



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 11:13 am BST

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

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

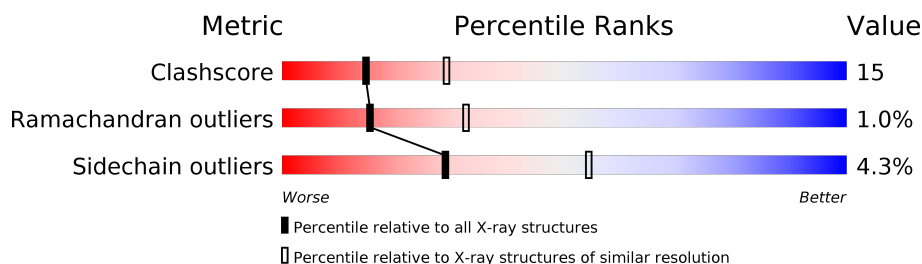
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)









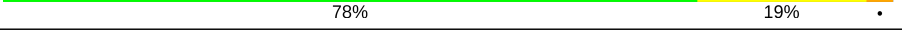

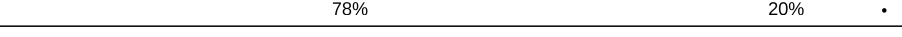







The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively.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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	514	
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
18	HEA	A	515	X	-	-	-
18	HEA	A	516	X	-	-	-
18	HEA	N	515	X	-	-	-
18	HEA	N	516	X	-	-	-
20	CHD	C	271	X	-	-	-
20	CHD	J	60	X	-	-	-
20	CHD	W	1060	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CHD	W	1271	X	-	-	-
22	TGL	L	522	-	-	X	-
24	DMU	C	272	X	-	-	-
24	DMU	M	526	X	-	-	-
24	DMU	P	1272	X	-	-	-
24	DMU	Z	1526	X	-	-	-
26	CDL	G	269	-	-	X	-
26	CDL	T	1269	-	-	X	-
9	SAC	V	1	-	X	-	-

2 Entry composition

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 14 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

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

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

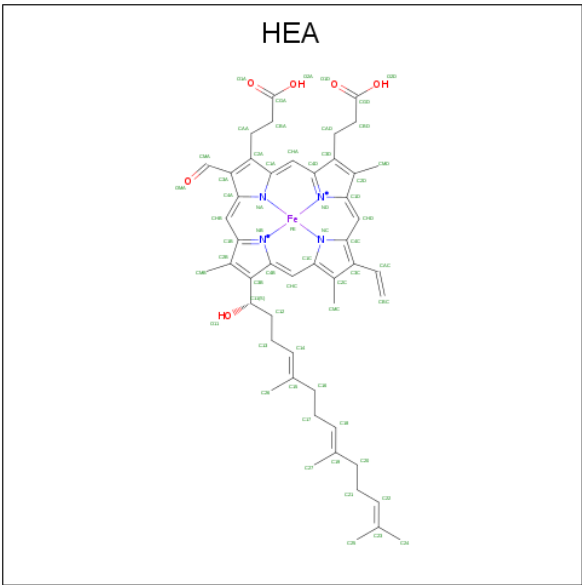
- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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



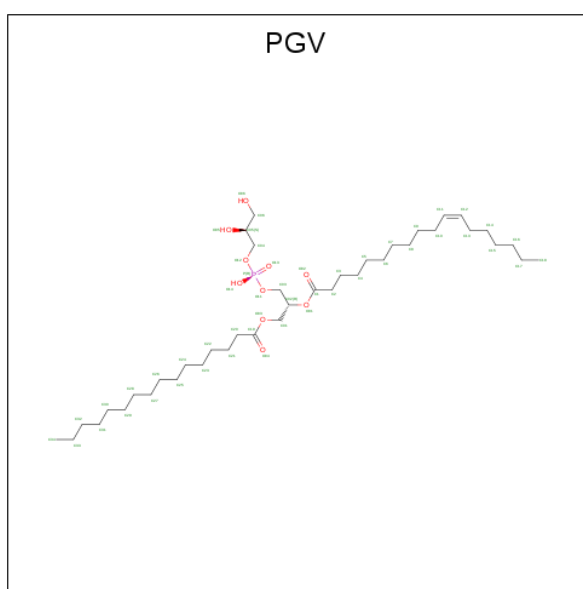
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

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

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



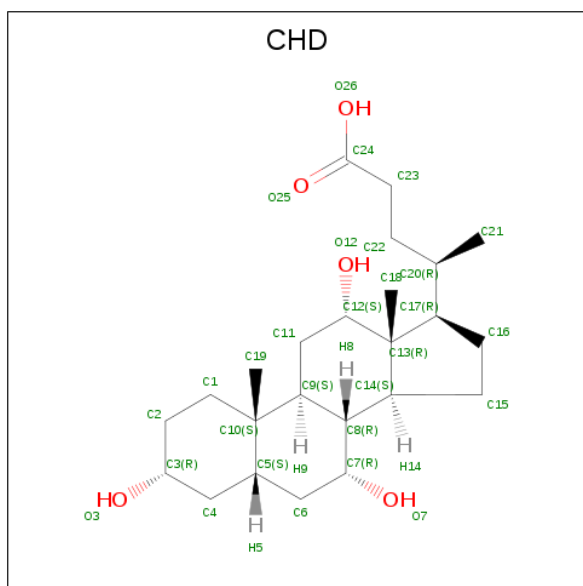
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P		
			51	40	10	1	0	0
19	C	1	Total	C	O	P		
			51	40	10	1	0	0
19	C	1	Total	C	O	P		
			51	40	10	1	0	0
19	C	1	Total	C	O	P		
			51	40	10	1	0	0
19	N	1	Total	C	O	P		
			51	40	10	1	0	0
19	P	1	Total	C	O	P		
			51	40	10	1	0	0
19	P	1	Total	C	O	P		
	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

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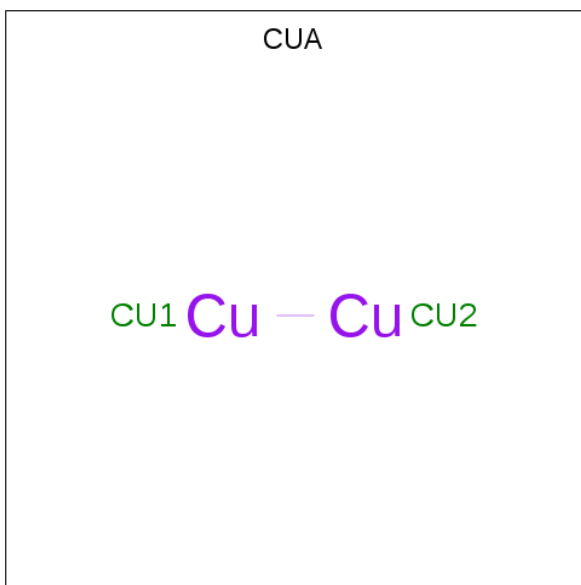
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	P	1	Total	C	O	P	0	0
			51	40	10	1		

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



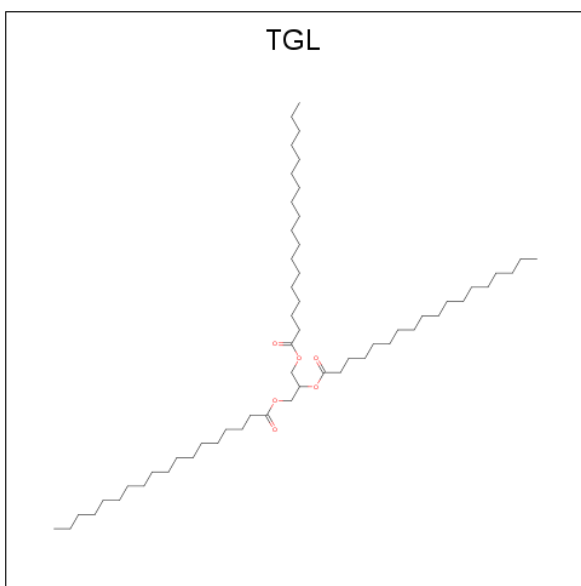
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O		0	0
			29	24	5			
20	B	1	Total	C	O		0	0
			29	24	5			
20	C	1	Total	C	O		0	0
			29	24	5			
20	J	1	Total	C	O		0	0
			29	24	5			
20	N	1	Total	C	O		0	0
			29	24	5			
20	P	1	Total	C	O		0	0
			29	24	5			
20	W	1	Total	C	O		0	0
			29	24	5			
20	W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

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).



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

- Molecule 22 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C₅₇H₁₁₀O₆).



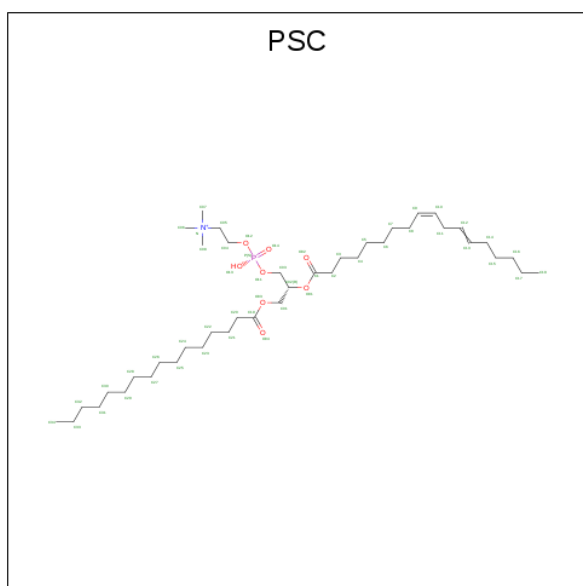
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	B	1	Total	C	O	0	0
			63	57	6		
22	D	1	Total	C	O	0	0
			63	57	6		

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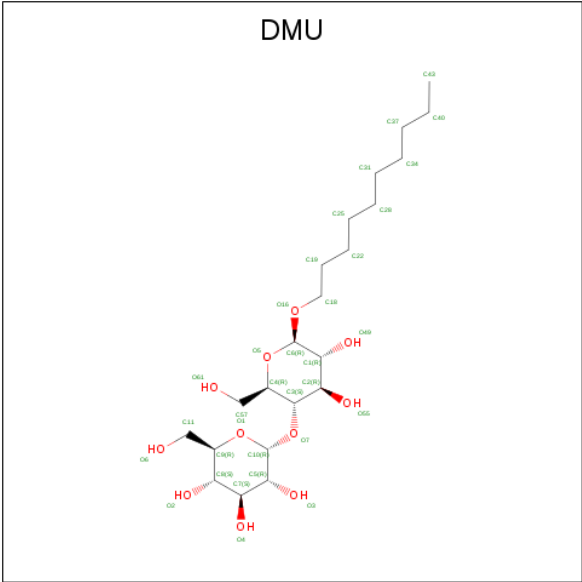
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
22	L	1	Total	C	O	0	0
			63	57	6		
22	N	1	Total	C	O	0	0
			63	57	6		
22	N	1	Total	C	O	0	0
			63	57	6		
22	O	1	Total	C	O	0	0
			63	57	6		

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



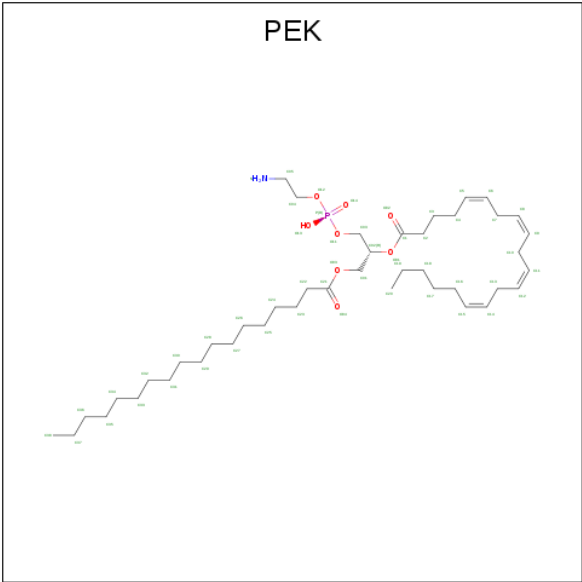
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
23	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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



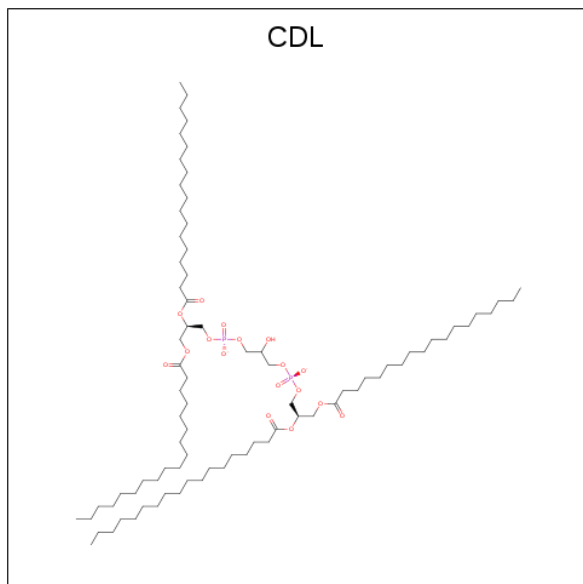
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			33	22	11		
24	M	1	Total	C	O	0	0
			33	22	11		
24	P	1	Total	C	O	0	0
			33	22	11		
24	Z	1	Total	C	O	0	0
			33	22	11		

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



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

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



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

- Molecule 27 is water.

