



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 01:45 PM EDT

PDB ID : 2EIJ / pdb_00002ejj
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 types of validation reports are described at

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

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

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

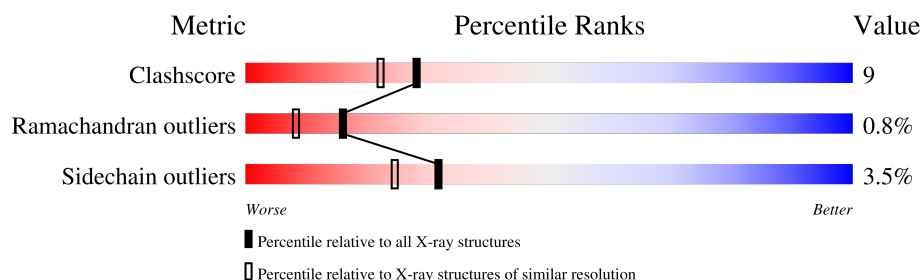
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

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

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CHD	C	271	X	-	-	-
22	CHD	J	60	X	-	-	-
22	CHD	P	1271	X	-	-	-
22	CHD	W	1060	X	-	-	-
23	DMU	C	272	X	-	-	-
23	DMU	M	526	X	-	-	-
23	DMU	P	1272	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	DMU	Z	1526	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 (CCD ID: CU) (formula: Cu).

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

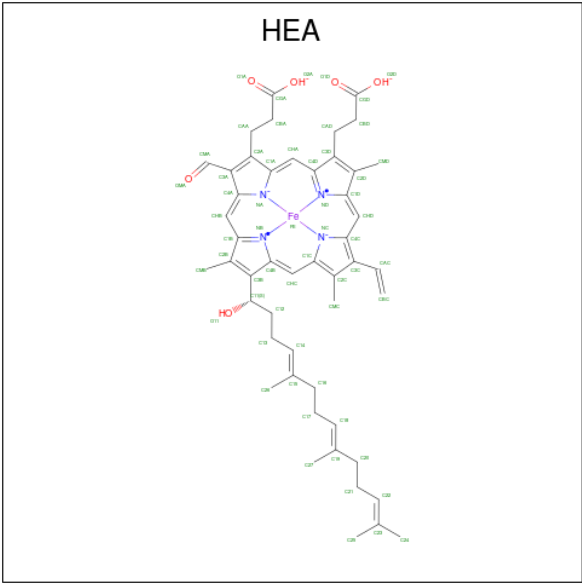
- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

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

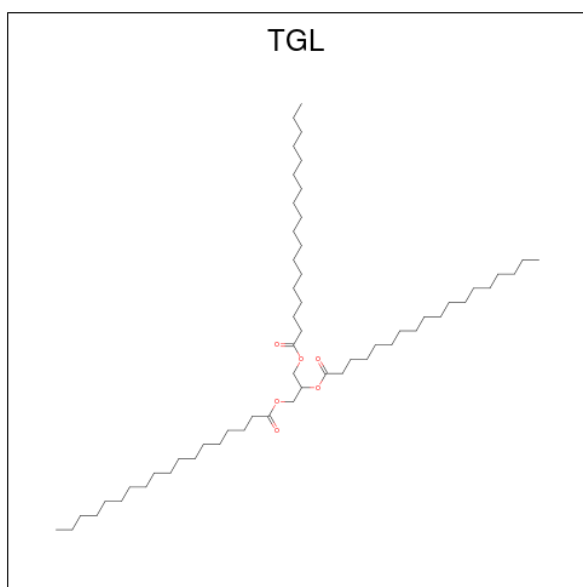
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Na	0	0
			1	1		
16	N	1	Total	Na	0	0
			1	1		

- Molecule 17 is HEME-A (CCD ID: HEA) (formula: C₄₉H₅₆FeN₄O₆).



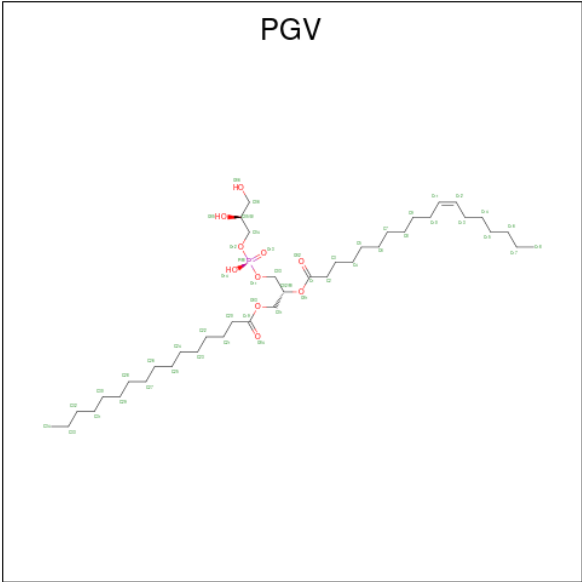
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
17	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 18 is TRISTEAROYLGLYCEROL (CCD ID: TGL) (formula: C₅₇H₁₁₀O₆).



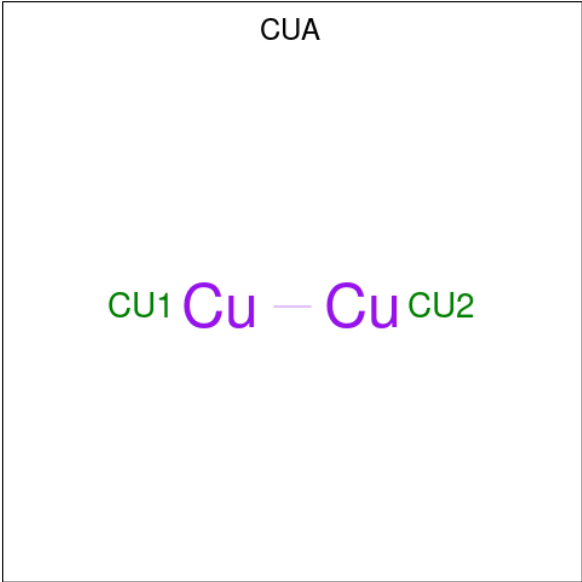
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			63	57	6		
18	B	1	Total	C	O	0	0
			63	57	6		
18	L	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		

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



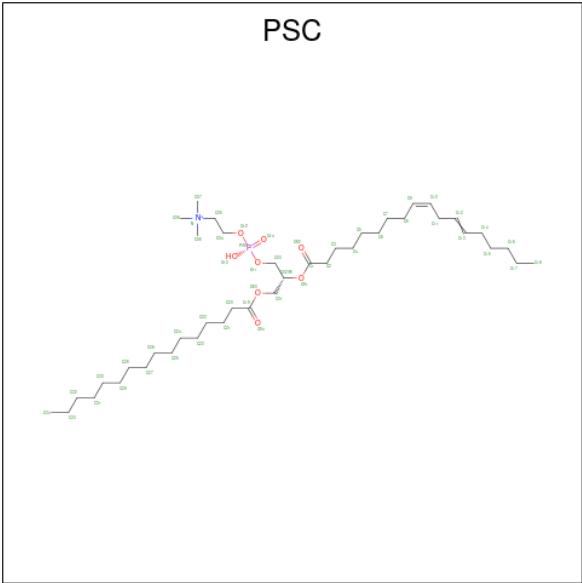
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

- Molecule 20 is DINUCLEAR COPPER ION (CCD ID: 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-[(PALMITO YLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (CCD ID: PSC) (formula: C₄₂H₈₁NO₈P).



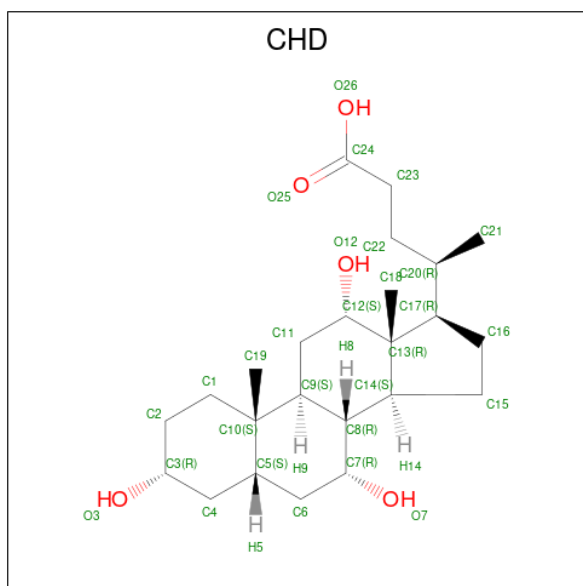
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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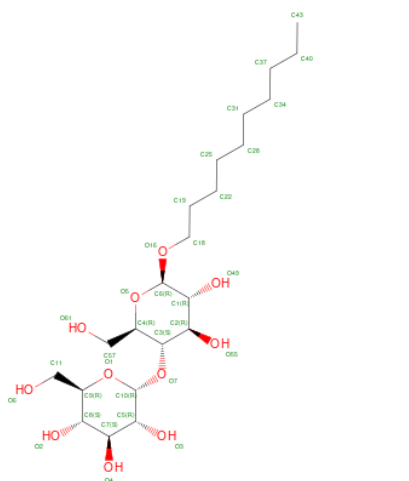
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
21	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 22 is CHOLIC ACID (CCD ID: 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 (CCD ID: DMU) (formula: $C_{22}H_{42}O_{11}$).

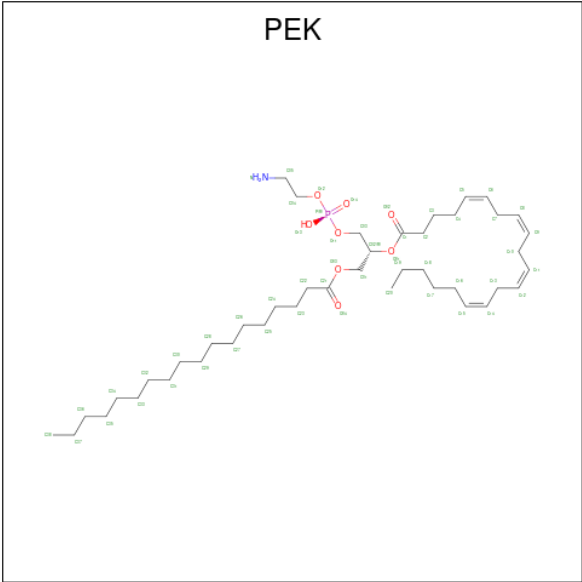


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total 33	C 22	O 11	0	0
23	M	1	Total 33	C 22	O 11	0	0
23	P	1	Total 33	C 22	O 11	0	0
23	Z	1	Total 33	C 22	O 11	0	0

- Molecule 24 is ZINC ION (CCD ID: ZN) (formula: Zn).

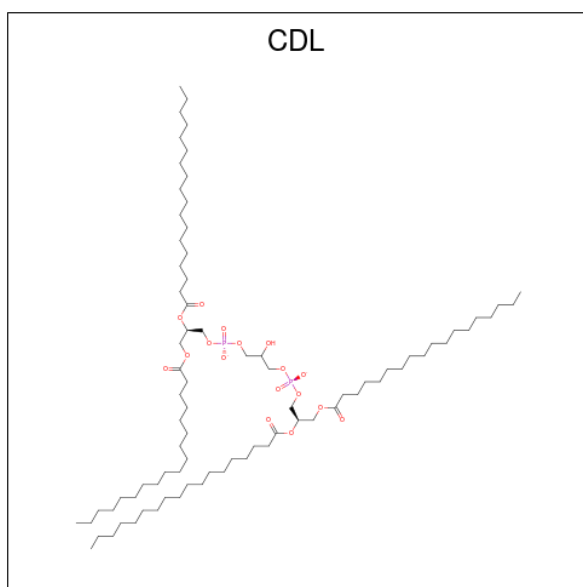
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	C	1	Total 1	Zn 1	0	0
24	F	1	Total 1	Zn 1	0	0
24	P	1	Total 1	Zn 1	0	0
24	S	1	Total 1	Zn 1	0	0

- Molecule 25 is (1S)-2-[[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (CCD ID: PEK) (formula: $C_{43}H_{78}NO_8P$).



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

- Molecule 26 is CARDIOLIPIN (CCD ID: CDL) (formula: 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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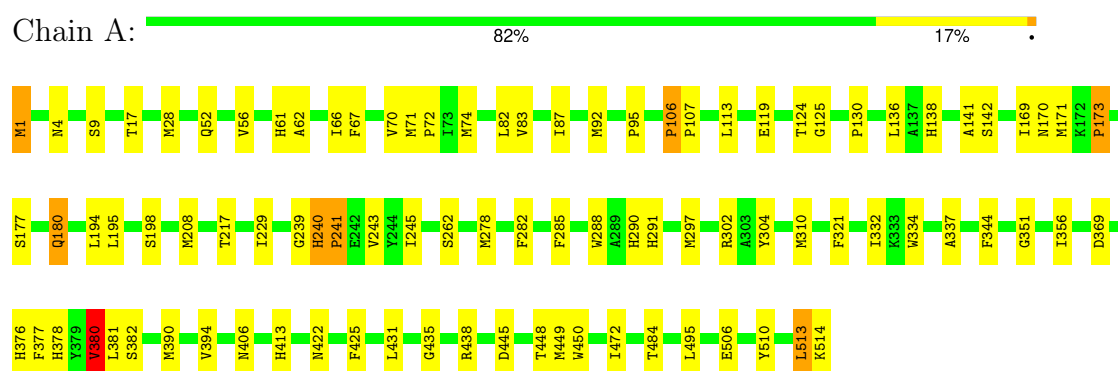
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	I	38	Total 38	O 38	0	0
27	J	23	Total 23	O 23	0	0
27	K	22	Total 22	O 22	0	0
27	L	27	Total 27	O 27	0	0
27	M	24	Total 24	O 24	0	0
27	N	218	Total 218	O 218	0	0
27	O	122	Total 122	O 122	0	0
27	P	112	Total 112	O 112	0	0
27	Q	53	Total 53	O 53	0	0
27	R	45	Total 45	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

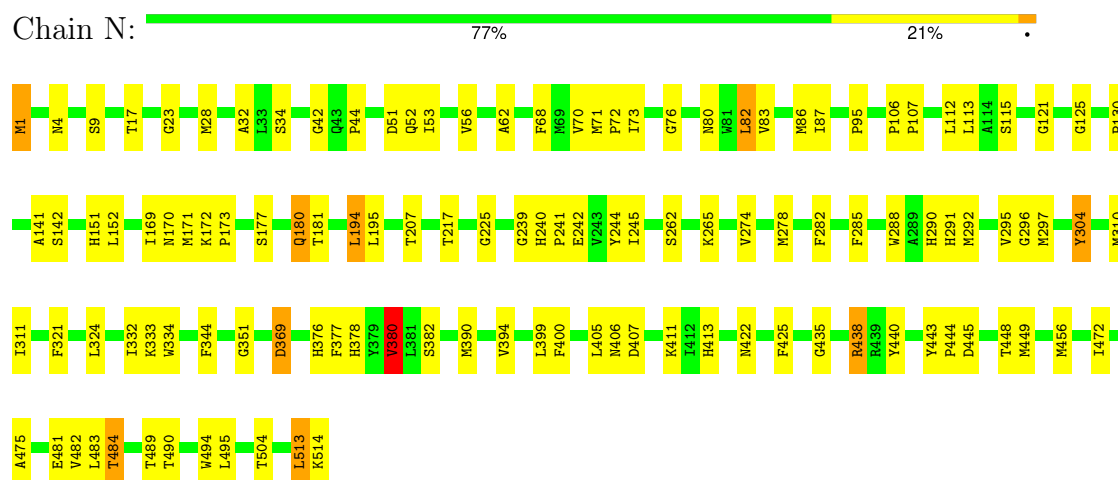
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

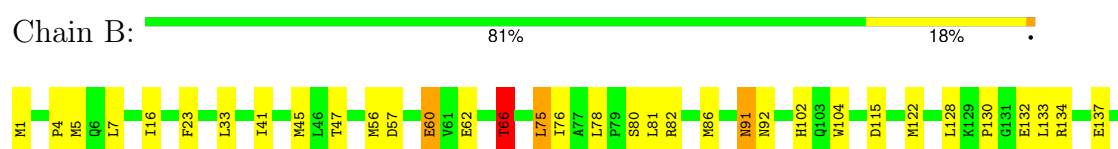
• Molecule 1: Cytochrome c oxidase subunit 1



• Molecule 1: Cytochrome c oxidase subunit 1



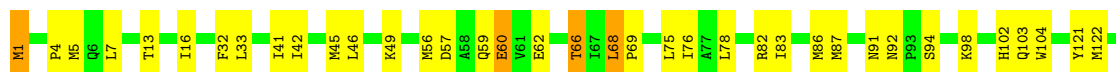
• Molecule 2: Cytochrome c oxidase subunit 2





• Molecule 2: Cytochrome c oxidase subunit 2

Chain O: 70% 25% .



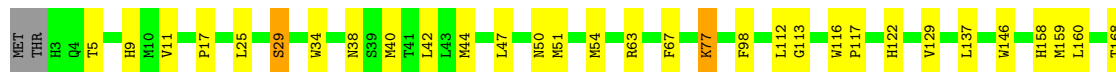
• Molecule 3: Cytochrome c oxidase subunit 3

Chain C: 85% 15% .



• Molecule 3: Cytochrome c oxidase subunit 3

Chain P: 84% 15% ..



• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D: 88% 10% .



• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q: 76% 20% ..



• Molecule 5: Cytochrome c oxidase polypeptide Va

Chain E:  83% 13% •



- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain R:  75% 21% •



- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F:  76% 21% ••



- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S:  76% 17% 6% •



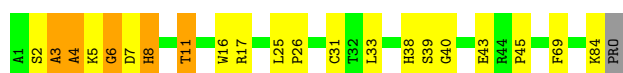
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G:  74% 15% 8% ••



- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T:  74% 19% 6% •



- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain H:  75% 15% 7% •



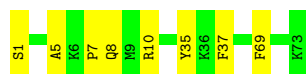
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain U:  69% 21% 7%



- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I:  89% 11%



- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V:  82% 18%



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain J:  90% 7% 2%



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain W:  90% 8% 2%



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K:  73% 14% 12%



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X:  73% 12% 12%



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:  79% 15% • •



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y:  79% 17% • •



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M:  72% 20% • 7%



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain Z:  61% 30% • 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: DMU, CDL, TPO, PSC, CU, CUA, SAC, PGV, PEK, FME, NA, TGL, ZN, MG, HEA, CHD

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	0.67	3/4156 (0.1%)	1.08	31/5678 (0.5%)
1	N	0.64	1/4156 (0.0%)	1.05	23/5678 (0.4%)
2	B	0.62	0/1860	1.04	5/2534 (0.2%)
2	O	0.63	1/1860 (0.1%)	1.07	5/2534 (0.2%)
3	C	0.59	0/2197	0.93	6/3005 (0.2%)
3	P	0.58	0/2197	0.96	9/3005 (0.3%)
4	D	0.58	0/1229	0.99	2/1658 (0.1%)
4	Q	0.60	0/1229	1.00	2/1658 (0.1%)
5	E	0.62	0/871	0.99	1/1182 (0.1%)
5	R	0.62	0/871	1.12	3/1182 (0.3%)
6	F	0.64	0/765	1.19	8/1038 (0.8%)
6	S	0.63	0/765	1.18	4/1038 (0.4%)
7	G	0.62	0/690	1.02	3/937 (0.3%)
7	T	0.65	0/690	1.04	3/937 (0.3%)
8	H	0.60	0/682	1.02	5/921 (0.5%)
8	U	0.57	0/682	1.06	3/921 (0.3%)
9	I	0.55	0/605	0.90	1/802 (0.1%)
9	V	0.53	0/605	0.86	1/802 (0.1%)
10	J	0.54	0/471	0.92	0/636
10	W	0.54	0/471	0.99	0/636
11	K	0.64	0/398	1.11	3/546 (0.5%)
11	X	0.60	0/398	1.02	1/546 (0.2%)
12	L	0.58	0/393	0.92	2/526 (0.4%)
12	Y	0.55	0/393	0.90	1/526 (0.2%)
13	M	0.60	0/345	0.95	1/470 (0.2%)
13	Z	0.53	0/345	0.93	1/470 (0.2%)
All	All	0.62	5/29324 (0.0%)	1.03	124/39866 (0.3%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	N	0	3
8	U	0	1
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	83	VAL	CA-CB	6.35	1.57	1.54
1	A	83	VAL	CA-CB	6.17	1.57	1.54
1	A	130	PRO	CA-C	5.39	1.57	1.52
2	O	103	GLN	CA-C	5.16	1.59	1.52
1	A	106	PRO	CA-C	5.09	1.56	1.52

All (124) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	133	GLY	N-CA-C	12.63	128.93	112.77
4	Q	133	GLY	N-CA-C	11.86	127.94	112.77
6	F	93	PRO	N-CA-C	10.68	126.60	111.33
6	S	93	PRO	N-CA-C	9.98	125.59	111.33
1	A	125	GLY	N-CA-C	-9.44	101.06	112.48
1	N	125	GLY	N-CA-C	-9.41	101.10	112.48
5	R	42	VAL	N-CA-C	-8.73	98.00	107.77
6	S	94	HIS	N-CA-C	8.20	128.27	110.80
1	N	130	PRO	N-CA-C	-7.97	100.97	110.70
6	F	94	HIS	N-CA-C	7.96	127.75	110.80
1	N	448	THR	N-CA-C	7.91	119.53	111.07
5	E	42	VAL	N-CA-C	-7.54	99.15	108.05
5	R	76	GLY	CA-C-N	7.51	127.22	119.64
5	R	76	GLY	C-N-CA	7.51	127.22	119.64
2	O	206	PHE	N-CA-C	7.39	120.35	110.88
1	A	130	PRO	N-CA-C	-7.25	101.86	110.70
1	N	70	VAL	N-CA-C	7.22	117.35	110.42
1	A	448	THR	N-CA-C	6.92	118.83	111.28
1	A	70	VAL	N-CA-C	6.80	116.90	110.30
8	H	64	CYS	N-CA-C	6.80	118.22	109.65
11	K	6	ALA	CA-C-N	6.72	127.09	119.83
11	K	6	ALA	C-N-CA	6.72	127.09	119.83
1	A	425	PHE	N-CA-C	6.62	121.57	112.90
8	U	64	CYS	N-CA-C	6.60	117.97	109.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	197	SER	N-CA-C	6.55	120.91	112.26
1	A	435	GLY	N-CA-C	6.52	125.16	115.64
6	S	93	PRO	CA-C-N	6.52	133.99	121.54
6	S	93	PRO	C-N-CA	6.52	133.99	121.54
1	A	82	LEU	N-CA-C	6.50	121.48	112.45
1	N	82	LEU	N-CA-C	6.48	121.45	112.45
1	N	425	PHE	N-CA-C	6.47	121.38	112.90
2	O	197	SER	N-CA-C	6.46	120.79	112.26
6	F	82	CYS	CA-C-N	6.46	126.39	119.28
6	F	82	CYS	C-N-CA	6.46	126.39	119.28
1	N	332	ILE	N-CA-C	6.45	117.64	108.93
1	A	141	ALA	N-CA-C	6.41	120.36	112.54
12	Y	20	ARG	N-CA-C	-6.37	104.42	111.36
1	A	332	ILE	N-CA-C	6.31	117.45	108.93
1	N	262	SER	N-CA-C	-6.25	105.29	113.17
1	A	169	ILE	CB-CA-C	-6.25	103.85	112.04
1	N	435	GLY	N-CA-C	6.24	124.75	115.64
1	A	170	ASN	N-CA-C	6.24	120.97	113.23
2	B	161	HIS	N-CA-C	-6.22	100.09	108.86
1	A	438	ARG	N-CA-C	-6.19	102.55	110.53
3	P	29	SER	N-CA-C	-6.16	104.48	111.07
1	A	262	SER	N-CA-C	-6.15	105.42	113.17
1	N	445	ASP	N-CA-C	6.14	118.76	111.33
1	N	438	ARG	N-CA-C	-6.08	102.68	110.53
11	X	36	ILE	N-CA-C	6.08	118.03	112.43
1	N	141	ALA	N-CA-C	6.06	119.94	112.54
1	A	217	THR	N-CA-C	-6.03	102.75	110.53
6	F	95	GLN	N-CA-C	5.96	123.49	110.80
2	B	66	THR	N-CA-C	-5.95	105.27	113.18
1	A	9	SER	N-CA-C	5.94	118.62	110.24
1	A	288	TRP	N-CA-C	5.91	119.32	111.75
12	L	20	ARG	N-CA-C	-5.90	104.93	111.36
3	P	113	GLY	N-CA-C	-5.89	107.04	115.64
1	N	171	MET	N-CA-C	5.85	120.11	111.87
1	A	495	LEU	N-CA-C	5.82	119.85	112.87
1	N	380	VAL	CB-CA-C	-5.80	104.43	112.02
1	A	380	VAL	CB-CA-C	-5.77	104.46	112.02
13	M	27	LEU	N-CA-C	5.77	118.78	111.69
8	H	10	ASN	CA-C-N	5.76	128.94	120.82
8	H	10	ASN	C-N-CA	5.76	128.94	120.82
1	N	288	TRP	N-CA-C	5.76	119.12	111.75
4	D	102	TYR	N-CA-C	5.74	120.56	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Z	27	LEU	N-CA-C	5.72	118.73	111.69
3	C	113	GLY	N-CA-C	-5.72	107.28	115.64
1	A	239	GLY	N-CA-C	5.72	119.56	112.64
1	N	217	THR	N-CA-C	-5.71	103.16	110.53
7	T	8	HIS	N-CA-C	5.68	122.89	110.80
1	A	445	ASP	N-CA-C	5.67	118.19	111.33
1	A	142	SER	N-CA-C	5.62	117.88	111.02
7	G	8	HIS	N-CA-C	5.59	122.70	110.80
12	L	3	TYR	N-CA-C	5.56	118.75	110.52
3	P	257	TYR	N-CA-C	5.55	117.41	111.36
7	G	69	PHE	N-CA-C	5.54	118.03	111.33
11	K	36	ILE	N-CA-C	5.53	117.52	112.43
1	N	495	LEU	N-CA-C	5.53	119.51	112.87
1	A	171	MET	N-CA-C	5.51	119.64	111.87
3	P	228	THR	N-CA-C	-5.47	101.93	110.42
1	A	506	GLU	N-CA-C	-5.46	105.43	111.71
2	B	133	LEU	N-CA-C	5.45	117.59	109.25
2	O	161	HIS	N-CA-C	-5.45	101.18	108.86
8	H	11	TYR	N-CA-C	5.44	118.21	110.10
2	B	47	THR	N-CA-C	5.40	119.02	111.30
3	C	256	ILE	N-CA-C	5.39	116.05	110.82
3	C	198	PHE	N-CA-C	5.39	118.07	111.82
1	N	239	GLY	N-CA-C	5.37	119.13	112.64
4	Q	102	TYR	N-CA-C	5.37	120.10	113.50
3	P	129	VAL	N-CA-CB	5.36	113.88	110.50
9	V	69	PHE	N-CA-C	5.33	118.92	109.96
8	H	54	GLU	N-CA-C	5.33	117.51	111.11
1	A	66	ILE	N-CA-C	5.31	115.57	110.74
8	U	22	ASN	N-CA-C	5.31	118.18	110.17
1	A	67	PHE	N-CA-C	5.27	118.87	112.23
9	I	69	PHE	N-CA-C	5.27	118.82	109.96
7	G	6	GLY	N-CA-C	5.24	125.60	113.18
1	N	443	TYR	N-CA-C	5.24	114.33	108.25
1	A	74	MET	N-CA-C	5.22	116.78	111.14
2	O	133	LEU	N-CA-C	5.22	117.24	109.25
3	P	198	PHE	N-CA-C	5.21	117.87	111.82
7	T	6	GLY	N-CA-C	5.21	125.53	113.18
6	F	4	GLY	N-CA-C	5.20	119.03	110.77
3	C	257	TYR	N-CA-C	5.19	117.02	111.36
6	F	39	THR	N-CA-C	-5.19	101.81	109.86
1	A	380	VAL	N-CA-C	5.19	115.41	110.53
1	A	173	PRO	N-CA-C	-5.18	105.50	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	HIS	CE1-NE2-CD2	-5.17	103.83	109.00
3	P	122	HIS	CA-C-N	5.17	125.45	119.92
3	P	122	HIS	C-N-CA	5.17	125.45	119.92
1	N	9	SER	N-CA-C	5.17	117.72	110.23
1	N	170	ASN	N-CA-C	5.15	119.83	113.50
7	T	69	PHE	N-CA-C	5.15	117.56	111.33
1	N	142	SER	N-CA-C	5.14	117.30	111.02
3	C	9	HIS	N-CA-C	5.14	117.11	108.73
6	F	12	GLN	N-CA-C	5.14	121.27	114.12
3	P	9	HIS	N-CA-C	5.09	117.03	108.73
1	A	198	SER	N-CA-C	5.09	117.60	111.40
1	A	119	GLU	CB-CA-C	-5.07	110.72	116.54
8	U	63	LEU	N-CA-C	5.06	119.49	112.45
3	C	29	SER	N-CA-C	-5.06	105.77	111.28
1	N	207	THR	N-CA-C	-5.05	105.86	111.36
2	O	203	ASN	N-CA-C	5.05	118.27	112.57

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	67	0
1	N	4027	0	4001	85	0
2	B	1824	0	1833	24	0
2	O	1824	0	1833	43	0
3	C	2110	0	2027	26	0
3	P	2110	0	2027	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1195	0	1183	11	0
4	Q	1195	0	1183	23	0
5	E	852	0	845	8	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	8	0
8	U	662	0	623	12	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	13	0
12	Y	380	0	380	9	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	3	0
17	N	120	0	108	4	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	12	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	550	0

