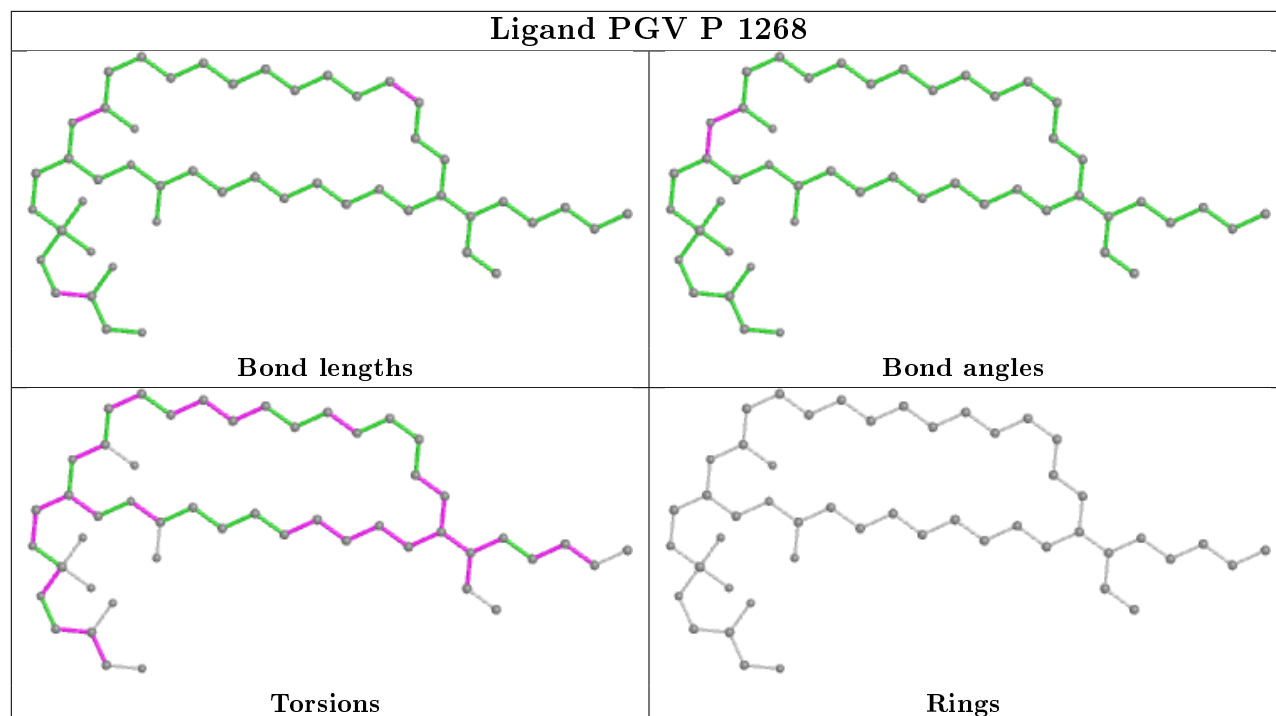




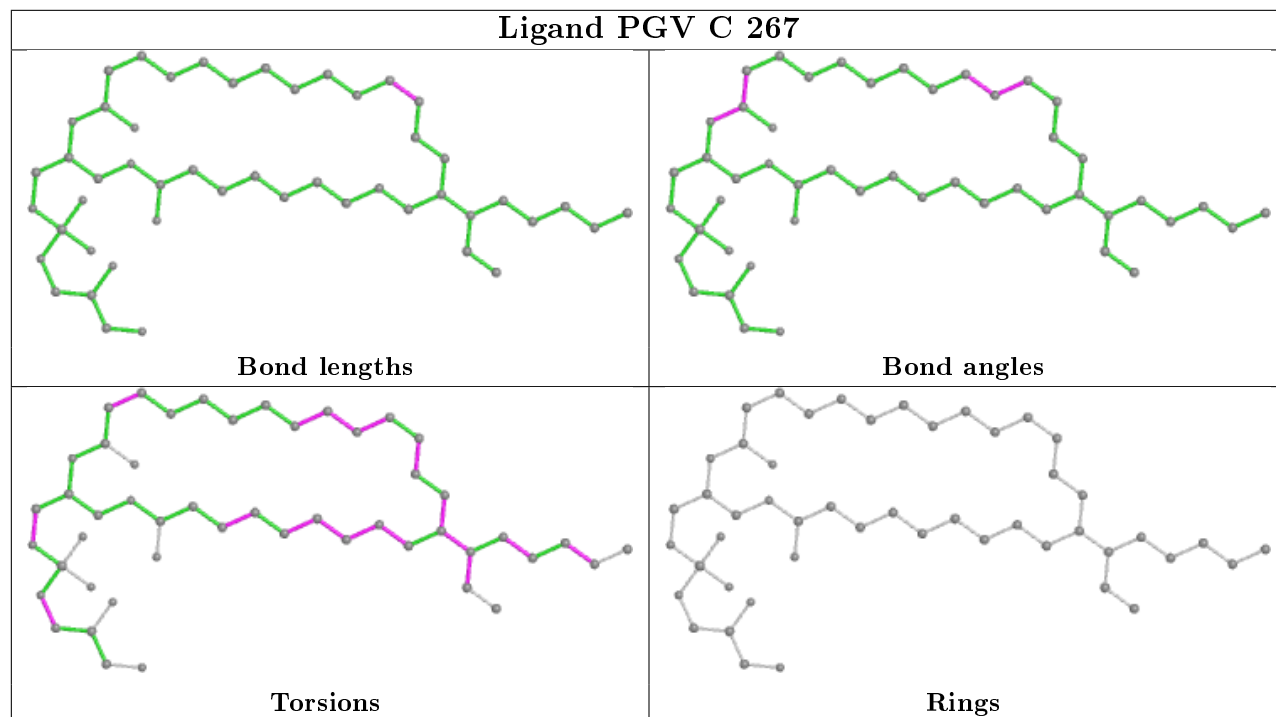