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

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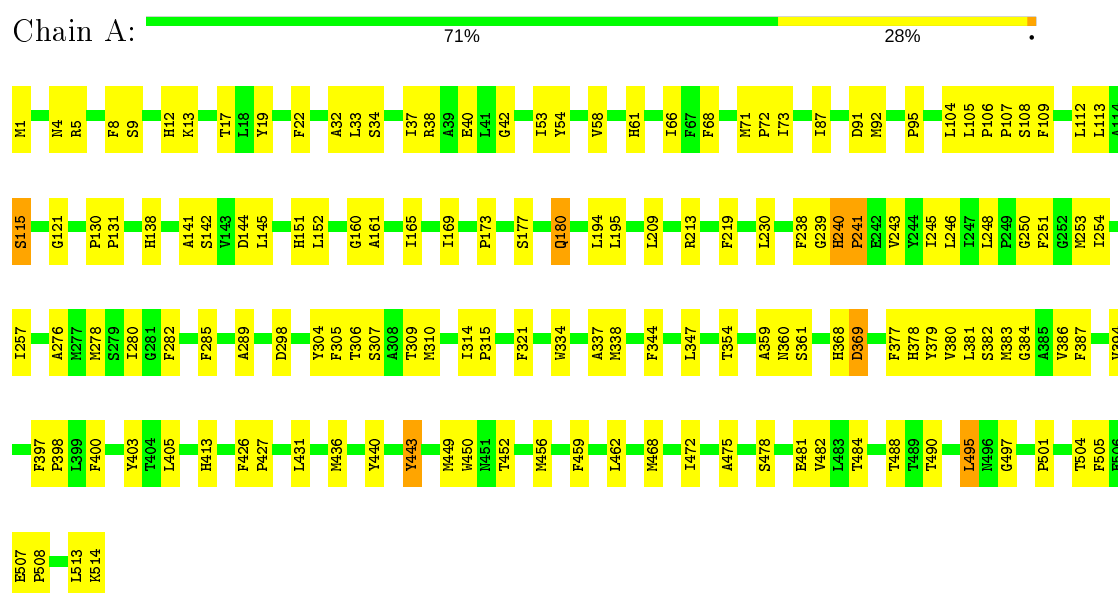
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	W	8	Total 8	O 8	0	0
27	X	18	Total 18	O 18	0	0
27	Y	14	Total 14	O 14	0	0
27	Z	11	Total 11	O 11	0	0

3 Residue-property plots

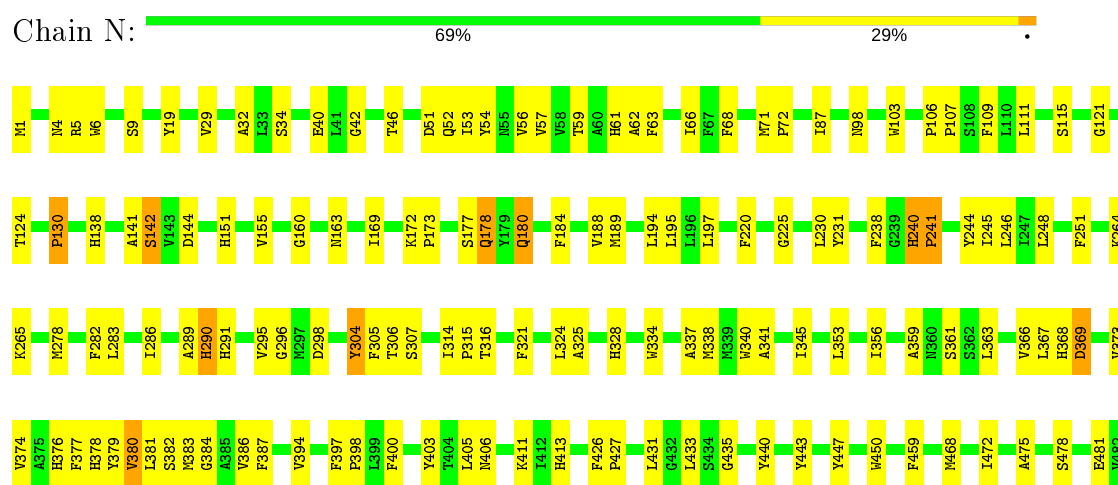
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: Cytochrome c oxidase subunit 1



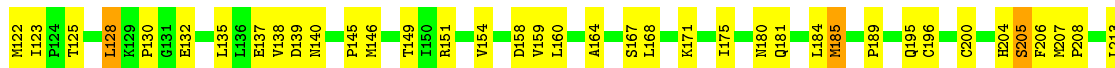
• Molecule 1: Cytochrome c oxidase subunit 1





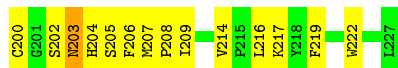
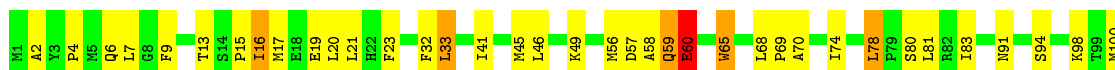
• Molecule 2: Cytochrome c oxidase subunit 2

Chain B: 65% 32%



• Molecule 2: Cytochrome c oxidase subunit 2

Chain O: 63% 34%



• Molecule 3: Cytochrome c oxidase subunit 3

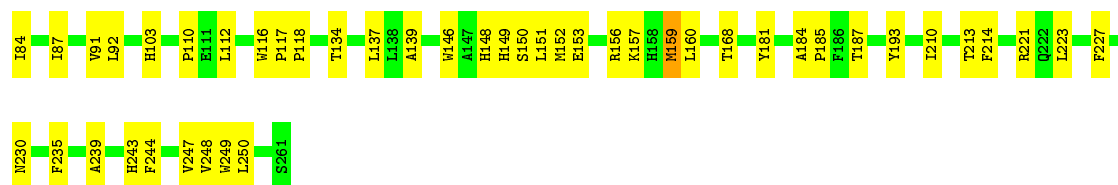
Chain C: 72% 26%



• Molecule 3: Cytochrome c oxidase subunit 3

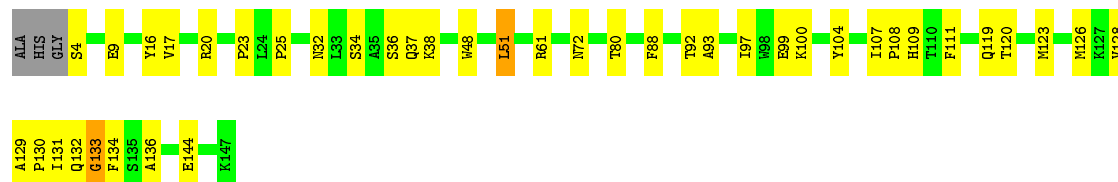
Chain P: 68% 30%





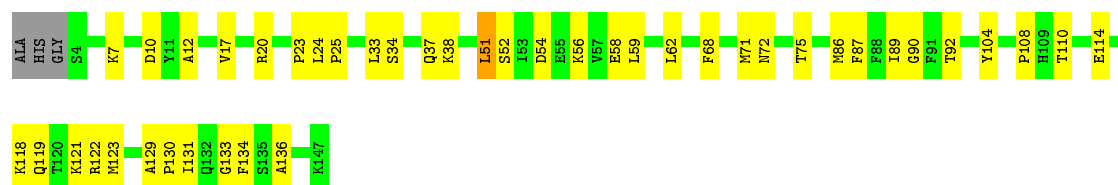
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain D: 70% 27% ..



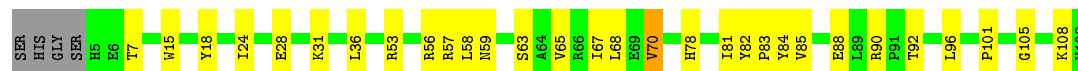
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

Chain Q: 69% 29% ..



- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain E: 69% 27% . .



- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain R: 81% 16% .




- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F: 67% 29% . .



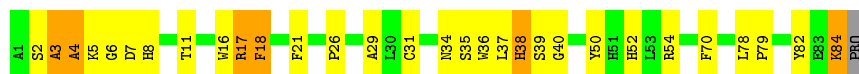
- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S:  77% 18% . .



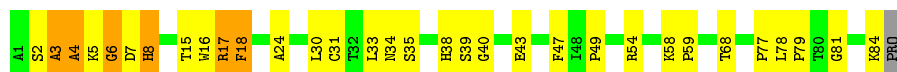
- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G:  64% 28% 7% .




- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T:  61% 31% 7% .



- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain H:  79% 11% 7% .



- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain U:  73% 20% 7% .




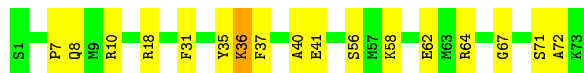
- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I:  78% 19% .




- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V:  77% 22% .



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain J:  78% 20% .



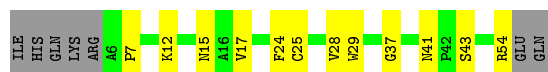
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain W:  75% 22% ..



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K:  66% 21% 13%



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X:  63% 25% 13%



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:  74% 23% .



- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y:  68% 28% ..



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain M:  63% 26% . 7%



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart

Chain Z:

67%

22%

•

7%



4 Data and refinement statistics

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

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.70	0/4156	0.78	1/5678 (0.0%)
1	N	0.64	0/4156	0.76	2/5678 (0.0%)
2	B	0.60	0/1860	0.83	1/2534 (0.0%)
2	O	0.59	0/1860	0.83	0/2534
3	C	0.68	0/2197	0.70	0/3005
3	P	0.63	0/2197	0.72	0/3005
4	D	0.60	0/1229	0.73	1/1658 (0.1%)
4	Q	0.64	0/1229	0.71	0/1658
5	E	0.62	0/871	0.73	0/1182
5	R	0.61	0/871	0.75	0/1182
6	F	0.60	0/765	0.86	2/1038 (0.2%)
6	S	0.59	0/765	0.86	2/1038 (0.2%)
7	G	0.61	0/690	0.77	1/937 (0.1%)
7	T	0.63	0/690	0.81	2/937 (0.2%)
8	H	0.64	0/682	0.71	0/921
8	U	0.57	0/682	0.72	0/921
9	I	0.62	0/605	0.70	0/802
9	V	0.60	0/605	0.68	0/802
10	J	0.59	0/471	0.74	0/636
10	W	0.59	0/471	0.73	0/636
11	K	0.71	0/398	0.75	0/546
11	X	0.59	0/398	0.74	0/546
12	L	0.63	0/393	0.69	0/526
12	Y	0.62	0/393	0.67	0/526
13	M	0.57	0/345	0.70	0/470
13	Z	0.60	0/345	0.70	0/470
All	All	0.63	0/29324	0.76	12/39866 (0.0%)

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

sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	N	0	5
2	B	0	1
2	O	0	1
All	All	0	10

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	S	94	HIS	N-CA-C	6.74	129.20	111.00
6	F	94	HIS	N-CA-C	6.46	128.43	111.00
2	B	128	LEU	CA-CB-CG	6.03	129.16	115.30
6	S	93	PRO	N-CA-C	5.74	127.02	112.10
7	T	33	LEU	CA-CB-CG	5.72	128.47	115.30
6	F	93	PRO	N-CA-C	5.72	126.98	112.10
7	T	6	GLY	N-CA-C	5.29	126.32	113.10
1	A	130	PRO	N-CA-C	-5.24	98.48	112.10
7	G	6	GLY	N-CA-C	5.12	125.89	113.10
4	D	133	GLY	N-CA-C	5.05	125.72	113.10
1	N	435	GLY	N-CA-C	5.03	125.68	113.10
1	N	130	PRO	N-CA-C	-5.00	99.09	112.10

There are no chirality outliers.