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

All (550) 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:H	7:G:84:LYS:HD2	1.18	1.05
7:T:84:LYS:HD2	7:T:84:LYS:H	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:H191	26:C:270:CDL:H642	1.50	0.93
18:N:1522:TGL:HC62	18:N:1522:TGL:HC22	1.52	0.92
25:C:264:PEK:H161	25:C:264:PEK:H102	1.51	0.91
26:P:1270:CDL:H191	26:P:1270:CDL:H642	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:113:LEU:HB3	27:N:4646:HOH:O	1.82	0.77
8:H:43:MET:HE1	8:U:43:MET:HE1	1.66	0.76
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:H242	18:N:1522:TGL:H202	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:H102	18:N:1521:TGL:C28	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:H241	18:N:1521:TGL:H201	1.74	0.68
26:G:269:CDL:H541	26:G:269:CDL:C23	2.23	0.68
1:A:1:FME:HE2	1:A:1:FME:HA	1.76	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
7:T:3:ALA:HB1	25:T:263:PEK:H382	1.77	0.67
7:T:84:LYS:HD2	7:T:84:LYS:N	2.04	0.66
2:B:41:ILE:HD13	21:B:230:PSC:H342	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HG3	11:X:54:ARG:NH2	2.09	0.66
4:D:34:SER:H	4:D:37:GLN:NE2	1.91	0.66
19:P:1267:PGV:H161	19:P:1267:PGV:H12	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:HD2	7:G:84:LYS:N	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:HH11	12:Y:20:ARG:HB3	1.63	0.64
18:A:523:TGL:HC21	18:A:523:TGL:HG11	1.80	0.64
3:P:160:LEU:HD13	22:P:1271:CHD:H181	1.80	0.64
2:O:217:LYS:HA	2:O:217:LYS:HE2	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:51:MET:HB3	26:P:1270:CDL:H622	1.80	0.62
3:P:168:THR:HG22	25:P:1265:PEK:H14	1.81	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
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:HG23	6:F:92:VAL:O	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
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.81	0.61
21:O:1230:PSC:H21	21:O:1230:PSC:H222	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H142	21:B:230:PSC:C34	2.27	0.59
21:B:230:PSC:H222	21:B:230:PSC:H21	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:H222	18:B:521:TGL:HA82	1.85	0.58
1:N:51:ASP:OD1	2:O:206:PHE:HE1	1.85	0.58
18:N:1521:TGL:H222	18:N:1521:TGL:HA82	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:H322	26:T:1269:CDL:HA62	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:390:MET:HE2	1:N:413:HIS:HE1	1.69	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:G:269:CDL:H322	26:G:269:CDL:HA62	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
2:B:82:ARG:NH1	2:B:86:MET:HE1	2.21	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
1:A:390:MET:HE2	1:A:413:HIS:HE1	1.70	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
3:C:50:ASN:HD22	3:C:51:MET:HE2	1.72	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
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
6:F:64:GLU:O	6:F:65:ASP:HB2	2.08	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
1:N:52:GLN:O	1:N:56:VAL:HG23	2.08	0.54
1:N:406:ASN:HD21	19:N:1524:PGV:H21	1.73	0.54
18:N:1521:TGL:HB91	2:O:32:PHE:CE2	2.42	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
1:A:1:FME:HE3	12:L:3:TYR:HE1	1.72	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:H642	26:C:270:CDL:C19	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
7:G:3:ALA:HB1	25:G:1263:PEK:H382	1.91	0.52
13:M:42:LYS:HA	13:M:42:LYS:CE	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
7:T:3:ALA:O	7:T:4:ALA:HB2	2.09	0.52
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.91	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
8:H:43:MET:CE	8:U:43:MET:HE1	2.39	0.52
2:O:59:GLN:O	2:O:59:GLN:HG3	2.10	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
18:N:1521:TGL:HC22	27:Q:3383:HOH:O	2.09	0.52
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.41	0.52
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
1:A:310:MET:HE2	1:A:356:ILE:HG23	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
4:D:86:MET:HE3	27:K:4869:HOH:O	2.11	0.51
1:N:290:HIS:CD2	1:N:291:HIS:CD2	2.99	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.92	0.51
3:C:54:MET:HE3	26:C:270:CDL:H612	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
2:B:82:ARG:HH11	2:B:86:MET:HE1	1.76	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
1:N:28:MET:HE3	12:Y:29:PHE:CD2	2.46	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
1:A:310:MET:HE1	2:B:76:ILE:HG21	1.94	0.50
7:G:3:ALA:O	7:G:4:ALA:HB2	2.11	0.50
2:O:82:ARG:NH1	2:O:86:MET:HE1	2.26	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:N	2:O:203:ASN:HD22	2.10	0.49
2:B:41:ILE:O	2:B:45:MET:HG2	2.13	0.49
18:L:522:TGL:H202	18:L:522:TGL:C24	2.41	0.49
1:A:297:MET:HE2	1:A:302:ARG:HG2	1.94	0.49
2:O:41:ILE:CD1	21:O:1230:PSC:H342	2.39	0.49
3:C:50:ASN:ND2	3:C:54:MET:HE2	2.28	0.49
1:N:310:MET:HE1	2:O:76:ILE:HB	1.93	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
19:N:1524:PGV:H311	13:Z:16:ALA:HA	1.95	0.49
6:S:51:SER:O	6:S:94:HIS:N	2.46	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
1:N:390:MET:HE2	1:N:413:HIS:CE1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:1265:PEK:H383	26:T:1269:CDL:H273	1.95	0.48
4:Q:86:MET:HE1	27:X:4838:HOH:O	2.12	0.48
4:D:9:GLU:CD	4:D:9:GLU:H	2.21	0.48
1:N:34:SER:HB2	17:N:515:HEA:C2B	2.44	0.48
1:N:113:LEU:HD12	18:N:1522:TGL:H292	1.93	0.48
2:O:62:GLU:O	2:O:66:THR:HB	2.13	0.48
4:Q:138:TRP:CH2	11:X:50:PRO:HG2	2.48	0.48
6:S:22:LEU:HD12	27:S:4871:HOH:O	2.13	0.48
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
9:V:35:TYR:C	9:V:37:PHE:H	2.22	0.48
1:A:208:MET:HE2	3:C:97:PHE:CD1	2.49	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
9:I:35:TYR:C	9:I:37:PHE:H	2.22	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:A:177:SER:H	1:A:180:GLN:NE2	2.11	0.47
1:N:76:GLY:O	1:N:80:ASN:HB2	2.14	0.47
1:N:274:VAL:HG12	1:N:278:MET:HE2	1.97	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
10:W:40:LEU:HD12	22:W:1060:CHD:H183	1.97	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
1:A:1:FME:HA	1:A:1:FME:CE	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:2:SER:O	7:T:3:ALA:HB3	2.15	0.47
22:W:1060:CHD:H212	22:W:1060:CHD:H161	1.75	0.47
3:C:244:PHE:HA	25:T:263:PEK:H9	1.98	0.46
18:L:522:TGL:H231	18:L:522:TGL:H272	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
1:N:351:GLY:C	1:N:380:VAL:HG13	2.41	0.46
26:P:1270:CDL:H561	26:P:1270:CDL:H532	1.63	0.46
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.50	0.46
3:C:116:TRP:HA	3:C:117:PRO:C	2.39	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
3:P:50:ASN:ND2	3:P:54:MET:HE2	2.30	0.46
6:S:92:VAL:O	6:S:92:VAL:HG23	2.16	0.46
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
1:A:344:PHE:CD1	1:A:344:PHE:C	2.94	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:390:MET:HE2	1:A:413:HIS:CE1	2.49	0.45
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
3:P:116:TRP:HA	3:P:117:PRO:C	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:377:PHE:CD1	17:N:516:HEA:HAD1	2.51	0.45
2:O:1:FME:HE1	2:O:133:LEU:HD22	1.99	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:28:MET:HE2	17:A:515:HEA:H271	1.99	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
3:P:187:THR:HG22	25:P:1264:PEK:H052	1.99	0.45
26:P:1270:CDL:H112	27:P:4853:HOH:O	2.16	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
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:71:MET:HE1	1:N:195:LEU:HD21	1.99	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:HC62	18:L:522:TGL:CC2	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:H202	26:P:1270:CDL:H171	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
26:G:269:CDL:H212	1:N:311:ILE:HD12	2.00	0.44
13:M:37:LEU:HA	13:M:37:LEU:HD23	1.75	0.44
18:N:1522:TGL:H272	18:N:1522:TGL:H231	1.99	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
1:A:351:GLY:C	1:A:380:VAL:HG13	2.43	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
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
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:34:TRP:NE1	23:P:1272:DMU:H29	2.34	0.43
3:P:158:HIS:NE2	25:P:1265:PEK:H051	2.34	0.43
5:R:81:ILE:HG12	9:V:7:PRO:HG2	2.00	0.43
1:A:282:PHE:HZ	26:T:1269:CDL:H761	1.84	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:304:TYR:HD1	26:T:1269:CDL:HB32	1.84	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:351:GLY:HA3	1:N:380:VAL:HG13	2.01	0.43
17:N:515:HEA:HMC1	17:N:515:HEA:HBC1	2.01	0.43
4:Q:48:TRP:HB2	5:R:96:LEU:O	2.19	0.43
7:T:38:HIS:CD2	26:T:1269:CDL:HA21	2.53	0.43
26:T:1269:CDL:H601	26:T:1269:CDL:H571	1.63	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
22:O:229:CHD:H12	22:O:229:CHD:H212	1.99	0.43
25:P:1265:PEK:H383	26:T:1269:CDL:C27	2.48	0.43
6:S:53:THR:HB	6:S:54:ASN:H	1.65	0.43
6:F:51:SER:HB2	6:F:91:LEU:HD11	2.00	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
3:C:173:PHE:CD2	3:C:173:PHE:C	2.97	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
8:H:60:TYR:CD1	8:H:60:TYR:C	2.96	0.42
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
1:N:369:ASP:C	1:N:438:ARG:HG3	2.45	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:HD23	7:T:25:LEU:HA	1.88	0.42
22:C:271:CHD:H162	22:C:271:CHD:H222	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
4:D:144:GLU:OE1	4:D:147:LYS:HE3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:N:514:LYS:HA	6:S:38:ALA:HB3	2.02	0.42
21:O:1230:PSC:H62	21:O:1230:PSC:H241	2.01	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:HD12	2:B:75:LEU:HA	1.89	0.42
26:C:270:CDL:H632	26:C:270:CDL:H602	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:310:MET:HE1	2:B:76:ILE:CG2	2.49	0.42
1:A:376:HIS:O	1:A:380:VAL:HG22	2.19	0.42
1:A:510:TYR:CD1	1:A:510:TYR:C	2.98	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
2:O:42:ILE:O	2:O:46:LEU:HG	2.19	0.41
2:O:164:ALA:O	2:O:194:GLY:HA3	2.19	0.41
3:P:137:LEU:HD23	3:P:137:LEU:HA	1.88	0.41
3:P:173:PHE:C	3:P:173:PHE:CD2	2.98	0.41
1:A:195:LEU:HD23	1:A:245:ILE:HD13	2.01	0.41
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
13:Z:32:TRP:CZ3	13:Z:40:TYR:OH	2.72	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
5:E:80:GLU:H	5:E:80:GLU:CD	2.29	0.41
1:N:71:MET:HB2	1:N:72:PRO:HD3	2.02	0.41
1:N:344:PHE:CD1	1:N:344:PHE:C	2.98	0.41
1:N:376:HIS:O	1:N:380:VAL:HG22	2.21	0.41
1:N:440:TYR:CZ	2:O:205:SER:HA	2.56	0.41
8:U:43:MET:HE2	8:U:52:VAL:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
19:N:1524:PGV:H322	13:Z:19:LEU:HD23	2.02	0.41
2:O:86:MET:HE3	2:O:86:MET:HB2	1.95	0.41
3:P:230:ASN:HB2	27:S:3287:HOH:O	2.20	0.41
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.55	0.41
25:G:1263:PEK:H042	3:P:77:LYS:NZ	2.36	0.41
23:P:1272:DMU:H30	23:P:1272:DMU:O1	2.21	0.41
1:A:124:THR:HB	27:A:4100:HOH:O	2.20	0.41
1:A:378:HIS:CD2	1:A:382:SER:OG	2.74	0.41
1:A:510:TYR:CD2	6:F:49:VAL:HG13	2.56	0.41
2:B:81:LEU:HD13	26:T:1269:CDL:H122	2.03	0.41
7:G:34:ASN:ND2	26:G:269:CDL:H151	2.35	0.41
26:P:1270:CDL:HB21	26:P:1270:CDL:CB3	2.51	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
1:A:297:MET:HE2	1:A:302:ARG:CG	2.51	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:H251	26:G:269:CDL:H222	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
4:Q:131:ILE:HD12	4:Q:131:ILE:H	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
2:O:132:GLU:HB3	2:O:137:GLU:HG3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	499 (98%)	13 (2%)	0	100	100
1	N	512/514 (100%)	501 (98%)	11 (2%)	0	100	100
2	B	225/227 (99%)	213 (95%)	10 (4%)	2 (1%)	14	6
2	O	225/227 (99%)	211 (94%)	12 (5%)	2 (1%)	14	6
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	5 (2%)	1 (0%)	30	22
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%)	3	0
6	S	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	3	0
7	G	81/85 (95%)	66 (82%)	8 (10%)	7 (9%)	0	0
7	T	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	0	0
8	H	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	4	1
8	U	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	4	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%)	16	8

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS

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Mol	Chain	Res	Type
7	G	39	SER
6	S	94	HIS
6	S	95	GLN
7	T	4	ALA
7	T	7	ASP
7	T	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
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%)	420 (99%)	6 (1%)	59	59
1	N	426/426 (100%)	414 (97%)	12 (3%)	38	32
2	B	210/210 (100%)	200 (95%)	10 (5%)	23	15
2	O	210/210 (100%)	195 (93%)	15 (7%)	13	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	224/226 (99%)	218 (97%)	6 (3%)	39	34
3	P	224/226 (99%)	220 (98%)	4 (2%)	51	50
4	D	128/129 (99%)	126 (98%)	2 (2%)	55	54
4	Q	128/129 (99%)	124 (97%)	4 (3%)	35	29
5	E	92/95 (97%)	90 (98%)	2 (2%)	45	42
5	R	92/95 (97%)	89 (97%)	3 (3%)	33	26
6	F	81/81 (100%)	78 (96%)	3 (4%)	30	22
6	S	81/81 (100%)	77 (95%)	4 (5%)	22	14
7	G	67/68 (98%)	63 (94%)	4 (6%)	17	9
7	T	67/68 (98%)	64 (96%)	3 (4%)	24	17
8	H	71/75 (95%)	68 (96%)	3 (4%)	26	19
8	U	71/75 (95%)	67 (94%)	4 (6%)	19	11
9	I	57/57 (100%)	56 (98%)	1 (2%)	51	50
9	V	57/57 (100%)	54 (95%)	3 (5%)	20	12
10	J	49/50 (98%)	48 (98%)	1 (2%)	48	46
10	W	49/50 (98%)	48 (98%)	1 (2%)	48	46
11	K	39/46 (85%)	38 (97%)	1 (3%)	40	35
11	X	39/46 (85%)	38 (97%)	1 (3%)	40	35
12	L	39/40 (98%)	38 (97%)	1 (3%)	40	35
12	Y	39/40 (98%)	37 (95%)	2 (5%)	21	13
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%)	32	24

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

Mol	Chain	Res	Type
1	A	138	HIS
1	A	180	GLN
1	A	241	PRO
1	A	369	ASP
1	A	380	VAL
1	A	513	LEU
2	B	16	ILE

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Mol	Chain	Res	Type
2	B	33	LEU
2	B	60	GLU
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
2	B	130	PRO
2	B	167	SER
3	C	13	PRO
3	C	17	PRO
3	C	77	LYS
3	C	127	LEU
3	C	179	SER
3	C	230	ASN
4	D	4	SER
4	D	51	LEU
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
6	F	95	GLN
6	F	96	LEU
7	G	17	ARG
7	G	36	TRP
7	G	43	GLU
7	G	84	LYS
8	H	8	ILE
8	H	29	CYS
8	H	60	TYR
9	I	8	GLN
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	152	LEU
1	N	180	GLN
1	N	194	LEU
1	N	241	PRO

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Mol	Chain	Res	Type
1	N	297	MET
1	N	369	ASP
1	N	380	VAL
1	N	394	VAL
1	N	444	PRO
1	N	484	THR
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
2	O	94	SER
2	O	130	PRO
2	O	148	MET
2	O	167	SER
2	O	203	ASN
2	O	205	SER
2	O	217	LYS
3	P	17	PRO
3	P	77	LYS
3	P	159	MET
3	P	230	ASN
4	Q	8	SER
4	Q	9	GLU
4	Q	51	LEU
4	Q	121	LYS
5	R	80	GLU
5	R	86	ILE
5	R	90	ARG
6	S	48	LEU
6	S	53	THR
6	S	54	ASN
6	S	80	GLN
7	T	26	PRO
7	T	33	LEU
7	T	43	GLU
8	U	21	PRO

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Mol	Chain	Res	Type
8	U	29	CYS
8	U	60	TYR
8	U	61	LYS
9	V	8	GLN
9	V	29	LEU
9	V	61	GLU
10	W	50	LEU
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) 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	10	GLN
2	B	91	ASN
2	B	92	ASN
2	B	140	ASN
2	B	181	GLN
3	C	3	HIS
3	C	50	ASN
3	C	68	GLN
3	C	76	GLN
3	C	161	GLN
4	D	37	GLN
4	D	109	HIS
4	D	119	GLN
4	D	143	ASN
5	E	94	ASN
7	G	34	ASN
8	H	31	GLN
9	I	53	ASN

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Mol	Chain	Res	Type
10	J	29	ASN
11	K	35	GLN
1	N	4	ASN
1	N	80	ASN
1	N	98	ASN
1	N	151	HIS
1	N	170	ASN
1	N	178	GLN
1	N	180	GLN
1	N	406	ASN
1	N	512	ASN
2	O	10	GLN
2	O	203	ASN
3	P	50	ASN
3	P	68	GLN
4	Q	37	GLN
4	Q	101	HIS
4	Q	109	HIS
4	Q	119	GLN
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
7	T	71	HIS
8	U	31	GLN
8	U	32	ASN
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	A	1	1	8,9,10	0.66	0	8,9,11	1.19	1 (12%)
2	FME	O	1	2	8,9,10	0.74	0	8,9,11	1.96	2 (25%)
7	TPO	T	11	7	8,10,11	1.29	2 (25%)	10,14,16	1.11	0
1	FME	N	1	1	8,9,10	0.81	0	8,9,11	1.73	2 (25%)
9	SAC	I	1	9	7,8,9	2.36	2 (28%)	7,9,11	1.66	2 (28%)
2	FME	B	1	2	8,9,10	0.79	0	8,9,11	1.98	2 (25%)
9	SAC	V	1	9	7,8,9	2.68	2 (28%)	7,9,11	1.92	3 (42%)
7	TPO	G	11	7	8,10,11	1.67	1 (12%)	10,14,16	1.07	1 (10%)

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	OAC-C1A	5.17	1.34	1.23
9	I	1	SAC	OAC-C1A	4.98	1.34	1.23
9	V	1	SAC	CA-N	4.47	1.53	1.46
9	I	1	SAC	CA-N	3.53	1.51	1.46
7	G	11	TPO	CB-CA	3.29	1.60	1.53
7	T	11	TPO	P-O1P	2.22	1.57	1.50
7	T	11	TPO	CB-CA	2.07	1.58	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	FME	C-CA-N	4.17	117.55	109.50
1	N	1	FME	CA-N-CN	-4.06	116.57	122.82
2	B	1	FME	C-CA-N	3.84	116.92	109.50
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	V	1	SAC	C2A-C1A-N	2.93	120.98	116.12
9	I	1	SAC	C-CA-N	-2.82	104.05	109.50
9	V	1	SAC	C-CA-N	-2.72	104.24	109.50
1	A	1	FME	CA-N-CN	-2.46	119.03	122.82
9	V	1	SAC	OAC-C1A-C2A	-2.29	117.98	122.05
9	I	1	SAC	C2A-C1A-N	2.17	119.72	116.12
1	N	1	FME	O-C-CA	-2.13	119.28	124.77
7	G	11	TPO	O3P-P-OG1	2.02	113.73	105.85

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
9	I	1	SAC	CB-CA-N-C1A
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
2	O	1	FME	O1-CN-N-CA
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	CB-CA-N-C1A
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
7	G	11	TPO	CB-OG1-P-O3P

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1	FME	4	0
2	O	1	FME	1	0
7	T	11	TPO	1	0
1	N	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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$
19	PGV	C	267	-	50,50,50	0.83	1 (2%)	53,56,56	0.87	2 (3%)
19	PGV	N	1266	-	50,50,50	0.92	3 (6%)	53,56,56	0.82	2 (3%)
23	DMU	C	272	-	34,34,34	2.75	12 (35%)	45,45,45	4.24	19 (42%)
21	PSC	B	230	-	51,51,51	1.23	3 (5%)	57,59,59	0.93	1 (1%)
22	CHD	B	1086	-	32,32,32	0.79	1 (3%)	51,51,51	1.78	13 (25%)
21	PSC	O	1230	-	51,51,51	1.22	3 (5%)	57,59,59	0.92	1 (1%)
22	CHD	P	1271	-	32,32,32	0.87	0	51,51,51	3.62	24 (47%)
18	TGL	A	523	-	62,62,62	0.75	1 (1%)	65,65,65	1.22	8 (12%)
22	CHD	P	1525	-	32,32,32	0.88	1 (3%)	51,51,51	1.54	9 (17%)
19	PGV	N	1524	-	50,50,50	1.09	3 (6%)	53,56,56	0.95	5 (9%)
17	HEA	N	516	1	67,67,67	1.28	7 (10%)	81,103,103	1.35	12 (14%)
25	PEK	C	265	-	52,52,52	1.63	10 (19%)	55,57,57	1.13	6 (10%)
17	HEA	A	516	1	67,67,67	1.34	7 (10%)	81,103,103	1.25	11 (13%)
19	PGV	P	1268	-	50,50,50	1.19	4 (8%)	53,56,56	0.84	1 (1%)
23	DMU	P	1272	-	34,34,34	2.87	11 (32%)	45,45,45	4.27	19 (42%)
23	DMU	M	526	-	34,34,34	3.27	8 (23%)	45,45,45	4.33	20 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CDL	P	1270	-	99,99,99	0.85	3 (3%)	105,111,111	0.92	5 (4%)
25	PEK	G	1263	-	52,52,52	1.79	9 (17%)	55,57,57	1.20	5 (9%)
22	CHD	C	271	-	32,32,32	0.93	1 (3%)	51,51,51	3.63	23 (45%)
25	PEK	P	1264	-	52,52,52	1.41	5 (9%)	55,57,57	0.98	3 (5%)
18	TGL	B	521	-	62,62,62	0.72	0	65,65,65	1.47	9 (13%)
26	CDL	C	270	-	99,99,99	0.82	3 (3%)	105,111,111	0.94	6 (5%)
26	CDL	T	1269	-	99,99,99	0.97	6 (6%)	105,111,111	0.98	7 (6%)
19	PGV	C	268	-	50,50,50	1.18	3 (6%)	53,56,56	0.82	0
25	PEK	T	263	-	52,52,52	1.83	11 (21%)	55,57,57	1.20	5 (9%)
22	CHD	O	229	-	32,32,32	0.77	1 (3%)	51,51,51	1.83	14 (27%)
26	CDL	G	269	-	99,99,99	0.99	7 (7%)	105,111,111	0.95	7 (6%)
18	TGL	N	1522	-	62,62,62	1.16	3 (4%)	65,65,65	1.66	13 (20%)
22	CHD	J	60	-	32,32,32	1.10	2 (6%)	51,51,51	3.44	30 (58%)
25	PEK	C	264	-	52,52,52	1.40	4 (7%)	55,57,57	0.97	3 (5%)
25	PEK	P	1265	-	52,52,52	1.64	11 (21%)	55,57,57	1.11	5 (9%)
22	CHD	C	525	-	32,32,32	0.85	0	51,51,51	1.57	8 (15%)
20	CUA	B	228	2	0,1,1	-	-	-		
20	CUA	O	228	2	0,1,1	-	-	-		
23	DMU	Z	1526	-	34,34,34	3.19	8 (23%)	45,45,45	4.28	20 (44%)
22	CHD	W	1060	-	32,32,32	1.20	3 (9%)	51,51,51	3.45	29 (56%)
17	HEA	A	515	1	67,67,67	1.11	4 (5%)	81,103,103	1.06	3 (3%)
17	HEA	N	515	1	67,67,67	1.21	7 (10%)	81,103,103	1.06	5 (6%)
18	TGL	N	1523	-	62,62,62	0.79	1 (1%)	65,65,65	1.21	5 (7%)
18	TGL	L	522	-	62,62,62	1.11	5 (8%)	65,65,65	1.70	14 (21%)
19	PGV	C	266	-	50,50,50	0.88	2 (4%)	53,56,56	0.76	1 (1%)
19	PGV	A	524	-	50,50,50	1.10	3 (6%)	53,56,56	0.97	5 (9%)
18	TGL	N	1521	-	62,62,62	0.77	1 (1%)	65,65,65	1.43	9 (13%)
19	PGV	P	1267	-	50,50,50	0.87	2 (4%)	53,56,56	0.80	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	PGV	C	267	-	-	17/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	DMU	C	272	-	6/6/10/10	9/19/59/59	0/2/2/2
19	PGV	N	1266	-	-	13/55/55/55	-
21	PSC	B	230	-	-	41/55/55/55	-
22	CHD	B	1086	-	-	2/9/74/74	0/4/4/4
21	PSC	O	1230	-	-	41/55/55/55	-
22	CHD	P	1271	-	5/5/12/12	8/9/74/74	0/4/4/4
18	TGL	A	523	-	-	13/65/65/65	-
22	CHD	P	1525	-	-	2/9/74/74	0/4/4/4
19	PGV	N	1524	-	-	32/55/55/55	-
17	HEA	N	516	1	-	7/36/76/76	-
25	PEK	C	265	-	-	16/56/56/56	-
17	HEA	A	516	1	-	7/36/76/76	-
19	PGV	P	1268	-	-	33/55/55/55	-
23	DMU	P	1272	-	6/6/10/10	10/19/59/59	0/2/2/2
23	DMU	M	526	-	5/5/10/10	12/19/59/59	0/2/2/2
26	CDL	P	1270	-	-	70/110/110/110	-
25	PEK	G	1263	-	-	29/56/56/56	-
22	CHD	C	271	-	5/5/12/12	8/9/74/74	0/4/4/4
25	PEK	P	1264	-	-	23/56/56/56	-
18	TGL	B	521	-	-	16/65/65/65	-
26	CDL	C	270	-	-	70/110/110/110	-
26	CDL	T	1269	-	-	61/110/110/110	-
19	PGV	C	268	-	-	33/55/55/55	-
25	PEK	T	263	-	-	29/56/56/56	-
22	CHD	O	229	-	-	2/9/74/74	0/4/4/4
26	CDL	G	269	-	-	60/110/110/110	-
18	TGL	N	1522	-	-	17/65/65/65	-
22	CHD	J	60	-	5/5/12/12	8/9/74/74	0/4/4/4
25	PEK	C	264	-	-	23/56/56/56	-
25	PEK	P	1265	-	-	16/56/56/56	-
22	CHD	C	525	-	-	2/9/74/74	0/4/4/4
23	DMU	Z	1526	-	5/5/10/10	11/19/59/59	0/2/2/2
22	CHD	W	1060	-	5/5/12/12	8/9/74/74	0/4/4/4
17	HEA	A	515	1	-	7/36/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	HEA	N	515	1	-	6/36/76/76	-
18	TGL	N	1523	-	-	13/65/65/65	-
18	TGL	L	522	-	-	16/65/65/65	-
19	PGV	C	266	-	-	13/55/55/55	-
19	PGV	A	524	-	-	32/55/55/55	-
18	TGL	N	1521	-	-	15/65/65/65	-
19	PGV	P	1267	-	-	16/55/55/55	-

All (180) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	M	526	DMU	O7-C3	-8.42	1.22	1.43
23	Z	1526	DMU	O7-C3	-7.92	1.23	1.43
23	M	526	DMU	O16-C6	-7.60	1.27	1.40
23	Z	1526	DMU	O16-C6	-7.47	1.27	1.40
23	M	526	DMU	O16-C18	-7.04	1.23	1.43
23	Z	1526	DMU	O16-C18	-6.79	1.24	1.43
23	P	1272	DMU	O1-C9	-6.63	1.28	1.44
23	M	526	DMU	O1-C9	-6.57	1.28	1.44
23	Z	1526	DMU	O1-C9	-6.46	1.28	1.44
23	M	526	DMU	O5-C4	-6.43	1.28	1.44
23	P	1272	DMU	O16-C6	-6.40	1.29	1.40
23	M	526	DMU	O7-C10	-6.30	1.24	1.41
23	P	1272	DMU	O7-C3	-6.25	1.28	1.43
23	Z	1526	DMU	O7-C10	-6.25	1.24	1.41
23	C	272	DMU	O1-C9	-6.22	1.29	1.44
23	P	1272	DMU	O16-C18	-6.19	1.26	1.43
23	Z	1526	DMU	O5-C4	-5.94	1.29	1.44
23	C	272	DMU	O16-C6	-5.86	1.30	1.40
17	A	516	HEA	FE-NC	5.74	2.14	1.95
23	C	272	DMU	O7-C3	-5.74	1.29	1.43
23	C	272	DMU	O16-C18	-5.74	1.27	1.43
23	M	526	DMU	O1-C10	-5.65	1.27	1.41
23	Z	1526	DMU	O1-C10	-5.61	1.27	1.41
18	N	1522	TGL	OG2-CB1	4.93	1.48	1.34
23	C	272	DMU	O5-C4	-4.88	1.32	1.44
25	G	1263	PEK	C12-C11	4.88	1.59	1.31
17	N	516	HEA	FE-NA	4.87	2.11	1.95
23	P	1272	DMU	O5-C4	-4.86	1.32	1.44
25	T	263	PEK	C12-C11	4.75	1.58	1.31
25	P	1264	PEK	C12-C11	4.73	1.58	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	264	PEK	C15-C14	4.72	1.58	1.31
18	L	522	TGL	OG2-CB1	4.68	1.47	1.34
25	P	1264	PEK	C15-C14	4.63	1.58	1.31
23	C	272	DMU	O1-C10	-4.60	1.30	1.41
23	P	1272	DMU	O7-C10	-4.59	1.28	1.41
25	C	264	PEK	C12-C11	4.59	1.57	1.31
23	M	526	DMU	O5-C6	-4.59	1.30	1.41
23	P	1272	DMU	O1-C10	-4.58	1.30	1.41
19	C	268	PGV	C12-C11	4.51	1.57	1.31
19	P	1268	PGV	C12-C11	4.50	1.57	1.31
25	C	265	PEK	C9-C8	4.45	1.57	1.31
25	T	263	PEK	C6-C5	4.44	1.56	1.31
23	Z	1526	DMU	O5-C6	-4.44	1.30	1.41
25	C	265	PEK	C15-C14	4.38	1.56	1.31
21	O	1230	PSC	C10-C9	4.37	1.56	1.31
25	C	265	PEK	C12-C11	4.37	1.56	1.31
25	T	263	PEK	C9-C8	4.35	1.56	1.31
25	P	1265	PEK	C12-C11	4.35	1.56	1.31
25	G	1263	PEK	C6-C5	4.33	1.56	1.31
25	P	1265	PEK	C6-C5	4.32	1.56	1.31
23	C	272	DMU	O7-C10	-4.32	1.29	1.41
25	T	263	PEK	C15-C14	4.31	1.56	1.31
21	B	230	PSC	C10-C9	4.31	1.56	1.31
25	G	1263	PEK	C9-C8	4.30	1.56	1.31
25	P	1265	PEK	C9-C8	4.24	1.55	1.31
25	P	1265	PEK	C15-C14	4.22	1.55	1.31
25	G	1263	PEK	C15-C14	4.22	1.55	1.31
21	O	1230	PSC	C13-C12	4.22	1.55	1.31
25	P	1264	PEK	C6-C5	4.16	1.55	1.31
25	C	264	PEK	C6-C5	4.14	1.55	1.31
23	P	1272	DMU	O5-C6	-4.14	1.31	1.41
19	N	1524	PGV	C12-C11	4.11	1.55	1.31
25	C	265	PEK	C6-C5	4.11	1.55	1.31
25	C	264	PEK	C9-C8	4.03	1.54	1.31
25	P	1264	PEK	C9-C8	4.02	1.54	1.31
21	B	230	PSC	C13-C12	3.98	1.54	1.31
25	G	1263	PEK	C03-C02	3.97	1.63	1.50
19	A	524	PGV	C12-C11	3.95	1.54	1.31
19	N	1266	PGV	C12-C11	3.95	1.54	1.31
17	A	515	HEA	FE-NA	3.93	2.08	1.95
22	W	1060	CHD	C13-C17	3.90	1.62	1.55
25	T	263	PEK	C03-C02	3.89	1.63	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	515	HEA	C11-C3B	-3.87	1.46	1.51
23	C	272	DMU	O5-C6	-3.84	1.31	1.41
19	C	266	PGV	C12-C11	3.83	1.53	1.31
18	N	1522	TGL	OG1-CA1	3.74	1.44	1.33
25	T	263	PEK	O03-C21	3.72	1.44	1.33
25	G	1263	PEK	C01-C02	3.53	1.61	1.50
26	T	1269	CDL	CB6-CB4	3.53	1.61	1.50
25	G	1263	PEK	O03-C21	3.53	1.43	1.33
19	A	524	PGV	O03-C19	3.36	1.43	1.33
19	P	1267	PGV	C12-C11	3.35	1.50	1.31
25	T	263	PEK	C01-C02	3.33	1.61	1.50
19	C	267	PGV	C12-C11	3.28	1.50	1.31
22	J	60	CHD	C13-C17	3.21	1.60	1.55
26	G	269	CDL	CB6-CB4	3.19	1.60	1.50
17	N	516	HEA	FE-ND	-3.17	1.85	1.94
19	P	1268	PGV	O01-C1	3.07	1.42	1.34
25	T	263	PEK	P-O11	3.04	1.71	1.59
17	N	515	HEA	CMA-C3A	-3.02	1.38	1.45
26	G	269	CDL	OA6-CA5	2.91	1.42	1.34
19	N	1524	PGV	O03-C19	2.91	1.41	1.33
17	N	515	HEA	FE-NA	2.87	2.04	1.95
25	P	1265	PEK	O03-C21	2.86	1.41	1.33
17	N	516	HEA	CMA-C3A	-2.85	1.39	1.45
19	C	268	PGV	O01-C1	2.84	1.42	1.34
25	G	1263	PEK	P-O11	2.81	1.70	1.59
18	L	522	TGL	OG1-CA1	2.80	1.41	1.33
17	A	516	HEA	CMA-C3A	-2.79	1.39	1.45
17	A	515	HEA	CMA-C3A	-2.73	1.39	1.45
25	C	265	PEK	O03-C21	2.71	1.41	1.33
18	L	522	TGL	CG1-CG2	2.70	1.59	1.50
26	T	1269	CDL	CB3-CB4	2.69	1.59	1.50
19	N	1266	PGV	C01-C02	2.68	1.59	1.50
18	N	1522	TGL	CG1-CG2	2.65	1.59	1.50
23	C	272	DMU	C3-C4	2.64	1.60	1.52
17	N	516	HEA	C3C-C4C	2.64	1.50	1.42
21	O	1230	PSC	C2-C1	2.60	1.58	1.50
17	A	516	HEA	FE-NA	2.59	2.03	1.95
25	T	263	PEK	O01-C1	2.59	1.41	1.34
19	C	266	PGV	C20-C19	2.55	1.58	1.50
26	G	269	CDL	CB3-CB4	2.55	1.58	1.50
26	G	269	CDL	C11-CA5	2.55	1.58	1.50
26	T	1269	CDL	C11-CA5	2.55	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	265	PEK	C03-C02	2.54	1.58	1.50
17	N	516	HEA	C4D-ND	2.53	1.43	1.38
17	N	516	HEA	FE-NC	2.53	2.03	1.95
21	B	230	PSC	C2-C1	2.53	1.58	1.50
25	P	1265	PEK	C22-C21	2.52	1.58	1.50
25	T	263	PEK	C2-C1	2.51	1.58	1.50
25	P	1265	PEK	C01-C02	2.51	1.58	1.50
26	P	1270	CDL	CA6-CA4	2.49	1.58	1.50
19	C	268	PGV	C04-C05	2.49	1.59	1.51
18	N	1521	TGL	OG2-CB1	2.48	1.41	1.34
19	N	1524	PGV	C20-C19	2.48	1.57	1.50
23	P	1272	DMU	C3-C4	2.48	1.59	1.52
25	P	1265	PEK	P-O11	2.45	1.69	1.59
25	C	265	PEK	C22-C21	2.44	1.57	1.50
22	P	1525	CHD	C8-C9	2.41	1.58	1.53
25	C	265	PEK	C01-C02	2.41	1.58	1.50
19	P	1268	PGV	C04-C05	2.40	1.59	1.51
17	A	515	HEA	FE-NC	2.40	2.03	1.95
22	W	1060	CHD	C20-C17	2.39	1.58	1.54
25	C	265	PEK	P-O11	2.37	1.68	1.59
25	P	1265	PEK	P-O12	2.34	1.68	1.59
26	T	1269	CDL	OA6-CA5	2.34	1.40	1.34
26	C	270	CDL	CA6-CA4	2.33	1.58	1.50
25	P	1265	PEK	C03-C02	2.31	1.58	1.50
17	A	516	HEA	C3C-C4C	2.30	1.49	1.42
18	N	1523	TGL	OG2-CB1	2.29	1.40	1.34
19	A	524	PGV	C20-C19	2.29	1.57	1.50
17	A	516	HEA	CAC-C3C	2.28	1.53	1.47
23	C	272	DMU	C7-C5	2.28	1.58	1.52
17	A	516	HEA	C4D-ND	2.27	1.43	1.38
23	C	272	DMU	C6-C1	2.27	1.59	1.52
22	O	229	CHD	C8-C9	2.27	1.58	1.53
26	P	1270	CDL	CA3-CA4	2.26	1.57	1.50
23	P	1272	DMU	C6-C1	2.25	1.59	1.52
18	L	522	TGL	CC2-CC1	2.24	1.57	1.50
26	G	269	CDL	CB2-C1	2.23	1.58	1.51
25	T	263	PEK	P-O12	2.23	1.68	1.59
26	G	269	CDL	CA6-CA4	2.21	1.57	1.50
17	N	515	HEA	C1D-C2D	2.21	1.49	1.44
17	N	515	HEA	FE-NC	2.21	2.02	1.95
25	C	265	PEK	P-O12	2.21	1.68	1.59
26	P	1270	CDL	C31-CA7	2.21	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	N	1266	PGV	C20-C19	2.20	1.57	1.50
25	G	1263	PEK	P-O12	2.20	1.68	1.59
23	P	1272	DMU	C7-C5	2.18	1.58	1.52
26	C	270	CDL	CA3-CA4	2.16	1.57	1.50
26	T	1269	CDL	CB2-C1	2.15	1.58	1.51
22	C	271	CHD	C19-C10	-2.12	1.50	1.54
25	P	1265	PEK	O01-C1	2.11	1.40	1.34
17	N	515	HEA	CMD-C2D	2.09	1.55	1.50
26	T	1269	CDL	CA6-CA4	2.06	1.57	1.50
17	N	516	HEA	CAC-C3C	2.05	1.52	1.47
25	P	1264	PEK	C2-C1	2.05	1.56	1.50
19	P	1268	PGV	P-O12	2.04	1.67	1.59
18	L	522	TGL	CG3-CG2	2.04	1.57	1.50
22	W	1060	CHD	C8-C7	2.03	1.57	1.53
17	N	515	HEA	C4D-C3D	2.03	1.48	1.45
22	B	1086	CHD	C13-C12	-2.01	1.51	1.54
23	C	272	DMU	C8-C7	2.01	1.57	1.52
26	G	269	CDL	C71-CB7	2.01	1.56	1.50
19	P	1267	PGV	C01-C02	2.01	1.57	1.50
17	A	515	HEA	FE-ND	2.01	2.01	1.94
22	J	60	CHD	C20-C17	2.01	1.57	1.54
26	C	270	CDL	C71-CB7	2.01	1.56	1.50
17	A	516	HEA	C4C-NC	-2.00	1.35	1.39
18	A	523	TGL	OG2-CB1	2.00	1.39	1.34