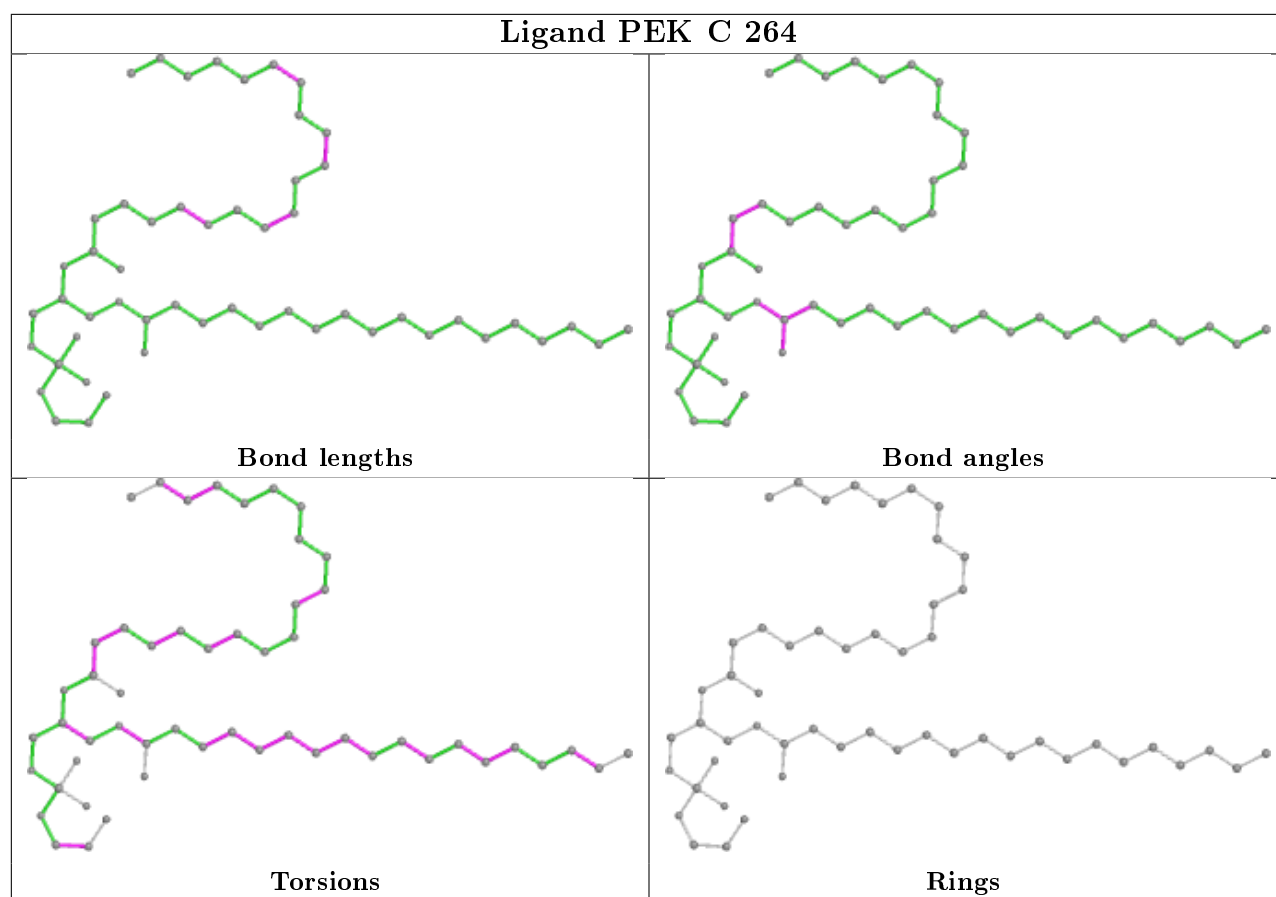


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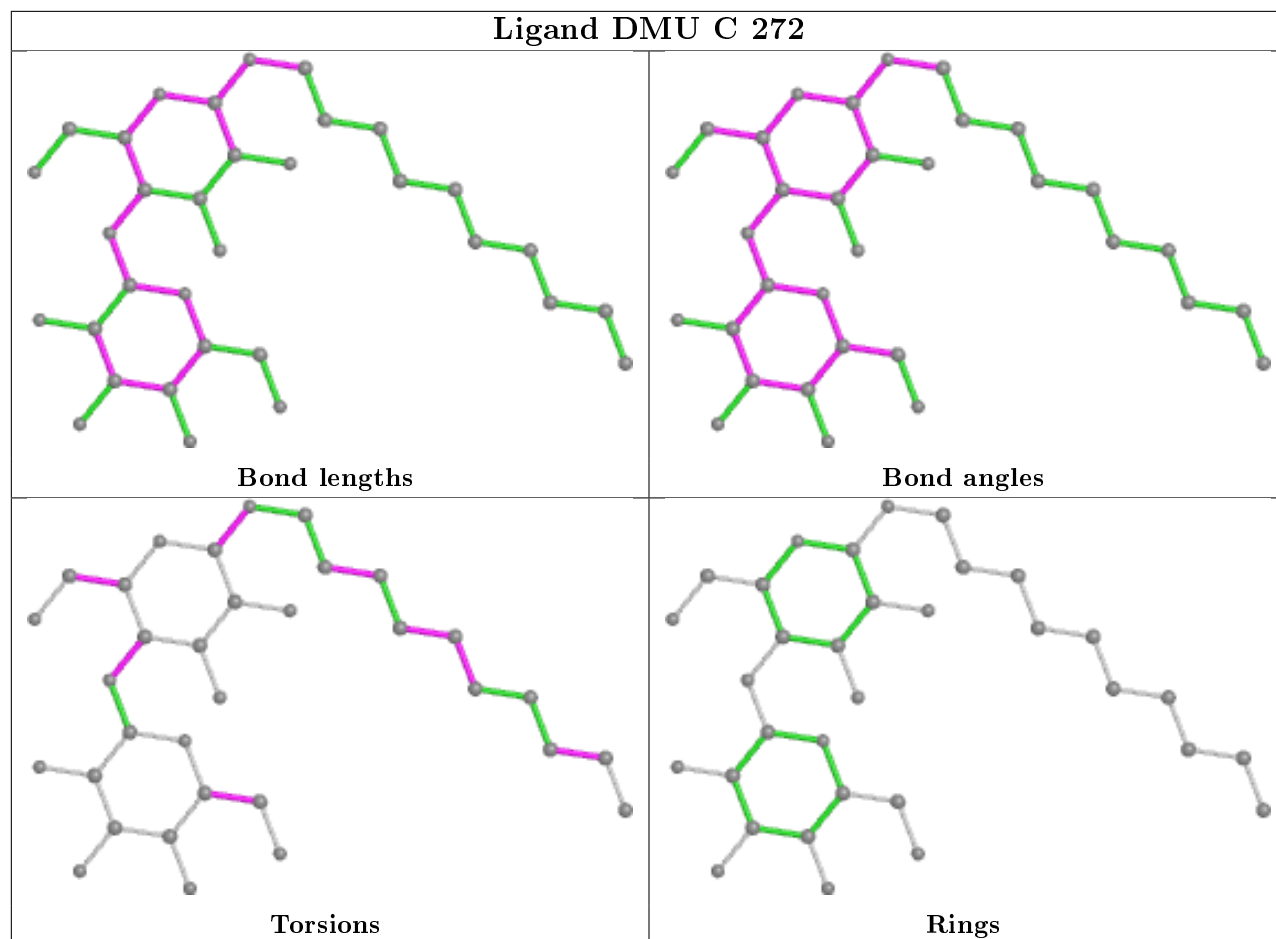