All (10) planarity outliers are listed below:

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

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	130	0
1	N	4027	0	4001	145	0
2	B	1824	0	1833	66	0
2	O	1824	0	1833	85	0
3	C	2110	0	2027	66	0
3	P	2110	0	2027	76	0
4	D	1195	0	1183	34	0
4	Q	1195	0	1183	37	0
5	E	852	0	845	23	0
5	R	852	0	845	11	0
6	F	748	0	728	24	0
6	S	748	0	728	16	0
7	G	675	0	644	35	0
7	T	675	0	644	40	0
8	H	662	0	623	8	0
8	U	662	0	623	14	0
9	I	601	0	613	14	0
9	V	601	0	613	16	0
10	J	460	0	459	12	0
10	W	460	0	459	11	0
11	K	384	0	366	8	0
11	X	384	0	366	9	0
12	L	380	0	380	21	0
12	Y	380	0	380	14	0
13	M	335	0	352	10	0
13	Z	335	0	352	11	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	F	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	S	1	0	0	0	0
18	A	120	0	108	9	0
18	N	120	0	108	12	0
19	A	51	0	76	7	0
19	C	153	0	228	12	0
19	N	51	0	76	10	0
19	P	153	0	228	11	0
20	A	29	0	39	1	0
20	B	29	0	39	1	0
20	C	29	0	39	2	0
20	J	29	0	37	5	0
20	N	29	0	39	2	0
20	P	29	0	39	2	0
20	W	58	0	76	5	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	63	0	110	6	0
22	D	63	0	110	5	0
22	L	63	0	110	27	0
22	N	126	0	220	22	0
22	O	63	0	110	8	0
23	B	52	0	80	19	0
23	O	52	0	80	18	0
24	C	33	0	36	3	0
24	M	33	0	38	1	0
24	P	33	0	37	4	0
24	Z	33	0	38	0	0
25	C	106	0	154	17	0
25	G	53	0	77	9	0
25	P	106	0	154	18	0
25	T	53	0	77	14	0
26	C	100	0	156	19	0
26	G	100	0	156	22	0
26	P	100	0	156	13	0
26	T	100	0	156	23	0
27	A	182	0	0	9	0
27	B	96	0	0	2	0
27	C	82	0	0	5	0
27	D	61	0	0	7	0
27	E	43	0	0	4	0
27	F	52	0	0	5	0
27	G	37	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	H	35	0	0	1	0
27	I	22	0	0	2	0
27	J	12	0	0	1	0
27	K	12	0	0	2	0
27	L	13	0	0	0	0
27	M	13	0	0	2	0
27	N	171	0	0	14	0
27	O	79	0	0	4	0
27	P	73	0	0	0	0
27	Q	42	0	0	1	0
27	R	30	0	0	2	0
27	S	42	0	0	0	0
27	T	30	0	0	3	0
27	U	30	0	0	0	0
27	V	19	0	0	3	0
27	W	8	0	0	0	0
27	X	18	0	0	1	0
27	Y	14	0	0	0	0
27	Z	11	0	0	2	0
All	All	31961	0	31295	945	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 15.