All (389) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	1271	CHD	C17-C13-C14	10.54	110.69	100.11
23	M	526	DMU	C10-C5-C7	10.44	131.97	110.01
22	C	271	CHD	C17-C13-C14	10.39	110.54	100.11
23	Z	1526	DMU	C10-C5-C7	10.24	131.55	110.01
22	P	1271	CHD	C10-C9-C8	10.15	123.15	111.84
23	P	1272	DMU	O16-C6-C1	9.76	123.09	108.27
22	C	271	CHD	C10-C9-C8	9.72	122.68	111.84
23	C	272	DMU	C1-C2-C3	9.68	131.66	109.68
23	P	1272	DMU	C1-C2-C3	9.43	131.08	109.68
23	C	272	DMU	C6-O5-C4	9.38	132.04	113.72
22	J	60	CHD	C17-C13-C14	9.30	109.45	100.11
23	C	272	DMU	O16-C6-C1	9.22	122.28	108.27
22	P	1271	CHD	C17-C13-C12	-8.99	109.58	117.67
23	M	526	DMU	C1-C2-C3	8.93	129.95	109.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	1060	CHD	C17-C13-C14	8.88	109.02	100.11
23	Z	1526	DMU	C1-C2-C3	8.83	129.73	109.68
23	P	1272	DMU	C6-O5-C4	8.74	130.79	113.72
23	C	272	DMU	C18-O16-C6	8.74	128.60	113.68
22	C	271	CHD	C17-C13-C12	-8.72	109.82	117.67
22	C	271	CHD	C19-C10-C9	-8.47	99.79	111.18
23	P	1272	DMU	O7-C3-C4	8.45	131.65	109.48
23	C	272	DMU	O1-C9-C11	8.24	126.87	106.44
23	M	526	DMU	C6-O5-C4	8.20	129.73	113.72
23	Z	1526	DMU	C6-O5-C4	8.17	129.68	113.72
22	P	1271	CHD	C19-C10-C9	-7.94	100.50	111.18
23	M	526	DMU	O5-C4-C3	7.94	126.14	109.72
23	M	526	DMU	C8-C7-C5	-7.94	96.90	110.83
23	P	1272	DMU	C18-O16-C6	7.90	127.17	113.68
23	Z	1526	DMU	C8-C7-C5	-7.85	97.06	110.83
23	Z	1526	DMU	O5-C4-C3	7.79	125.83	109.72
23	C	272	DMU	O7-C3-C4	7.65	129.55	109.48
23	Z	1526	DMU	O1-C9-C11	7.62	125.32	106.44
23	Z	1526	DMU	C7-C8-C9	7.61	124.03	110.23
23	M	526	DMU	C7-C8-C9	7.61	124.02	110.23
23	M	526	DMU	O1-C9-C11	7.48	124.96	106.44
23	P	1272	DMU	O1-C9-C11	7.47	124.94	106.44
23	P	1272	DMU	O5-C4-C3	7.47	125.16	109.72
23	M	526	DMU	O1-C9-C8	7.37	122.98	109.70
23	P	1272	DMU	C8-C7-C5	7.33	123.69	110.83
23	C	272	DMU	O5-C4-C3	7.10	124.41	109.72
23	Z	1526	DMU	O1-C9-C8	7.03	122.36	109.70
23	Z	1526	DMU	O5-C6-O16	6.88	126.30	110.04
23	Z	1526	DMU	O5-C4-C57	6.74	123.15	106.44
23	P	1272	DMU	O1-C9-C8	6.67	121.72	109.70
22	W	1060	CHD	C13-C17-C20	6.55	127.42	119.48
23	M	526	DMU	O5-C6-O16	6.51	125.43	110.04
22	J	60	CHD	C13-C17-C20	6.49	127.35	119.48
23	M	526	DMU	O5-C4-C57	6.48	122.49	106.44
22	W	1060	CHD	C10-C9-C8	6.36	118.93	111.84
22	C	271	CHD	C1-C10-C5	6.31	116.80	107.75
23	C	272	DMU	O5-C4-C57	6.29	122.04	106.44
22	J	60	CHD	C10-C9-C8	6.29	118.85	111.84
23	C	272	DMU	O7-C10-C5	6.28	123.54	108.09
23	M	526	DMU	C18-O16-C6	6.21	124.29	113.68
23	P	1272	DMU	O7-C10-C5	6.19	123.32	108.09
22	P	1271	CHD	C1-C10-C5	6.19	116.63	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	271	CHD	C19-C10-C1	-6.16	98.52	108.31
22	J	60	CHD	C4-C3-C2	6.14	118.11	110.62
23	M	526	DMU	O7-C3-C2	6.13	122.80	107.23
23	Z	1526	DMU	O7-C3-C2	6.08	122.67	107.23
23	C	272	DMU	O7-C3-C2	6.06	122.63	107.23
23	P	1272	DMU	O5-C4-C57	6.02	121.37	106.44
22	W	1060	CHD	C6-C5-C10	5.96	119.00	112.66
23	Z	1526	DMU	C18-O16-C6	5.93	123.81	113.68
22	W	1060	CHD	C4-C3-C2	5.89	117.80	110.62
22	P	1271	CHD	C19-C10-C1	-5.89	98.95	108.31
22	W	1060	CHD	C15-C14-C8	-5.62	110.65	118.36
23	P	1272	DMU	O7-C3-C2	5.59	121.44	107.23
22	J	60	CHD	C6-C5-C10	5.59	118.61	112.66
22	W	1060	CHD	C11-C12-C13	5.57	116.93	111.26
23	C	272	DMU	O1-C9-C8	5.55	119.70	109.70
22	J	60	CHD	C15-C14-C8	-5.51	110.80	118.36
22	J	60	CHD	C11-C12-C13	5.46	116.81	111.26
22	J	60	CHD	C11-C9-C10	5.45	119.23	113.70
23	C	272	DMU	C10-O1-C9	5.45	124.36	113.72
18	B	521	TGL	CG2-OG2-CB1	5.38	130.68	117.80
22	W	1060	CHD	C11-C9-C10	5.29	119.07	113.70
23	P	1272	DMU	C10-O1-C9	5.20	123.88	113.72
22	O	229	CHD	C10-C9-C8	5.18	117.61	111.84
22	P	1271	CHD	C15-C14-C8	-5.15	111.30	118.36
22	C	271	CHD	C4-C5-C10	5.12	118.11	112.66
22	J	60	CHD	C5-C6-C7	5.10	120.46	114.40
22	W	1060	CHD	C5-C6-C7	5.05	120.40	114.40
22	C	271	CHD	C15-C14-C8	-5.01	111.49	118.36
18	N	1521	TGL	CG2-OG2-CB1	4.99	129.75	117.80
22	C	271	CHD	C4-C3-C2	4.95	116.66	110.62
18	L	522	TGL	C12-C11-C10	-4.87	89.74	114.37
22	C	271	CHD	C14-C13-C12	4.84	111.84	107.42
22	J	60	CHD	C2-C1-C10	4.80	120.84	112.74
23	Z	1526	DMU	O5-C6-C1	4.79	120.22	110.37
18	N	1522	TGL	C12-C11-C10	-4.79	90.17	114.37
22	P	1271	CHD	C4-C5-C10	4.76	117.73	112.66
22	W	1060	CHD	C2-C1-C10	4.75	120.75	112.74
22	P	1271	CHD	C14-C13-C12	4.72	111.73	107.42
23	M	526	DMU	O5-C6-C1	4.69	120.00	110.37
22	J	60	CHD	C18-C13-C14	-4.64	103.93	111.20
22	W	1060	CHD	C18-C13-C14	-4.64	103.94	111.20
22	C	271	CHD	C9-C8-C7	4.61	117.66	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	J	60	CHD	C1-C10-C5	4.57	114.31	107.75
22	J	60	CHD	C9-C8-C7	4.54	117.57	111.86
22	P	1271	CHD	C9-C8-C7	4.53	117.56	111.86
22	W	1060	CHD	C9-C8-C7	4.51	117.53	111.86
22	W	1060	CHD	C1-C10-C5	4.50	114.20	107.75
22	P	1271	CHD	C4-C3-C2	4.49	116.10	110.62
23	Z	1526	DMU	O7-C3-C4	4.47	121.21	109.48
23	M	526	DMU	O7-C3-C4	4.41	121.05	109.48
23	P	1272	DMU	O5-C6-C1	4.37	119.35	110.37
18	N	1522	TGL	CB9-CB8-CB7	-4.32	92.52	114.37
23	C	272	DMU	O5-C6-C1	4.31	119.23	110.37
23	M	526	DMU	O7-C10-C5	4.27	118.60	108.09
23	C	272	DMU	C8-C7-C5	4.22	118.24	110.83
22	P	1525	CHD	C1-C10-C5	4.22	113.80	107.75
23	M	526	DMU	O16-C6-C1	4.14	114.55	108.27
18	L	522	TGL	CB9-CB8-CB7	-4.12	93.57	114.37
22	W	1060	CHD	C18-C13-C12	-4.01	105.05	109.06
22	C	525	CHD	C14-C13-C12	-3.97	103.78	107.42
22	P	1271	CHD	C1-C10-C9	3.95	117.47	111.34
22	B	1086	CHD	C10-C9-C8	3.94	116.23	111.84
18	B	521	TGL	CG1-OG1-CA1	-3.92	102.77	117.12
23	Z	1526	DMU	O7-C10-C5	3.92	117.74	108.09
25	T	263	PEK	O03-C01-C02	3.89	119.60	108.40
25	G	1263	PEK	O03-C01-C02	3.88	119.58	108.40
23	P	1272	DMU	O7-C10-O1	3.87	120.89	110.69
22	B	1086	CHD	C15-C14-C8	-3.87	113.05	118.36
18	L	522	TGL	C15-CC9-CC8	3.82	133.67	114.37
22	W	1060	CHD	C5-C4-C3	3.82	118.47	112.71
23	C	272	DMU	O7-C10-O1	3.79	120.66	110.69
18	N	1522	TGL	C15-CC9-CC8	3.78	133.49	114.37
23	M	526	DMU	C10-O7-C3	3.76	126.90	117.98
22	B	1086	CHD	C16-C17-C13	-3.75	99.91	103.54
22	B	1086	CHD	C1-C10-C5	3.74	113.12	107.75
22	C	271	CHD	C1-C10-C9	3.74	117.14	111.34
18	L	522	TGL	C16-C15-CC9	3.73	133.24	114.37
22	J	60	CHD	C5-C4-C3	3.73	118.33	112.71
18	N	1522	TGL	C16-C15-CC9	3.72	133.16	114.37
18	L	522	TGL	CG2-OG2-CB1	3.69	126.64	117.80
18	N	1521	TGL	CG1-OG1-CA1	-3.69	103.63	117.12
25	G	1263	PEK	P-O11-C03	3.65	142.29	121.35
25	T	263	PEK	P-O11-C03	3.64	142.21	121.35
22	C	525	CHD	C1-C10-C5	3.62	112.94	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	272	DMU	C10-O7-C3	3.61	126.52	117.98
22	O	229	CHD	C15-C14-C8	-3.57	113.46	118.36
18	L	522	TGL	C11-C10-CB9	3.55	132.32	114.37
22	P	1271	CHD	C5-C6-C7	3.54	118.61	114.40
22	P	1525	CHD	C15-C14-C8	-3.52	113.53	118.36
22	C	271	CHD	C5-C6-C7	3.52	118.58	114.40
18	N	1522	TGL	CG2-OG2-CB1	3.52	126.22	117.80
18	N	1522	TGL	C11-C10-CB9	3.50	132.05	114.37
22	J	60	CHD	C1-C2-C3	3.49	115.10	110.48
22	P	1525	CHD	C13-C17-C20	3.47	123.69	119.48
23	C	272	DMU	O5-C6-O16	3.46	118.23	110.04
22	C	525	CHD	C15-C14-C8	-3.45	113.62	118.36
22	J	60	CHD	C6-C5-C4	3.45	115.16	111.23
22	C	271	CHD	C18-C13-C12	-3.44	105.61	109.06
22	W	1060	CHD	C6-C5-C4	3.43	115.14	111.23
23	Z	1526	DMU	O16-C6-C1	3.42	113.47	108.27
22	W	1060	CHD	C1-C2-C3	3.42	115.01	110.48
22	W	1060	CHD	C17-C13-C12	-3.39	114.62	117.67
17	N	516	HEA	C3C-C4C-NC	3.38	112.65	109.80
22	B	1086	CHD	C15-C14-C13	-3.38	100.26	103.54
22	C	271	CHD	C14-C8-C7	3.38	116.34	111.85
22	J	60	CHD	C17-C13-C12	-3.38	114.63	117.67
22	P	1271	CHD	C5-C4-C3	3.37	117.79	112.71
22	W	1060	CHD	C13-C14-C8	3.35	118.96	114.72
18	N	1521	TGL	CG3-OG3-CC1	3.34	129.31	117.12
22	J	60	CHD	C18-C13-C12	-3.30	105.75	109.06
22	J	60	CHD	C13-C14-C8	3.30	118.89	114.72
25	G	1263	PEK	C02-O01-C1	3.29	125.66	117.80
17	A	516	HEA	CMB-C2B-C3B	-3.26	123.98	130.28
26	P	1270	CDL	PA1-OA5-CA3	3.25	139.99	121.35
18	B	521	TGL	CG3-OG3-CC1	3.24	128.97	117.12
22	O	229	CHD	C1-C10-C5	3.24	112.40	107.75
22	O	229	CHD	C16-C17-C13	-3.24	100.40	103.54
18	N	1522	TGL	CC3-CC2-CC1	3.24	125.55	113.69
18	L	522	TGL	CC3-CC2-CC1	3.23	125.53	113.69
25	C	265	PEK	P-O11-C03	3.23	139.85	121.35
22	B	1086	CHD	C9-C11-C12	3.23	118.52	114.29
22	P	1271	CHD	C14-C8-C7	3.22	116.12	111.85
22	C	525	CHD	C10-C9-C8	3.21	115.42	111.84
17	A	516	HEA	C27-C19-C20	3.21	120.80	115.23
25	P	1265	PEK	P-O11-C03	3.21	139.72	121.35
22	W	1060	CHD	C9-C11-C12	3.20	118.48	114.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	1523	TGL	CG3-OG3-CC1	3.20	128.81	117.12
22	O	229	CHD	C9-C11-C12	3.19	118.47	114.29
18	N	1523	TGL	CG1-OG1-CA1	-3.19	105.45	117.12
26	C	270	CDL	PA1-OA5-CA3	3.19	139.64	121.35
23	C	272	DMU	C2-C3-C4	-3.18	103.87	110.93
22	J	60	CHD	C14-C8-C9	3.17	114.18	109.75
22	W	1060	CHD	C16-C15-C14	3.17	111.34	105.14
22	W	1060	CHD	C14-C8-C9	3.16	114.16	109.75
25	T	263	PEK	C02-O01-C1	3.16	125.36	117.80
23	Z	1526	DMU	O7-C10-O1	3.13	118.92	110.69
23	Z	1526	DMU	C10-O7-C3	3.12	125.38	117.98
18	A	523	TGL	CB3-CB2-CB1	3.12	125.11	113.69
22	B	1086	CHD	C1-C2-C3	3.10	114.59	110.48
18	A	523	TGL	CG3-OG3-CC1	3.10	128.43	117.12
23	P	1272	DMU	C2-C3-C4	-3.09	104.08	110.93
17	N	516	HEA	C27-C19-C20	3.08	120.58	115.23
22	J	60	CHD	C4-C5-C10	3.07	115.93	112.66
22	O	229	CHD	C5-C6-C7	3.06	118.03	114.40
23	M	526	DMU	C2-C3-C4	-3.04	104.18	110.93
25	C	264	PEK	O03-C21-C22	-3.04	102.58	111.83
26	C	270	CDL	OB6-CB5-C51	-3.03	104.92	111.48
21	B	230	PSC	C01-O03-C19	-3.03	106.05	117.12
23	P	1272	DMU	O5-C6-O16	3.02	117.18	110.04
22	J	60	CHD	C9-C11-C12	2.99	118.21	114.29
22	J	60	CHD	C16-C15-C14	2.98	110.98	105.14
18	A	523	TGL	CG1-OG1-CA1	-2.98	106.23	117.12
18	N	1523	TGL	OG2-CG2-CG3	2.97	119.02	108.34
17	N	516	HEA	C1D-ND-C4D	-2.97	101.69	105.21
22	C	525	CHD	C13-C17-C20	2.97	123.08	119.48
21	O	1230	PSC	C01-O03-C19	-2.94	106.36	117.12
23	Z	1526	DMU	C2-C3-C4	-2.94	104.40	110.93
26	T	1269	CDL	C23-C22-C21	2.94	129.21	114.37
26	T	1269	CDL	C22-C21-C20	2.91	129.08	114.37
25	P	1264	PEK	C3-C2-C1	-2.90	103.06	113.69
22	W	1060	CHD	C4-C5-C10	2.89	115.74	112.66
26	G	269	CDL	C22-C21-C20	2.89	128.96	114.37
22	P	1271	CHD	C15-C16-C17	2.88	110.79	105.14
26	G	269	CDL	C23-C22-C21	2.88	128.91	114.37
25	P	1264	PEK	O03-C21-C22	-2.88	103.07	111.83
22	C	525	CHD	C14-C8-C9	-2.86	105.75	109.75
22	C	271	CHD	C15-C16-C17	2.86	110.74	105.14
22	P	1271	CHD	C6-C5-C10	2.86	115.70	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1086	CHD	C17-C13-C14	2.84	102.96	100.11
18	N	1522	TGL	C13-C12-C11	2.84	128.73	114.37
25	C	265	PEK	C24-C23-C22	2.84	123.56	113.13
22	J	60	CHD	C15-C16-C17	2.83	110.68	105.14
22	C	271	CHD	C5-C4-C3	2.83	116.97	112.71
22	P	1525	CHD	C14-C8-C9	-2.82	105.81	109.75
22	O	229	CHD	C14-C13-C12	-2.82	104.84	107.42
22	B	1086	CHD	C18-C13-C12	-2.82	106.23	109.06
18	L	522	TGL	C20-CA9-CA8	2.79	128.48	114.37
22	C	271	CHD	C16-C15-C14	2.79	110.60	105.14
18	B	521	TGL	CG3-CG2-CG1	2.78	118.26	111.78
23	M	526	DMU	O7-C10-O1	2.78	118.00	110.69
22	P	1271	CHD	C18-C13-C12	-2.78	106.28	109.06
22	P	1271	CHD	C16-C15-C14	2.77	110.56	105.14
22	J	60	CHD	C19-C10-C5	-2.76	105.82	110.44
25	C	264	PEK	C3-C2-C1	-2.75	103.64	113.69
18	L	522	TGL	OG1-CG1-CG2	2.74	116.31	108.40
22	O	229	CHD	C15-C14-C13	-2.74	100.88	103.54
22	W	1060	CHD	C19-C10-C5	-2.74	105.86	110.44
25	P	1265	PEK	P-O12-C04	2.73	134.27	121.26
22	C	271	CHD	C6-C5-C10	2.71	115.54	112.66
22	J	60	CHD	C19-C10-C9	-2.70	107.54	111.18
18	L	522	TGL	CC4-CC3-CC2	2.70	123.06	113.13
22	O	229	CHD	C1-C2-C3	2.69	114.05	110.48
22	W	1060	CHD	C15-C16-C17	2.69	110.41	105.14
17	N	516	HEA	CHA-C4D-C3D	-2.69	120.86	124.77
22	C	271	CHD	C9-C11-C12	2.68	117.80	114.29
18	N	1523	TGL	CB3-CB2-CB1	2.67	123.47	113.69
26	P	1270	CDL	CB6-OB8-CB7	-2.67	107.37	117.12
18	N	1522	TGL	OG1-CG1-CG2	2.66	116.07	108.40
22	W	1060	CHD	C14-C13-C12	2.65	109.83	107.42
25	T	263	PEK	C03-C02-C01	2.64	117.95	111.78
26	P	1270	CDL	OB6-CB5-C51	-2.64	105.77	111.48
18	N	1522	TGL	C20-CA9-CA8	2.64	127.71	114.37
18	L	522	TGL	C13-C12-C11	2.64	127.70	114.37
18	A	523	TGL	OG2-CG2-CG3	2.64	117.80	108.34
17	N	516	HEA	CHA-C4D-ND	2.63	127.26	124.42
23	M	526	DMU	C10-O1-C9	2.63	118.86	113.72
17	N	516	HEA	C17-C18-C19	2.63	133.64	127.62
25	P	1265	PEK	C24-C23-C22	2.62	122.76	113.13
18	N	1521	TGL	CG3-CG2-CG1	2.62	117.89	111.78
17	A	516	HEA	C1D-ND-C4D	-2.61	102.11	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	1265	PEK	C11-C10-C9	2.61	124.87	112.02
17	N	516	HEA	CMB-C2B-C3B	-2.61	125.23	130.28
22	O	229	CHD	C5-C4-C3	2.60	116.63	112.71
22	P	1271	CHD	C1-C2-C3	2.59	113.92	110.48
25	C	265	PEK	C11-C10-C9	2.58	124.73	112.02
26	C	270	CDL	CB6-OB8-CB7	-2.57	107.71	117.12
22	C	271	CHD	C1-C2-C3	2.57	113.88	110.48
25	C	265	PEK	P-O12-C04	2.56	133.44	121.26
23	P	1272	DMU	C10-O7-C3	2.56	124.04	117.98
22	P	1271	CHD	C9-C11-C12	2.56	117.64	114.29
19	C	267	PGV	O01-C1-C2	-2.56	105.95	111.48
22	P	1525	CHD	C5-C6-C7	2.55	117.44	114.40
22	P	1525	CHD	C1-C2-C3	2.54	113.84	110.48
26	C	270	CDL	OB6-CB5-OB7	2.53	129.61	123.70
25	G	1263	PEK	C03-C02-C01	2.52	117.67	111.78
19	A	524	PGV	C02-O01-C1	2.52	123.83	117.80
17	A	516	HEA	C4A-C3A-C2A	-2.52	104.63	106.81
18	A	523	TGL	OG1-CG1-CG2	2.52	115.65	108.40
19	N	1524	PGV	C02-O01-C1	2.51	123.80	117.80
17	N	516	HEA	C2D-C1D-ND	2.51	112.72	109.84
19	N	1524	PGV	C3-C2-C1	-2.50	104.53	113.69
17	A	515	HEA	C26-C15-C16	2.50	119.56	115.23
18	N	1521	TGL	OG2-CG2-CG3	2.48	117.26	108.34
22	P	1525	CHD	C14-C13-C12	-2.48	105.14	107.42
22	O	229	CHD	C19-C10-C1	-2.48	104.36	108.31
18	N	1521	TGL	C10-CB9-CB8	2.47	126.85	114.37
19	N	1266	PGV	O01-C1-C2	-2.47	106.15	111.48
17	A	515	HEA	C2D-C1D-ND	2.44	112.64	109.84
18	N	1522	TGL	CC4-CC3-CC2	2.44	122.09	113.13
22	W	1060	CHD	C19-C10-C1	-2.42	104.46	108.31
22	P	1271	CHD	C18-C13-C14	-2.41	107.43	111.20
25	P	1264	PEK	O03-C21-O04	2.40	129.62	123.63
19	N	1266	PGV	O03-C01-C02	2.39	115.29	108.40
25	C	264	PEK	O03-C21-O04	2.38	129.58	123.63
25	C	265	PEK	O03-C01-C02	2.37	115.23	108.40
18	B	521	TGL	OG2-CG2-CG3	2.37	116.84	108.34
23	Z	1526	DMU	C10-O1-C9	2.36	118.33	113.72
22	O	229	CHD	C18-C13-C12	-2.35	106.70	109.06
19	C	267	PGV	C9-C10-C11	-2.35	99.45	112.60
18	B	521	TGL	C10-CB9-CB8	2.35	126.22	114.37
18	B	521	TGL	CA8-CA7-CA6	-2.34	102.52	114.37
22	B	1086	CHD	C14-C13-C12	-2.34	105.27	107.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	P	1265	PEK	O03-C01-C02	2.33	115.11	108.40
19	C	266	PGV	O01-C1-C2	-2.33	106.44	111.48
26	G	269	CDL	C19-C18-C17	2.32	126.11	114.37
17	N	515	HEA	C26-C15-C16	2.32	119.25	115.23
22	B	1086	CHD	C14-C8-C9	-2.31	106.52	109.75
19	A	524	PGV	C04-C05-C06	2.31	119.56	111.77
26	T	1269	CDL	OB8-CB6-CB4	2.31	115.07	108.40
25	T	263	PEK	P-O12-C04	2.31	132.26	121.26
19	N	1524	PGV	C04-C05-C06	2.31	119.54	111.77
19	P	1267	PGV	C9-C10-C11	-2.31	99.68	112.60
26	T	1269	CDL	OB8-CB7-C71	-2.31	104.80	111.83
22	O	229	CHD	C17-C13-C14	2.31	102.43	100.11
17	A	516	HEA	C4B-NB-C1B	-2.31	102.48	105.21
26	T	1269	CDL	C19-C18-C17	2.30	126.00	114.37
17	A	516	HEA	C2B-C1B-NB	2.30	112.56	109.90
22	B	1086	CHD	C19-C10-C1	-2.30	104.65	108.31
26	P	1270	CDL	OB6-CB5-OB7	2.30	129.08	123.70
26	G	269	CDL	C20-C19-C18	2.28	125.90	114.37
17	N	516	HEA	C26-C15-C16	2.28	119.18	115.23
19	A	524	PGV	C3-C2-C1	-2.27	105.38	113.69
18	N	1521	TGL	CA8-CA7-CA6	-2.27	102.91	114.37
22	W	1060	CHD	C14-C8-C7	2.26	114.84	111.85
25	G	1263	PEK	P-O12-C04	2.25	131.98	121.26
26	C	270	CDL	OA8-CA6-CA4	2.25	114.88	108.40
22	C	525	CHD	C5-C6-C7	2.24	117.07	114.40
22	J	60	CHD	C14-C13-C12	2.24	109.47	107.42
22	W	1060	CHD	C19-C10-C9	-2.24	108.16	111.18
22	P	1525	CHD	C9-C11-C12	2.24	117.23	114.29
23	P	1272	DMU	O1-C10-C5	2.24	114.97	110.37
19	N	1524	PGV	O01-C02-C03	2.24	116.37	108.34
22	J	60	CHD	C14-C8-C7	2.24	114.82	111.85
22	J	60	CHD	C19-C10-C1	-2.23	104.76	108.31
22	C	271	CHD	C18-C13-C14	-2.23	107.71	111.20
19	N	1524	PGV	C03-C02-C01	2.23	116.98	111.78
23	C	272	DMU	O1-C10-C5	2.22	114.93	110.37
22	P	1525	CHD	C10-C9-C8	2.22	114.31	111.84
17	A	516	HEA	C20-C19-C18	-2.22	116.19	121.17
17	A	516	HEA	CHA-C4D-C3D	-2.21	121.55	124.77
22	C	271	CHD	C9-C10-C5	2.20	111.58	108.51
18	L	522	TGL	OG2-CB1-OB1	2.20	128.85	123.70
22	C	525	CHD	C19-C10-C9	-2.19	108.24	111.18
17	N	516	HEA	C4C-C3C-C2C	-2.18	104.58	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1086	CHD	C5-C4-C3	2.18	116.00	112.71
18	N	1523	TGL	OG1-CG1-CG2	2.17	114.65	108.40
26	C	270	CDL	C52-C51-CB5	-2.15	105.82	113.69
26	T	1269	CDL	C20-C19-C18	2.14	125.20	114.37
17	N	516	HEA	C4B-NB-C1B	-2.14	102.67	105.21
17	A	516	HEA	C26-C15-C16	2.14	118.94	115.23
17	N	515	HEA	C12-C11-C3B	2.14	115.46	112.12
18	B	521	TGL	OG1-CG1-CG2	2.14	114.55	108.40
19	A	524	PGV	O01-C02-C03	2.13	115.98	108.34
19	A	524	PGV	C03-C02-C01	2.13	116.74	111.78
17	N	515	HEA	C2D-C1D-ND	2.13	112.28	109.84
26	G	269	CDL	OB8-CB6-CB4	2.13	114.52	108.40
17	N	515	HEA	C1D-C2D-C3D	-2.12	104.75	106.98
26	G	269	CDL	C79-C78-C77	2.12	125.11	114.37
22	P	1271	CHD	C2-C1-C10	2.12	116.32	112.74
26	T	1269	CDL	C79-C78-C77	2.12	125.07	114.37
17	N	515	HEA	OMA-CMA-C3A	-2.11	120.87	125.62
22	J	60	CHD	O7-C7-C6	2.10	115.08	109.86
17	A	515	HEA	C4A-C3A-C2A	-2.10	104.99	106.81
26	P	1270	CDL	OA8-CA6-CA4	2.10	114.44	108.40
18	N	1521	TGL	CA6-CA5-CA4	-2.10	103.78	114.37
22	O	229	CHD	C13-C17-C20	-2.09	116.95	119.48
19	P	1268	PGV	C02-O01-C1	-2.09	112.80	117.80
18	A	523	TGL	OG2-CG2-CG1	2.08	115.82	108.34
25	C	265	PEK	C03-C02-C01	2.08	116.64	111.78
17	N	516	HEA	C20-C19-C18	-2.08	116.50	121.17
18	L	522	TGL	C10-CB9-CB8	2.08	124.87	114.37
18	N	1522	TGL	C10-CB9-CB8	2.08	124.86	114.37
17	A	516	HEA	CMB-C2B-C1B	2.07	128.27	125.03
26	G	269	CDL	OB8-CB7-C71	-2.06	105.55	111.83
18	A	523	TGL	CA3-CA2-CA1	-2.05	106.17	113.69
18	N	1521	TGL	OG1-CG1-CG2	2.05	114.30	108.40
18	B	521	TGL	CA6-CA5-CA4	-2.05	104.02	114.37
19	P	1267	PGV	O01-C1-C2	-2.03	107.08	111.48
18	N	1522	TGL	OG2-CB1-OB1	2.03	128.46	123.70
18	L	522	TGL	CC7-CC6-CC5	2.03	124.63	114.37
18	A	523	TGL	CB4-CB3-CB2	2.03	120.57	113.13
22	P	1271	CHD	O12-C12-C13	2.02	114.44	111.02
17	A	516	HEA	C17-C18-C19	2.02	132.25	127.62