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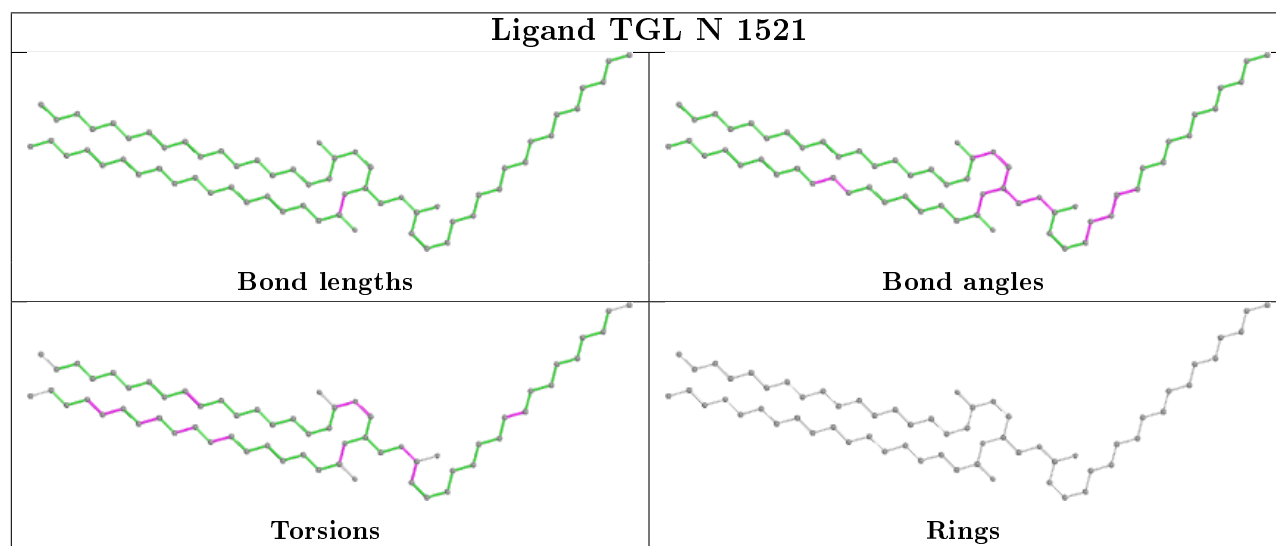