All (945) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:33:ARG:HG2	20:W:1060:CHD:H152	1.29	1.14
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.19	1.07
3:P:63:ARG:HE	26:P:1270:CDL:HA22	1.30	0.97
23:O:1230:PSC:H142	23:O:1230:PSC:H343	1.46	0.97
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.49	0.95
23:B:230:PSC:H142	23:B:230:PSC:H343	1.51	0.93
4:D:34:SER:H	4:D:37:GLN:HE21	1.04	0.93
7:G:84:LYS:HD2	7:G:84:LYS:H	1.33	0.93
7:T:84:LYS:HD2	7:T:84:LYS:H	1.34	0.92
7:G:31:CYS:SG	26:G:269:CDL:H532	2.10	0.92
6:S:94:HIS:CD2	6:S:95:GLN:H	1.89	0.90
12:L:20:ARG:HH12	22:L:522:TGL:HC61	1.34	0.90
26:T:1269:CDL:H231	26:T:1269:CDL:H541	1.54	0.90
26:G:269:CDL:H541	26:G:269:CDL:H231	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:L:522:TGL:HC62	22:L:522:TGL:HC22	1.55	0.88
25:C:264:PEK:H161	25:C:264:PEK:H102	1.54	0.88
1:N:151:HIS:CD2	25:P:1264:PEK:H382	2.09	0.88
23:O:1230:PSC:H071	9:V:10:ARG:HE	1.39	0.88
7:G:5:LYS:HG3	25:G:1263:PEK:H383	1.57	0.87
10:J:33:ARG:HG2	20:J:60:CHD:H152	1.56	0.85
22:N:1522:TGL:HC62	22:N:1522:TGL:HC22	1.60	0.84
22:L:522:TGL:H242	22:L:522:TGL:H202	1.60	0.83
7:G:5:LYS:HB2	25:G:1263:PEK:H362	1.60	0.83
4:D:34:SER:H	4:D:37:GLN:NE2	1.77	0.82
1:N:151:HIS:HD2	25:P:1264:PEK:H382	1.44	0.82
1:N:472:ILE:HG21	22:N:1522:TGL:HA92	1.59	0.82
25:P:1264:PEK:H102	25:P:1264:PEK:H161	1.62	0.81
1:N:225:GLY:HA3	3:P:112:LEU:HD21	1.61	0.81
4:D:120:THR:HA	27:D:4164:HOH:O	1.78	0.81
7:G:5:LYS:HD3	1:N:278:MET:HB3	1.64	0.80
7:T:31:CYS:SG	26:T:1269:CDL:H532	2.21	0.80
22:N:1522:TGL:H242	22:N:1522:TGL:H202	1.63	0.79
12:L:13:PHE:HA	22:L:522:TGL:HC31	1.63	0.79
2:O:41:ILE:HD13	23:O:1230:PSC:H342	1.63	0.79
2:O:15:PRO:HD2	27:O:3142:HOH:O	1.83	0.79
26:G:269:CDL:H622	19:P:1268:PGV:H152	1.62	0.79
1:A:472:ILE:HG21	22:L:522:TGL:HA92	1.64	0.79
13:M:42:LYS:HE3	13:M:42:LYS:HA	1.64	0.79
23:O:1230:PSC:H222	23:O:1230:PSC:H21	1.64	0.78
3:C:80:ARG:NH1	25:T:263:PEK:H032	1.99	0.78
22:N:1522:TGL:HC31	12:Y:13:PHE:HA	1.64	0.78
12:L:24:MET:SD	22:L:522:TGL:H162	2.24	0.78
22:N:1522:TGL:H361	22:N:1522:TGL:HB91	1.66	0.78
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.32	0.78
23:B:230:PSC:H222	23:B:230:PSC:H21	1.66	0.77
3:C:80:ARG:HH11	25:T:263:PEK:H032	1.48	0.77
7:T:3:ALA:HB1	25:T:263:PEK:H382	1.65	0.77
22:B:521:TGL:H281	22:B:521:TGL:H102	1.67	0.76
3:C:160:LEU:HD13	20:C:271:CHD:H181	1.68	0.76
22:B:521:TGL:C28	22:B:521:TGL:H102	2.15	0.76
12:L:20:ARG:NH1	22:L:522:TGL:HC61	2.00	0.76
22:O:1521:TGL:H102	22:O:1521:TGL:C28	2.15	0.76
26:P:1270:CDL:H642	26:P:1270:CDL:H191	1.67	0.76
7:T:47:PHE:CD2	7:T:81:GLY:HA2	2.22	0.75
4:Q:130:PRO:HG2	4:Q:131:ILE:HD12	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.21	0.74
22:O:1521:TGL:H102	22:O:1521:TGL:H281	1.67	0.74
19:C:268:PGV:H152	26:T:1269:CDL:H622	1.70	0.74
26:C:270:CDL:H642	26:C:270:CDL:H191	1.67	0.74
6:F:51:SER:HB2	6:F:91:LEU:HD11	1.70	0.74
3:C:168:THR:HG22	25:C:265:PEK:H14	1.70	0.74
1:N:1:FME:HCN	1:N:4:ASN:H	1.53	0.73
27:A:4014:HOH:O	12:L:3:TYR:HB3	1.88	0.73
22:B:521:TGL:H201	22:B:521:TGL:H241	1.71	0.73
26:G:269:CDL:H541	26:G:269:CDL:C23	2.20	0.72
1:A:1:FME:HCN	1:A:4:ASN:H	1.54	0.72
3:P:168:THR:HG22	25:P:1265:PEK:H14	1.72	0.72
2:B:41:ILE:HD13	23:B:230:PSC:H342	1.71	0.71
3:P:168:THR:HG21	25:P:1265:PEK:H12	1.71	0.71
4:D:130:PRO:HG2	4:D:131:ILE:HD12	1.72	0.71
7:T:38:HIS:NE2	26:T:1269:CDL:H111	2.05	0.70
1:A:278:MET:SD	7:T:5:LYS:HB3	2.31	0.70
22:O:1521:TGL:H201	22:O:1521:TGL:H241	1.73	0.70
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.74	0.70
1:A:160:GLY:HA3	27:A:2064:HOH:O	1.91	0.70
1:A:377:PHE:CD1	18:A:516:HEA:HAD1	2.27	0.69
3:P:47:LEU:O	3:P:51:MET:HG2	1.92	0.69
12:L:20:ARG:HH22	22:L:522:TGL:HC61	1.55	0.69
1:A:87:ILE:O	1:A:173:PRO:HD3	1.91	0.69
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.75	0.69
3:C:149:HIS:HA	3:C:152:MET:HE2	1.74	0.69
7:G:5:LYS:HB3	1:N:278:MET:SD	2.33	0.69
1:A:484:THR:HB	13:M:2:THR:OG1	1.92	0.68
1:N:296:GLY:HA2	8:U:23:GLN:OE1	1.93	0.68
6:F:92:VAL:HG23	6:F:92:VAL:O	1.94	0.68
10:J:12:PHE:O	10:J:23:LYS:HE2	1.94	0.68
26:G:269:CDL:H522	26:G:269:CDL:H202	1.76	0.68
1:N:472:ILE:HG21	22:N:1522:TGL:CA9	2.22	0.68
3:P:34:TRP:CZ2	24:P:1272:DMU:H29	2.28	0.68
7:T:5:LYS:HG3	25:T:263:PEK:H383	1.76	0.68
5:E:68:LEU:HD12	5:E:101:PRO:HD3	1.76	0.68
3:C:210:ILE:HG23	19:C:267:PGV:H102	1.75	0.67
3:P:160:LEU:HD13	20:W:1271:CHD:H181	1.76	0.67
4:D:48:TRP:HA	4:D:51:LEU:HD22	1.77	0.67
4:D:16:TYR:CE1	4:D:25:PRO:HG2	2.29	0.67
1:N:177:SER:H	1:N:180:GLN:HE21	1.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:41:ILE:CD1	23:O:1230:PSC:H342	2.24	0.67
12:Y:20:ARG:HB3	12:Y:20:ARG:HH11	1.59	0.67
3:C:67:PHE:HE1	26:C:270:CDL:H1	1.59	0.67
26:T:1269:CDL:H541	26:T:1269:CDL:C23	2.24	0.67
8:U:49:ASP:O	8:U:52:VAL:HG22	1.95	0.67
26:C:270:CDL:H431	27:J:4266:HOH:O	1.95	0.67
3:P:148:HIS:CE1	3:P:152:MET:SD	2.87	0.66
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.30	0.66
1:N:514:LYS:HE3	27:N:3395:HOH:O	1.94	0.66
1:N:328:HIS:O	2:O:56:MET:HE1	1.95	0.66
12:Y:26:THR:HG23	13:Z:25:SER:HB2	1.77	0.66
7:T:47:PHE:CE2	7:T:81:GLY:HA2	2.31	0.66
1:A:219:PHE:HE2	3:C:196:THR:HG22	1.60	0.66
3:C:168:THR:CG2	25:C:265:PEK:H14	2.25	0.66
3:P:34:TRP:HZ2	24:P:1272:DMU:H29	1.61	0.66
4:D:34:SER:N	4:D:37:GLN:HE21	1.87	0.65
2:B:98:LYS:HD3	8:H:63:LEU:O	1.95	0.65
7:T:34:ASN:ND2	26:T:1269:CDL:H151	2.11	0.65
9:V:58:LYS:O	9:V:62:GLU:HG3	1.96	0.65
7:G:3:ALA:HB1	25:G:1263:PEK:H382	1.78	0.65
19:N:1524:PGV:H322	13:Z:19:LEU:HD23	1.79	0.65
2:O:160:LEU:HD23	2:O:176:PRO:HD2	1.78	0.65
3:P:67:PHE:HE1	26:P:1270:CDL:H1	1.61	0.65
3:P:80:ARG:O	3:P:84:ILE:HD12	1.96	0.65
1:A:32:ALA:HB3	12:L:36:PRO:HG2	1.78	0.65
1:A:73:ILE:HD11	18:A:515:HEA:H22	1.79	0.65
1:N:440:TYR:HE2	2:O:204:HIS:CE1	2.15	0.65
6:S:94:HIS:CD2	6:S:95:GLN:N	2.62	0.65
7:G:2:SER:OG	25:G:1263:PEK:H301	1.96	0.64
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.79	0.64
19:N:1524:PGV:H062	27:Z:3160:HOH:O	1.96	0.64
3:P:210:ILE:HG23	19:P:1267:PGV:H102	1.79	0.64
19:C:267:PGV:H182	26:C:270:CDL:H673	1.80	0.64
1:N:334:TRP:CZ3	22:N:1523:TGL:HA51	2.33	0.64
22:L:522:TGL:HB91	22:L:522:TGL:H361	1.80	0.64
26:G:269:CDL:HB32	1:N:304:TYR:HD1	1.61	0.64
19:A:524:PGV:H062	27:M:2160:HOH:O	1.98	0.64
3:C:34:TRP:HZ2	24:C:272:DMU:H29	1.63	0.64
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.79	0.64
1:A:33:LEU:HD23	12:L:36:PRO:HB3	1.78	0.63
12:L:20:ARG:NH2	22:L:522:TGL:HC32	2.14	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:1269:CDL:H172	26:T:1269:CDL:H511	1.80	0.63
5:E:57:ARG:HH11	5:E:57:ARG:HG3	1.63	0.63
1:N:381:LEU:HD13	18:N:516:HEA:HBC2	1.81	0.63
6:F:1:ALA:HB2	27:N:4346:HOH:O	1.99	0.63
5:R:87:GLN:HG2	5:R:88:GLU:N	2.13	0.63
2:B:184:LEU:HD23	2:B:185:MET:N	2.14	0.63
1:N:376:HIS:O	1:N:380:VAL:HG22	1.98	0.63
22:O:1521:TGL:HC92	27:O:4117:HOH:O	1.99	0.63
4:Q:130:PRO:O	4:Q:136:ALA:HB2	1.99	0.62
1:N:341:ALA:O	1:N:345:ILE:HG13	2.00	0.62
23:O:1230:PSC:H142	23:O:1230:PSC:C34	2.27	0.62
12:L:20:ARG:NH2	22:L:522:TGL:HC61	2.14	0.62
23:O:1230:PSC:C07	9:V:10:ARG:HE	2.09	0.62
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.30	0.62
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.82	0.62
23:B:230:PSC:H072	9:I:10:ARG:HH21	1.65	0.62
7:G:37:LEU:HD21	26:G:269:CDL:H361	1.81	0.62
1:A:354:THR:HG21	27:A:2228:HOH:O	1.99	0.62
1:A:368:HIS:CD2	1:A:369:ASP:HB2	2.34	0.62
1:N:406:ASN:HD21	19:N:1524:PGV:C2	2.13	0.62
1:A:452:THR:O	1:A:456:MET:HG3	1.99	0.62
26:G:269:CDL:H511	26:G:269:CDL:H172	1.81	0.62
26:T:1269:CDL:H522	26:T:1269:CDL:H202	1.80	0.62
3:P:25:LEU:O	3:P:29:SER:HB2	2.01	0.61
1:N:321:PHE:CD2	23:O:1230:PSC:H341	2.36	0.61
1:A:472:ILE:HG21	22:L:522:TGL:CA9	2.30	0.61
1:N:87:ILE:O	1:N:173:PRO:HD3	2.00	0.61
6:F:85:CYS:SG	6:F:87:THR:HG23	2.41	0.61
1:N:324:LEU:HD13	2:O:41:ILE:HG22	1.82	0.61
6:S:22:LEU:O	6:S:25:ARG:HB3	2.00	0.61
1:A:306:THR:HG23	1:A:359:ALA:O	2.01	0.61
19:A:524:PGV:H311	13:M:16:ALA:HA	1.82	0.61
3:C:25:LEU:O	3:C:29:SER:HB2	2.01	0.61
19:N:1524:PGV:H311	13:Z:16:ALA:HA	1.83	0.61