All (42) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
22	C	271	CHD	C12
22	C	271	CHD	C14
22	C	271	CHD	C9
22	C	271	CHD	C8
22	C	271	CHD	C3
22	J	60	CHD	C17
22	J	60	CHD	C12
22	J	60	CHD	C14
22	J	60	CHD	C9
22	J	60	CHD	C8
22	P	1271	CHD	C12
22	P	1271	CHD	C14
22	P	1271	CHD	C9
22	P	1271	CHD	C8
22	P	1271	CHD	C3
22	W	1060	CHD	C17
22	W	1060	CHD	C12
22	W	1060	CHD	C14
22	W	1060	CHD	C9
22	W	1060	CHD	C8
23	C	272	DMU	C10
23	C	272	DMU	C2
23	C	272	DMU	C4
23	C	272	DMU	C6
23	C	272	DMU	C5
23	C	272	DMU	C9
23	M	526	DMU	C4
23	M	526	DMU	C6
23	M	526	DMU	C2
23	M	526	DMU	C9
23	M	526	DMU	C5
23	P	1272	DMU	C10
23	P	1272	DMU	C2
23	P	1272	DMU	C4
23	P	1272	DMU	C6
23	P	1272	DMU	C5
23	P	1272	DMU	C9
23	Z	1526	DMU	C4
23	Z	1526	DMU	C6
23	Z	1526	DMU	C2
23	Z	1526	DMU	C9
23	Z	1526	DMU	C5

All (867) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	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
19	N	1524	PGV	C04-O12-P-O11
19	N	1524	PGV	C04-O12-P-O13
19	N	1524	PGV	C04-O12-P-O14
19	N	1524	PGV	C02-C03-O11-P
19	N	1524	PGV	C05-C04-O12-P
19	N	1524	PGV	C04-C05-C06-O06
19	N	1524	PGV	O05-C05-C06-O06
19	N	1524	PGV	O02-C1-O01-C02
19	N	1524	PGV	C20-C19-O03-C01
19	P	1268	PGV	C04-O12-P-O11
19	P	1268	PGV	C04-O12-P-O13
19	P	1268	PGV	C04-O12-P-O14
21	B	230	PSC	C03-O11-P-O14
21	B	230	PSC	C04-O12-P-O11
21	B	230	PSC	C04-O12-P-O14
21	B	230	PSC	O02-C1-O01-C02
21	O	1230	PSC	C03-O11-P-O14
21	O	1230	PSC	C04-O12-P-O11
21	O	1230	PSC	C04-O12-P-O14
21	O	1230	PSC	O02-C1-O01-C02
22	J	60	CHD	C16-C17-C20-C21
22	J	60	CHD	C16-C17-C20-C22
22	W	1060	CHD	C16-C17-C20-C21
22	W	1060	CHD	C16-C17-C20-C22
23	M	526	DMU	O5-C6-O16-C18
23	Z	1526	DMU	O5-C6-O16-C18
25	C	264	PEK	O12-C04-C05-N
25	C	265	PEK	C04-O12-P-O11
25	C	265	PEK	C04-O12-P-O13
25	C	265	PEK	C04-O12-P-O14

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Mol	Chain	Res	Type	Atoms
25	C	265	PEK	C11-C12-C13-C14
25	G	1263	PEK	C03-O11-P-O12
25	G	1263	PEK	C03-O11-P-O14
25	G	1263	PEK	O12-C04-C05-N
25	P	1264	PEK	O12-C04-C05-N
25	P	1265	PEK	C04-O12-P-O11
25	P	1265	PEK	C04-O12-P-O13
25	P	1265	PEK	C04-O12-P-O14
25	P	1265	PEK	C11-C12-C13-C14
25	T	263	PEK	C03-O11-P-O12
25	T	263	PEK	C03-O11-P-O14
25	T	263	PEK	O12-C04-C05-N
26	C	270	CDL	CA2-C1-CB2-OB2
26	C	270	CDL	CA2-OA2-PA1-OA3
26	C	270	CDL	CA2-OA2-PA1-OA4
26	C	270	CDL	CA2-OA2-PA1-OA5
26	C	270	CDL	CA4-CA3-OA5-PA1
26	C	270	CDL	C11-CA5-OA6-CA4
26	C	270	CDL	CB2-OB2-PB2-OB3
26	C	270	CDL	CB2-OB2-PB2-OB4
26	G	269	CDL	CB2-C1-CA2-OA2
26	G	269	CDL	CA2-OA2-PA1-OA3
26	G	269	CDL	C1-CB2-OB2-PB2
26	G	269	CDL	CB3-OB5-PB2-OB2
26	G	269	CDL	CB3-OB5-PB2-OB3
26	G	269	CDL	CB3-OB5-PB2-OB4
26	G	269	CDL	OB6-CB4-CB6-OB8
26	P	1270	CDL	CA2-C1-CB2-OB2
26	P	1270	CDL	CA2-OA2-PA1-OA3
26	P	1270	CDL	CA2-OA2-PA1-OA4
26	P	1270	CDL	CA2-OA2-PA1-OA5
26	P	1270	CDL	CA4-CA3-OA5-PA1
26	P	1270	CDL	C11-CA5-OA6-CA4
26	P	1270	CDL	CB2-OB2-PB2-OB3
26	P	1270	CDL	CB2-OB2-PB2-OB4
26	T	1269	CDL	CB2-C1-CA2-OA2
26	T	1269	CDL	CA2-OA2-PA1-OA3
26	T	1269	CDL	C1-CB2-OB2-PB2
26	T	1269	CDL	CB3-OB5-PB2-OB2
26	T	1269	CDL	CB3-OB5-PB2-OB3
26	T	1269	CDL	CB3-OB5-PB2-OB4
26	T	1269	CDL	OB6-CB4-CB6-OB8

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Mol	Chain	Res	Type	Atoms
19	A	524	PGV	O04-C19-O03-C01
19	N	1524	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
18	N	1521	TGL	OB1-CB1-OG2-CG2
26	C	270	CDL	OA7-CA5-OA6-CA4
26	G	269	CDL	C31-CA7-OA8-CA6
26	T	1269	CDL	C31-CA7-OA8-CA6
18	N	1521	TGL	CB2-CB1-OG2-CG2
19	A	524	PGV	C2-C1-O01-C02
19	N	1524	PGV	C2-C1-O01-C02
18	N	1521	TGL	OA1-CA1-OG1-CG1
18	A	523	TGL	CC2-CC1-OG3-CG3
18	B	521	TGL	CA2-CA1-OG1-CG1
18	N	1521	TGL	CA2-CA1-OG1-CG1
18	N	1523	TGL	CC2-CC1-OG3-CG3
26	P	1270	CDL	C57-C58-C59-C60
23	C	272	DMU	O6-C11-C9-O1
26	C	270	CDL	C80-C81-C82-C83
18	B	521	TGL	OA1-CA1-OG1-CG1
26	G	269	CDL	OA9-CA7-OA8-CA6
26	T	1269	CDL	OA9-CA7-OA8-CA6
26	P	1270	CDL	OA7-CA5-OA6-CA4
26	C	270	CDL	C40-C41-C42-C43
26	C	270	CDL	C57-C58-C59-C60
26	G	269	CDL	C20-C21-C22-C23
26	T	1269	CDL	C20-C21-C22-C23
26	T	1269	CDL	C77-C78-C79-C80
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	C40-C41-C42-C43
26	P	1270	CDL	C60-C61-C62-C63
26	P	1270	CDL	C80-C81-C82-C83
26	T	1269	CDL	C17-C18-C19-C20
26	T	1269	CDL	C57-C58-C59-C60
26	T	1269	CDL	C60-C61-C62-C63
26	G	269	CDL	O1-C1-CA2-OA2
26	T	1269	CDL	O1-C1-CA2-OA2
26	C	270	CDL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	C37-C38-C39-C40
18	B	521	TGL	CB2-CB1-OG2-CG2
26	C	270	CDL	C37-C38-C39-C40
26	C	270	CDL	C60-C61-C62-C63
26	G	269	CDL	C37-C38-C39-C40
26	G	269	CDL	C40-C41-C42-C43
26	G	269	CDL	C80-C81-C82-C83
26	T	1269	CDL	C80-C81-C82-C83
26	C	270	CDL	C77-C78-C79-C80
26	G	269	CDL	C60-C61-C62-C63
26	T	1269	CDL	C37-C38-C39-C40
18	B	521	TGL	C16-C15-CC9-CC8
18	N	1521	TGL	C16-C15-CC9-CC8
26	P	1270	CDL	C77-C78-C79-C80
26	T	1269	CDL	C40-C41-C42-C43
18	N	1522	TGL	OA1-CA1-OG1-CG1
26	C	270	CDL	C17-C18-C19-C20
26	P	1270	CDL	C17-C18-C19-C20
18	A	523	TGL	C21-C20-CA9-CA8
18	N	1522	TGL	C21-C20-CA9-CA8
18	N	1523	TGL	C21-C20-CA9-CA8
18	L	522	TGL	OA1-CA1-OG1-CG1
18	L	522	TGL	C21-C20-CA9-CA8
18	B	521	TGL	C21-C20-CA9-CA8
18	N	1521	TGL	C21-C20-CA9-CA8
18	A	523	TGL	C11-C10-CB9-CB8
18	A	523	TGL	C16-C15-CC9-CC8
18	N	1523	TGL	C11-C10-CB9-CB8
18	N	1523	TGL	C16-C15-CC9-CC8
18	L	522	TGL	C16-C15-CC9-CC8
18	N	1522	TGL	C16-C15-CC9-CC8
19	A	524	PGV	O12-C04-C05-C06
19	N	1524	PGV	O12-C04-C05-C06
18	L	522	TGL	CA2-CA1-OG1-CG1
18	N	1522	TGL	CA2-CA1-OG1-CG1
21	B	230	PSC	C20-C19-O03-C01
21	O	1230	PSC	C20-C19-O03-C01
18	B	521	TGL	C11-C10-CB9-CB8
18	L	522	TGL	C11-C10-CB9-CB8
18	N	1521	TGL	C11-C10-CB9-CB8
18	N	1522	TGL	C11-C10-CB9-CB8
23	M	526	DMU	O5-C4-C57-O61

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Mol	Chain	Res	Type	Atoms
23	C	272	DMU	C3-C4-C57-O61
23	C	272	DMU	C1-C6-O16-C18
19	A	524	PGV	O12-C04-C05-O05
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
26	T	1269	CDL	O1-C1-CB2-OB2
23	Z	1526	DMU	O5-C4-C57-O61
22	J	60	CHD	C13-C17-C20-C22
23	P	1272	DMU	O6-C11-C9-O1
22	W	1060	CHD	C13-C17-C20-C22
23	M	526	DMU	O6-C11-C9-C8
23	P	1272	DMU	C3-C4-C57-O61
19	A	524	PGV	C19-C20-C21-C22
19	N	1524	PGV	C19-C20-C21-C22
21	B	230	PSC	C1-C2-C3-C4
21	O	1230	PSC	C1-C2-C3-C4
21	B	230	PSC	O04-C19-O03-C01
21	B	230	PSC	C2-C1-O01-C02
21	O	1230	PSC	O04-C19-O03-C01
23	Z	1526	DMU	O6-C11-C9-C8
18	L	522	TGL	CC3-CC4-CC5-CC6
19	C	268	PGV	O12-C04-C05-O05
19	P	1268	PGV	O12-C04-C05-O05
18	N	1521	TGL	OC1-CC1-OG3-CG3
26	C	270	CDL	CB7-C71-C72-C73
26	G	269	CDL	CA5-C11-C12-C13
26	P	1270	CDL	CB7-C71-C72-C73
18	A	523	TGL	CA2-CA1-OG1-CG1
18	N	1523	TGL	CA2-CA1-OG1-CG1
19	P	1268	PGV	C2-C1-O01-C02
21	O	1230	PSC	C2-C1-O01-C02
18	B	521	TGL	OC1-CC1-OG3-CG3
23	P	1272	DMU	O5-C4-C57-O61
18	N	1522	TGL	CC3-CC4-CC5-CC6
17	A	516	HEA	C4D-C3D-CAD-CBD
26	T	1269	CDL	CA5-C11-C12-C13
26	G	269	CDL	OA7-CA5-OA6-CA4
26	T	1269	CDL	OA7-CA5-OA6-CA4
19	C	268	PGV	O12-C04-C05-C06
19	P	1268	PGV	O12-C04-C05-C06

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Mol	Chain	Res	Type	Atoms
26	G	269	CDL	CA2-C1-CB2-OB2
26	T	1269	CDL	CA2-C1-CB2-OB2
25	G	1263	PEK	C28-C29-C30-C31
21	B	230	PSC	C20-C21-C22-C23
25	T	263	PEK	C28-C29-C30-C31
22	J	60	CHD	C13-C17-C20-C21
22	C	271	CHD	C17-C20-C22-C23
22	P	1271	CHD	C17-C20-C22-C23
19	C	268	PGV	C2-C1-O01-C02
26	G	269	CDL	C11-CA5-OA6-CA4
26	T	1269	CDL	C11-CA5-OA6-CA4
21	B	230	PSC	C22-C23-C24-C25
19	C	268	PGV	O02-C1-O01-C02
19	P	1268	PGV	O02-C1-O01-C02
22	W	1060	CHD	C13-C17-C20-C21
23	P	1272	DMU	C1-C6-O16-C18
21	O	1230	PSC	C20-C21-C22-C23
25	C	264	PEK	C22-C21-O03-C01
19	P	1268	PGV	C04-C05-C06-O06
21	O	1230	PSC	C22-C23-C24-C25
23	Z	1526	DMU	O6-C11-C9-O1
23	P	1272	DMU	O5-C6-O16-C18
25	G	1263	PEK	O03-C01-C02-O01
25	T	263	PEK	O03-C01-C02-O01
25	P	1264	PEK	C22-C21-O03-C01
26	C	270	CDL	CA5-C11-C12-C13
26	G	269	CDL	C15-C16-C17-C18
18	A	523	TGL	OA1-CA1-OG1-CG1
18	N	1523	TGL	OA1-CA1-OG1-CG1
22	W	1060	CHD	C17-C20-C22-C23
18	N	1522	TGL	CB4-CB5-CB6-CB7
19	C	266	PGV	C23-C24-C25-C26
21	B	230	PSC	C2-C3-C4-C5
21	O	1230	PSC	C2-C3-C4-C5
21	O	1230	PSC	C29-C30-C31-C32
23	Z	1526	DMU	C25-C28-C31-C34
26	C	270	CDL	C16-C17-C18-C19
26	G	269	CDL	C72-C73-C74-C75
26	P	1270	CDL	C16-C17-C18-C19
19	A	524	PGV	C24-C25-C26-C27
19	P	1268	PGV	C24-C25-C26-C27
21	B	230	PSC	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
23	M	526	DMU	C25-C28-C31-C34
26	G	269	CDL	C13-C14-C15-C16
26	G	269	CDL	C56-C57-C58-C59
26	G	269	CDL	C58-C59-C60-C61
19	C	268	PGV	O05-C05-C06-O06
19	P	1268	PGV	O05-C05-C06-O06
18	L	522	TGL	CB4-CB5-CB6-CB7
26	T	1269	CDL	C72-C73-C74-C75
22	W	1060	CHD	C21-C20-C22-C23
26	P	1270	CDL	CA5-C11-C12-C13
19	C	268	PGV	C24-C25-C26-C27
26	C	270	CDL	C51-C52-C53-C54
26	T	1269	CDL	C13-C14-C15-C16
26	T	1269	CDL	C56-C57-C58-C59
26	T	1269	CDL	C58-C59-C60-C61
19	C	266	PGV	C6-C7-C8-C9
19	N	1524	PGV	C4-C5-C6-C7
25	G	1263	PEK	C27-C28-C29-C30
25	C	264	PEK	C1-C2-C3-C4
25	P	1264	PEK	C1-C2-C3-C4
19	N	1524	PGV	C24-C25-C26-C27
19	N	1266	PGV	C6-C7-C8-C9
25	T	263	PEK	C27-C28-C29-C30
18	N	1522	TGL	CC2-CC3-CC4-CC5
19	N	1266	PGV	C23-C24-C25-C26
19	P	1268	PGV	C22-C23-C24-C25
26	C	270	CDL	C59-C60-C61-C62
26	C	270	CDL	C73-C74-C75-C76
26	P	1270	CDL	C59-C60-C61-C62
18	L	522	TGL	CC2-CC3-CC4-CC5
22	C	271	CHD	C21-C20-C22-C23
19	A	524	PGV	C4-C5-C6-C7
26	P	1270	CDL	C51-C52-C53-C54
17	N	516	HEA	C4D-C3D-CAD-CBD
19	C	268	PGV	C22-C23-C24-C25
26	P	1270	CDL	C73-C74-C75-C76
25	C	264	PEK	O03-C01-C02-C03
25	P	1264	PEK	O03-C01-C02-C03
19	P	1268	PGV	C13-C14-C15-C16
25	P	1265	PEK	C16-C17-C18-C19
26	P	1270	CDL	C55-C56-C57-C58
25	T	263	PEK	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
19	C	268	PGV	C13-C14-C15-C16
25	C	265	PEK	C16-C17-C18-C19
25	T	263	PEK	C25-C26-C27-C28
26	C	270	CDL	C55-C56-C57-C58
26	T	1269	CDL	C15-C16-C17-C18
25	G	1263	PEK	C25-C26-C27-C28
22	J	60	CHD	C21-C20-C22-C23
22	P	1271	CHD	C21-C20-C22-C23
25	P	1265	PEK	C25-C26-C27-C28
26	G	269	CDL	C79-C80-C81-C82
26	T	1269	CDL	C79-C80-C81-C82
26	P	1270	CDL	C72-C73-C74-C75
25	C	265	PEK	C25-C26-C27-C28
22	J	60	CHD	C17-C20-C22-C23
26	C	270	CDL	C72-C73-C74-C75
25	C	264	PEK	O04-C21-O03-C01
25	P	1264	PEK	O04-C21-O03-C01
19	N	1524	PGV	C22-C23-C24-C25
26	C	270	CDL	OB7-CB5-OB6-CB4
25	P	1264	PEK	C31-C32-C33-C34
19	A	524	PGV	C22-C23-C24-C25
18	B	521	TGL	CC2-CC1-OG3-CG3
18	N	1521	TGL	CC2-CC1-OG3-CG3
23	P	1272	DMU	C25-C28-C31-C34
19	P	1268	PGV	C30-C31-C32-C33
19	C	268	PGV	C30-C31-C32-C33
19	P	1267	PGV	C22-C23-C24-C25
25	T	263	PEK	C29-C30-C31-C32
25	G	1263	PEK	C1-C2-C3-C4
19	A	524	PGV	C28-C29-C30-C31
19	C	267	PGV	C22-C23-C24-C25
19	N	1524	PGV	C28-C29-C30-C31
25	C	264	PEK	C31-C32-C33-C34
25	G	1263	PEK	C29-C30-C31-C32
26	C	270	CDL	C51-CB5-OB6-CB4
26	P	1270	CDL	C51-CB5-OB6-CB4
26	P	1270	CDL	OB7-CB5-OB6-CB4
25	C	264	PEK	C23-C24-C25-C26
26	C	270	CDL	C74-C75-C76-C77
26	P	1270	CDL	C75-C76-C77-C78
25	C	264	PEK	C25-C26-C27-C28
21	O	1230	PSC	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	C	266	PGV	C29-C30-C31-C32
21	O	1230	PSC	C04-C05-N-C08
23	P	1272	DMU	O6-C11-C9-C8
25	P	1264	PEK	C25-C26-C27-C28
19	N	1266	PGV	C29-C30-C31-C32
19	P	1268	PGV	C27-C28-C29-C30
19	C	268	PGV	C27-C28-C29-C30
25	P	1264	PEK	C23-C24-C25-C26
25	C	265	PEK	C29-C30-C31-C32
19	P	1267	PGV	C7-C8-C9-C10
23	C	272	DMU	C25-C28-C31-C34
26	C	270	CDL	C75-C76-C77-C78
26	P	1270	CDL	C13-C14-C15-C16
26	P	1270	CDL	C74-C75-C76-C77
19	C	268	PGV	C1-C2-C3-C4
19	P	1268	PGV	C1-C2-C3-C4
25	C	265	PEK	C21-C22-C23-C24
19	C	267	PGV	C7-C8-C9-C10
25	P	1264	PEK	C16-C17-C18-C19
26	C	270	CDL	C13-C14-C15-C16
19	C	268	PGV	C3-C4-C5-C6
25	P	1265	PEK	C29-C30-C31-C32
26	T	1269	CDL	C43-C44-C45-C46
25	C	265	PEK	C31-C32-C33-C34
26	C	270	CDL	C61-C62-C63-C64
25	C	264	PEK	C16-C17-C18-C19
25	P	1265	PEK	C31-C32-C33-C34
26	G	269	CDL	C43-C44-C45-C46
19	P	1268	PGV	C3-C4-C5-C6
26	P	1270	CDL	C61-C62-C63-C64
18	B	521	TGL	CB6-CB7-CB8-CB9
19	N	1266	PGV	C5-C6-C7-C8
26	C	270	CDL	C18-C19-C20-C21
26	P	1270	CDL	C18-C19-C20-C21
26	T	1269	CDL	C54-C55-C56-C57
25	P	1265	PEK	C21-C22-C23-C24
26	G	269	CDL	C82-C83-C84-C85
19	C	268	PGV	C25-C26-C27-C28
25	T	263	PEK	C34-C35-C36-C37
25	C	264	PEK	C22-C23-C24-C25
19	C	268	PGV	C11-C10-C9-C8
19	P	1268	PGV	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
19	P	1268	PGV	C12-C13-C14-C15
25	G	1263	PEK	C2-C3-C4-C5
25	G	1263	PEK	C15-C16-C17-C18
25	G	1263	PEK	C30-C31-C32-C33
25	G	1263	PEK	C34-C35-C36-C37
25	P	1264	PEK	C22-C23-C24-C25
26	T	1269	CDL	C82-C83-C84-C85
25	G	1263	PEK	C01-C02-C03-O11
25	T	263	PEK	C01-C02-C03-O11
26	C	270	CDL	OB5-CB3-CB4-CB6
26	P	1270	CDL	OB5-CB3-CB4-CB6
18	L	522	TGL	OB1-CB1-OG2-CG2
26	C	270	CDL	C32-C33-C34-C35
19	C	266	PGV	C5-C6-C7-C8
18	N	1521	TGL	CB6-CB7-CB8-CB9
26	G	269	CDL	C73-C74-C75-C76
26	P	1270	CDL	C71-C72-C73-C74
26	C	270	CDL	C71-C72-C73-C74
19	N	1266	PGV	C7-C8-C9-C10
19	C	266	PGV	C7-C8-C9-C10
19	P	1268	PGV	C25-C26-C27-C28
25	T	263	PEK	C30-C31-C32-C33
26	G	269	CDL	C54-C55-C56-C57
26	P	1270	CDL	C32-C33-C34-C35
26	T	1269	CDL	C73-C74-C75-C76
18	N	1522	TGL	OB1-CB1-OG2-CG2
25	G	1263	PEK	O03-C01-C02-C03
25	T	263	PEK	O03-C01-C02-C03
26	C	270	CDL	CB3-CB4-CB6-OB8
26	G	269	CDL	CB3-CB4-CB6-OB8
26	P	1270	CDL	CB3-CB4-CB6-OB8
26	T	1269	CDL	CB3-CB4-CB6-OB8
19	N	1524	PGV	C11-C10-C9-C8
21	O	1230	PSC	C13-C14-C15-C16
19	P	1267	PGV	C13-C14-C15-C16
26	P	1270	CDL	C78-C79-C80-C81
19	C	267	PGV	C13-C14-C15-C16
23	M	526	DMU	O6-C11-C9-O1
19	C	267	PGV	C25-C26-C27-C28
26	T	1269	CDL	C41-C42-C43-C44
26	C	270	CDL	C78-C79-C80-C81
26	G	269	CDL	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
19	P	1267	PGV	C25-C26-C27-C28
25	P	1264	PEK	C27-C28-C29-C30
26	G	269	CDL	C41-C42-C43-C44
25	C	264	PEK	C27-C28-C29-C30
25	P	1264	PEK	C24-C25-C26-C27
25	G	1263	PEK	C26-C27-C28-C29
25	T	263	PEK	C26-C27-C28-C29
26	G	269	CDL	C21-C22-C23-C24
26	T	1269	CDL	C33-C34-C35-C36
25	C	264	PEK	C24-C25-C26-C27
26	T	1269	CDL	C21-C22-C23-C24
19	A	524	PGV	C03-C02-O01-C1
19	N	1524	PGV	C03-C02-O01-C1
26	C	270	CDL	C42-C43-C44-C45
26	P	1270	CDL	C63-C64-C65-C66
19	A	524	PGV	C11-C10-C9-C8
19	A	524	PGV	C12-C13-C14-C15
19	C	267	PGV	C11-C10-C9-C8
19	C	268	PGV	C12-C13-C14-C15
19	N	1524	PGV	C12-C13-C14-C15
19	P	1267	PGV	C11-C10-C9-C8
21	B	230	PSC	C13-C14-C15-C16
25	T	263	PEK	C2-C3-C4-C5
17	A	515	HEA	C2A-C3A-CMA-OMA
26	P	1270	CDL	C42-C43-C44-C45
21	B	230	PSC	C11-C12-C13-C14
26	C	270	CDL	C63-C64-C65-C66
23	P	1272	DMU	C34-C37-C40-C43
21	O	1230	PSC	O03-C01-C02-O01
26	G	269	CDL	OA6-CA4-CA6-OA8
26	C	270	CDL	C44-C45-C46-C47
19	C	268	PGV	C28-C29-C30-C31
18	N	1522	TGL	CC2-CC1-OG3-CG3
26	G	269	CDL	C44-C45-C46-C47
26	T	1269	CDL	C44-C45-C46-C47
18	N	1523	TGL	CA9-C20-C21-C22
19	C	267	PGV	C15-C16-C17-C18
19	P	1267	PGV	C15-C16-C17-C18
23	Z	1526	DMU	C34-C37-C40-C43
18	A	523	TGL	CA9-C20-C21-C22
21	O	1230	PSC	C27-C28-C29-C30
26	P	1270	CDL	C44-C45-C46-C47

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Mol	Chain	Res	Type	Atoms
26	C	270	CDL	C84-C85-C86-C87
21	B	230	PSC	C27-C28-C29-C30
25	C	264	PEK	C32-C33-C34-C35
19	N	1524	PGV	C20-C21-C22-C23
22	C	271	CHD	C13-C17-C20-C22
26	P	1270	CDL	C84-C85-C86-C87
26	C	270	CDL	C36-C37-C38-C39
26	P	1270	CDL	C23-C24-C25-C26
19	P	1268	PGV	C5-C6-C7-C8
19	P	1268	PGV	C28-C29-C30-C31
26	P	1270	CDL	C36-C37-C38-C39
23	M	526	DMU	C19-C18-O16-C6
23	Z	1526	DMU	C19-C18-O16-C6
26	C	270	CDL	C23-C24-C25-C26
19	C	268	PGV	C5-C6-C7-C8
23	M	526	DMU	C34-C37-C40-C43
23	Z	1526	DMU	O16-C18-C19-C22
17	N	516	HEA	C2D-C3D-CAD-CBD
22	P	1271	CHD	C13-C17-C20-C22
26	C	270	CDL	C64-C65-C66-C67
18	N	1522	TGL	CC7-CC8-CC9-C15
19	P	1268	PGV	C14-C15-C16-C17
21	B	230	PSC	C3-C4-C5-C6
21	B	230	PSC	C24-C25-C26-C27
19	A	524	PGV	C01-C02-C03-O11
26	C	270	CDL	OA5-CA3-CA4-CA6
26	G	269	CDL	OA5-CA3-CA4-CA6
26	T	1269	CDL	OA5-CA3-CA4-CA6
25	P	1264	PEK	C32-C33-C34-C35
26	G	269	CDL	C53-C54-C55-C56
19	A	524	PGV	C20-C21-C22-C23
21	B	230	PSC	C04-C05-N-C08
26	P	1270	CDL	C64-C65-C66-C67
19	C	268	PGV	C31-C32-C33-C34
19	A	524	PGV	C5-C6-C7-C8
21	B	230	PSC	C23-C24-C25-C26
19	C	268	PGV	C14-C15-C16-C17
19	P	1268	PGV	C4-C5-C6-C7
21	O	1230	PSC	C3-C4-C5-C6
26	T	1269	CDL	C53-C54-C55-C56
22	C	271	CHD	C13-C17-C20-C21
22	P	1271	CHD	C13-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
19	N	1266	PGV	C30-C31-C32-C33
19	C	268	PGV	C4-C5-C6-C7
19	P	1268	PGV	C31-C32-C33-C34
23	Z	1526	DMU	C22-C25-C28-C31
17	A	516	HEA	C2D-C3D-CAD-CBD
23	M	526	DMU	C22-C25-C28-C31
19	C	268	PGV	C20-C19-O03-C01
18	L	522	TGL	CC7-CC8-CC9-C15
19	C	266	PGV	C30-C31-C32-C33
19	N	1524	PGV	C5-C6-C7-C8
25	P	1264	PEK	C26-C27-C28-C29
23	C	272	DMU	C34-C37-C40-C43
21	O	1230	PSC	C23-C24-C25-C26
21	O	1230	PSC	C24-C25-C26-C27
21	O	1230	PSC	C04-C05-N-C07
26	P	1270	CDL	OB5-CB3-CB4-OB6
18	L	522	TGL	CC2-CC1-OG3-CG3
25	C	264	PEK	C26-C27-C28-C29
19	A	524	PGV	C26-C27-C28-C29
19	C	268	PGV	C23-C24-C25-C26
21	B	230	PSC	O03-C01-C02-O01
26	C	270	CDL	OB6-CB4-CB6-OB8
26	P	1270	CDL	OB6-CB4-CB6-OB8
26	T	1269	CDL	OA6-CA4-CA6-OA8
21	B	230	PSC	C9-C10-C11-C12
21	O	1230	PSC	C9-C10-C11-C12
25	C	264	PEK	C5-C6-C7-C8
25	C	264	PEK	C9-C10-C11-C12
25	G	1263	PEK	C6-C7-C8-C9
25	P	1264	PEK	C5-C6-C7-C8
25	P	1264	PEK	C9-C10-C11-C12
25	T	263	PEK	C6-C7-C8-C9
25	P	1264	PEK	C17-C18-C19-C20
19	C	268	PGV	C15-C16-C17-C18
25	C	264	PEK	C17-C18-C19-C20
19	C	267	PGV	C20-C21-C22-C23
26	T	1269	CDL	C19-C20-C21-C22
19	P	1267	PGV	C20-C21-C22-C23
26	G	269	CDL	C19-C20-C21-C22
19	C	267	PGV	C23-C24-C25-C26
19	N	1266	PGV	C26-C27-C28-C29
26	P	1270	CDL	C39-C40-C41-C42