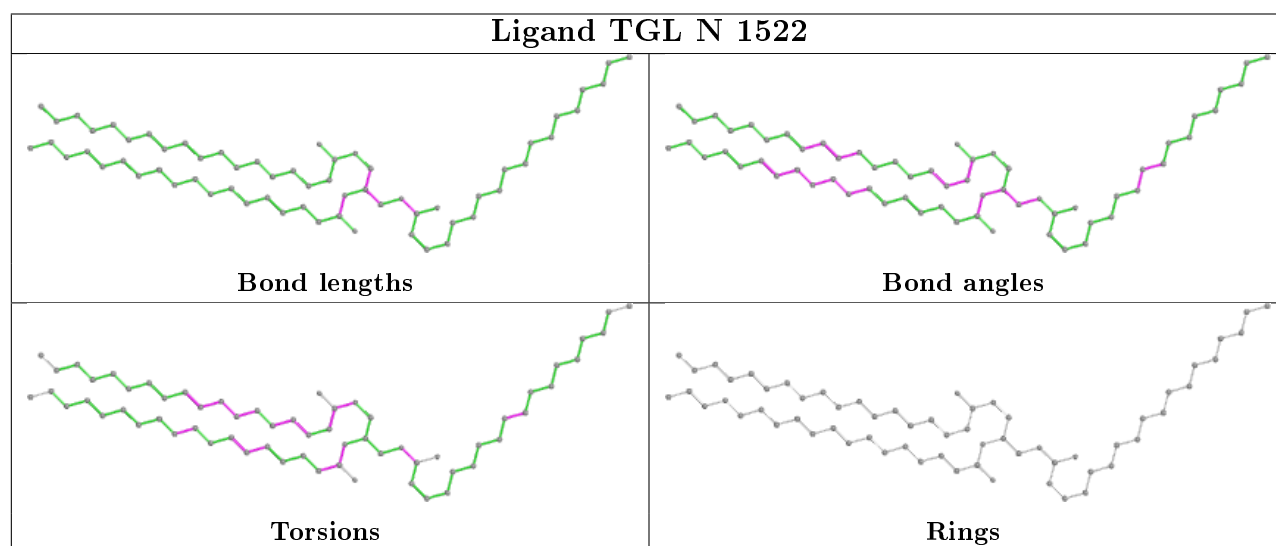
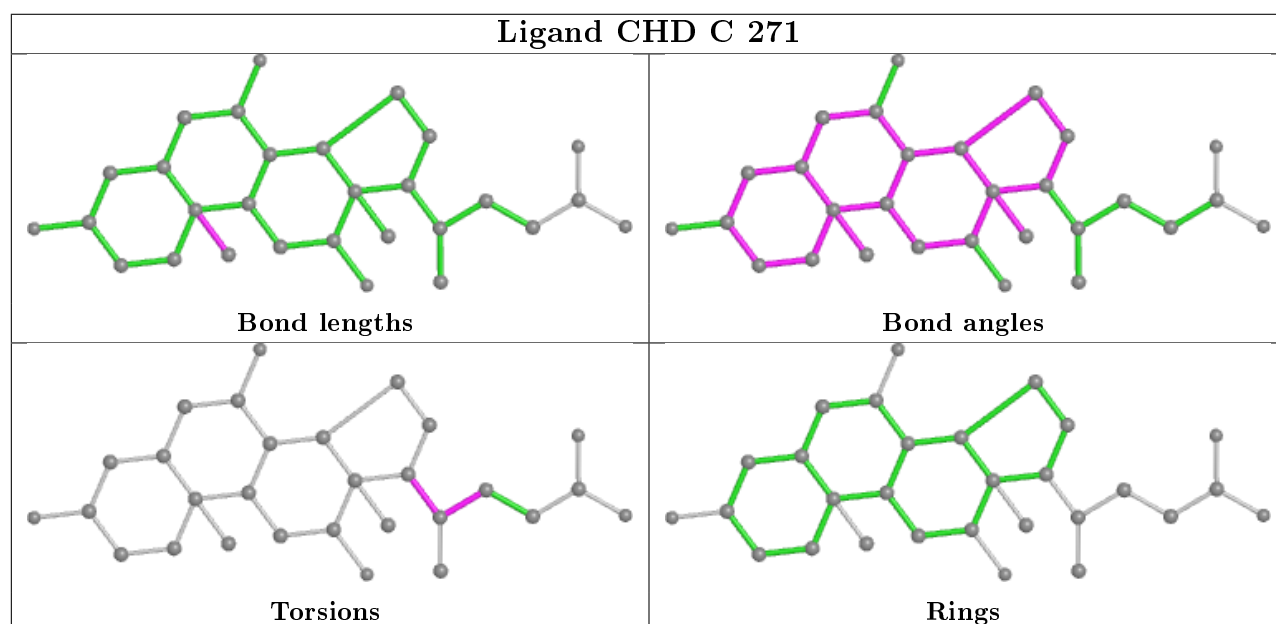