1:N:160:GLY:HA3	27:N:3064:HOH:O	2.00	0.61
12:L:20:ARG:HH22	22:L:522:TGL:HC32	1.65	0.61
2:O:163:TRP:NE1	2:O:209:ILE:HG12	2.15	0.61
2:B:99:THR:HG23	2:B:154:VAL:HG13	1.83	0.60
22:N:1523:TGL:H271	2:O:46:LEU:HD12	1.83	0.60
3:P:168:THR:CG2	25:P:1265:PEK:H14	2.31	0.60
8:H:60:TYR:C	8:H:60:TYR:CD1	2.74	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:68:LEU:CB	2:O:69:PRO:HD3	2.31	0.60
1:A:253:MET:O	1:A:257:ILE:HG13	2.01	0.60
7:G:84:LYS:H	7:G:84:LYS:CD	2.07	0.60
2:O:32:PHE:HE2	22:O:1521:TGL:HB91	1.66	0.60
12:Y:20:ARG:NH1	12:Y:20:ARG:HB3	2.15	0.60
3:C:47:LEU:O	3:C:51:MET:HG2	2.00	0.60
24:P:1272:DMU:H25	25:P:1264:PEK:H341	1.84	0.60
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.37	0.60
6:F:8:THR:OG1	6:F:11:GLU:HG3	2.01	0.60
2:B:123:ILE:HG22	2:B:128:LEU:HD23	1.84	0.60
6:S:16:LEU:O	6:S:20:VAL:HG23	2.01	0.60
3:C:28:THR:HG22	19:C:266:PGV:H182	1.84	0.59
2:B:65:TRP:CZ3	23:B:230:PSC:H331	2.37	0.59
23:B:230:PSC:H032	27:E:2129:HOH:O	2.02	0.59
1:N:367:LEU:HD21	1:N:433:LEU:HD23	1.84	0.59
1:N:5:ARG:O	1:N:9:SER:HB2	2.01	0.59
2:O:116:LEU:HD21	2:O:222:TRP:CH2	2.37	0.59
1:A:151:HIS:CD2	25:C:264:PEK:H382	2.37	0.59
4:D:20:ARG:HG2	4:D:72:ASN:HD21	1.68	0.59
4:D:9:GLU:CD	4:D:9:GLU:H	2.05	0.59
19:P:1267:PGV:H182	26:P:1270:CDL:H673	1.85	0.59
1:N:240:HIS:HB3	1:N:241:PRO:HD3	1.84	0.59
1:A:488:THR:HB	1:A:495:LEU:HD13	1.84	0.59
1:N:289:ALA:HB3	1:N:305:PHE:CD1	2.37	0.59
4:Q:20:ARG:HD2	4:Q:72:ASN:OD1	2.03	0.59
3:C:40:MET:O	3:C:44:MET:HG2	2.01	0.59
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.00	0.59
2:B:145:PRO:HA	2:B:214:VAL:O	2.03	0.58
3:C:122:HIS:HB3	27:C:4324:HOH:O	2.02	0.58
3:C:34:TRP:CZ2	24:C:272:DMU:H29	2.37	0.58
8:H:46:LYS:HB2	8:U:52:VAL:HG12	1.85	0.58
22:B:521:TGL:HC22	27:I:2383:HOH:O	2.02	0.58
10:W:16:ASN:ND2	10:W:18:LEU:HD12	2.19	0.58
2:B:15:PRO:HB2	27:B:4350:HOH:O	2.04	0.58
1:N:378:HIS:O	1:N:382:SER:HB2	2.02	0.58
3:P:250:LEU:HD22	26:T:1269:CDL:C67	2.34	0.58
1:A:508:PRO:HD2	3:C:5:THR:OG1	2.04	0.58
7:G:2:SER:O	25:G:1263:PEK:H322	2.04	0.58
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.67	0.58
2:B:122:MET:SD	2:B:206:PHE:HB3	2.43	0.58
6:F:51:SER:CB	6:F:91:LEU:HD11	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:CD2	12:L:36:PRO:HB3	2.34	0.58
1:A:361:SER:OG	2:B:84:LEU:HD13	2.04	0.58
1:N:177:SER:H	1:N:180:GLN:NE2	2.00	0.57
1:N:377:PHE:HA	1:N:380:VAL:CG2	2.34	0.57
3:P:40:MET:O	3:P:44:MET:HG2	2.03	0.57
7:G:17:ARG:HD2	27:N:2309:HOH:O	2.04	0.57
2:O:134:ARG:HD3	4:Q:110:THR:OG1	2.04	0.57
2:O:7:LEU:HD11	22:O:1521:TGL:H161	1.86	0.57
27:B:4027:HOH:O	25:P:1265:PEK:H292	2.03	0.57
1:N:6:TRP:CD2	12:Y:12:PRO:HB3	2.39	0.57
3:P:41:THR:O	3:P:45:ILE:HG13	2.04	0.57
2:B:164:ALA:HB2	2:B:171:LYS:HG3	1.85	0.57
1:N:51:ASP:OD1	2:O:206:PHE:HE1	1.88	0.57
7:T:8:HIS:HE1	27:T:4411:HOH:O	1.86	0.57
19:C:267:PGV:H172	26:C:270:CDL:H662	1.86	0.57
9:I:36:LYS:HA	9:I:40:ALA:HB3	1.87	0.57
12:L:20:ARG:HH22	22:L:522:TGL:CC6	2.17	0.57
22:N:1522:TGL:C24	22:N:1522:TGL:H202	2.34	0.57
1:N:368:HIS:CD2	1:N:369:ASP:HB2	2.40	0.57
10:W:16:ASN:OD1	10:W:23:LYS:HE3	2.04	0.57
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.86	0.57
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.40	0.57
22:B:521:TGL:H222	22:B:521:TGL:HA82	1.87	0.56
2:O:146:MET:SD	2:O:189:PRO:HB3	2.45	0.56
11:K:24:PHE:O	11:K:28:VAL:HG12	2.04	0.56
12:Y:21:LEU:O	12:Y:25:MET:HG3	2.05	0.56
22:D:523:TGL:HC61	27:D:4382:HOH:O	2.05	0.56
26:G:269:CDL:C54	26:G:269:CDL:H231	2.33	0.56
22:L:522:TGL:C24	22:L:522:TGL:H202	2.34	0.56
6:S:54:ASN:HD22	6:S:54:ASN:C	2.08	0.56
1:A:177:SER:H	1:A:180:GLN:HE21	1.54	0.56
22:O:1521:TGL:HA82	22:O:1521:TGL:H222	1.87	0.56
1:A:42:GLY:HA3	4:D:104:TYR:OH	2.05	0.56
1:A:397:PHE:HB3	1:A:398:PRO:HD3	1.86	0.56
4:D:107:ILE:HD12	4:D:111:PHE:CD1	2.41	0.56
2:B:56:MET:HG2	23:B:230:PSC:H211	1.87	0.56
2:O:9:PHE:HB2	2:O:21:LEU:HD21	1.88	0.56
7:G:50:TYR:HB3	7:G:52:HIS:CE1	2.40	0.56
10:J:40:LEU:HD12	20:J:60:CHD:H183	1.87	0.56
1:N:406:ASN:HD21	19:N:1524:PGV:H22	1.70	0.56
2:B:135:LEU:HD22	2:B:206:PHE:CD2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:C:265:PEK:H371	26:G:269:CDL:H261	1.88	0.55
12:L:20:ARG:HH12	22:L:522:TGL:CC6	2.14	0.55
2:B:74:ILE:O	2:B:78:LEU:HD22	2.06	0.55
3:P:244:PHE:O	3:P:248:VAL:HG23	2.07	0.55
6:S:40:SER:OG	6:S:42:THR:HG23	2.06	0.55
1:N:481:GLU:HB2	13:Z:4:LYS:HE2	1.88	0.55
1:N:483:LEU:HD21	13:Z:4:LYS:HG2	1.88	0.55
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.89	0.55
22:N:1523:TGL:HC21	22:N:1523:TGL:HG11	1.89	0.55
1:A:66:ILE:HG23	1:A:246:LEU:HD21	1.87	0.55
25:C:264:PEK:C16	25:C:264:PEK:H102	2.33	0.55
3:P:87:ILE:O	3:P:91:VAL:HG23	2.06	0.55
1:A:379:TYR:O	1:A:383:MET:HB2	2.07	0.55
2:B:214:VAL:HB	2:B:215:PRO:CD	2.36	0.55
2:O:146:MET:CE	9:V:56:SER:HB2	2.37	0.55
1:A:306:THR:O	1:A:310:MET:HG3	2.07	0.55
5:E:24:ILE:O	5:E:58:LEU:HD21	2.05	0.55
1:N:431:LEU:HD21	1:N:450:TRP:HB2	1.88	0.55
6:S:94:HIS:CG	6:S:95:GLN:H	2.13	0.55
1:N:406:ASN:ND2	19:N:1524:PGV:H032	2.21	0.55
1:N:459:PHE:HB3	4:Q:92:THR:CG2	2.37	0.55
26:C:270:CDL:C19	26:C:270:CDL:H642	2.37	0.55
12:L:20:ARG:CZ	22:L:522:TGL:HC61	2.37	0.55
6:S:13:ALA:O	6:S:18:ARG:HD2	2.07	0.55
1:A:405:LEU:HD23	1:A:475:ALA:HB2	1.89	0.54
6:F:18:ARG:HB3	27:F:4412:HOH:O	2.08	0.54
4:D:130:PRO:O	4:D:136:ALA:HB2	2.06	0.54
1:A:334:TRP:CZ3	22:D:523:TGL:HA51	2.42	0.54
23:B:230:PSC:H142	23:B:230:PSC:C34	2.31	0.54
3:C:146:TRP:CE2	7:G:17:ARG:HG3	2.42	0.54
19:N:1524:PGV:H152	19:N:1524:PGV:H321	1.89	0.54
1:N:440:TYR:HE2	2:O:204:HIS:NE2	2.05	0.54
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.37	0.54
23:B:230:PSC:C07	9:I:10:ARG:HH21	2.20	0.54
1:A:161:ALA:O	1:A:165:ILE:HG13	2.07	0.54
12:L:25:MET:HG2	22:L:522:TGL:HA62	1.90	0.54
2:O:98:LYS:HE3	2:O:109:GLU:HB2	1.90	0.54
9:V:36:LYS:HA	9:V:40:ALA:HB3	1.88	0.54
1:A:243:VAL:HA	1:A:246:LEU:HD12	1.89	0.54
5:E:57:ARG:NH1	5:E:57:ARG:HG3	2.23	0.54
1:A:115:SER:HA	1:A:145:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:63:GLU:HG3	27:F:4360:HOH:O	2.07	0.54
2:O:100:MET:HB2	2:O:107:SER:OG	2.08	0.54
1:A:282:PHE:HA	7:T:4:ALA:CB	2.38	0.54
1:N:380:VAL:O	1:N:384:GLY:HA3	2.07	0.54
1:A:377:PHE:O	1:A:381:LEU:HB3	2.08	0.53
25:C:265:PEK:H231	7:G:21:PHE:CD2	2.43	0.53
3:P:187:THR:HG22	25:P:1264:PEK:H052	1.90	0.53
1:A:34:SER:HB3	1:A:61:HIS:CE1	2.43	0.53
1:A:12:HIS:CD2	1:A:91:ASP:HA	2.43	0.53
1:N:197:LEU:O	3:P:92:LEU:HD12	2.08	0.53
2:B:114:GLU:HG3	2:B:227:LEU:HD11	1.90	0.53
22:L:522:TGL:H272	22:L:522:TGL:H231	1.91	0.53
2:O:56:MET:HA	23:O:1230:PSC:H202	1.91	0.53
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.91	0.53
3:P:66:THR:HG23	19:P:1267:PGV:O05	2.09	0.53
1:A:472:ILE:HD13	22:L:522:TGL:HA91	1.91	0.53
1:N:169:ILE:HD11	1:N:189:MET:SD	2.48	0.53
1:N:289:ALA:HB3	1:N:305:PHE:CG	2.44	0.53
2:O:203:ASN:HD22	2:O:203:ASN:N	2.05	0.53
3:P:157:LYS:NZ	25:P:1265:PEK:H052	2.23	0.53
1:N:459:PHE:HB3	4:Q:92:THR:HG23	1.90	0.53
11:K:25:CYS:O	11:K:29:TRP:HD1	1.92	0.53
22:N:1522:TGL:HC21	22:N:1522:TGL:OA1	2.08	0.53
3:C:168:THR:HG21	25:C:265:PEK:H12	1.89	0.53
1:N:314:ILE:HB	1:N:315:PRO:CD	2.39	0.53
1:N:400:PHE:HB3	22:N:1522:TGL:H283	1.91	0.53
3:P:250:LEU:HD22	26:T:1269:CDL:H673	1.90	0.53
3:C:80:ARG:HH11	25:T:263:PEK:C03	2.18	0.53
5:E:53:ARG:NH2	5:E:92:THR:HG23	2.23	0.53
26:P:1270:CDL:H642	26:P:1270:CDL:C19	2.38	0.52
1:A:240:HIS:O	1:A:243:VAL:HG22	2.09	0.52
1:A:347:LEU:HD13	1:A:383:MET:SD	2.49	0.52
3:C:51:MET:SD	26:C:270:CDL:H622	2.49	0.52
2:O:122:MET:SD	2:O:206:PHE:HB3	2.49	0.52
2:O:74:ILE:O	2:O:78:LEU:HD22	2.10	0.52
2:O:146:MET:HE3	9:V:56:SER:HB2	1.91	0.52
4:Q:131:ILE:HD12	4:Q:131:ILE:N	2.25	0.52
1:A:165:ILE:O	1:A:169:ILE:HG12	2.08	0.52
4:Q:134:PHE:HE1	11:X:44:PRO:HD2	1.74	0.52
2:B:23:PHE:CZ	2:B:80:SER:HB2	2.44	0.52
3:C:68:GLN:HB2	3:C:70:HIS:HD2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:440:TYR:CG	2:B:205:SER:HB3	2.45	0.52
7:G:79:PRO:HD2	27:G:2136:HOH:O	2.10	0.52
10:J:12:PHE:HD2	10:J:23:LYS:HG2	1.75	0.52
1:N:468:MET:HG2	1:N:468:MET:O	2.09	0.52
2:O:145:PRO:HB2	2:O:148:MET:HG3	1.90	0.52
11:X:31:TYR:HB2	27:X:4091:HOH:O	2.08	0.52