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Mol	Chain	Res	Type	Atoms
25	T	263	PEK	C15-C16-C17-C18
23	Z	1526	DMU	C3-C4-C57-O61
26	C	270	CDL	C34-C35-C36-C37
23	C	272	DMU	O5-C6-O16-C18
26	G	269	CDL	C14-C15-C16-C17
19	N	1524	PGV	C26-C27-C28-C29
19	P	1267	PGV	C24-C25-C26-C27
19	P	1267	PGV	C23-C24-C25-C26
19	P	1268	PGV	C23-C24-C25-C26
19	P	1268	PGV	C15-C16-C17-C18
26	C	270	CDL	C39-C40-C41-C42
26	P	1270	CDL	C34-C35-C36-C37
26	T	1269	CDL	C14-C15-C16-C17
23	M	526	DMU	O16-C18-C19-C22
25	P	1265	PEK	C32-C33-C34-C35
26	G	269	CDL	C35-C36-C37-C38
21	O	1230	PSC	C4-C5-C6-C7
19	N	1524	PGV	C01-C02-C03-O11
26	P	1270	CDL	OA5-CA3-CA4-CA6
18	B	521	TGL	C12-C13-C14-C29
19	C	267	PGV	C24-C25-C26-C27
26	G	269	CDL	CB5-C51-C52-C53
26	T	1269	CDL	CB5-C51-C52-C53
26	T	1269	CDL	C71-C72-C73-C74
26	G	269	CDL	C64-C65-C66-C67
21	B	230	PSC	C4-C5-C6-C7
23	P	1272	DMU	C22-C25-C28-C31
21	B	230	PSC	C31-C32-C33-C34
19	P	1268	PGV	C20-C19-O03-C01
25	T	263	PEK	C22-C21-O03-C01
18	N	1521	TGL	C12-C13-C14-C29
19	C	268	PGV	O04-C19-O03-C01
26	T	1269	CDL	C35-C36-C37-C38
26	C	270	CDL	C24-C25-C26-C27
26	P	1270	CDL	C24-C25-C26-C27
26	T	1269	CDL	C64-C65-C66-C67
19	C	266	PGV	C4-C5-C6-C7
19	N	1266	PGV	C4-C5-C6-C7
21	O	1230	PSC	C31-C32-C33-C34
26	G	269	CDL	C24-C25-C26-C27
25	T	263	PEK	O04-C21-O03-C01
19	N	1266	PGV	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
25	G	1263	PEK	C16-C17-C18-C19
19	P	1268	PGV	O04-C19-O03-C01
25	G	1263	PEK	O04-C21-O03-C01
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	266	PGV	C31-C32-C33-C34
21	B	230	PSC	O03-C01-C02-C03
21	O	1230	PSC	O03-C01-C02-C03
26	T	1269	CDL	C39-C40-C41-C42
26	G	269	CDL	C71-C72-C73-C74
18	N	1523	TGL	OG2-CG2-CG3-OG3
19	N	1524	PGV	O03-C01-C02-O01
26	T	1269	CDL	C24-C25-C26-C27
26	C	270	CDL	C38-C39-C40-C41
21	B	230	PSC	C14-C15-C16-C17
25	C	265	PEK	C32-C33-C34-C35
21	B	230	PSC	C04-C05-N-C07
21	O	1230	PSC	C14-C15-C16-C17
25	G	1263	PEK	C22-C21-O03-C01
25	G	1263	PEK	C31-C32-C33-C34
22	C	271	CHD	C16-C17-C20-C22
26	P	1270	CDL	C38-C39-C40-C41
23	C	272	DMU	C22-C25-C28-C31
25	T	263	PEK	C31-C32-C33-C34
26	P	1270	CDL	C56-C57-C58-C59
19	C	268	PGV	C26-C27-C28-C29
22	P	1271	CHD	C16-C17-C20-C22
26	P	1270	CDL	C11-C12-C13-C14
19	P	1268	PGV	C01-C02-C03-O11
19	P	1268	PGV	C26-C27-C28-C29
26	P	1270	CDL	C76-C77-C78-C79
26	C	270	CDL	C11-C12-C13-C14
26	C	270	CDL	C56-C57-C58-C59
26	T	1269	CDL	C31-C32-C33-C34
18	N	1521	TGL	CG2-CG3-OG3-CC1
26	T	1269	CDL	CB4-CB3-OB5-PB2
25	T	263	PEK	C16-C17-C18-C19
26	C	270	CDL	C76-C77-C78-C79
25	T	263	PEK	O01-C02-C03-O11
23	Z	1526	DMU	C28-C31-C34-C37
19	C	266	PGV	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
21	O	1230	PSC	C04-C05-N-C06
25	P	1264	PEK	C29-C30-C31-C32
26	T	1269	CDL	C12-C13-C14-C15
17	A	515	HEA	C4A-C3A-CMA-OMA
17	N	515	HEA	C4A-C3A-CMA-OMA
26	G	269	CDL	C31-C32-C33-C34
26	G	269	CDL	C39-C40-C41-C42
18	A	523	TGL	OG2-CG2-CG3-OG3
19	A	524	PGV	O03-C01-C02-O01
25	C	264	PEK	O03-C01-C02-O01
25	P	1264	PEK	O03-C01-C02-O01
19	A	524	PGV	O03-C01-C02-C03
19	N	1524	PGV	O03-C01-C02-C03
26	G	269	CDL	CA3-CA4-CA6-OA8
26	T	1269	CDL	CA3-CA4-CA6-OA8
22	C	271	CHD	C16-C17-C20-C21
22	P	1271	CHD	C16-C17-C20-C21
18	N	1522	TGL	CC5-CC6-CC7-CC8
25	P	1265	PEK	C30-C31-C32-C33
21	B	230	PSC	C03-O11-P-O12
21	B	230	PSC	C03-O11-P-O13
21	B	230	PSC	C04-O12-P-O13
21	B	230	PSC	C04-C05-N-C06
21	O	1230	PSC	C03-O11-P-O12
21	O	1230	PSC	C03-O11-P-O13
21	O	1230	PSC	C04-O12-P-O13
25	G	1263	PEK	C03-O11-P-O13
25	T	263	PEK	C03-O11-P-O13
26	C	270	CDL	CA3-OA5-PA1-OA3
26	C	270	CDL	CB2-OB2-PB2-OB5
26	P	1270	CDL	CA3-OA5-PA1-OA3
26	P	1270	CDL	CB2-OB2-PB2-OB5
19	C	267	PGV	C02-C03-O11-P
19	P	1267	PGV	C02-C03-O11-P
25	G	1263	PEK	C02-C03-O11-P
25	T	263	PEK	C02-C03-O11-P
26	G	269	CDL	CB4-CB3-OB5-PB2
25	G	1263	PEK	C21-C22-C23-C24
19	P	1267	PGV	C31-C32-C33-C34
26	G	269	CDL	C12-C13-C14-C15
25	C	265	PEK	C30-C31-C32-C33
19	C	267	PGV	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	B	230	PSC	C03-C02-O01-C1
21	O	1230	PSC	C03-C02-O01-C1
19	C	267	PGV	C31-C32-C33-C34
17	N	515	HEA	C2A-C3A-CMA-OMA
19	C	268	PGV	C01-C02-C03-O11
18	B	521	TGL	CG2-CG3-OG3-CC1
26	G	269	CDL	CB7-C71-C72-C73
19	C	268	PGV	O01-C02-C03-O11
19	P	1268	PGV	O01-C02-C03-O11
25	G	1263	PEK	O01-C02-C03-O11
23	P	1272	DMU	C4-C3-O7-C10
25	T	263	PEK	C21-C22-C23-C24
19	C	268	PGV	O03-C01-C02-O01
19	P	1268	PGV	O03-C01-C02-O01
21	O	1230	PSC	C21-C22-C23-C24
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	P	1267	PGV	C11-C12-C13-C14
25	C	265	PEK	C3-C4-C5-C6
25	P	1265	PEK	C3-C4-C5-C6
26	T	1269	CDL	CB7-C71-C72-C73
18	L	522	TGL	CC5-CC6-CC7-CC8
21	B	230	PSC	C21-C22-C23-C24
23	M	526	DMU	C28-C31-C34-C37
26	P	1270	CDL	C22-C23-C24-C25
19	C	267	PGV	C14-C15-C16-C17
26	G	269	CDL	C38-C39-C40-C41
19	P	1267	PGV	C14-C15-C16-C17
25	G	1263	PEK	C32-C33-C34-C35
23	M	526	DMU	C3-C4-C57-O61
26	C	270	CDL	C22-C23-C24-C25
22	P	1271	CHD	C22-C23-C24-O25
22	C	271	CHD	C22-C23-C24-O25
25	T	263	PEK	C32-C33-C34-C35
25	C	265	PEK	C35-C36-C37-C38
22	C	271	CHD	C22-C23-C24-O26
22	O	229	CHD	C22-C23-C24-O25
25	C	264	PEK	C35-C36-C37-C38
22	P	1271	CHD	C22-C23-C24-O26
25	P	1265	PEK	C17-C18-C19-C20
25	P	1265	PEK	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
17	A	515	HEA	CAD-CBD-CGD-O1D
17	N	516	HEA	CAA-CBA-CGA-O1A
22	B	1086	CHD	C22-C23-C24-O25
26	T	1269	CDL	C38-C39-C40-C41
25	P	1264	PEK	C3-C4-C5-C6
25	C	265	PEK	O03-C01-C02-O01
17	N	515	HEA	CAD-CBD-CGD-O1D
26	C	270	CDL	C15-C16-C17-C18
17	A	516	HEA	CAA-CBA-CGA-O1A
26	P	1270	CDL	C15-C16-C17-C18
25	C	264	PEK	C3-C4-C5-C6
18	B	521	TGL	C10-C11-C12-C13
25	C	265	PEK	C17-C18-C19-C20
19	N	1266	PGV	C25-C26-C27-C28
25	C	265	PEK	C26-C27-C28-C29
26	C	270	CDL	C52-C53-C54-C55
17	A	516	HEA	CAA-CBA-CGA-O2A
19	C	268	PGV	C02-C03-O11-P
26	C	270	CDL	C1-CA2-OA2-PA1
26	P	1270	CDL	C1-CA2-OA2-PA1
18	N	1522	TGL	OC1-CC1-OG3-CG3
17	A	515	HEA	CAD-CBD-CGD-O2D
18	N	1522	TGL	CC6-CC7-CC8-CC9
22	B	1086	CHD	C22-C23-C24-O26
17	N	516	HEA	CAD-CBD-CGD-O2D
17	N	515	HEA	C26-C15-C16-C17
17	N	515	HEA	CAD-CBD-CGD-O2D
23	C	272	DMU	C18-C19-C22-C25
17	A	516	HEA	CAD-CBD-CGD-O2D
18	N	1521	TGL	C10-C11-C12-C13
22	J	60	CHD	C22-C23-C24-O25
25	P	1265	PEK	O03-C01-C02-O01
17	N	516	HEA	CAA-CBA-CGA-O2A
19	C	266	PGV	O03-C19-C20-C21
25	G	1263	PEK	C14-C15-C16-C17
19	P	1268	PGV	C02-C03-O11-P
22	W	1060	CHD	C22-C23-C24-O25
23	C	272	DMU	C4-C3-O7-C10
18	L	522	TGL	OG2-CB1-CB2-CB3
19	C	267	PGV	C29-C30-C31-C32
19	C	266	PGV	C9-C10-C11-C12
19	N	1266	PGV	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
21	B	230	PSC	C7-C8-C9-C10
21	O	1230	PSC	C7-C8-C9-C10
25	P	1265	PEK	C26-C27-C28-C29
22	O	229	CHD	C22-C23-C24-O26
17	A	516	HEA	CAD-CBD-CGD-O1D
17	N	516	HEA	CAD-CBD-CGD-O1D
19	A	524	PGV	C25-C26-C27-C28
18	N	1522	TGL	OG2-CB1-CB2-CB3
18	A	523	TGL	CG1-CG2-OG2-CB1
18	N	1523	TGL	CG1-CG2-OG2-CB1
19	P	1267	PGV	C29-C30-C31-C32
19	N	1266	PGV	C9-C10-C11-C12
25	G	1263	PEK	C3-C4-C5-C6
25	T	263	PEK	C3-C4-C5-C6
18	L	522	TGL	CC6-CC7-CC8-CC9
17	N	515	HEA	C14-C15-C16-C17
19	C	266	PGV	C11-C12-C13-C14
19	P	1267	PGV	C9-C10-C11-C12
25	T	263	PEK	C14-C15-C16-C17
19	C	267	PGV	C05-C04-O12-P
19	N	1266	PGV	O03-C19-C20-C21
19	C	267	PGV	C1-C2-C3-C4
17	N	516	HEA	C26-C15-C16-C17
26	P	1270	CDL	C12-C11-CA5-OA6
17	A	515	HEA	C14-C15-C16-C17
25	P	1264	PEK	C35-C36-C37-C38
26	P	1270	CDL	C52-C53-C54-C55
21	B	230	PSC	C15-C16-C17-C18
26	C	270	CDL	C82-C83-C84-C85
19	C	267	PGV	C9-C10-C11-C12
19	N	1524	PGV	C9-C10-C11-C12
18	L	522	TGL	OG3-CC1-CC2-CC3
21	B	230	PSC	C01-C02-C03-O11
21	O	1230	PSC	C01-C02-C03-O11
26	G	269	CDL	C78-C79-C80-C81
18	N	1522	TGL	OG3-CC1-CC2-CC3
26	G	269	CDL	CA7-C31-C32-C33
17	A	515	HEA	C2C-C3C-CAC-CBC
25	C	264	PEK	O01-C1-C2-C3
19	A	524	PGV	C9-C10-C11-C12
18	A	523	TGL	OG2-CB1-CB2-CB3
26	C	270	CDL	C12-C11-CA5-OA6

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Mol	Chain	Res	Type	Atoms
22	C	525	CHD	C22-C23-C24-O26
19	C	266	PGV	C25-C26-C27-C28
21	B	230	PSC	O03-C19-C20-C21
21	O	1230	PSC	O03-C19-C20-C21
21	O	1230	PSC	C15-C16-C17-C18
19	N	1524	PGV	O01-C1-C2-C3
26	T	1269	CDL	C36-C37-C38-C39
25	P	1264	PEK	O01-C1-C2-C3
26	C	270	CDL	C32-C31-CA7-OA8
26	P	1270	CDL	C32-C31-CA7-OA8
22	P	1525	CHD	C22-C23-C24-O26
17	A	515	HEA	C26-C15-C16-C17
18	N	1523	TGL	OG2-CB1-CB2-CB3
19	A	524	PGV	O01-C1-C2-C3
22	J	60	CHD	C22-C23-C24-O26
19	N	1524	PGV	C25-C26-C27-C28
19	A	524	PGV	C2-C3-C4-C5
26	P	1270	CDL	C82-C83-C84-C85
21	O	1230	PSC	O01-C1-C2-C3
26	T	1269	CDL	C78-C79-C80-C81
23	M	526	DMU	C19-C22-C25-C28
17	A	516	HEA	C26-C15-C16-C17
21	B	230	PSC	O01-C1-C2-C3
26	C	270	CDL	C52-C51-CB5-OB6
18	N	1523	TGL	OG1-CG1-CG2-OG2
22	W	1060	CHD	C22-C23-C24-O26
25	T	263	PEK	C33-C34-C35-C36
19	P	1267	PGV	C1-C2-C3-C4
26	G	269	CDL	C36-C37-C38-C39
21	B	230	PSC	C26-C27-C28-C29
26	P	1270	CDL	C14-C15-C16-C17
26	C	270	CDL	CB2-C1-CA2-OA2
26	P	1270	CDL	C52-C51-CB5-OB6
18	B	521	TGL	CG1-CG2-OG2-CB1
21	O	1230	PSC	C26-C27-C28-C29
26	G	269	CDL	C11-C12-C13-C14
18	N	1521	TGL	OG1-CA1-CA2-CA3
19	N	1524	PGV	C2-C3-C4-C5
21	B	230	PSC	O04-C19-C20-C21
26	C	270	CDL	C14-C15-C16-C17
26	T	1269	CDL	CA7-C31-C32-C33
25	C	264	PEK	O02-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
18	N	1521	TGL	C13-C14-C29-C30
18	B	521	TGL	OG1-CA1-CA2-CA3
22	C	525	CHD	C22-C23-C24-O25
22	P	1525	CHD	C22-C23-C24-O25
25	G	1263	PEK	C33-C34-C35-C36
21	O	1230	PSC	O04-C19-C20-C21
25	P	1264	PEK	O02-C1-C2-C3
26	P	1270	CDL	C32-C31-CA7-OA9
18	B	521	TGL	C13-C14-C29-C30
18	A	523	TGL	OC1-CC1-CC2-CC3
18	N	1523	TGL	OC1-CC1-CC2-CC3
26	C	270	CDL	C32-C31-CA7-OA9
18	N	1522	TGL	CB5-CB6-CB7-CB8
19	N	1524	PGV	O02-C1-C2-C3
21	B	230	PSC	O02-C1-C2-C3
21	O	1230	PSC	O02-C1-C2-C3
26	T	1269	CDL	C22-C23-C24-C25
26	P	1270	CDL	CB2-C1-CA2-OA2
19	A	524	PGV	O02-C1-C2-C3
26	T	1269	CDL	OB9-CB7-OB8-CB6
26	T	1269	CDL	C11-C12-C13-C14
26	G	269	CDL	C22-C23-C24-C25
21	B	230	PSC	C12-C13-C14-C15
21	O	1230	PSC	C12-C13-C14-C15
18	A	523	TGL	C21-C22-C23-C24
18	L	522	TGL	OC1-CC1-CC2-CC3

There are no ring outliers.

36 monomers are involved in 232 short contacts:

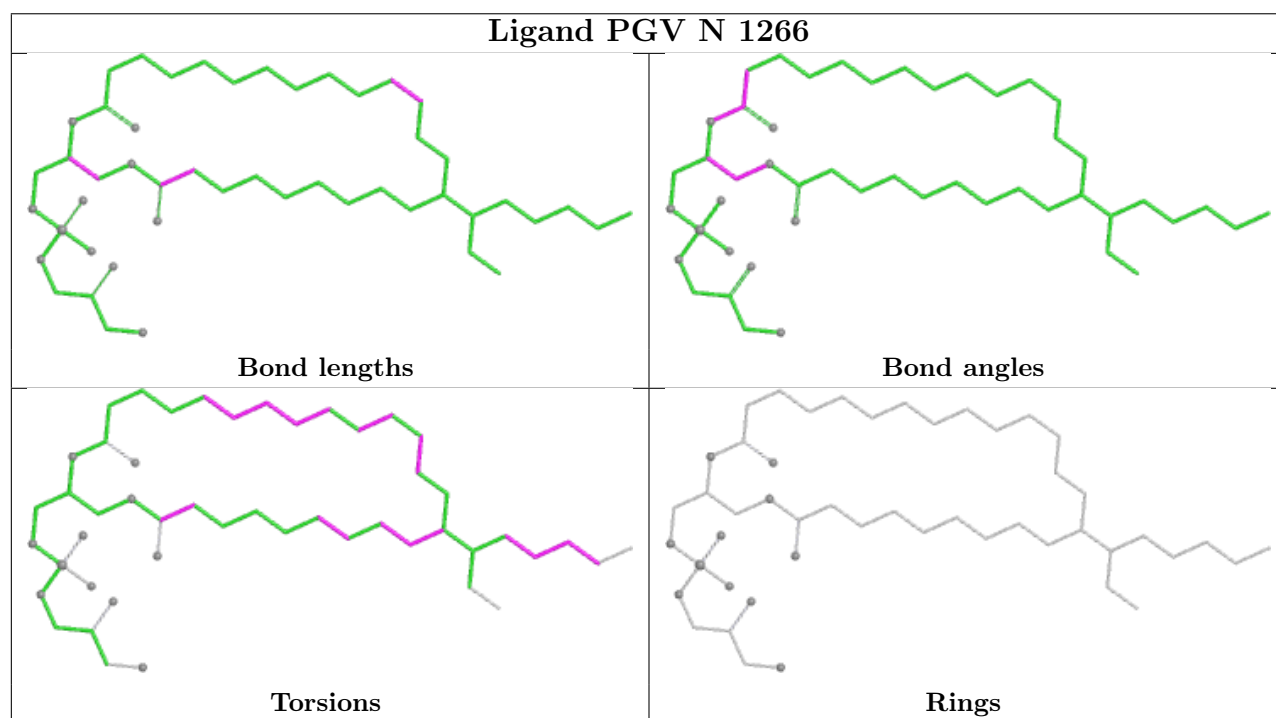
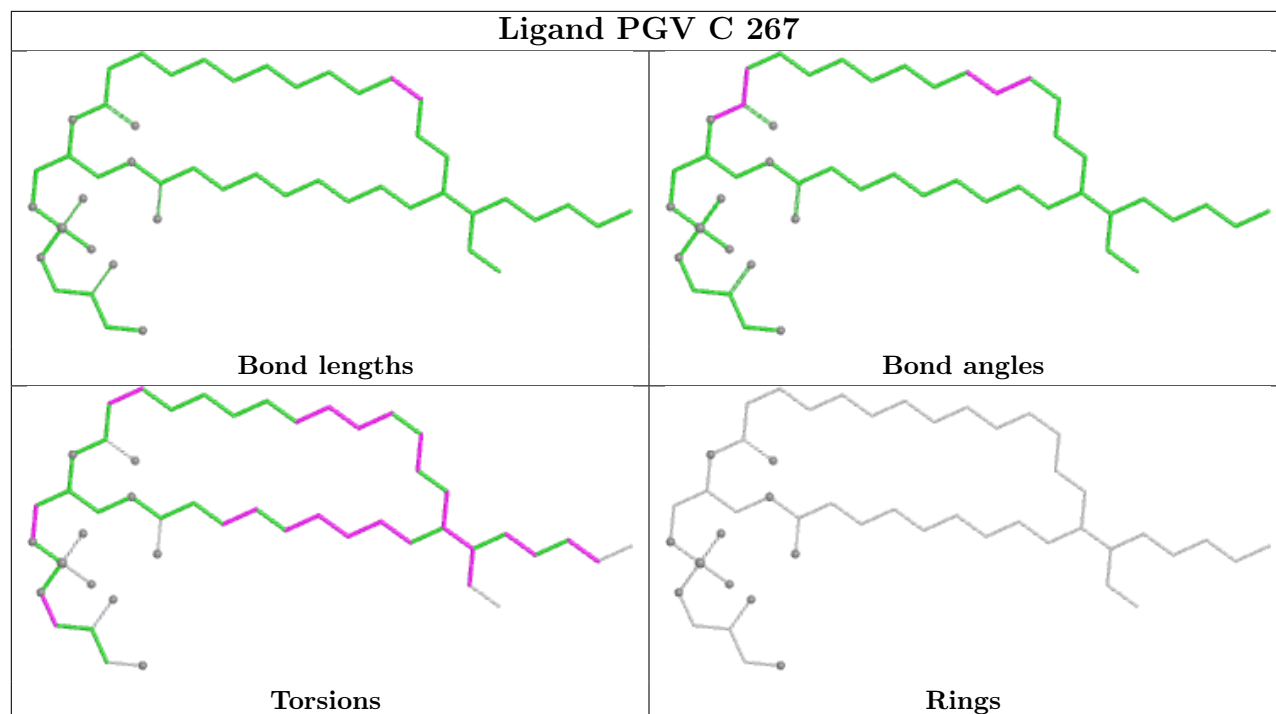
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	267	PGV	5	0
23	C	272	DMU	3	0
21	B	230	PSC	11	0
22	B	1086	CHD	1	0
21	O	1230	PSC	15	0
22	P	1271	CHD	1	0
18	A	523	TGL	4	0
19	N	1524	PGV	8	0
17	N	516	HEA	1	0
25	C	265	PEK	7	0
17	A	516	HEA	1	0

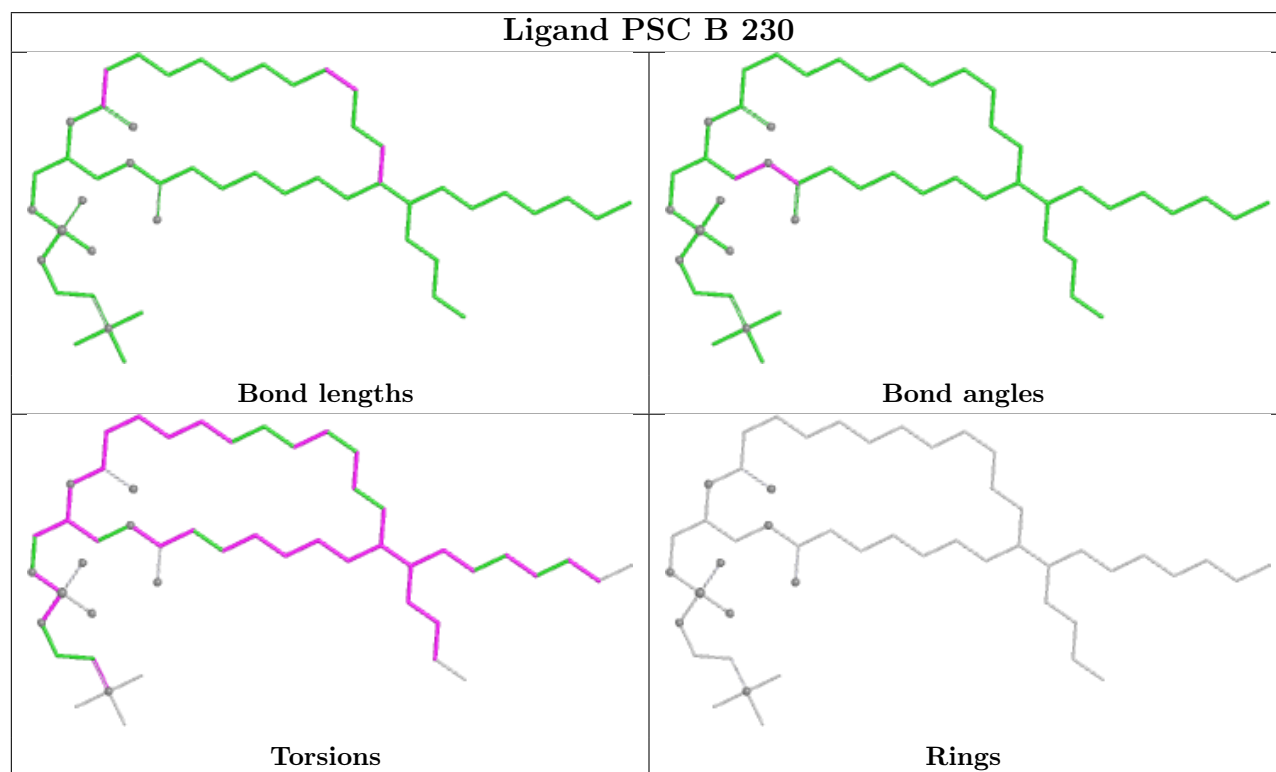
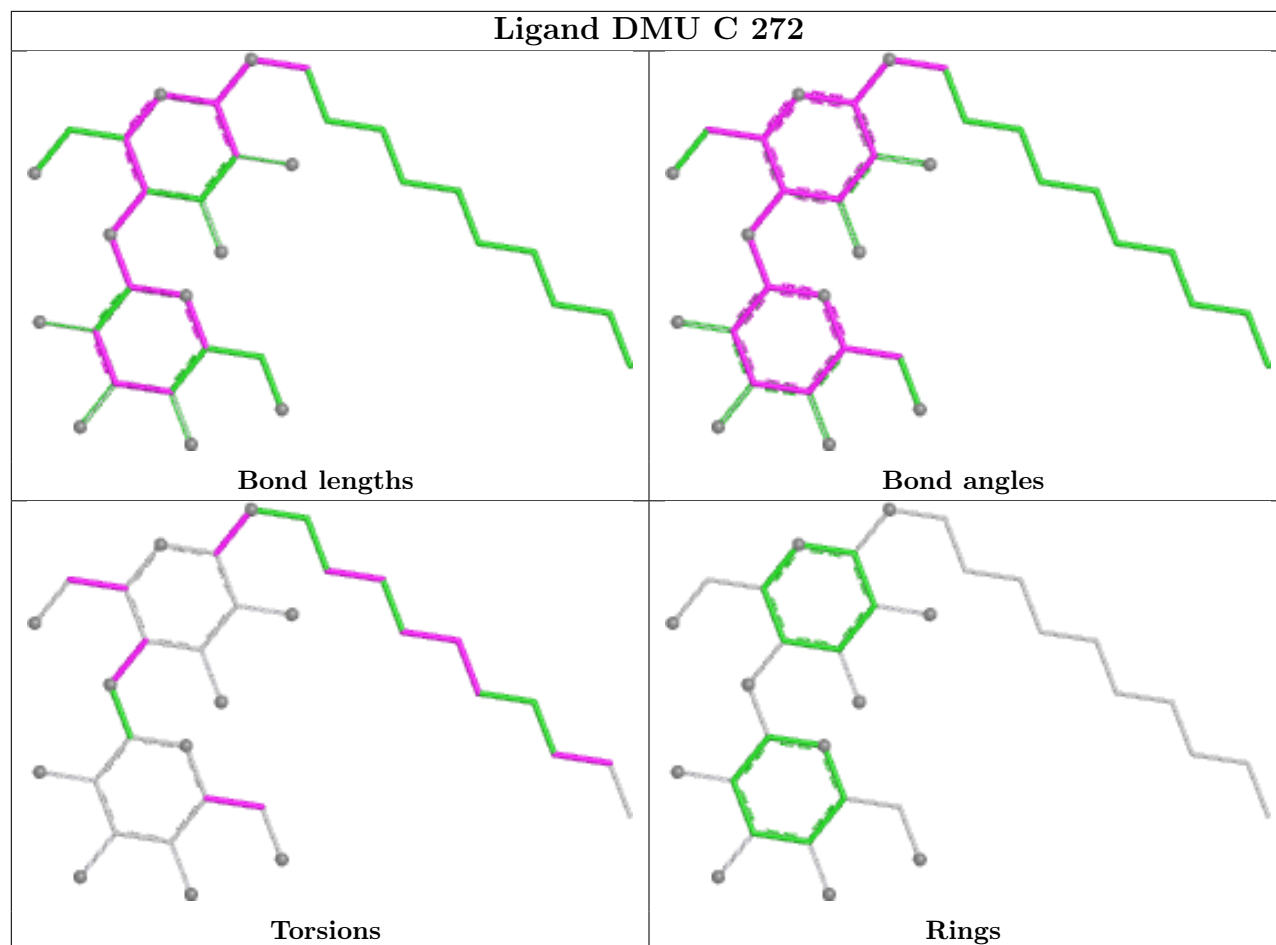
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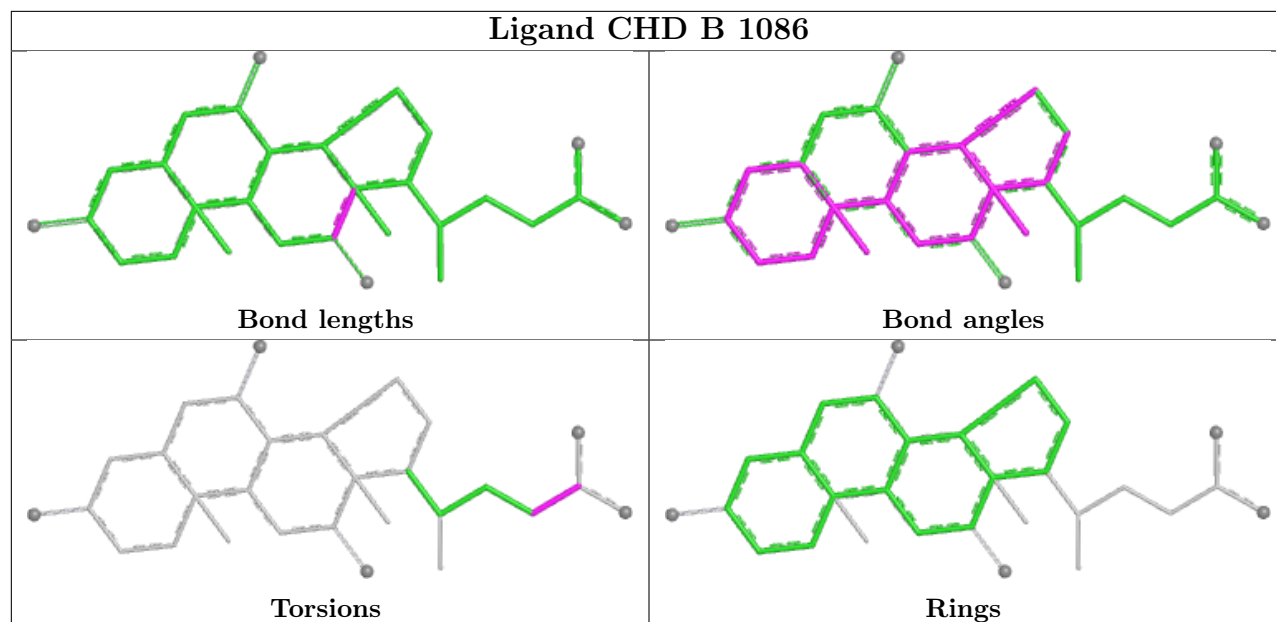
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	P	1268	PGV	1	0
23	P	1272	DMU	8	0
26	P	1270	CDL	15	0
25	G	1263	PEK	10	0
22	C	271	CHD	3	0
25	P	1264	PEK	6	0
18	B	521	TGL	7	0
26	C	270	CDL	12	0
26	T	1269	CDL	19	0
19	C	268	PGV	1	0
25	T	263	PEK	6	0
22	O	229	CHD	1	0
26	G	269	CDL	18	0
18	N	1522	TGL	14	0
22	J	60	CHD	2	0
25	C	264	PEK	4	0
25	P	1265	PEK	7	0
22	W	1060	CHD	4	0
17	A	515	HEA	2	0
17	N	515	HEA	3	0
18	N	1523	TGL	4	0
18	L	522	TGL	20	0
19	A	524	PGV	7	0
18	N	1521	TGL	9	0
19	P	1267	PGV	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