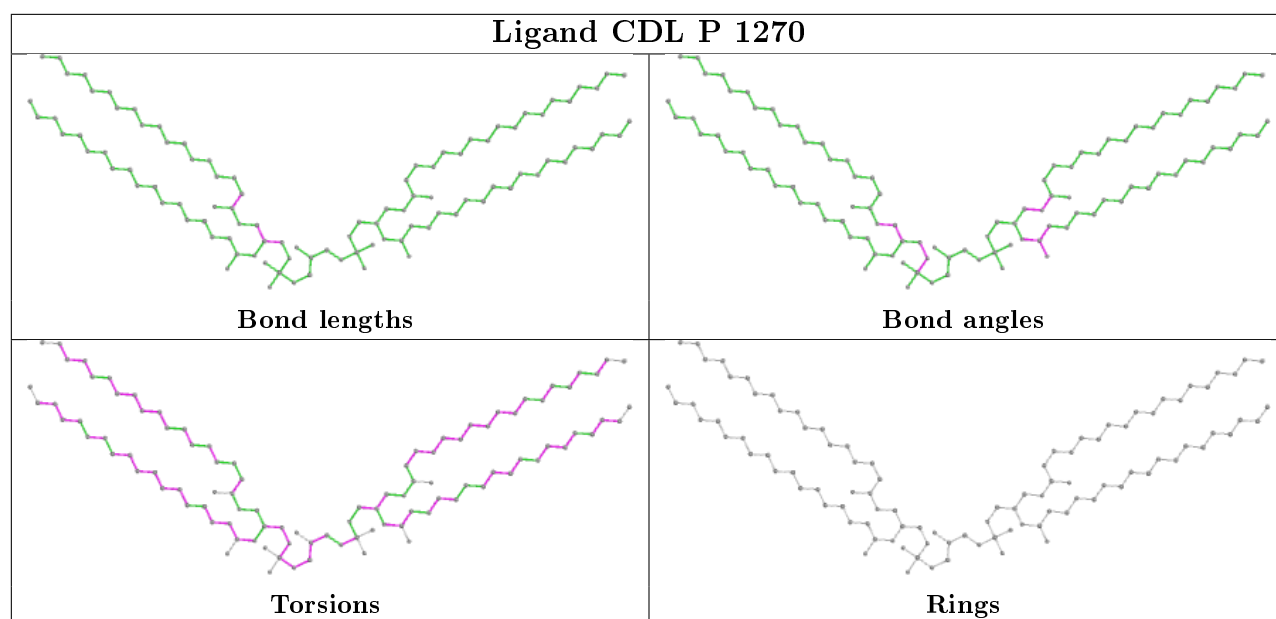


Ligand DMU C 272

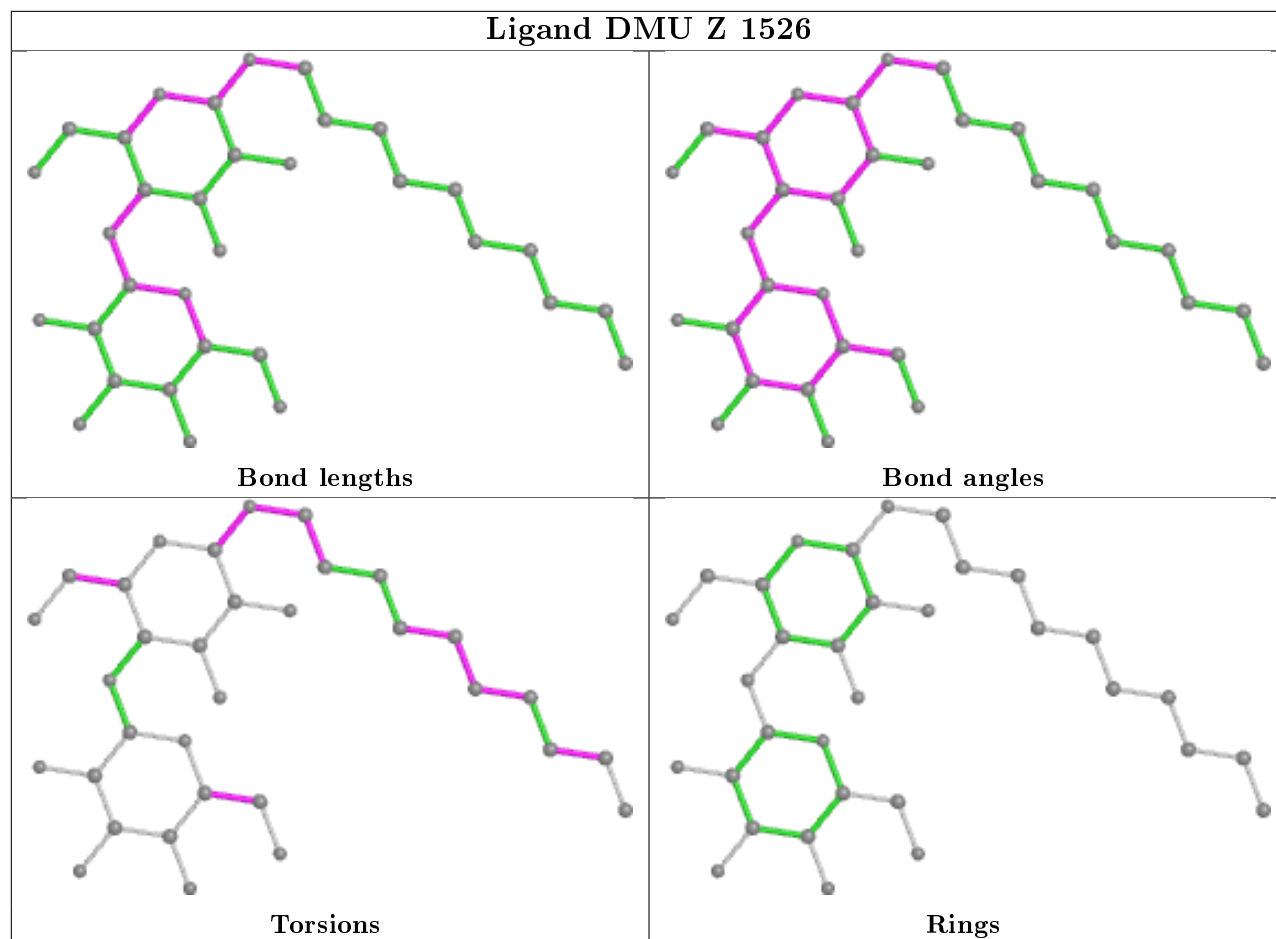