1:N:52:GLN:O	1:N:56:VAL:HG23	2.10	0.52
2:O:121:TYR:O	2:O:138:VAL:HA	2.09	0.52
1:A:33:LEU:HB3	1:A:61:HIS:HB2	1.91	0.52
4:D:144:GLU:HB2	27:D:4097:HOH:O	2.10	0.52
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.92	0.52
1:A:248:LEU:O	1:A:251:PHE:HB2	2.10	0.52
1:A:40:GLU:HG2	1:A:54:TYR:CD2	2.45	0.52
11:K:7:PRO:O	11:K:12:LYS:HE3	2.10	0.52
22:L:522:TGL:OA1	22:L:522:TGL:HC21	2.10	0.52
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.91	0.51
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.92	0.51
7:G:34:ASN:O	7:G:37:LEU:HB3	2.09	0.51
7:G:34:ASN:HD22	26:G:269:CDL:H151	1.76	0.51
1:A:482:VAL:HG22	13:M:1:ILE:HD11	1.92	0.51
2:O:163:TRP:CD1	2:O:209:ILE:HG12	2.46	0.51
2:O:4:PRO:HB2	11:X:43:SER:HA	1.91	0.51
25:C:265:PEK:H22	27:C:4087:HOH:O	2.09	0.51
4:D:80:THR:HA	11:K:17:VAL:HG11	1.93	0.51
19:P:1267:PGV:H172	26:P:1270:CDL:H662	1.91	0.51
3:C:51:MET:SD	26:C:270:CDL:C62	2.99	0.51
1:N:62:ALA:HB2	18:N:515:HEA:HBD1	1.93	0.51
3:P:28:THR:HG22	19:P:1266:PGV:H182	1.91	0.51
1:A:314:ILE:HB	1:A:315:PRO:CD	2.41	0.51
22:D:523:TGL:HC21	22:D:523:TGL:HG11	1.92	0.51
5:E:84:TYR:O	5:E:88:GLU:HG2	2.10	0.51
26:G:269:CDL:H182	1:N:307:SER:CB	2.39	0.51
2:B:81:LEU:HD13	26:T:1269:CDL:H122	1.93	0.51
1:A:1:FME:HA	1:A:1:FME:CE	2.41	0.51
2:B:123:ILE:CG2	2:B:128:LEU:HD23	2.40	0.51
2:B:200:CYS:SG	2:B:204:HIS:HA	2.50	0.51
4:Q:52:SER:O	4:Q:56:LYS:HG3	2.10	0.51
2:O:222:TRP:HB2	9:V:71:SER:HB2	1.92	0.51
4:Q:118:LYS:HB3	11:X:53:TRP:HB3	1.93	0.51
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.91	0.51
3:P:62:ILE:HG23	3:P:221:ARG:HH21	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:THR:HG22	1:A:309:THR:O	2.10	0.51
1:A:459:PHE:O	1:A:462:LEU:HB3	2.11	0.51
7:G:31:CYS:HG	26:G:269:CDL:H532	1.74	0.51
1:N:151:HIS:O	1:N:155:VAL:HG23	2.11	0.51
1:N:411:LYS:HD3	22:N:1523:TGL:HB21	1.93	0.51
6:S:94:HIS:HD2	6:S:95:GLN:N	2.09	0.51
7:G:37:LEU:HD23	7:G:38:HIS:CE1	2.46	0.50
1:N:377:PHE:CD1	18:N:516:HEA:HAD1	2.46	0.50
1:A:398:PRO:HA	1:A:403:TYR:O	2.12	0.50
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.41	0.50
2:O:59:GLN:O	2:O:59:GLN:HG3	2.11	0.50
2:O:20:LEU:HD21	2:O:83:ILE:HG21	1.93	0.50
2:B:39:LEU:HD22	22:B:521:TGL:H141	1.92	0.50
6:F:47:ASN:HB2	6:F:89:TYR:CD1	2.46	0.50
1:N:115:SER:O	1:N:121:GLY:HA2	2.11	0.50
18:N:516:HEA:HMD1	18:N:516:HEA:HBD2	1.94	0.50
4:Q:129:ALA:HB1	4:Q:133:GLY:HA3	1.93	0.50
19:A:524:PGV:H321	19:A:524:PGV:H152	1.93	0.50
4:D:93:ALA:O	4:D:97:ILE:HG13	2.11	0.50
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.94	0.50
7:G:3:ALA:O	7:G:4:ALA:HB2	2.11	0.50
26:G:269:CDL:H182	1:N:307:SER:HB3	1.93	0.50
2:O:57:ASP:H	23:O:1230:PSC:H201	1.76	0.50
4:Q:58:GLU:O	4:Q:62:LEU:HG	2.11	0.50
1:A:382:SER:O	1:A:386:VAL:HB	2.12	0.50
3:P:65:SER:HB2	19:P:1267:PGV:H041	1.94	0.50
5:R:8:ASP:HB3	9:V:10:ARG:CZ	2.41	0.50
1:A:240:HIS:HB3	1:A:241:PRO:HD3	1.93	0.50
3:C:157:LYS:NZ	25:C:265:PEK:H052	2.27	0.50
2:B:4:PRO:HB2	11:K:43:SER:HA	1.94	0.50
6:F:81:ARG:HG2	6:F:88:HIS:CD2	2.46	0.50
4:Q:75:THR:HG22	27:Q:4352:HOH:O	2.11	0.50
1:N:29:VAL:HG22	12:Y:32:GLY:O	2.12	0.50
19:A:524:PGV:P	19:A:524:PGV:H061	2.52	0.49
1:A:37:ILE:HD11	1:A:58:VAL:HA	1.93	0.49
1:N:298:ASP:HB3	27:N:3389:HOH:O	2.12	0.49
3:C:212:SER:O	3:C:216:ILE:HG13	2.11	0.49
4:D:34:SER:O	4:D:38:LYS:HG3	2.12	0.49
7:G:18:PHE:O	7:G:18:PHE:HD2	1.95	0.49
1:N:440:TYR:CE2	2:O:204:HIS:NE2	2.80	0.49
4:Q:90:GLY:O	11:X:28:VAL:HG11	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:C:267:PGV:H161	19:C:267:PGV:H12	1.94	0.49
6:S:92:VAL:HG23	6:S:92:VAL:O	2.12	0.49
7:T:17:ARG:HD2	27:T:3309:HOH:O	2.11	0.49
3:P:239:ALA:O	3:P:243:HIS:CD2	2.65	0.49
1:A:131:PRO:HG3	27:A:4333:HOH:O	2.13	0.49
1:A:5:ARG:O	1:A:9:SER:HB2	2.12	0.49
23:B:230:PSC:O01	23:B:230:PSC:H212	2.12	0.49
4:D:48:TRP:CH2	5:E:56:ARG:HA	2.47	0.49
4:Q:12:ALA:HA	6:S:73:TRP:CD1	2.48	0.49
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.78	0.49
2:O:56:MET:HA	23:O:1230:PSC:C20	2.42	0.49
1:A:304:TYR:HD1	26:T:1269:CDL:HB32	1.77	0.49
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.94	0.49
2:B:214:VAL:HB	2:B:215:PRO:HD2	1.95	0.49
25:G:1263:PEK:H9	3:P:244:PHE:HA	1.93	0.49
1:N:405:LEU:HD23	1:N:475:ALA:HB2	1.95	0.49
1:A:195:LEU:CD2	1:A:245:ILE:HD13	2.43	0.49
1:N:377:PHE:HA	1:N:380:VAL:HG23	1.93	0.49
9:V:67:GLY:HA2	27:V:3310:HOH:O	2.11	0.49
25:C:265:PEK:C38	26:G:269:CDL:H273	2.43	0.49
26:G:269:CDL:HA62	26:G:269:CDL:H322	1.93	0.49
9:I:23:GLY:O	9:I:27:VAL:HG23	2.13	0.49
19:N:1524:PGV:H012	27:N:4191:HOH:O	2.11	0.49
1:N:381:LEU:CD1	18:N:516:HEA:HBC2	2.42	0.49
7:T:78:LEU:HB3	7:T:79:PRO:HD2	1.94	0.49
3:P:50:ASN:O	3:P:54:MET:HG3	2.13	0.49
1:A:383:MET:O	1:A:387:PHE:HB2	2.12	0.48
1:N:71:MET:HE3	1:N:195:LEU:HD21	1.95	0.48
1:N:398:PRO:HA	1:N:403:TYR:O	2.12	0.48
2:O:172:THR:HG21	2:O:180:ASN:HB3	1.94	0.48
4:Q:33:LEU:HA	4:Q:37:GLN:NE2	2.28	0.48
1:N:507:GLU:HG3	3:P:5:THR:OG1	2.13	0.48
1:A:380:VAL:O	1:A:384:GLY:HA3	2.13	0.48
2:B:93:PRO:HA	2:B:149:THR:HG22	1.94	0.48
7:G:78:LEU:HB3	7:G:79:PRO:CD	2.42	0.48
1:N:115:SER:HB2	1:N:142:SER:O	2.13	0.48
3:P:59:ARG:HG3	26:P:1270:CDL:H512	1.94	0.48
26:T:1269:CDL:H322	26:T:1269:CDL:HA62	1.95	0.48
1:A:449:MET:SD	2:B:5:MET:HG2	2.53	0.48
10:J:31:LEU:HD12	10:J:31:LEU:HA	1.66	0.48
23:O:1230:PSC:O01	23:O:1230:PSC:H212	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.48	0.48
4:Q:129:ALA:HB3	4:Q:134:PHE:H	1.77	0.48
2:B:135:LEU:HD22	2:B:206:PHE:HD2	1.77	0.48
1:N:337:ALA:HB2	1:N:394:VAL:HG23	1.96	0.48
2:O:2:ALA:HA	2:O:6:GLN:OE1	2.13	0.48
2:B:151:ARG:CD	2:B:181:GLN:HE21	2.26	0.48
2:O:156:SER:HB3	2:O:176:PRO:HD3	1.96	0.48
3:P:151:LEU:HB2	3:P:159:MET:HG3	1.95	0.48
3:P:16:TRP:HA	3:P:16:TRP:CE3	2.49	0.48
4:Q:33:LEU:HB2	4:Q:38:LYS:HG2	1.94	0.48
1:A:104:LEU:C	1:A:107:PRO:HD2	2.34	0.48
1:A:115:SER:HB2	1:A:142:SER:O	2.14	0.48
2:B:41:ILE:CD1	23:B:230:PSC:H342	2.41	0.48
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.01	0.48
1:N:68:PHE:C	1:N:72:PRO:HG2	2.34	0.48
6:F:95:GLN:HG3	27:F:4316:HOH:O	2.13	0.48
19:P:1267:PGV:H161	19:P:1267:PGV:H12	1.94	0.48
7:T:3:ALA:O	7:T:4:ALA:HB2	2.14	0.48
1:A:497:GLY:HA3	27:A:2398:HOH:O	2.14	0.48
3:C:57:TRP:CZ2	19:C:266:PGV:H21	2.49	0.48
4:D:129:ALA:HB1	4:D:133:GLY:HA3	1.96	0.48
22:N:1522:TGL:H231	22:N:1522:TGL:H272	1.95	0.48
1:N:380:VAL:HG23	1:N:381:LEU:H	1.78	0.48
1:N:492:LEU:HD12	1:N:492:LEU:O	2.14	0.48
2:O:122:MET:HE2	27:O:4368:HOH:O	2.13	0.48
1:A:501:PRO:HG2	1:A:504:THR:HG22	1.94	0.47
1:N:103:TRP:O	1:N:106:PRO:HD2	2.14	0.47
26:G:269:CDL:H761	1:N:282:PHE:HZ	1.78	0.47
1:N:316:THR:HG21	18:N:516:HEA:H14	1.95	0.47
25:P:1264:PEK:H102	25:P:1264:PEK:C16	2.38	0.47
1:A:400:PHE:HB3	22:L:522:TGL:H283	1.96	0.47
1:A:61:HIS:CE1	18:A:515:HEA:NB	2.82	0.47
22:L:522:TGL:HC62	22:L:522:TGL:CC2	2.30	0.47
1:N:130:PRO:HD2	1:N:231:TYR:CD1	2.49	0.47
1:N:184:PHE:O	1:N:188:VAL:HG23	2.15	0.47
1:N:306:THR:HG23	1:N:359:ALA:O	2.14	0.47
26:T:1269:CDL:H231	26:T:1269:CDL:C54	2.36	0.47
7:G:78:LEU:HB3	7:G:79:PRO:HD2	1.97	0.47
2:O:68:LEU:HB3	2:O:69:PRO:HD3	1.97	0.47
10:W:16:ASN:CG	10:W:18:LEU:HD12	2.35	0.47
1:A:436:MET:HE3	1:A:443:TYR:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:MET:HB3	27:A:4144:HOH:O	2.13	0.47
6:F:92:VAL:O	6:F:92:VAL:CG2	2.63	0.47
3:P:61:VAL:HG22	19:P:1266:PGV:H061	1.96	0.47
3:P:43:LEU:O	3:P:47:LEU:HG	2.13	0.47
4:Q:131:ILE:HD12	4:Q:131:ILE:H	1.79	0.47
1:A:282:PHE:HZ	26:T:1269:CDL:H761	1.80	0.47
5:R:12:ASP:CG	9:V:10:ARG:HH22	2.18	0.47
2:B:114:GLU:HB3	2:B:227:LEU:HD21	1.96	0.47
24:P:1272:DMU:O1	24:P:1272:DMU:H30	2.15	0.47
19:C:267:PGV:H182	26:C:270:CDL:C67	2.43	0.47
7:G:4:ALA:CB	1:N:282:PHE:HA	2.45	0.47
5:R:37:VAL:HG11	5:R:70:VAL:HG21	1.96	0.47
1:A:33:LEU:HD12	1:A:61:HIS:HA	1.97	0.47
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.97	0.47
6:F:49:VAL:O	6:F:91:LEU:HD12	2.15	0.47
7:T:2:SER:O	25:T:263:PEK:H322	2.14	0.47
7:T:6:GLY:O	25:T:263:PEK:H311	2.15	0.47
1:A:195:LEU:HG	1:A:245:ILE:HD13	1.97	0.47
4:D:109:HIS:HD2	27:D:2159:HOH:O	1.97	0.47
13:M:4:LYS:HE3	27:M:4199:HOH:O	2.15	0.47
1:N:124:THR:HB	27:N:4378:HOH:O	2.14	0.47