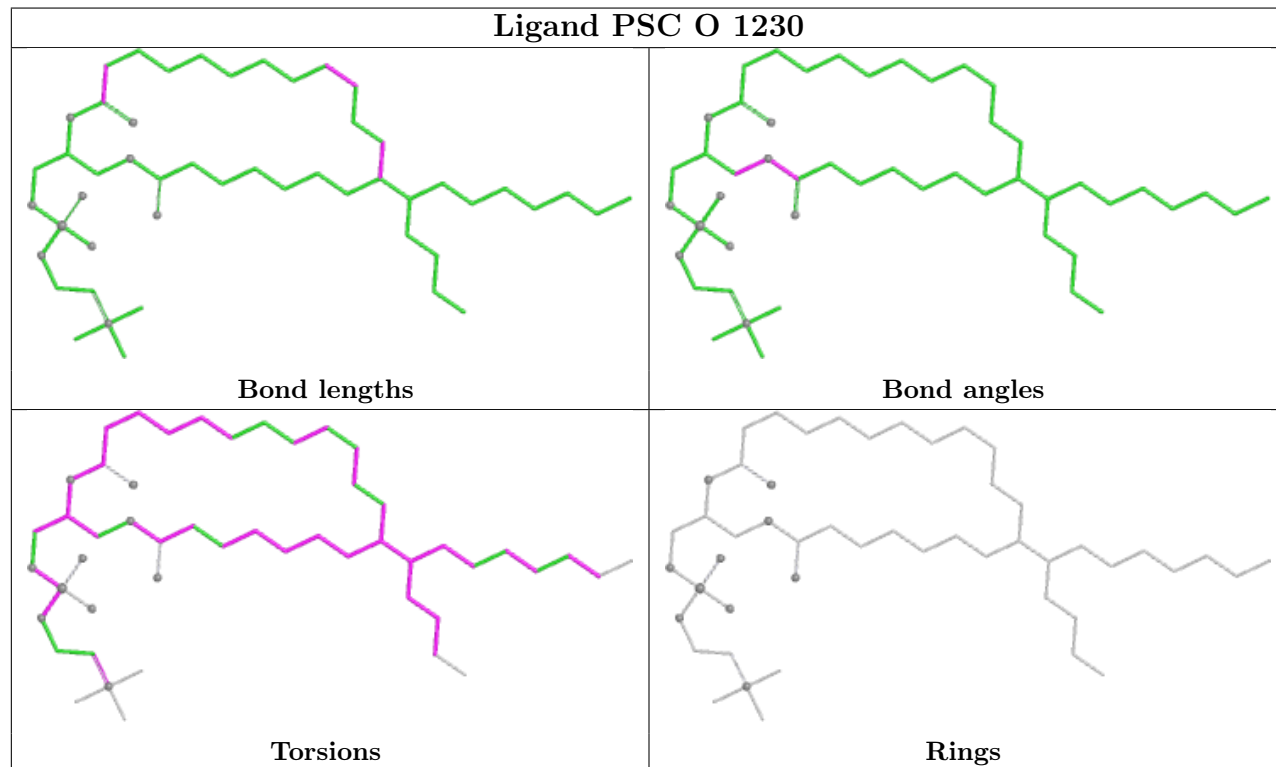




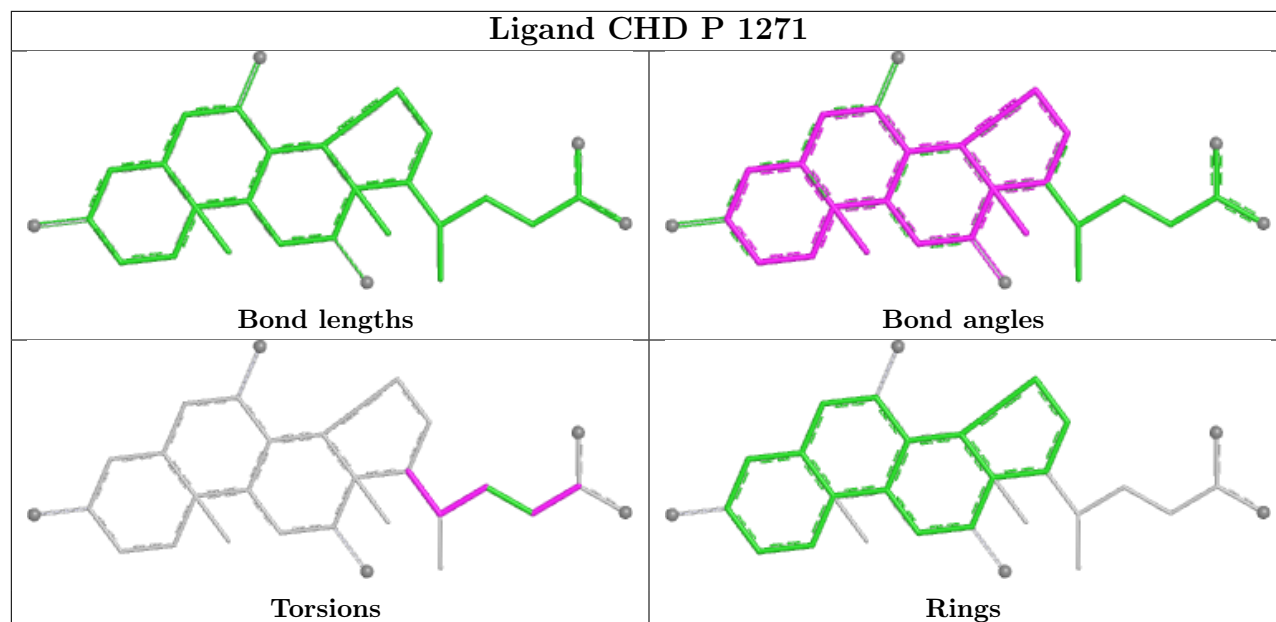
Ligand CHD B 1086



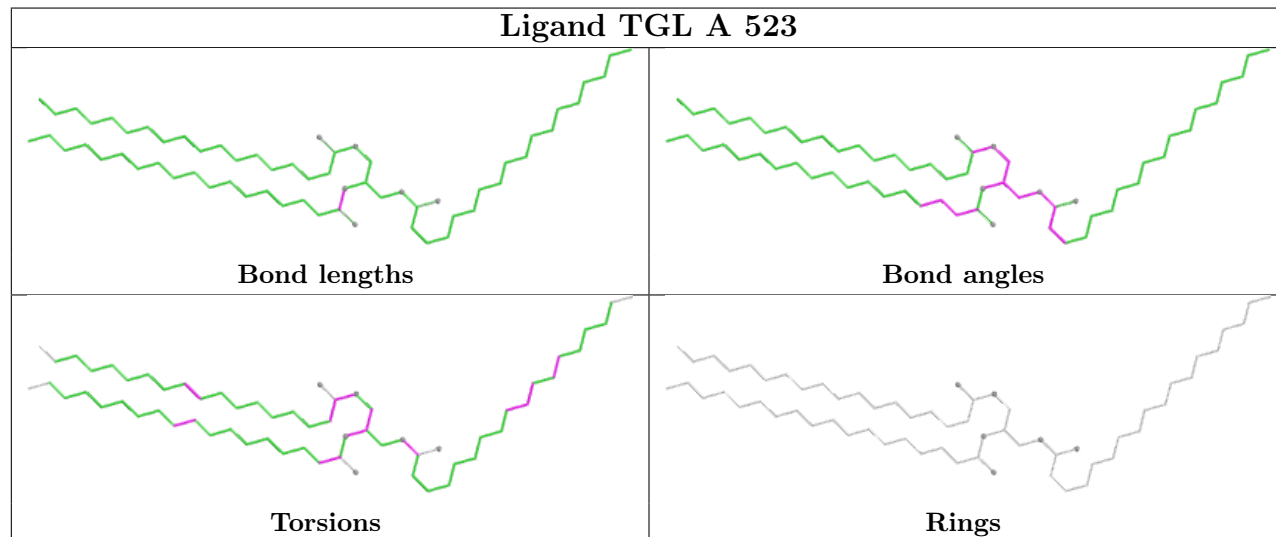
Ligand PSC O 1230



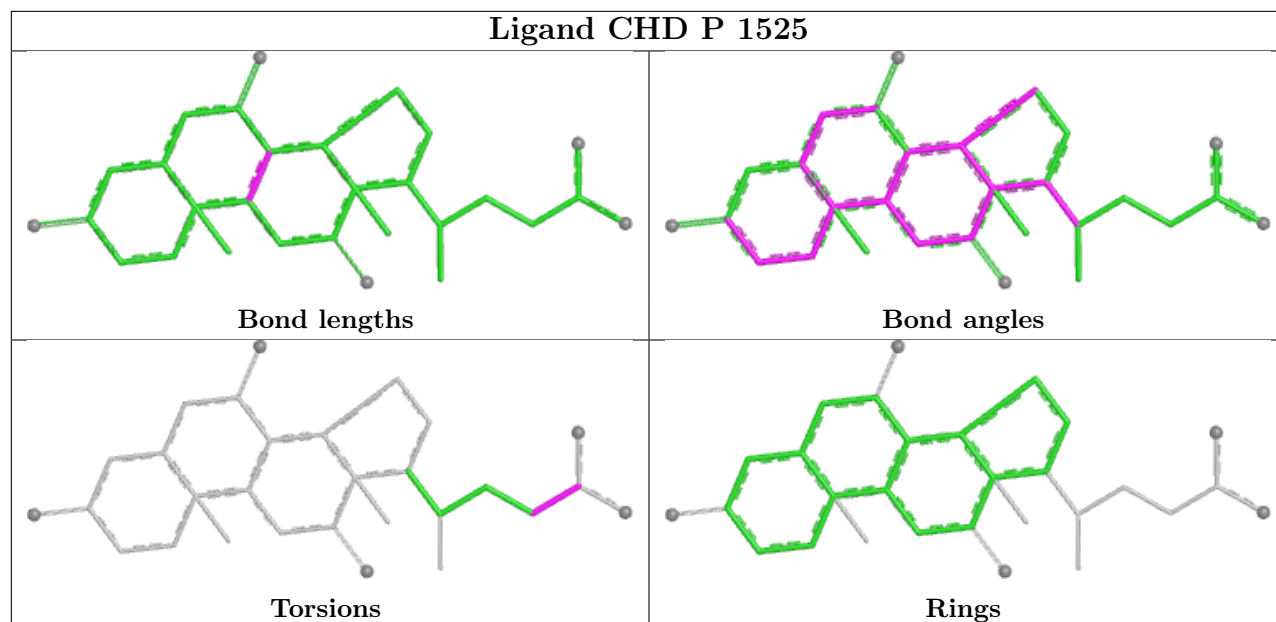
Ligand CHD P 1271



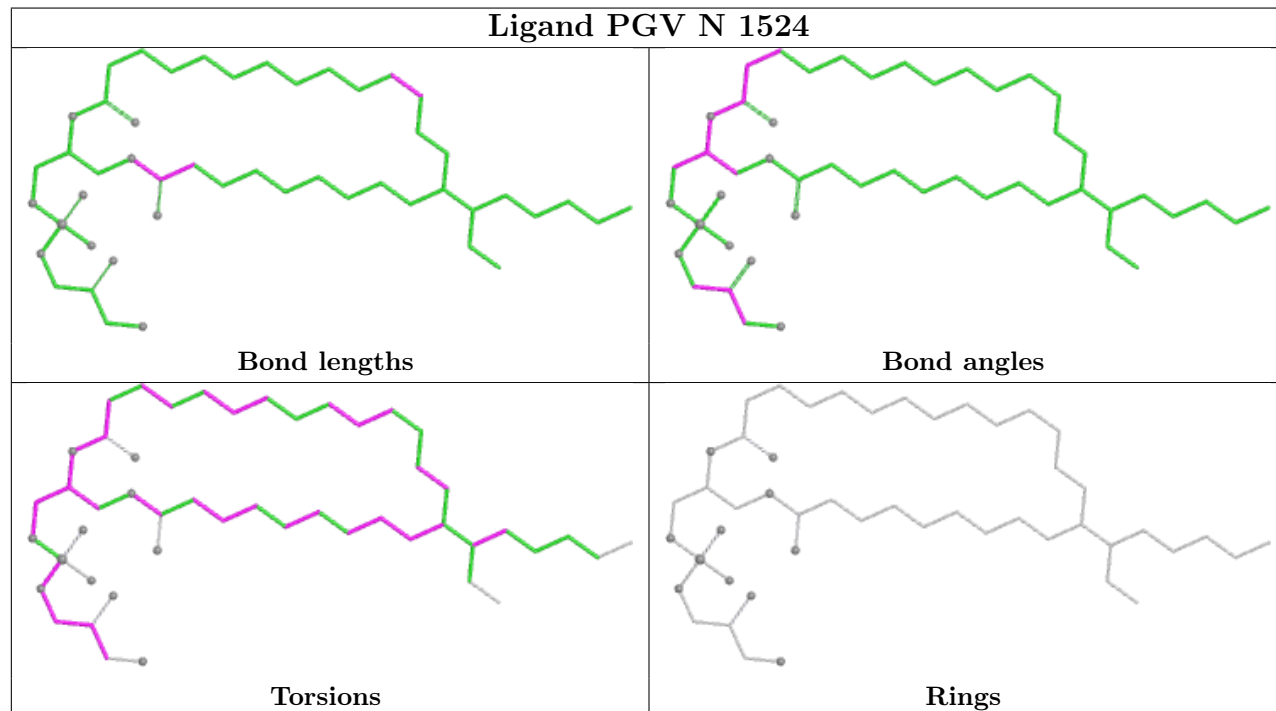
Ligand TGL A 523

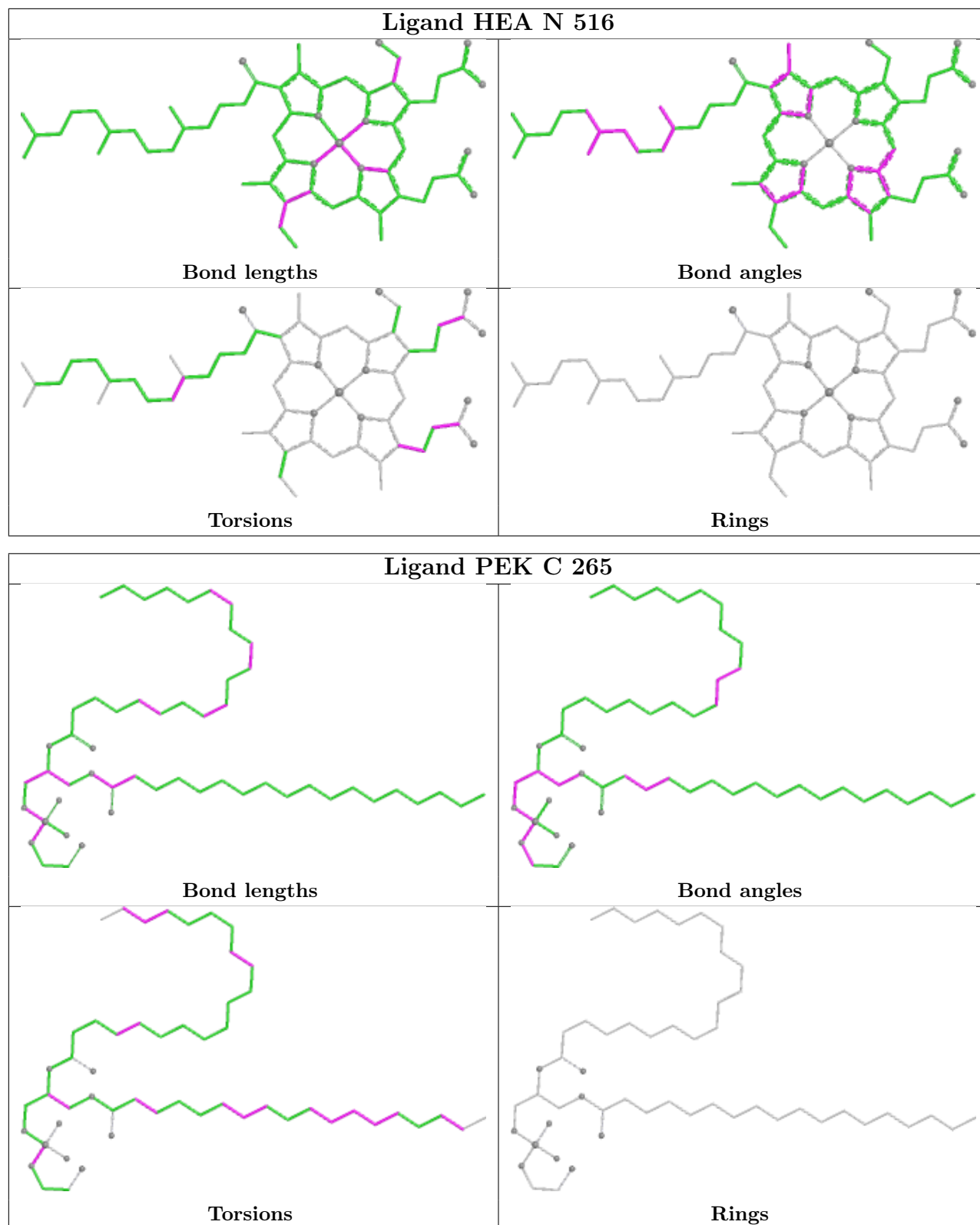


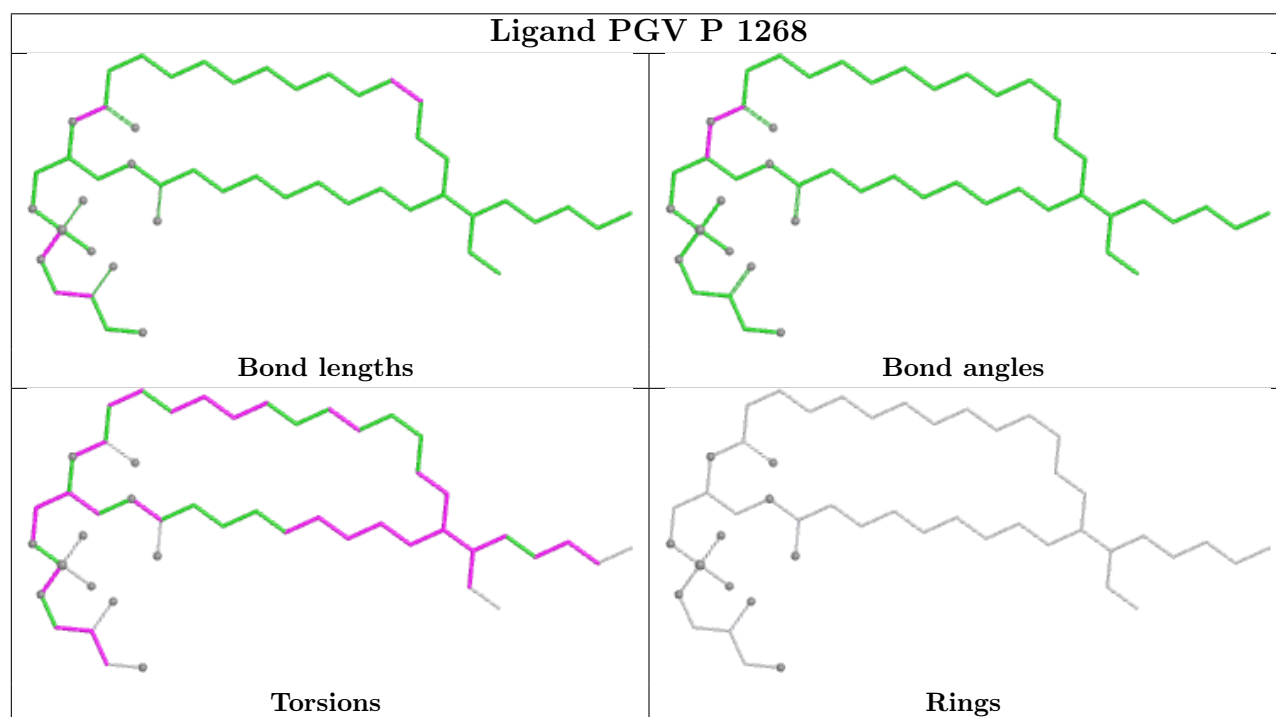
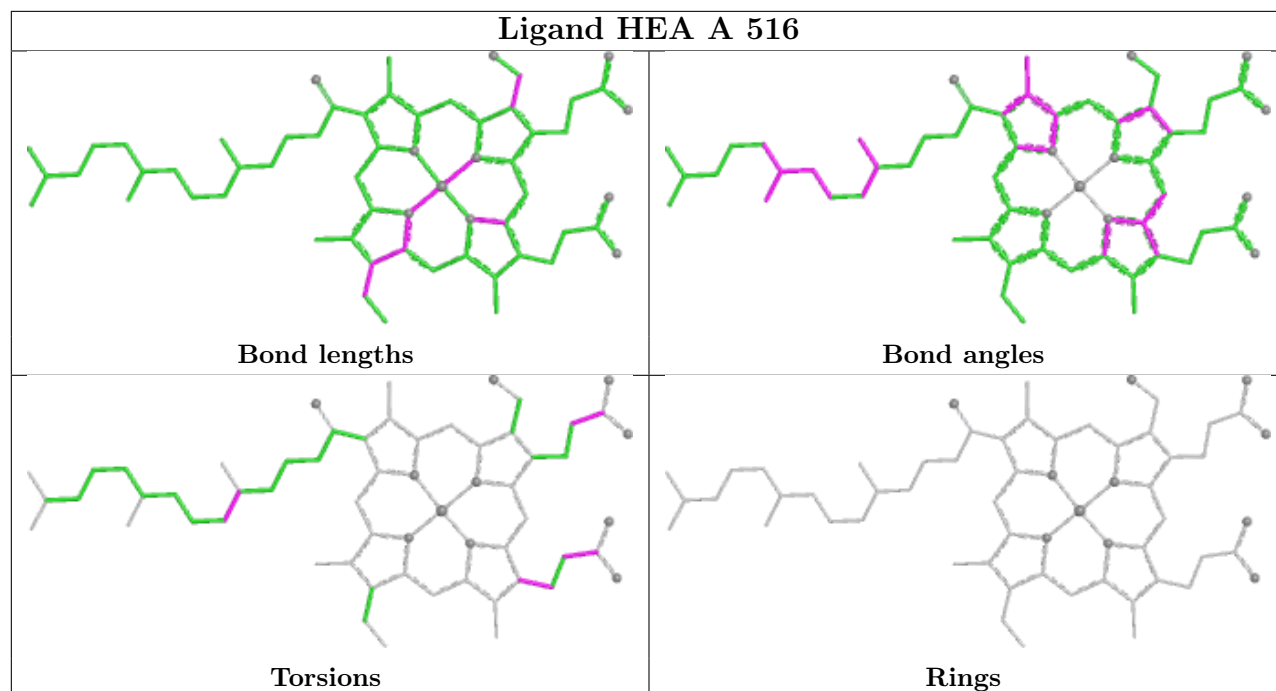
Ligand CHD P 1525