Ligand TGL N 1521

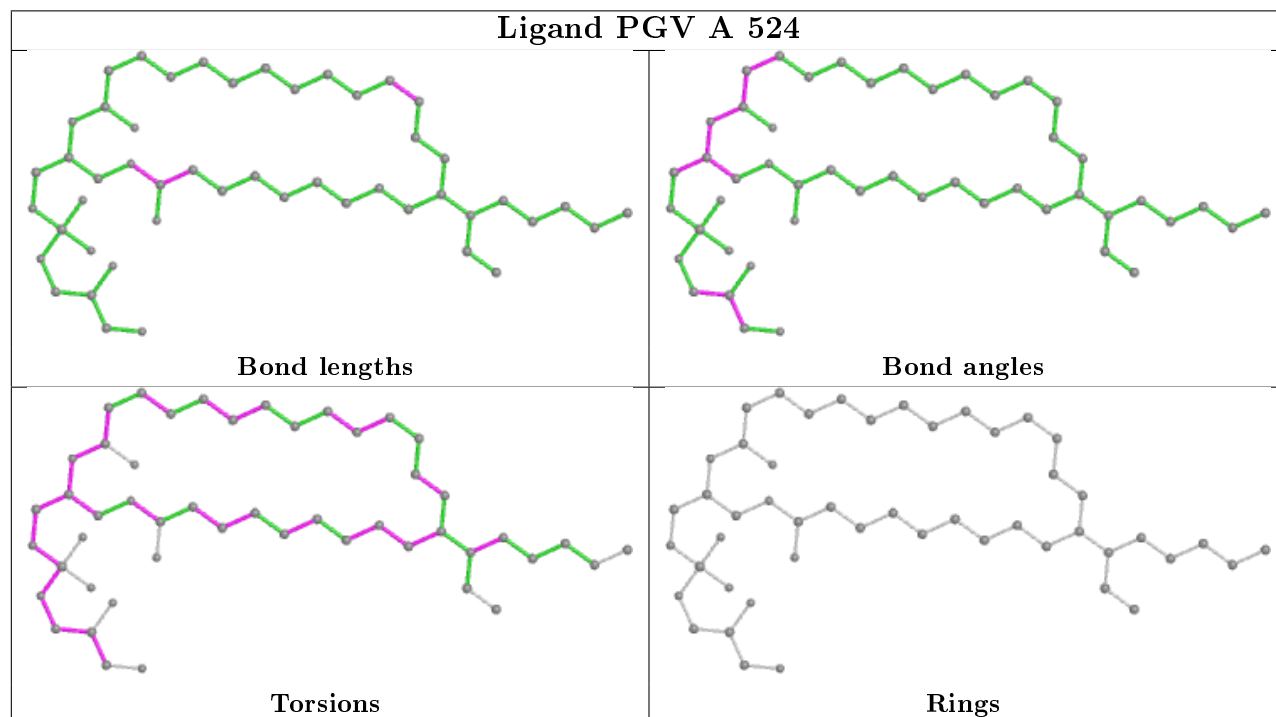




Ligand DMU Z 1526



Ligand PGV A 524



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 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.