9:V:64:ARG:HG3	9:V:72:ALA:O	2.15	0.47
4:D:88:PHE:HZ	13:M:19:LEU:HD21	1.80	0.47
1:N:151:HIS:HD2	25:P:1264:PEK:C38	2.22	0.47
2:O:20:LEU:CD2	2:O:83:ILE:HG21	2.45	0.47
25:P:1265:PEK:H041	6:S:1:ALA:N	2.30	0.47
7:T:2:SER:OG	25:T:263:PEK:H301	2.14	0.47
1:A:177:SER:H	1:A:180:GLN:NE2	2.12	0.46
4:D:129:ALA:HB3	4:D:134:PHE:H	1.79	0.46
23:O:1230:PSC:H032	27:R:3129:HOH:O	2.15	0.46
22:O:1521:TGL:HC22	27:V:3383:HOH:O	2.15	0.46
1:N:230:LEU:HD13	3:P:103:HIS:CG	2.50	0.46
3:P:9:HIS:CE1	3:P:11:VAL:HG22	2.50	0.46
1:A:17:THR:OG1	22:L:522:TGL:H281	2.15	0.46
2:B:79:PRO:O	2:B:83:ILE:HG13	2.14	0.46
2:O:110:TYR:CD2	2:O:110:TYR:N	2.83	0.46
3:P:221:ARG:NH1	3:P:227:PHE:HE1	2.13	0.46
18:A:516:HEA:HMD1	18:A:516:HEA:HBD2	1.97	0.46
1:N:304:TYR:HD2	1:N:305:PHE:CD2	2.33	0.46
1:A:426:PHE:N	1:A:427:PRO:CD	2.79	0.46
3:C:109:THR:HB	3:C:110:PRO:HD2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:159:MET:C	3:C:159:MET:SD	2.94	0.46
3:C:244:PHE:HA	25:T:263:PEK:H9	1.98	0.46
1:N:59:THR:HG22	1:N:63:PHE:CE2	2.50	0.46
10:W:30:ILE:O	10:W:34:VAL:HG23	2.15	0.46
1:A:194:LEU:CB	1:A:245:ILE:HD11	2.46	0.46
1:N:472:ILE:HD13	22:N:1522:TGL:HA91	1.97	0.46
26:T:1269:CDL:H601	26:T:1269:CDL:H571	1.45	0.46
1:A:115:SER:O	1:A:121:GLY:HA2	2.15	0.46
1:N:488:THR:HB	1:N:495:LEU:HD13	1.96	0.46
9:V:18:ARG:HG2	9:V:18:ARG:HH11	1.80	0.46
22:D:523:TGL:HG31	27:D:4040:HOH:O	2.16	0.46
5:E:105:GLY:O	5:E:108:LYS:HG2	2.16	0.46
3:P:51:MET:HB3	26:P:1270:CDL:H622	1.98	0.46
3:P:139:ALA:CB	7:T:24:ALA:HB1	2.45	0.46
1:N:398:PRO:HG3	27:N:4079:HOH:O	2.15	0.46
7:T:38:HIS:CD2	26:T:1269:CDL:HA21	2.50	0.46
20:W:1060:CHD:H161	20:W:1060:CHD:H212	1.76	0.46
4:D:131:ILE:HG22	4:D:132:GLN:HG3	1.98	0.46
4:D:23:PRO:HB3	5:E:70:VAL:HG21	1.97	0.46
3:P:213:THR:HG23	26:P:1270:CDL:H762	1.97	0.46
1:A:239:GLY:O	1:A:243:VAL:HG13	2.16	0.45
2:B:139:ASP:OD2	2:B:140:ASN:N	2.49	0.45
23:B:230:PSC:H212	23:B:230:PSC:C02	2.47	0.45
19:N:1524:PGV:P	19:N:1524:PGV:H061	2.56	0.45
1:A:514:LYS:HE2	27:F:2339:HOH:O	2.16	0.45
2:B:168:LEU:HD13	2:B:184:LEU:HG	1.98	0.45
5:E:65:VAL:HG13	5:E:101:PRO:HG3	1.98	0.45
1:N:325:ALA:HA	23:O:1230:PSC:H291	1.98	0.45
3:P:187:THR:CB	7:T:68:THR:HG21	2.46	0.45
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.16	0.45
3:C:184:ALA:HA	3:C:185:PRO:HD2	1.88	0.45
26:C:270:CDL:H641	26:C:270:CDL:H672	1.80	0.45
1:N:513:LEU:HD22	1:N:513:LEU:HA	1.80	0.45
18:N:515:HEA:HMC1	18:N:515:HEA:HBC1	1.98	0.45
2:O:170:LEU:HD23	27:O:4107:HOH:O	2.15	0.45
1:N:295:VAL:HG12	2:O:173:ASP:OD2	2.16	0.45
2:O:200:CYS:SG	2:O:204:HIS:HA	2.56	0.45
2:O:65:TRP:CZ3	23:O:1230:PSC:H331	2.51	0.45
25:P:1264:PEK:H71	25:P:1264:PEK:H32	1.97	0.45
4:Q:23:PRO:HD2	5:R:34:ASN:OD1	2.17	0.45
1:A:481:GLU:O	13:M:3:ALA:HB1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:HD21	3:C:100:ALA:HA	1.98	0.45
3:C:55:TYR:CD1	26:C:270:CDL:H532	2.52	0.45
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.82	0.45
2:O:113:TYR:HE1	8:U:11:TYR:O	2.00	0.45
2:O:145:PRO:HA	2:O:214:VAL:O	2.16	0.45
3:P:134:THR:OG1	3:P:249:TRP:NE1	2.41	0.45
3:P:50:ASN:ND2	3:P:54:MET:CE	2.80	0.45
3:P:68:GLN:HE21	3:P:70:HIS:CD2	2.34	0.45
7:T:8:HIS:ND1	25:T:263:PEK:H312	2.32	0.45
10:W:5:VAL:O	10:W:9:GLN:HG3	2.16	0.45
1:A:321:PHE:CD2	23:B:230:PSC:H341	2.51	0.45
3:C:246:ASP:HB2	27:C:4141:HOH:O	2.15	0.45
3:C:16:TRP:HA	3:C:16:TRP:CE3	2.51	0.45
25:P:1265:PEK:H371	26:T:1269:CDL:H261	1.98	0.45
2:O:98:LYS:HD3	8:U:63:LEU:O	2.17	0.45
20:W:1271:CHD:H112	20:W:1271:CHD:H12A	1.61	0.45
1:A:194:LEU:HD12	1:A:245:ILE:HG13	1.99	0.45
3:C:171:VAL:HA	27:C:4409:HOH:O	2.16	0.45
5:E:56:ARG:HG2	5:E:96:LEU:HD22	1.99	0.45
26:G:269:CDL:H122	2:O:81:LEU:HD13	1.99	0.45
2:O:172:THR:CG2	2:O:180:ASN:HB3	2.46	0.45
7:T:47:PHE:CD2	7:T:77:PRO:HB2	2.52	0.45
1:A:276:ALA:O	1:A:280:ILE:HG13	2.17	0.45
3:C:116:TRP:HA	3:C:117:PRO:C	2.37	0.45
2:O:58:ALA:O	2:O:60:GLU:N	2.48	0.45
3:P:213:THR:HG21	19:P:1267:PGV:H11	1.98	0.45
4:Q:24:LEU:HD12	5:R:33:MET:HB2	1.99	0.45
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.99	0.45
1:A:306:THR:HG23	1:A:360:ASN:HA	1.99	0.45
2:B:146:MET:SD	2:B:189:PRO:HB3	2.57	0.45
3:C:166:THR:HG22	3:C:215:LEU:HD13	1.99	0.45
3:C:158:HIS:NE2	25:C:265:PEK:H051	2.32	0.45
12:Y:42:HIS:NE2	12:Y:46:LYS:HD2	2.32	0.45
7:G:34:ASN:ND2	26:G:269:CDL:H151	2.31	0.45
9:I:15:ARG:HD3	9:I:16:ARG:N	2.32	0.45
3:P:243:HIS:O	3:P:247:VAL:HG23	2.16	0.45
2:B:74:ILE:HD11	26:T:1269:CDL:H452	1.98	0.45
9:V:37:PHE:HA	9:V:41:GLU:HB2	1.99	0.45
2:B:184:LEU:HD23	2:B:184:LEU:C	2.37	0.44
2:B:62:GLU:HA	2:B:65:TRP:CD1	2.52	0.44
3:C:187:THR:HG22	25:C:264:PEK:H052	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:HIS:CD2	9:I:12:LEU:HD13	2.53	0.44
6:F:64:GLU:O	6:F:65:ASP:HB2	2.17	0.44
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.16	0.44
3:C:63:ARG:NH1	10:J:20:VAL:O	2.49	0.44
1:N:489:THR:HA	6:S:71:TRP:O	2.18	0.44
4:Q:119:GLN:O	4:Q:123:MET:HG3	2.17	0.44
1:A:505:PHE:HB3	27:A:2194:HOH:O	2.18	0.44
1:A:321:PHE:HB3	2:B:65:TRP:CZ3	2.52	0.44
3:C:51:MET:HB3	26:C:270:CDL:H622	1.98	0.44
1:N:220:PHE:CE1	1:N:231:TYR:HB2	2.52	0.44
22:N:1523:TGL:H311	4:Q:89:ILE:HD13	2.00	0.44
7:T:2:SER:O	7:T:3:ALA:HB3	2.18	0.44
7:T:79:PRO:HD2	27:T:3136:HOH:O	2.17	0.44
1:A:377:PHE:CE2	1:A:378:HIS:CE1	3.04	0.44
2:B:160:LEU:O	2:B:200:CYS:HB3	2.15	0.44
23:B:230:PSC:H221	23:B:230:PSC:H251	1.71	0.44
2:B:58:ALA:O	2:B:60:GLU:N	2.49	0.44
9:I:35:TYR:C	9:I:37:PHE:H	2.21	0.44
3:P:184:ALA:HA	3:P:185:PRO:HD2	1.85	0.44
8:H:46:LYS:CB	8:U:52:VAL:HG12	2.48	0.44
11:X:36:ILE:HG13	11:X:38:ILE:HG13	1.99	0.44
2:B:70:ALA:O	2:B:74:ILE:HG13	2.18	0.44
4:D:99:GLU:HB3	27:D:4113:HOH:O	2.17	0.44
5:E:63:SER:O	5:E:67:ILE:HG13	2.18	0.44
6:F:13:ALA:O	6:F:18:ARG:HD2	2.17	0.44
11:K:15:ASN:HB2	27:K:2386:HOH:O	2.16	0.44
1:N:106:PRO:HB2	1:N:107:PRO:HD3	2.00	0.44
25:P:1265:PEK:C38	26:T:1269:CDL:H273	2.47	0.44
3:P:187:THR:HB	7:T:68:THR:HG21	2.00	0.44
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.17	0.44
20:A:525:CHD:H112	20:A:525:CHD:H12A	1.78	0.44
2:B:78:LEU:HD12	2:B:78:LEU:HA	1.83	0.44
18:N:516:HEA:HMB1	18:N:516:HEA:H11	1.94	0.44
1:N:66:ILE:O	1:N:71:MET:HG3	2.17	0.44
3:P:156:ARG:HH22	3:P:223:LEU:HA	1.81	0.44
3:P:193:TYR:CD2	3:P:193:TYR:C	2.90	0.44
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.53	0.44
20:B:1086:CHD:H212	20:B:1086:CHD:H12	1.99	0.44
1:N:383:MET:O	1:N:387:PHE:HB2	2.18	0.44
2:O:203:ASN:ND2	2:O:203:ASN:N	2.66	0.44
10:W:36:MET:HB3	20:W:1060:CHD:H181	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:LEU:CD2	2:B:213:LEU:N	2.81	0.44
3:C:68:GLN:HB3	27:C:2153:HOH:O	2.18	0.44
4:D:107:ILE:HB	4:D:108:PRO:HD2	1.98	0.44
6:F:95:GLN:NE2	27:F:4185:HOH:O	2.49	0.44
27:N:3090:HOH:O	3:P:13:PRO:HG3	2.17	0.44
1:A:145:LEU:HD21	3:C:32:THR:HG21	2.00	0.44
3:C:221:ARG:NH1	3:C:227:PHE:CE1	2.86	0.44
3:C:63:ARG:O	3:C:68:GLN:HG3	2.17	0.44
5:E:28:GLU:HG2	27:E:4385:HOH:O	2.17	0.44
26:G:269:CDL:HB32	1:N:304:TYR:CD1	2.49	0.44
1:A:53:ILE:CD1	12:L:44:LEU:HD23	2.48	0.44
1:N:40:GLU:OE1	1:N:46:THR:HA	2.18	0.44
1:N:68:PHE:HA	1:N:72:PRO:HG2	2.00	0.44
1:N:68:PHE:O	1:N:72:PRO:HG2	2.18	0.44
2:O:216:LEU:O	2:O:219:PHE:HB3	2.18	0.44
1:A:307:SER:CB	26:T:1269:CDL:H182	2.48	0.44
7:T:5:LYS:HD2	25:T:263:PEK:H371	2.00	0.44
1:A:92:MET:O	1:A:95:PRO:HD3	2.18	0.44
3:C:233:PHE:N	19:C:267:PGV:O14	2.47	0.44
4:D:23:PRO:HB3	5:E:70:VAL:CG2	2.48	0.44
1:N:34:SER:HB3	1:N:61:HIS:CE1	2.53	0.44
1:N:506:GLU:HB2	27:N:4072:HOH:O	2.18	0.44
2:O:41:ILE:O	2:O:45:MET:HG2	2.17	0.44
7:T:78:LEU:HB3	7:T:79:PRO:CD	2.48	0.44
23:B:230:PSC:H12	23:B:230:PSC:H322	2.01	0.43
2:B:65:TRP:HZ3	23:B:230:PSC:H331	1.81	0.43
8:H:27:ARG:NH1	27:H:2303:HOH:O	2.48	0.43
1:N:382:SER:O	1:N:386:VAL:HB	2.18	0.43
18:A:516:HEA:H11	18:A:516:HEA:HMB1	1.89	0.43
4:D:126:MET:HG3	4:D:128:VAL:HG23	1.99	0.43
6:F:54:ASN:OD1	6:F:76:LYS:HD2	2.17	0.43
1:N:356:ILE:HD13	1:N:356:ILE:HA	1.83	0.43
1:N:363:LEU:HA	1:N:363:LEU:HD23	1.88	0.43
1:N:366:VAL:HG12	27:N:3400:HOH:O	2.18	0.43
2:O:132:GLU:HA	4:Q:122:ARG:NH1	2.34	0.43
4:Q:51:LEU:HD21	4:Q:59:LEU:HD11	1.99	0.43