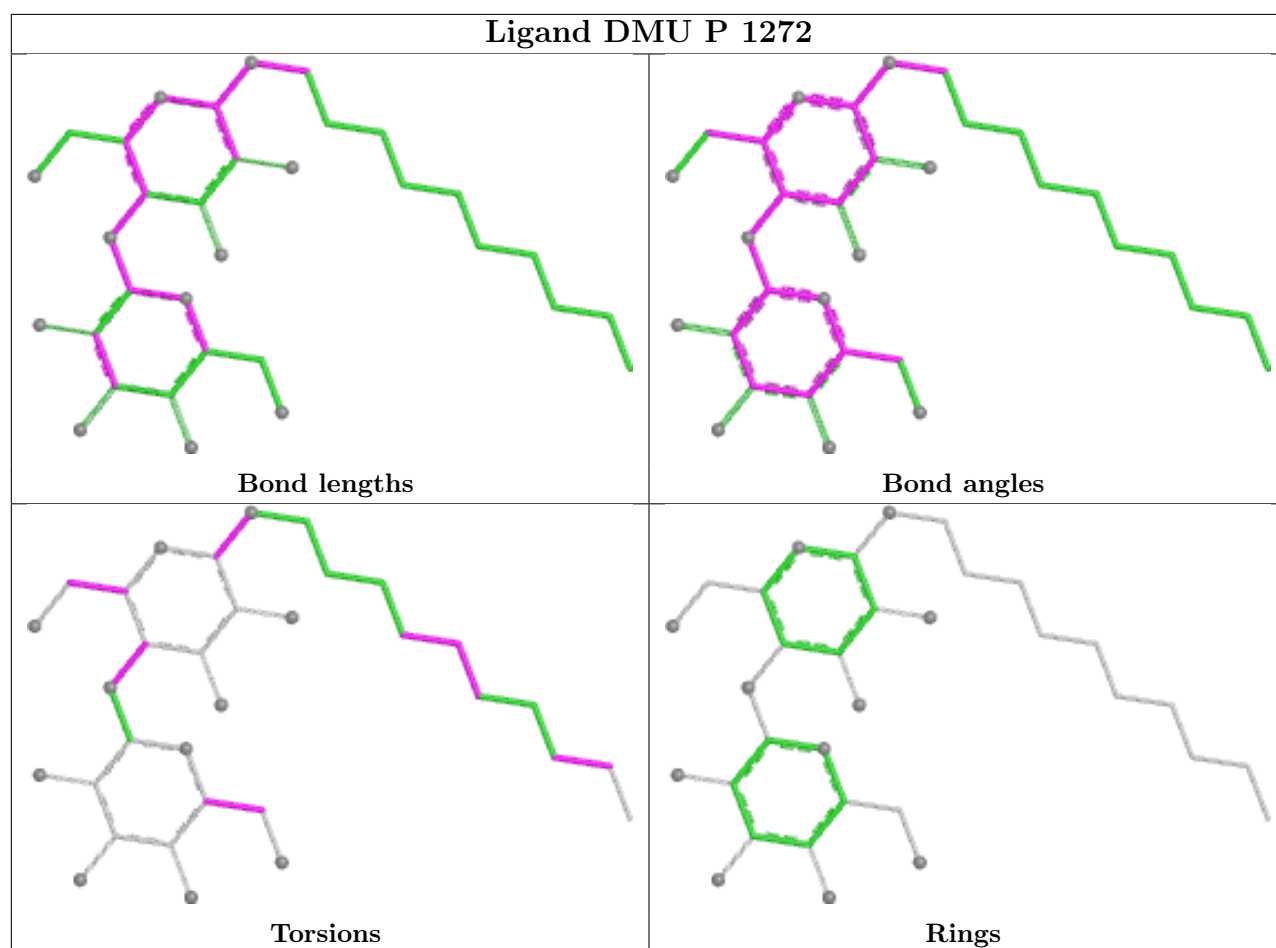


Ligand PGV N 1524

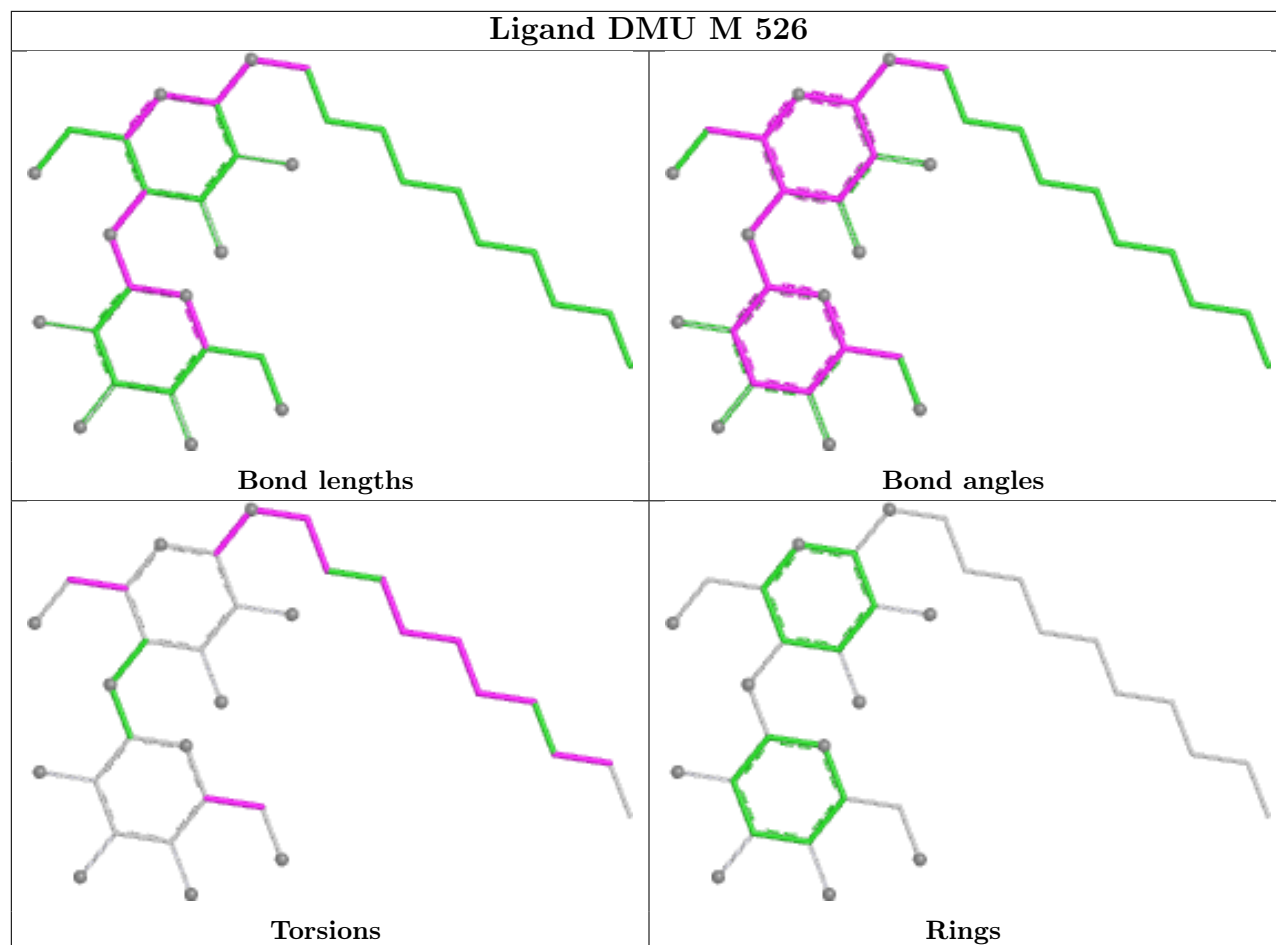




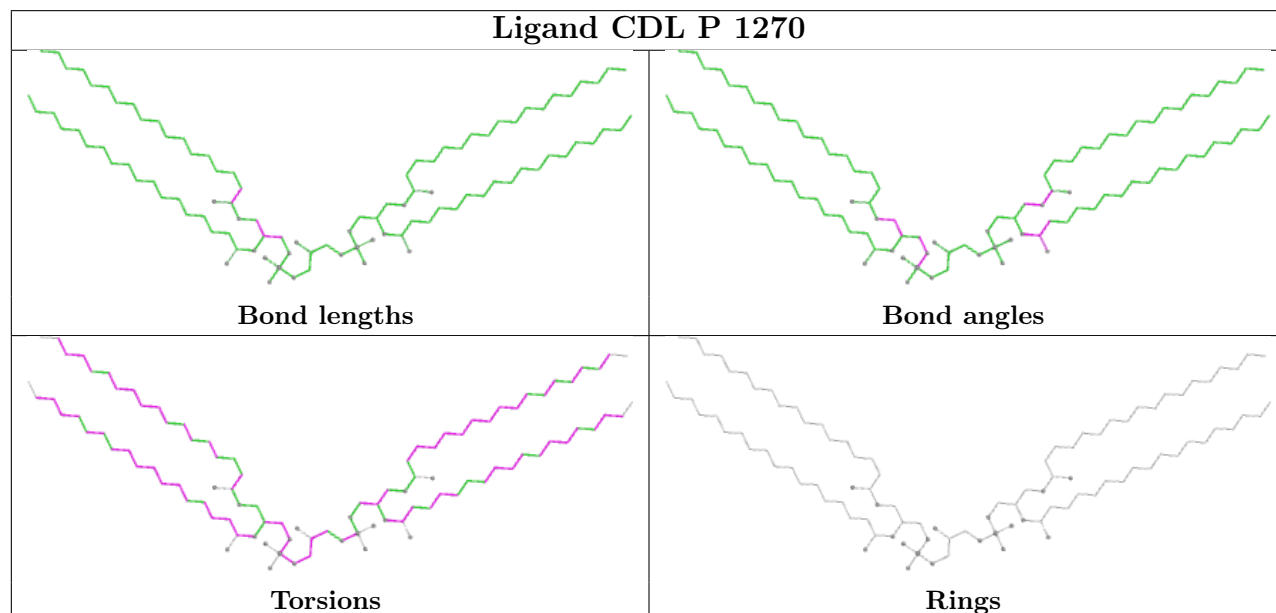




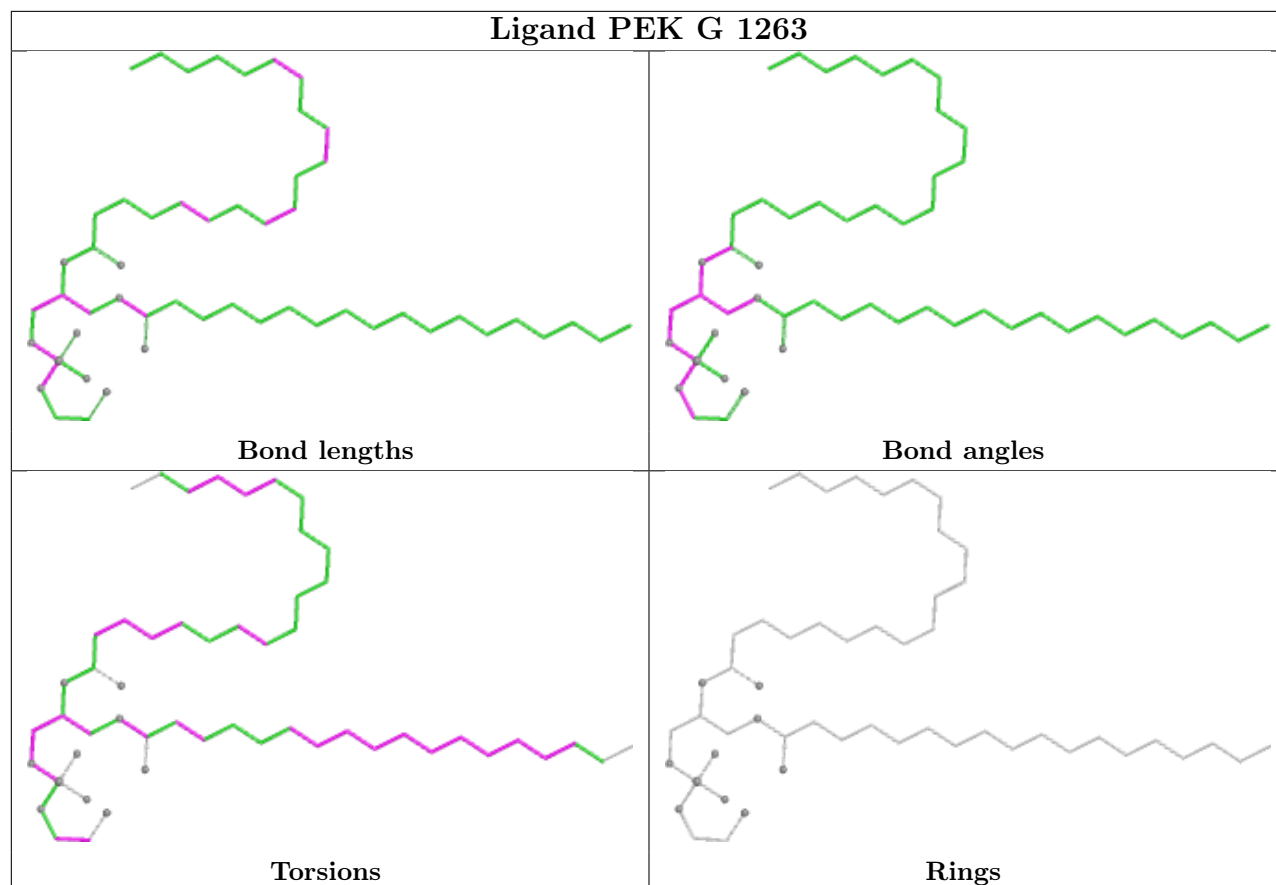
Ligand DMU M 526



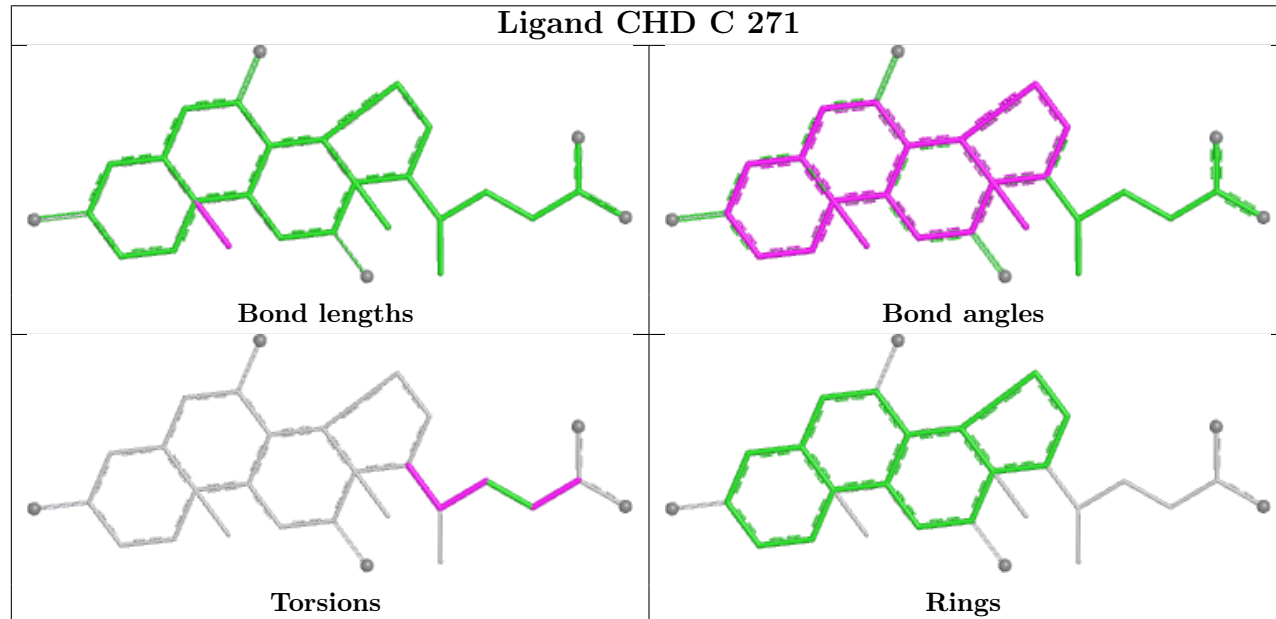
Ligand CDL P 1270

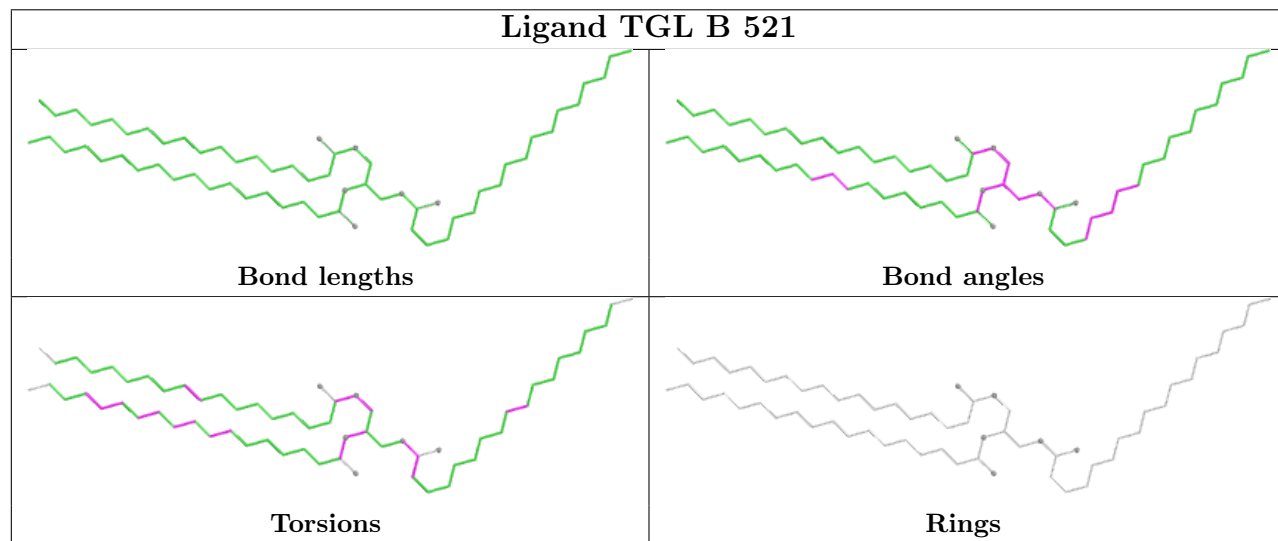
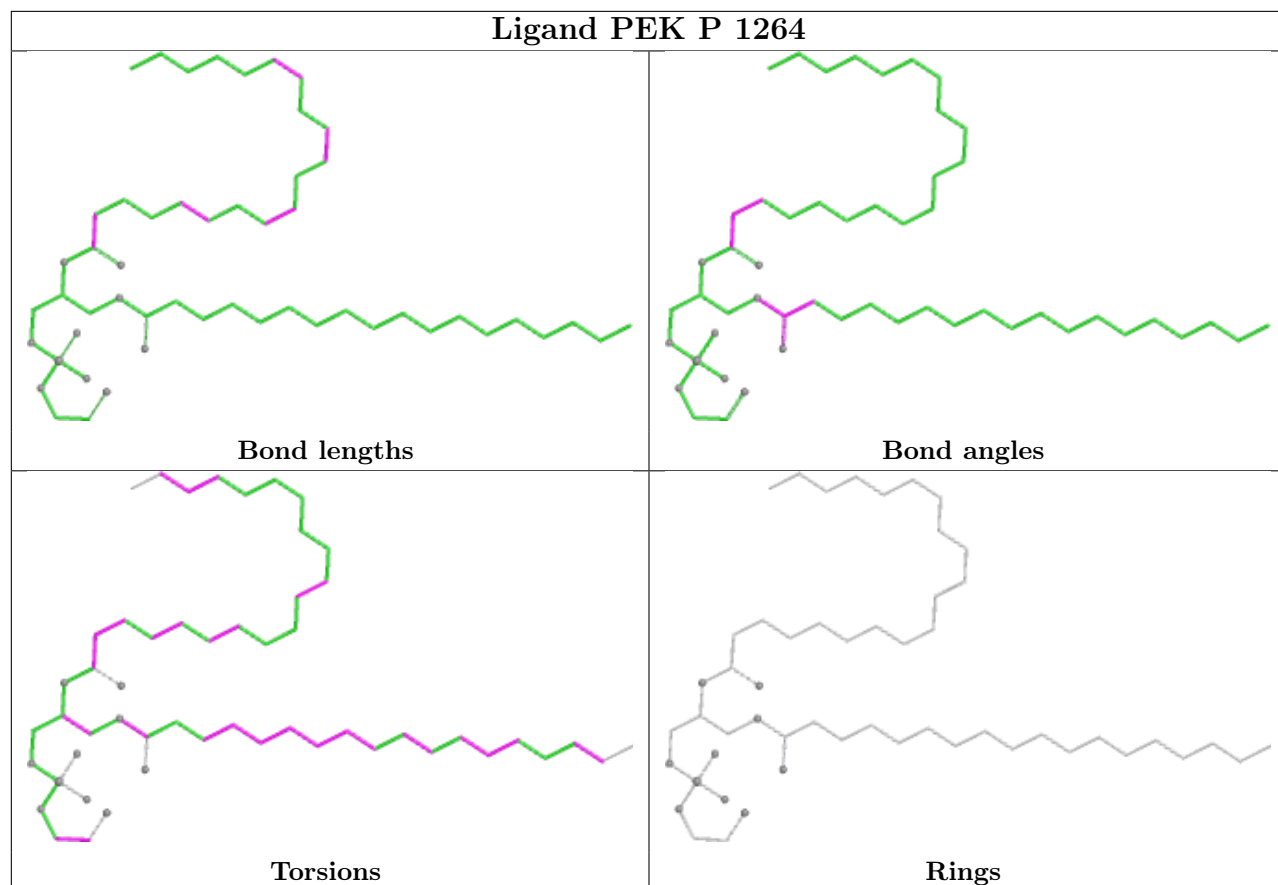


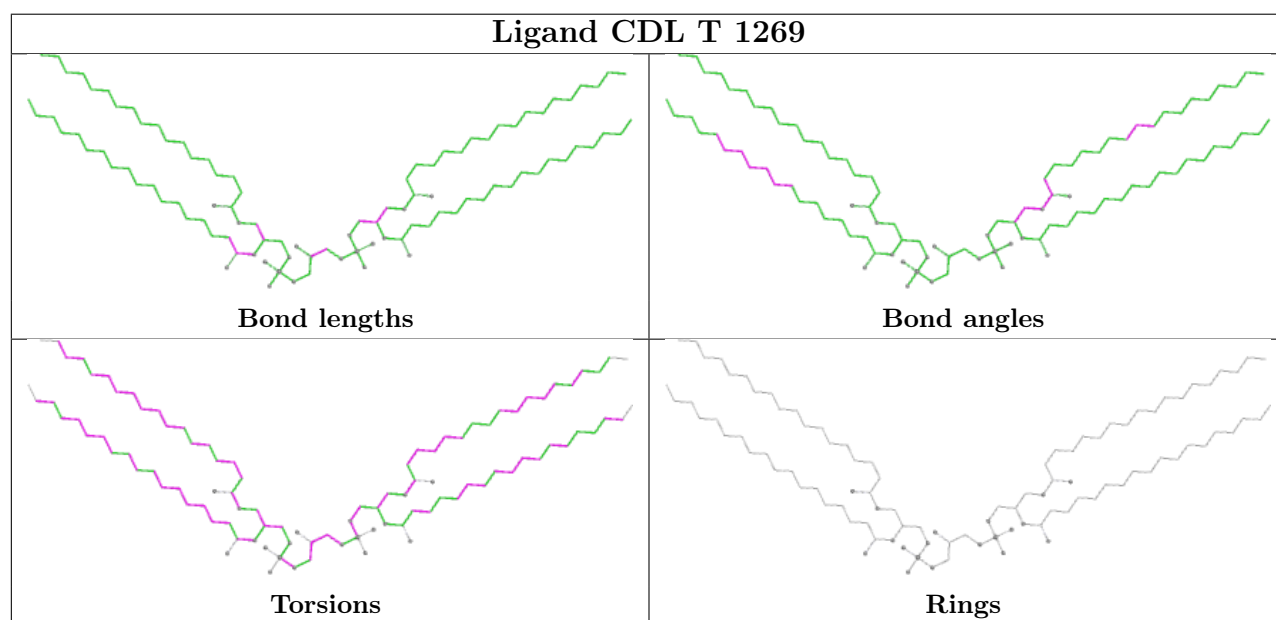
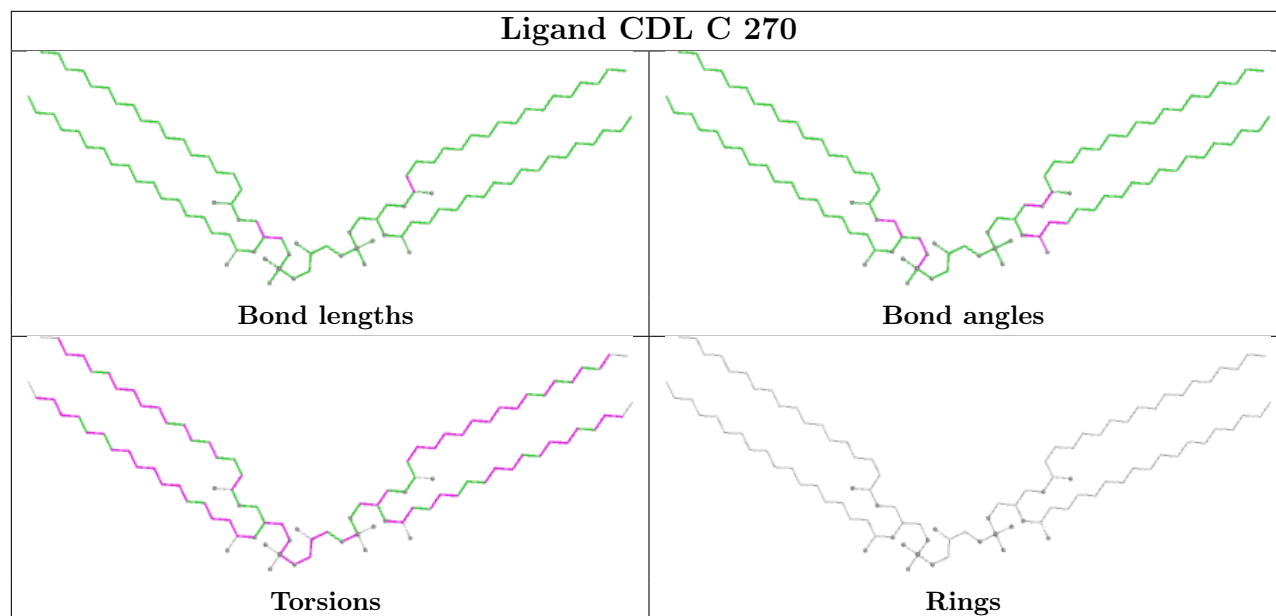
Ligand PEK G 1263

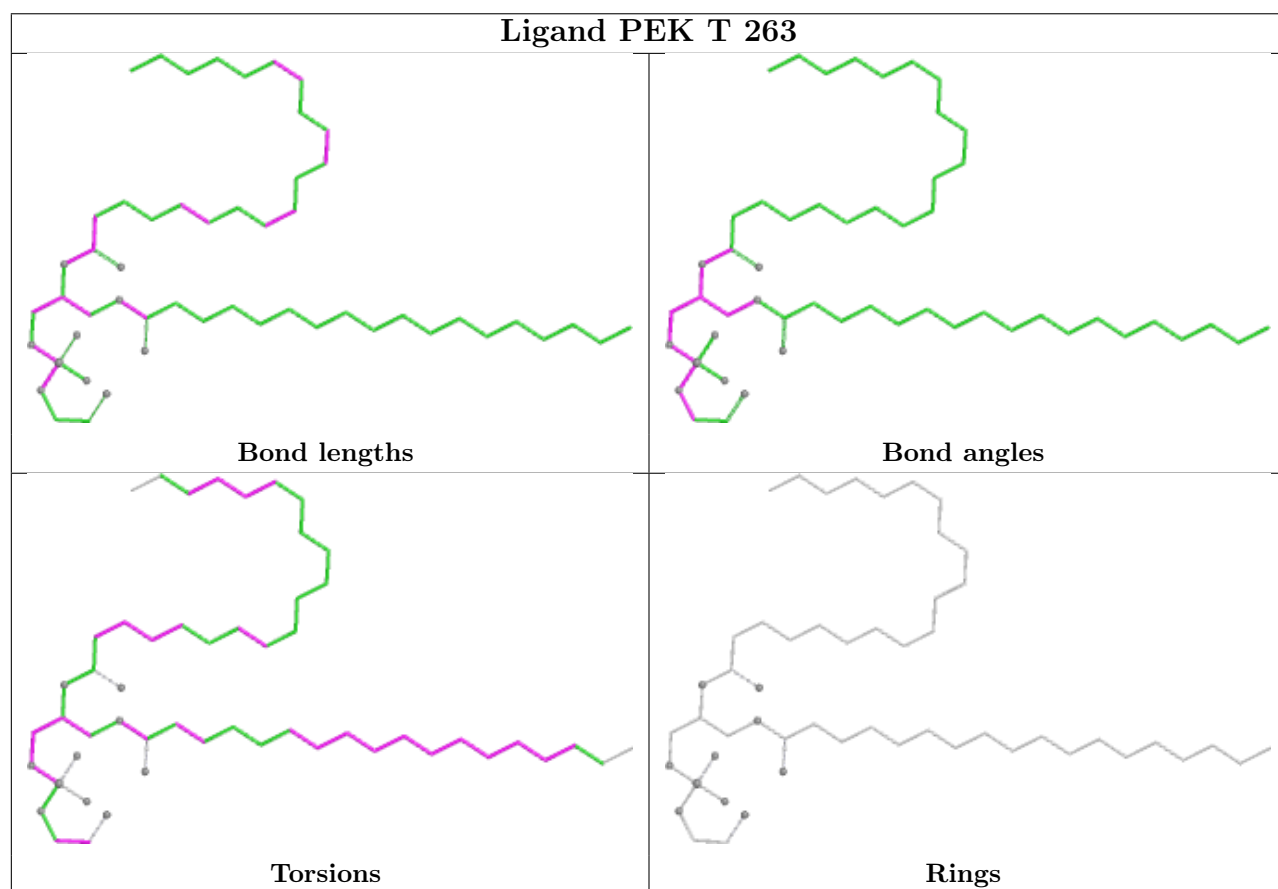
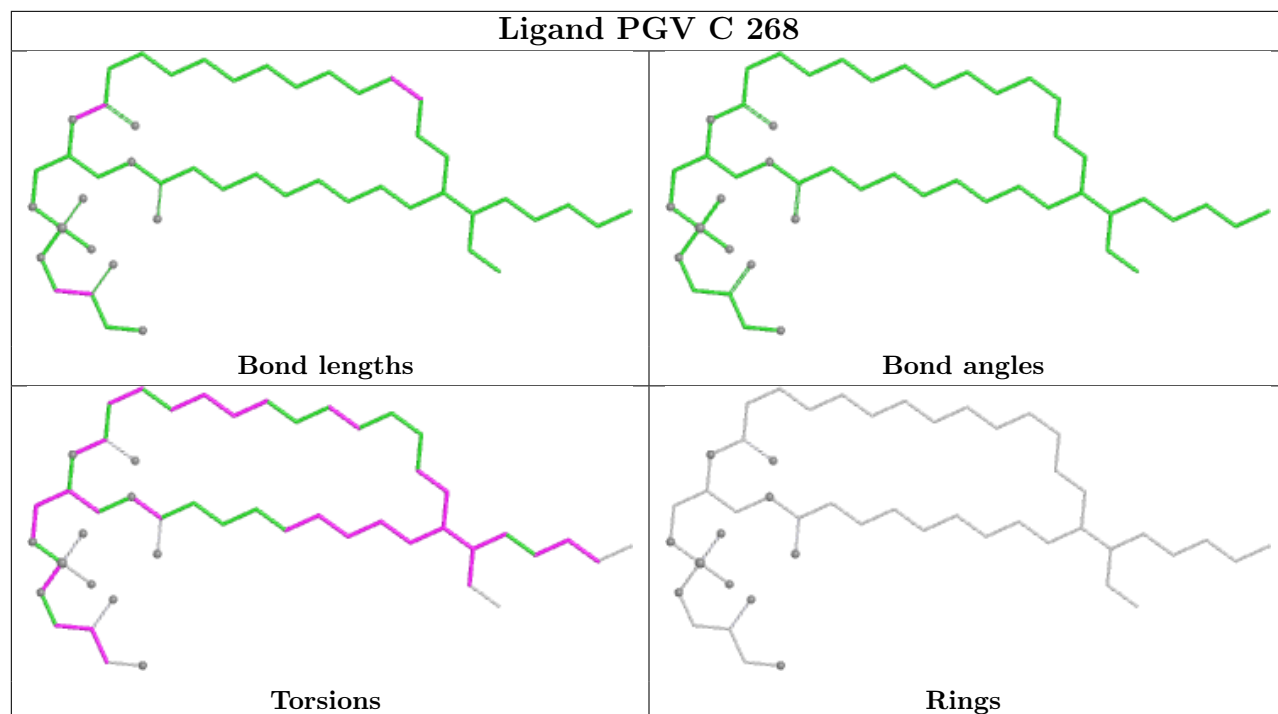


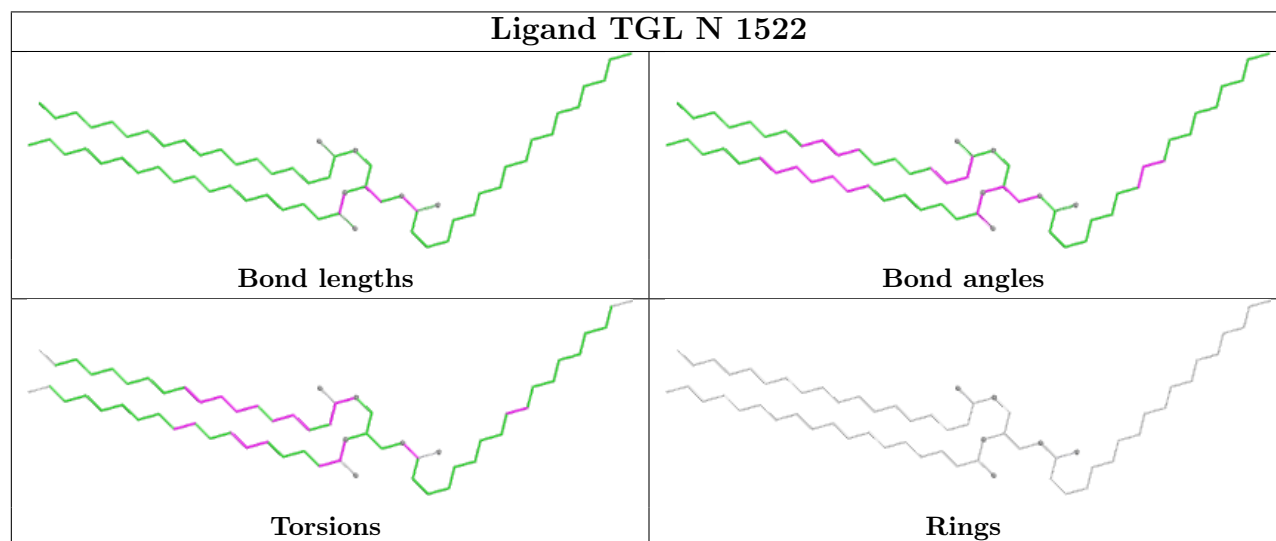
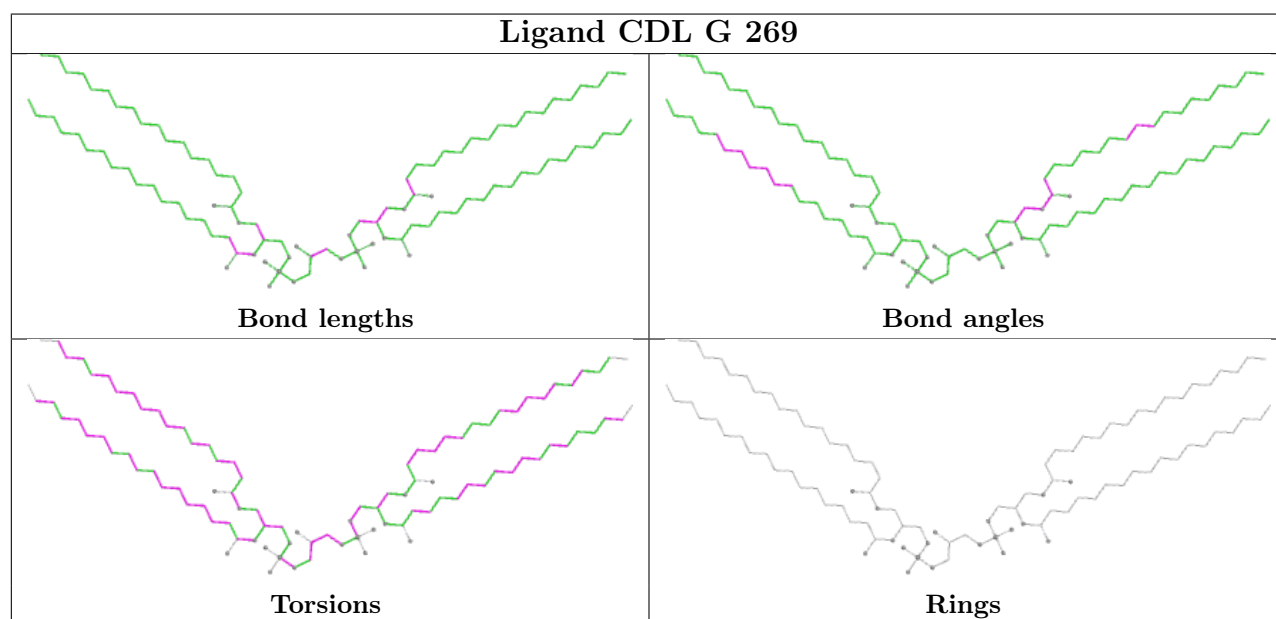
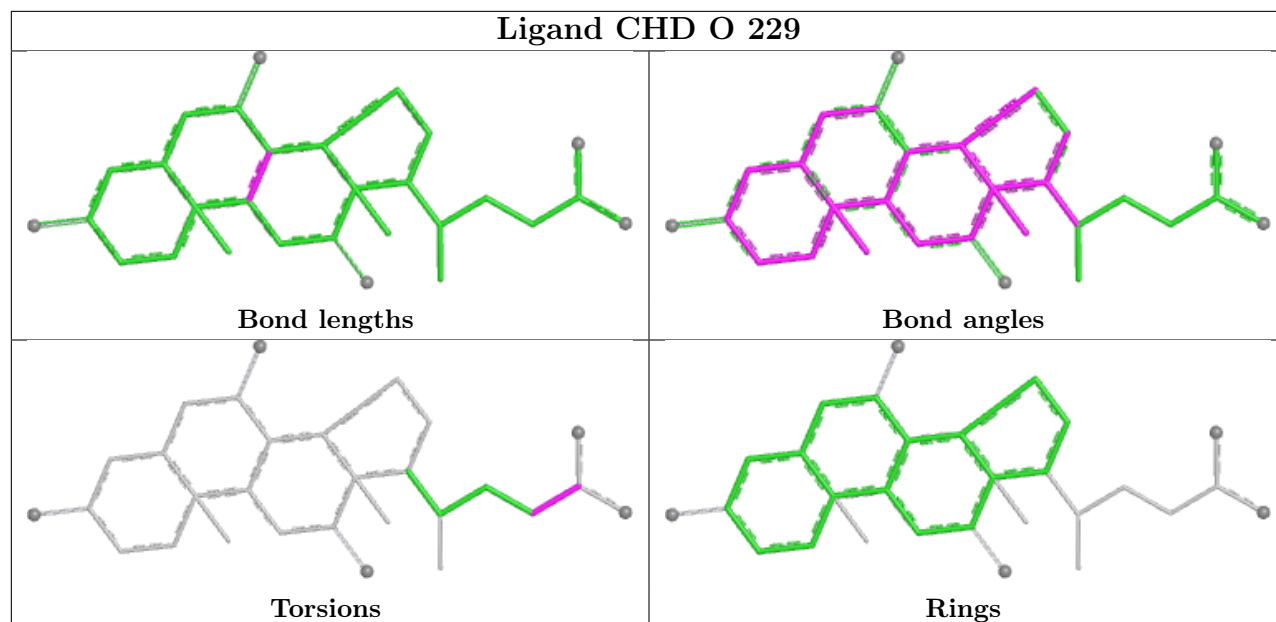
Ligand CHD C 271



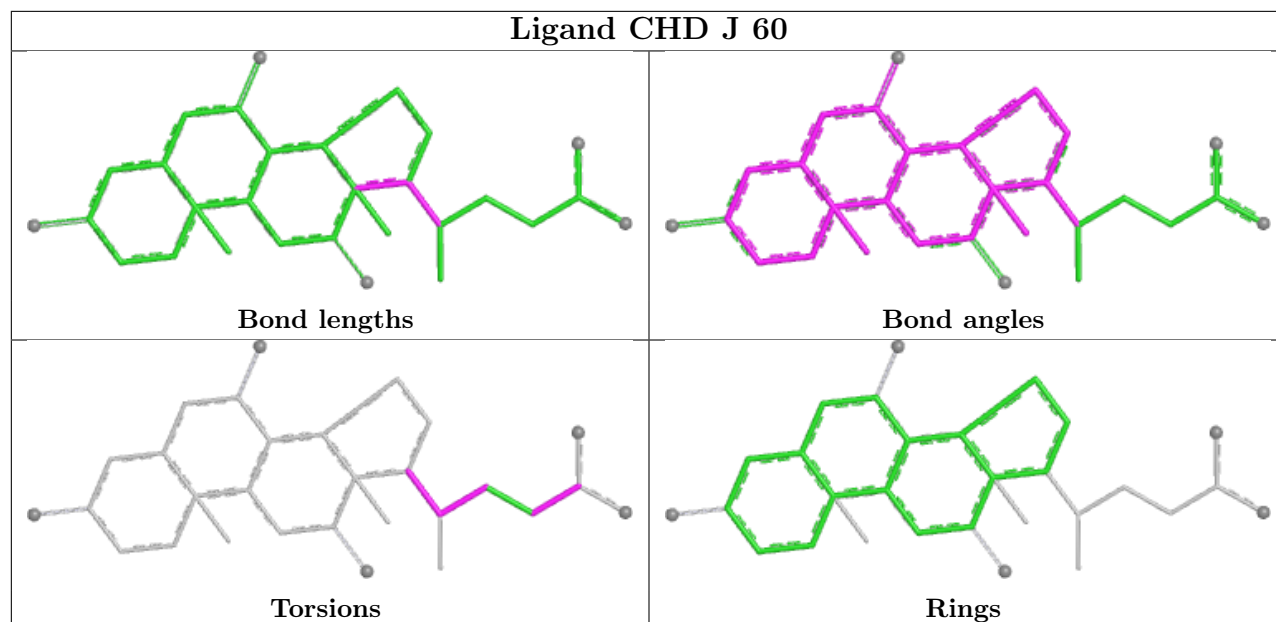




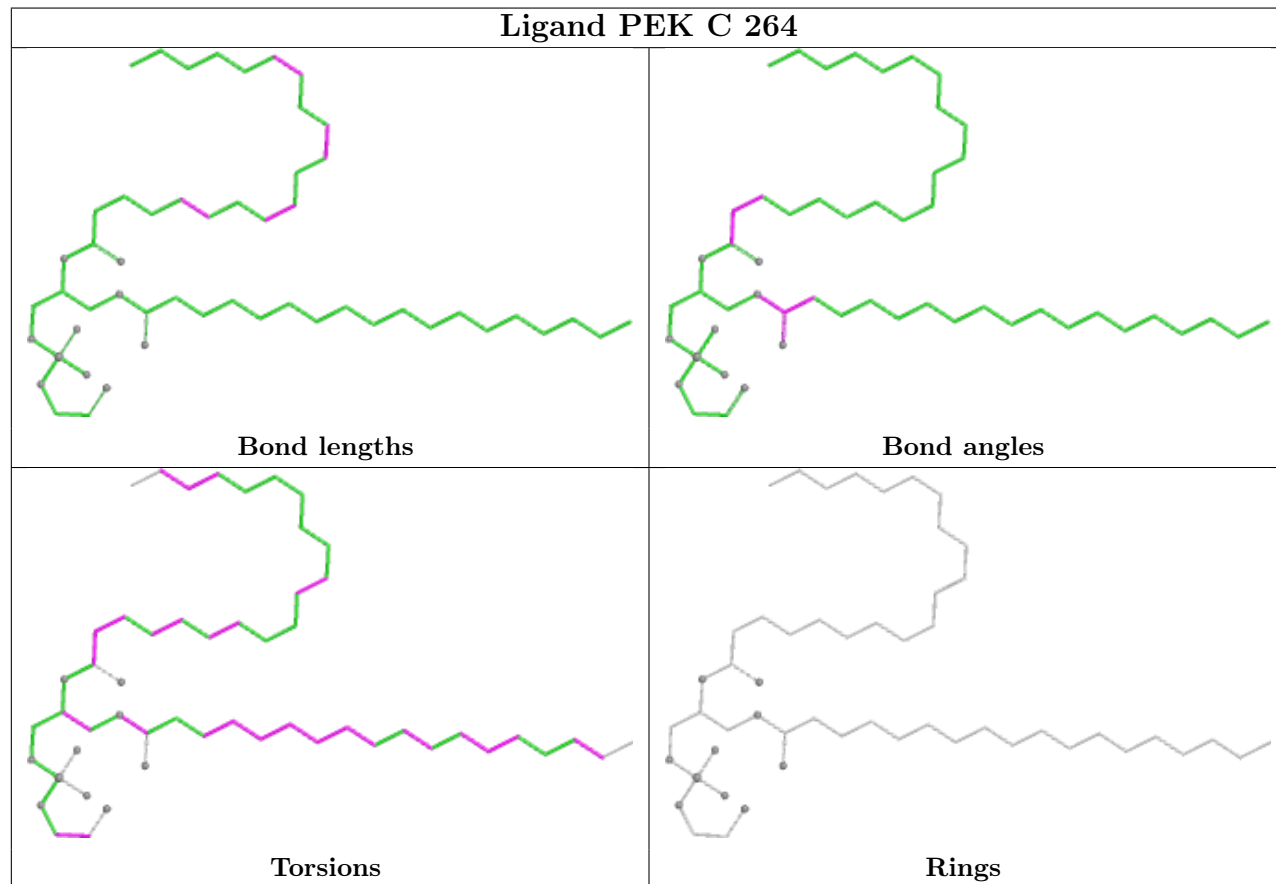




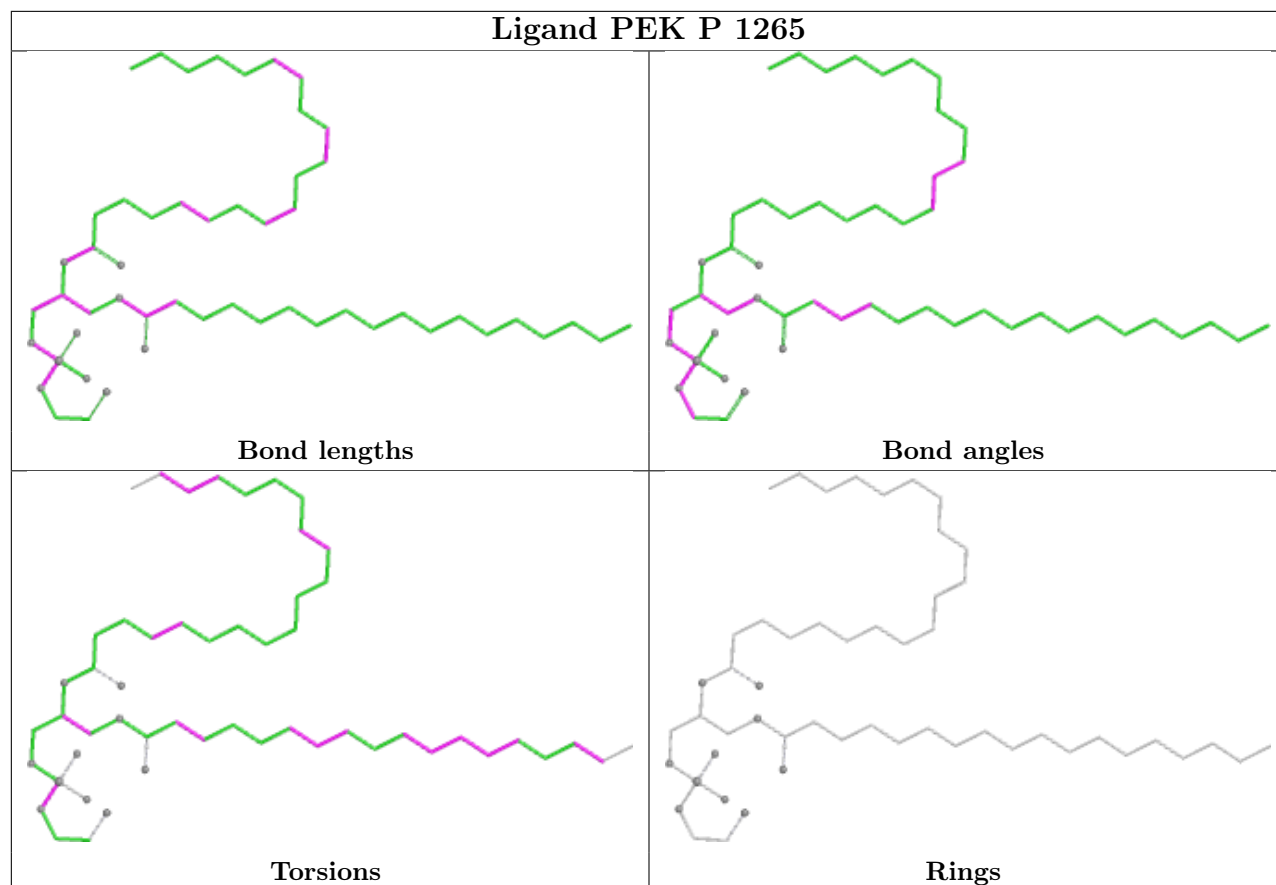
Ligand CHD J 60



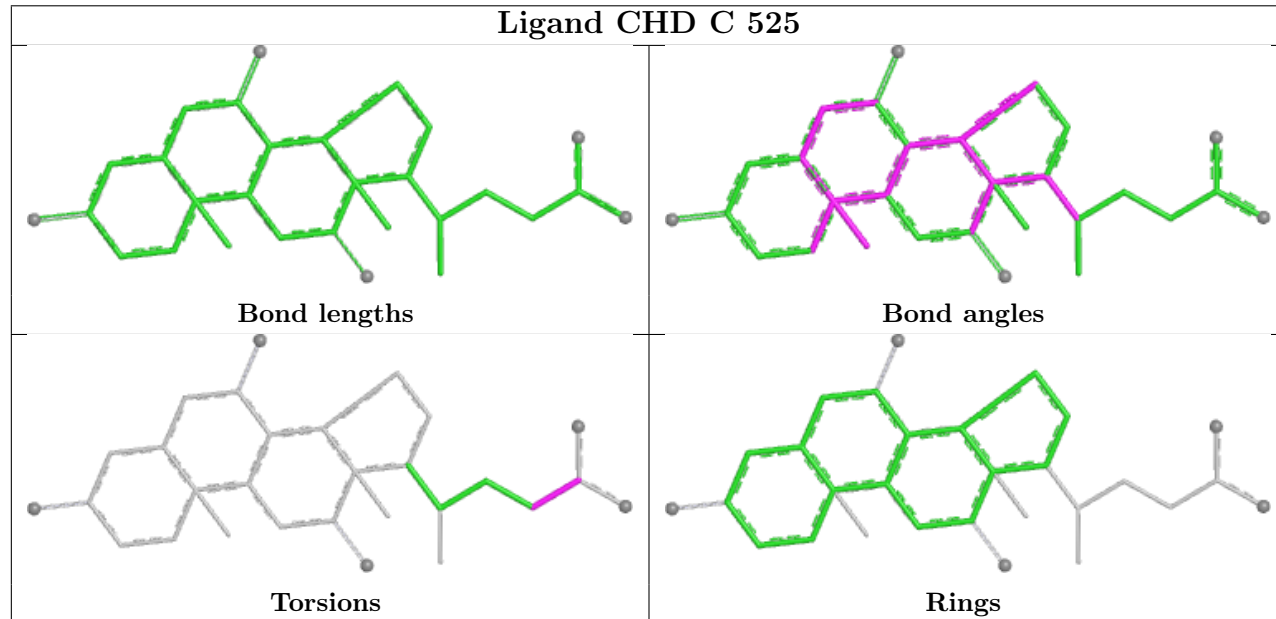
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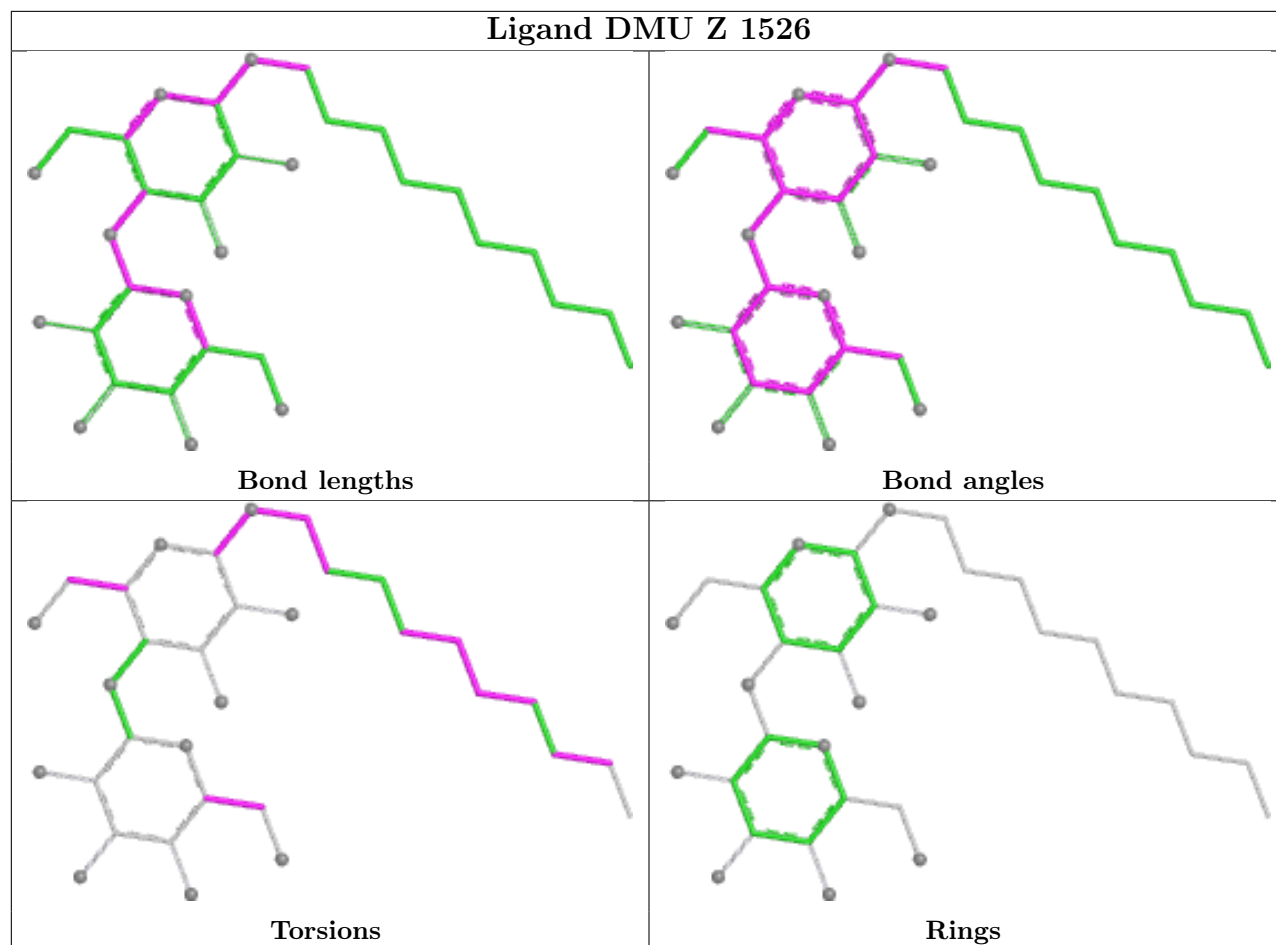
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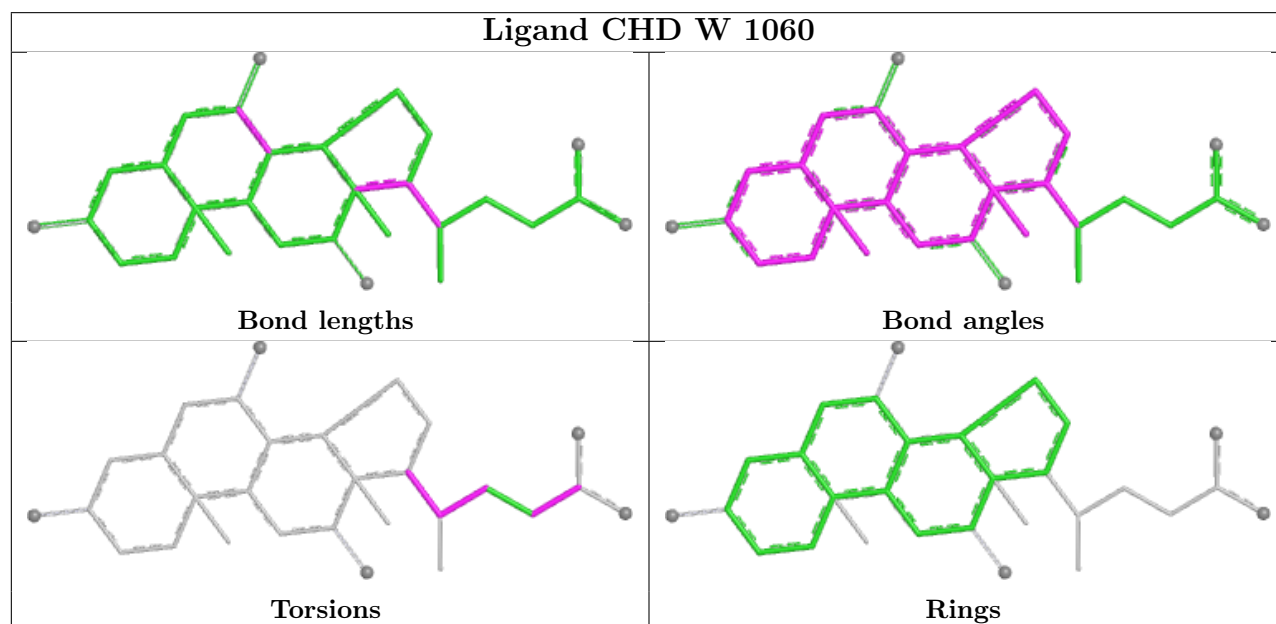
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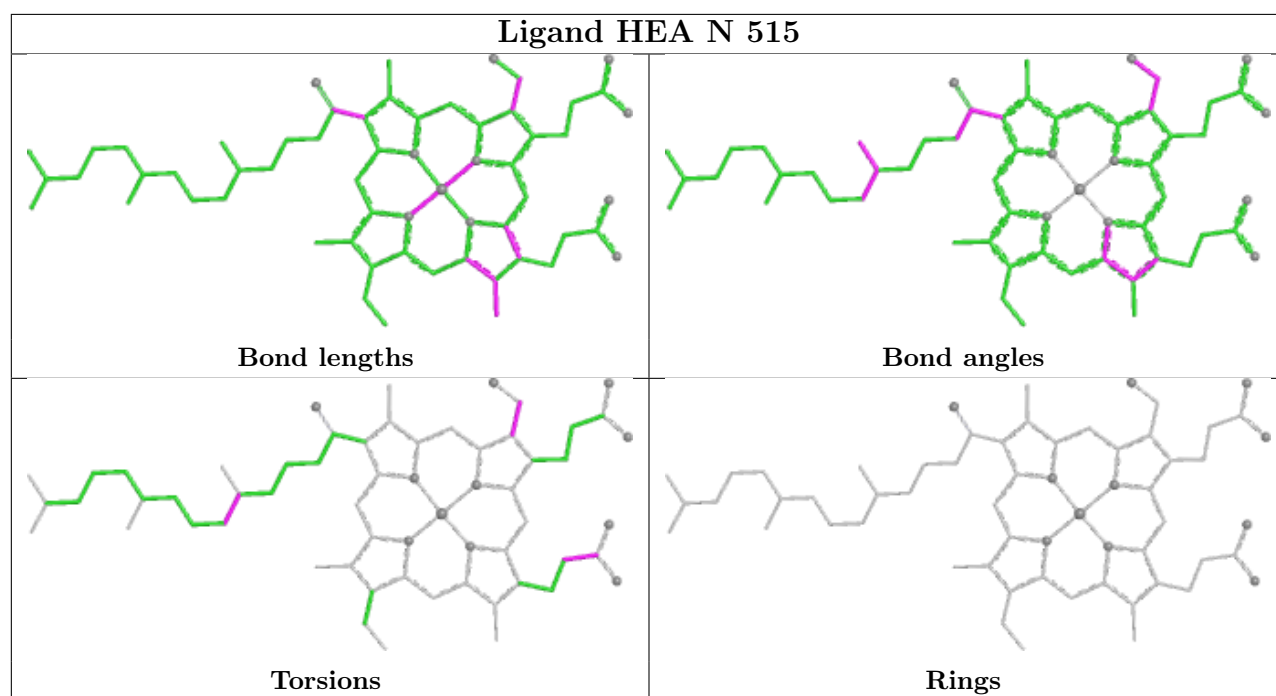
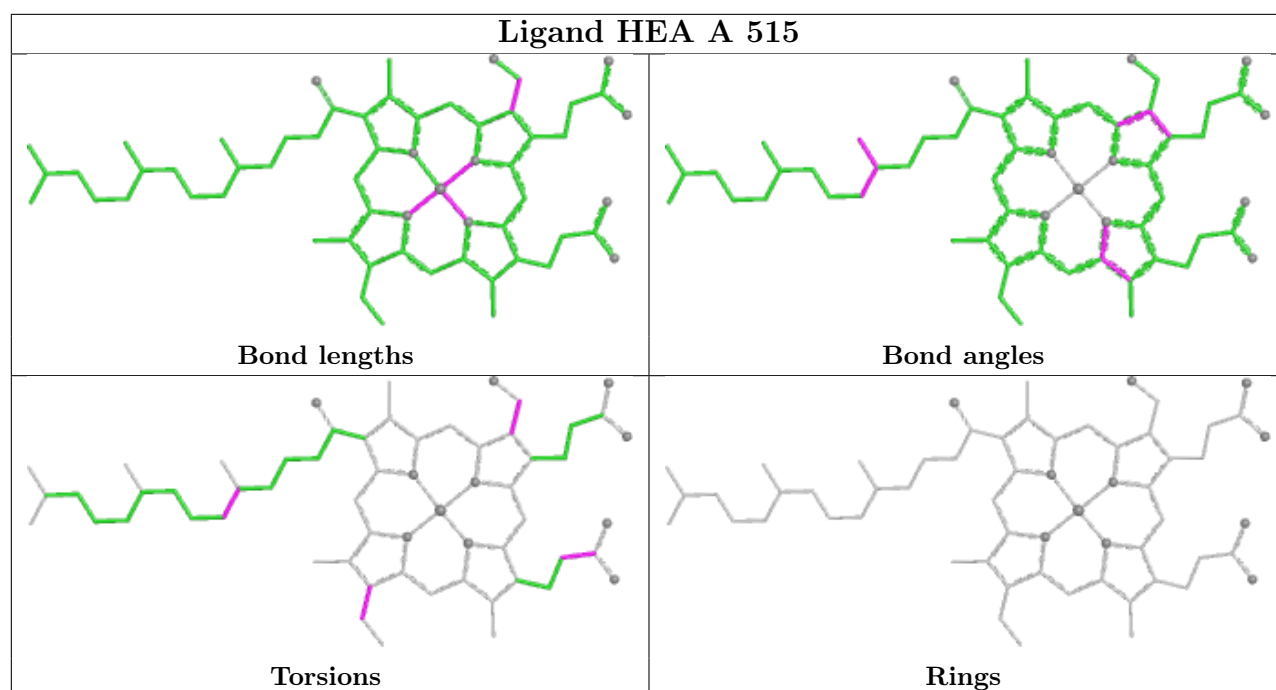


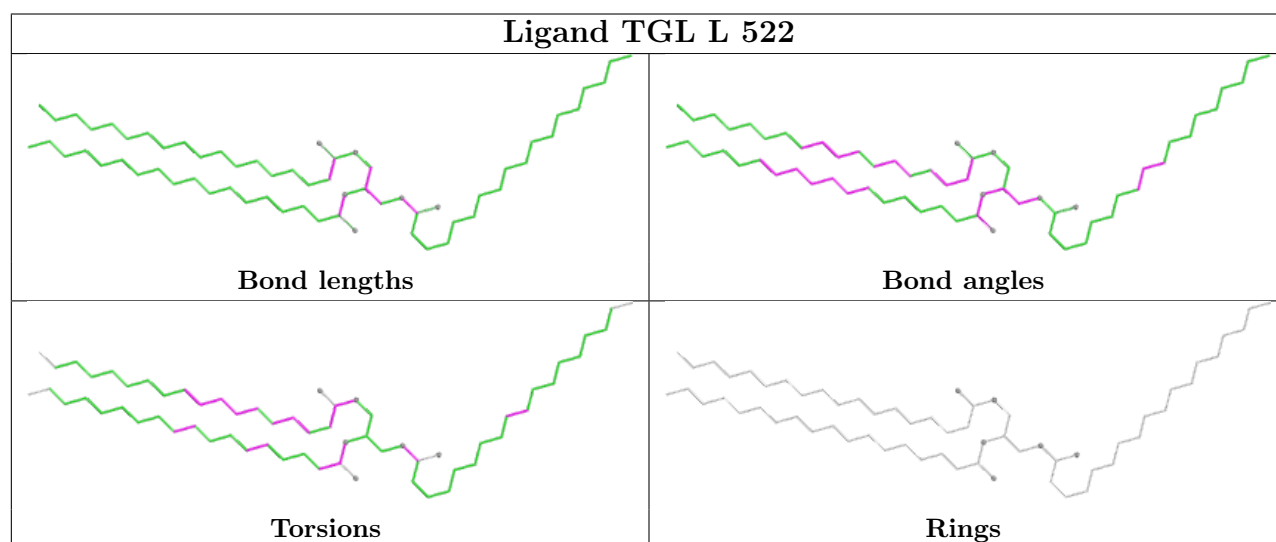
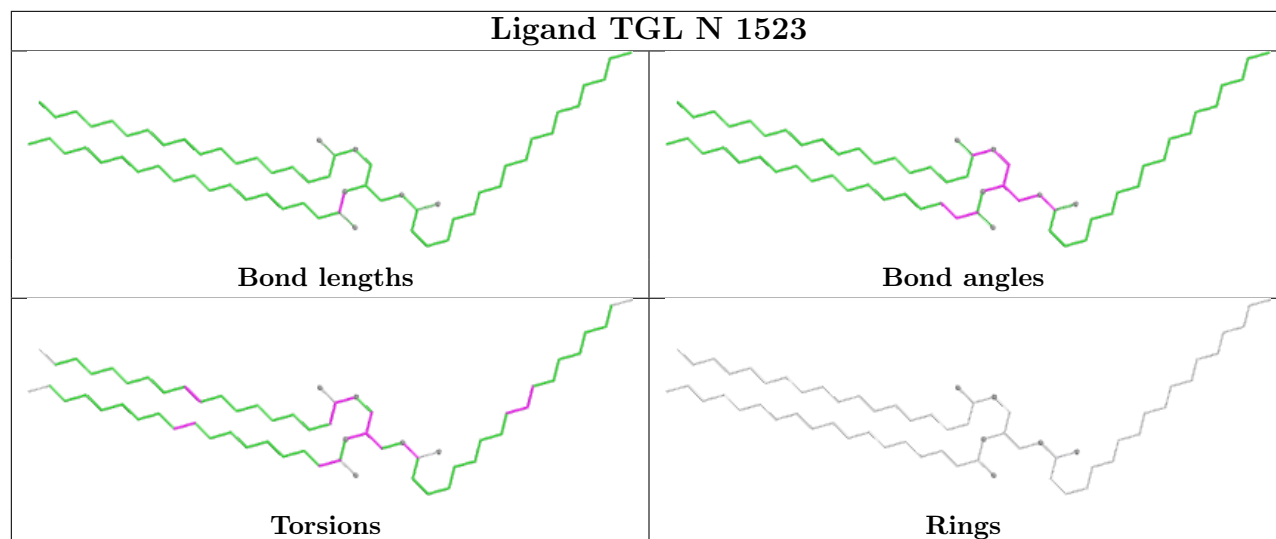
Ligand DMU Z 1526

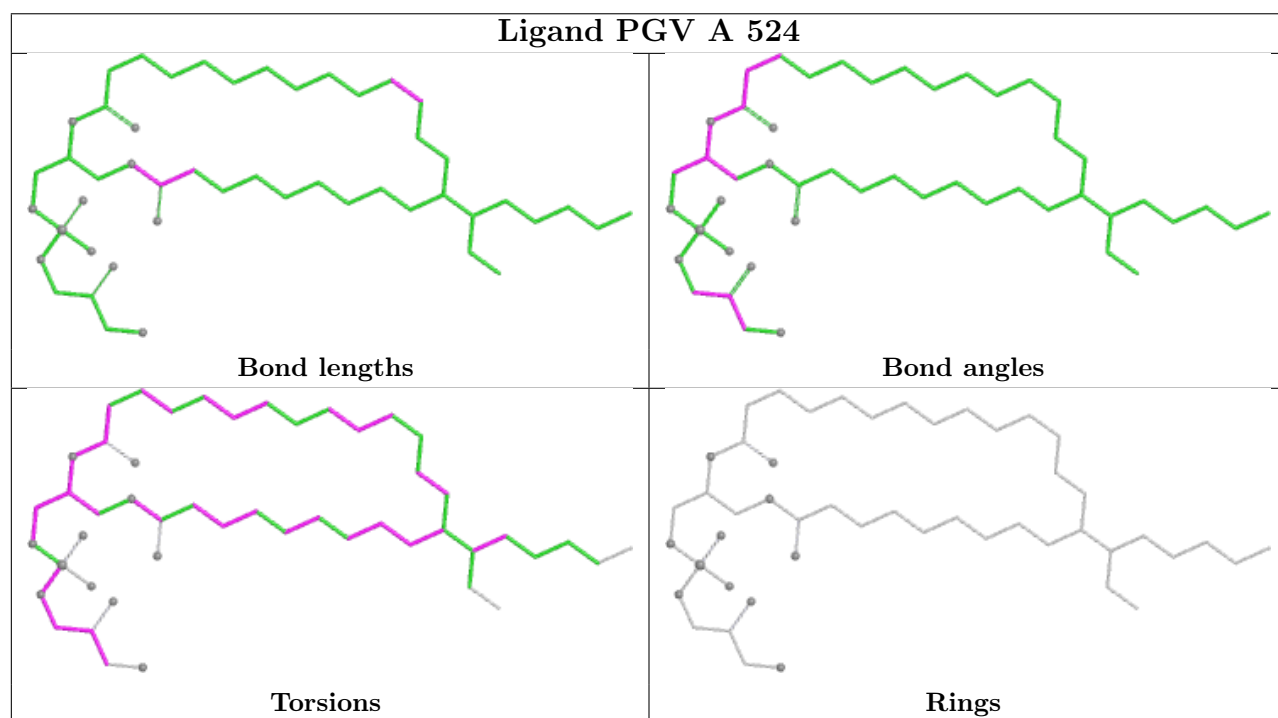
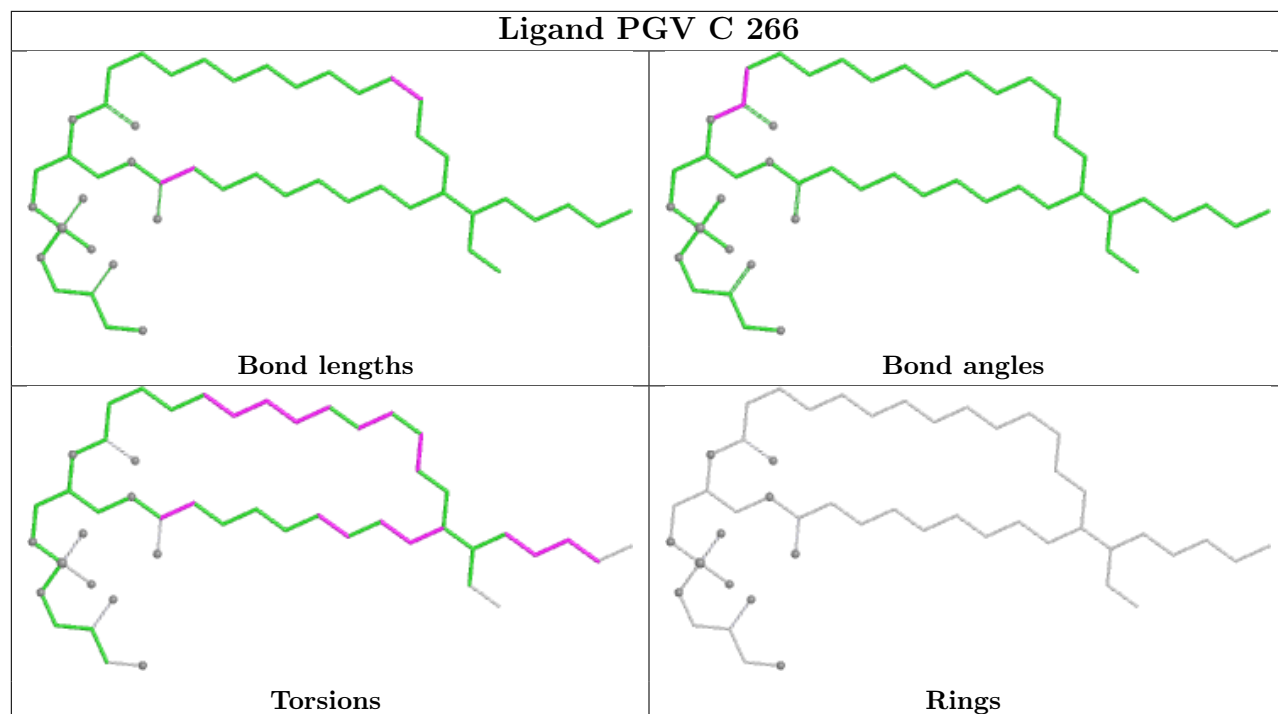


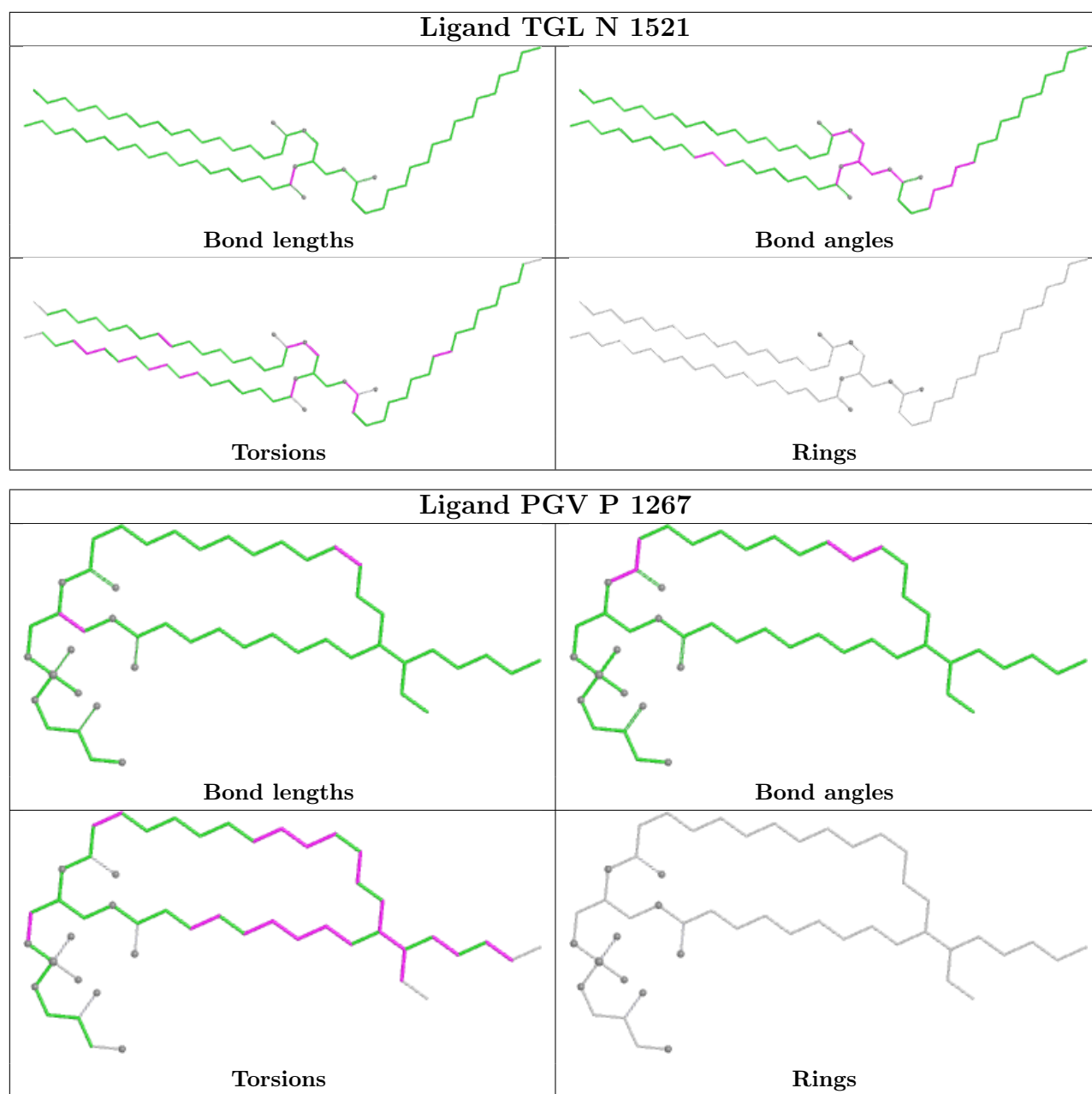
Ligand CHD W 1060











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.