7:T:49:PRO:HD2	8:U:80:THR:HG22	2.00	0.43
10:W:50:LEU:HD22	10:W:50:LEU:O	2.19	0.43
26:C:270:CDL:H171	26:C:270:CDL:H202	1.79	0.43
20:N:1604:CHD:H12	20:N:1604:CHD:H212	2.00	0.43
3:P:63:ARG:NH1	10:W:20:VAL:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:ARG:NE	2:B:181:GLN:NE2	2.66	0.43
3:C:218:CYS:SG	3:C:235:PHE:HA	2.59	0.43
10:J:36:MET:HG2	20:J:60:CHD:H222	1.99	0.43
4:Q:129:ALA:CB	4:Q:134:PHE:H	2.31	0.43
1:A:68:PHE:HA	1:A:72:PRO:HG2	1.99	0.43
2:B:102:HIS:O	2:B:104:TRP:HA	2.19	0.43
2:B:175:ILE:HD12	2:B:180:ASN:HD21	1.82	0.43
3:C:16:TRP:HA	3:C:16:TRP:HE3	1.83	0.43
4:D:119:GLN:O	4:D:123:MET:HG3	2.18	0.43
12:L:46:LYS:O	12:L:47:LYS:HB2	2.19	0.43
1:N:321:PHE:CZ	23:O:1230:PSC:H171	2.54	0.43
23:O:1230:PSC:C02	23:O:1230:PSC:H212	2.48	0.43
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.99	0.43
4:Q:34:SER:N	4:Q:37:GLN:HE21	2.08	0.43
1:A:141:ALA:O	1:A:144:ASP:N	2.51	0.43
11:K:41:ASN:ND2	27:K:2283:HOH:O	2.48	0.43
1:N:498:CYS:HA	1:N:499:PRO:HA	1.85	0.43
3:P:149:HIS:O	3:P:153:GLU:HG3	2.18	0.43
3:P:16:TRP:HE3	3:P:16:TRP:HA	1.82	0.43
8:U:39:CYS:O	8:U:43:MET:HG2	2.18	0.43
19:A:524:PGV:H301	19:A:524:PGV:H152	2.01	0.43
1:N:377:PHE:CE2	1:N:378:HIS:CE1	3.06	0.43
1:N:443:TYR:HB2	1:N:447:TYR:HD2	1.83	0.43
1:N:53:ILE:O	1:N:57:VAL:HG23	2.19	0.43
1:A:108:SER:HB2	1:A:152:LEU:HB2	2.01	0.43
2:O:161:HIS:CE1	2:O:200:CYS:HB2	2.54	0.43
2:O:160:LEU:O	2:O:200:CYS:HB3	2.19	0.43
3:P:139:ALA:HB1	7:T:24:ALA:HB1	2.00	0.43
3:P:157:LYS:HZ1	25:P:1265:PEK:H052	1.84	0.43
7:T:3:ALA:CB	25:T:263:PEK:H382	2.43	0.43
1:A:309:THR:CG2	18:A:516:HEA:HMB2	2.49	0.43
20:P:1525:CHD:H12A	20:P:1525:CHD:H112	1.82	0.43
6:S:54:ASN:ND2	6:S:55:LYS:HG2	2.34	0.43
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.19	0.43
2:B:189:PRO:HG2	9:I:63:MET:HE3	2.01	0.43
5:E:84:TYR:HE1	27:E:4265:HOH:O	2.01	0.43
25:C:264:PEK:H041	7:G:70:PHE:HB2	2.01	0.43
7:T:30:LEU:HA	7:T:30:LEU:HD23	1.87	0.43
8:U:78:GLU:O	8:U:78:GLU:HG2	2.19	0.43
22:N:1522:TGL:HB62	12:Y:28:PHE:CZ	2.53	0.43
1:A:413:HIS:NE2	1:A:468:MET:HB2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:507:GLU:HA	3:C:5:THR:OG1	2.19	0.42
10:J:45:TYR:O	10:J:48:TYR:HB3	2.19	0.42
1:N:505:PHE:HB3	27:N:3194:HOH:O	2.19	0.42
8:U:37:HIS:CD2	8:U:76:ARG:CZ	3.02	0.42
1:A:307:SER:HB3	26:T:1269:CDL:H182	2.00	0.42
1:A:71:MET:HB2	1:A:72:PRO:HD3	2.01	0.42
2:B:121:TYR:O	2:B:138:VAL:HA	2.19	0.42
7:G:26:PRO:O	7:G:29:ALA:HB3	2.19	0.42
1:N:34:SER:HB2	18:N:515:HEA:C2B	2.49	0.42
1:N:501:PRO:HG2	1:N:504:THR:HG22	2.01	0.42
2:O:9:PHE:HB2	2:O:21:LEU:CD2	2.48	0.42
25:G:1263:PEK:H132	3:P:247:VAL:CG1	2.49	0.42
8:U:58:ARG:HD2	8:U:58:ARG:HA	1.73	0.42
6:F:6:VAL:HA	6:F:7:PRO:HD2	1.92	0.42
8:H:57:ARG:O	8:H:61:LYS:HB2	2.19	0.42
7:T:58:LYS:HA	7:T:59:PRO:HD2	1.92	0.42
1:A:106:PRO:N	1:A:107:PRO:CD	2.83	0.42
4:D:61:ARG:HA	4:D:61:ARG:HD3	1.83	0.42
4:D:100:LYS:HE2	11:K:37:GLY:O	2.19	0.42
1:N:106:PRO:N	1:N:107:PRO:CD	2.83	0.42
1:N:40:GLU:HG2	1:N:54:TYR:CD2	2.54	0.42
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.54	0.42
6:S:35:ALA:HA	6:S:36:PRO:HD2	1.94	0.42
18:A:515:HEA:HBC1	18:A:515:HEA:HMC1	2.02	0.42
23:B:230:PSC:H042	27:E:2401:HOH:O	2.20	0.42
8:H:9:LYS:HB3	8:H:10:ASN:H	1.61	0.42
4:Q:17:VAL:O	4:Q:25:PRO:HG3	2.19	0.42
13:Z:38:ASP:HB2	27:Z:4321:HOH:O	2.20	0.42
1:A:289:ALA:HB3	1:A:305:PHE:CG	2.55	0.42
3:C:158:HIS:CE1	25:C:265:PEK:H051	2.55	0.42
6:F:48:LEU:O	6:F:50:PRO:HD3	2.19	0.42
1:A:478:SER:HA	13:M:8:THR:O	2.19	0.42
1:N:111:LEU:HA	1:N:111:LEU:HD23	1.78	0.42
4:Q:68:PHE:HA	4:Q:71:MET:HG2	2.02	0.42
5:E:81:ILE:O	5:E:85:VAL:HG23	2.20	0.42
7:G:5:LYS:CB	25:G:1263:PEK:H362	2.40	0.42
1:N:353:LEU:O	1:N:356:ILE:HB	2.20	0.42
2:O:20:LEU:HD23	2:O:83:ILE:HD13	2.02	0.42
2:O:68:LEU:CB	2:O:69:PRO:CD	2.98	0.42
26:P:1270:CDL:H202	26:P:1270:CDL:H171	1.79	0.42
3:P:31:LEU:HD23	3:P:31:LEU:HA	1.69	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:81:ILE:HG12	9:V:7:PRO:HG2	2.01	0.42
6:S:95:GLN:O	6:S:96:LEU:HB3	2.18	0.42
2:B:41:ILE:O	2:B:45:MET:HG2	2.19	0.42
3:C:216:ILE:O	3:C:219:PHE:HB3	2.20	0.42
3:C:223:LEU:HD23	3:C:223:LEU:HA	1.83	0.42
1:N:172:LYS:NZ	1:N:178:GLN:HE22	2.18	0.42
1:N:194:LEU:HD12	1:N:245:ILE:HG13	2.01	0.42
2:O:128:LEU:HD11	2:O:134:ARG:HA	2.02	0.42
2:O:13:THR:HB	2:O:168:LEU:HD23	2.01	0.42
3:P:156:ARG:HG3	3:P:156:ARG:HH11	1.84	0.42
10:W:40:LEU:O	10:W:44:LEU:HG	2.19	0.42
1:A:8:PHE:CE2	3:C:15:PRO:HB3	2.55	0.42
2:B:56:MET:HA	23:B:230:PSC:H202	2.02	0.42
3:C:63:ARG:HE	26:C:270:CDL:CA2	2.09	0.42
5:E:15:TRP:O	5:E:18:TYR:HB3	2.19	0.42
5:E:56:ARG:NH2	5:E:59:ASN:OD1	2.48	0.42
22:N:1523:TGL:HG11	22:N:1523:TGL:CC2	2.50	0.42
1:N:426:PHE:N	1:N:427:PRO:CD	2.82	0.42
2:O:100:MET:HB2	2:O:107:SER:HG	1.83	0.42
8:U:9:LYS:HB2	8:U:9:LYS:HE2	1.85	0.42
13:Z:34:LEU:HA	13:Z:34:LEU:HD12	1.89	0.42
1:A:250:GLY:O	1:A:254:ILE:HG12	2.20	0.41
19:A:524:PGV:H011	19:A:524:PGV:H202	1.94	0.41
1:A:440:TYR:OH	2:B:195:GLN:HB3	2.20	0.41
3:C:99:TRP:CE2	19:C:268:PGV:H232	2.55	0.41
1:A:459:PHE:HB3	4:D:92:THR:CG2	2.50	0.41
5:E:15:TRP:CD2	5:E:36:LEU:HD13	2.55	0.41
5:E:31:LYS:HE3	6:F:83:PRO:O	2.19	0.41
1:N:472:ILE:CG2	22:N:1522:TGL:HA92	2.42	0.41
1:N:246:LEU:HD13	1:N:381:LEU:HD21	2.02	0.41
1:A:13:LYS:NZ	27:A:2081:HOH:O	2.53	0.41
12:L:24:MET:SD	22:L:522:TGL:C16	3.04	0.41
1:N:283:LEU:HD23	1:N:286:ILE:HD11	2.02	0.41
1:N:468:MET:O	1:N:472:ILE:HG13	2.20	0.41
1:N:53:ILE:HG12	27:N:3076:HOH:O	2.18	0.41
2:B:125:THR:HA	2:B:128:LEU:HG	2.02	0.41
23:B:230:PSC:C07	9:I:10:ARG:HE	2.33	0.41
8:H:33:TYR:HE1	8:H:69:VAL:HG13	1.85	0.41
13:M:42:LYS:CE	13:M:42:LYS:HA	2.36	0.41
7:G:2:SER:HB3	1:N:197:LEU:HD11	2.01	0.41
2:O:110:TYR:HD2	2:O:110:TYR:N	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:440:TYR:CZ	2:O:205:SER:HA	2.55	0.41
2:O:33:LEU:HD12	2:O:33:LEU:HA	1.87	0.41
5:R:53:ARG:HD2	27:R:4076:HOH:O	2.20	0.41
9:V:31:PHE:HA	27:V:4259:HOH:O	2.20	0.41
1:A:33:LEU:HD13	1:A:61:HIS:N	2.35	0.41
4:D:17:VAL:HA	27:D:4085:HOH:O	2.21	0.41
4:D:32:ASN:HA	4:D:32:ASN:HD22	1.70	0.41
22:N:1523:TGL:H271	2:O:46:LEU:CD1	2.49	0.41
8:U:50:VAL:HG12	8:U:50:VAL:O	2.20	0.41
9:V:35:TYR:C	9:V:37:PHE:H	2.23	0.41
4:Q:114:GLU:HG3	11:X:51:LYS:HZ2	1.85	0.41
24:C:272:DMU:H25	25:C:264:PEK:H341	2.03	0.41
5:E:57:ARG:CG	5:E:57:ARG:HH11	2.33	0.41
6:F:59:GLY:HA2	6:F:70:ILE:O	2.20	0.41
1:A:113:LEU:CD1	22:L:522:TGL:H292	2.50	0.41
1:N:381:LEU:HD13	18:N:516:HEA:CBC	2.49	0.41
2:O:153:LEU:HD23	2:O:181:GLN:HA	2.02	0.41
2:O:59:GLN:O	2:O:59:GLN:CG	2.68	0.41
2:O:98:LYS:HE3	2:O:98:LYS:HB2	1.90	0.41
3:P:22:LEU:HD23	3:P:22:LEU:HA	1.89	0.41
3:P:146:TRP:CE2	7:T:17:ARG:HG3	2.56	0.41
1:A:309:THR:HG22	18:A:516:HEA:HMB2	2.02	0.41
3:C:23:SER:HB2	3:C:49:THR:OG1	2.21	0.41
3:C:3:HIS:HE1	6:F:31:TYR:OH	2.04	0.41
26:P:1270:CDL:H561	26:P:1270:CDL:H532	1.80	0.41
3:P:137:LEU:HA	3:P:137:LEU:HD23	1.81	0.41
1:A:209:LEU:O	1:A:213:ARG:HG3	2.21	0.41
1:A:33:LEU:HD23	1:A:33:LEU:HA	1.78	0.41
2:B:146:MET:CE	9:I:56:SER:HB2	2.50	0.41
1:A:334:TRP:CZ2	2:B:46:LEU:HB3	2.56	0.41
3:C:172:TYR:O	3:C:176:LEU:HG	2.21	0.41
7:G:38:HIS:NE2	26:G:269:CDL:H111	2.36	0.41
26:G:269:CDL:H601	26:G:269:CDL:H571	1.51	0.41
3:C:41:THR:HG21	10:J:45:TYR:CE2	2.56	0.41
20:N:1604:CHD:H112	20:N:1604:CHD:H12A	1.90	0.41
2:O:158:ASP:O	2:O:176:PRO:HG3	2.21	0.41
3:P:134:THR:HG22	26:T:1269:CDL:H591	2.02	0.41
19:N:1524:PGV:H12	4:Q:87:PHE:CD2	2.55	0.41
1:A:337:ALA:HB2	1:A:394:VAL:CG2	2.51	0.41
1:A:344:PHE:CD1	1:A:344:PHE:C	2.93	0.41
20:J:60:CHD:H161	20:J:60:CHD:H212	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:248:LEU:O	1:N:251:PHE:HB2	2.20	0.41
1:N:340:TRP:HZ2	1:N:413:HIS:ND1	2.18	0.41
3:P:181:TYR:O	25:P:1264:PEK:C04	2.69	0.41
19:P:1267:PGV:H182	26:P:1270:CDL:C67	2.49	0.41
1:N:42:GLY:HA3	4:Q:104:TYR:OH	2.20	0.41
5:R:61:PHE:O	5:R:64:ALA:HB3	2.20	0.41
11:X:6:ALA:HA	11:X:7:PRO:HD2	1.92	0.41
2:B:78:LEU:CB	2:B:79:PRO:CD	2.98	0.41
1:A:219:PHE:CE2	3:C:196:THR:HG22	2.48	0.41
1:N:374:VAL:HA	1:N:377:PHE:CE1	2.56	0.41
1:N:483:LEU:HB2	13:Z:2:THR:OG1	2.20	0.41
1:N:500:PRO:HB3	27:N:3186:HOH:O	2.19	0.41
7:T:15:THR:O	7:T:18:PHE:HB3	2.21	0.41
1:A:22:PHE:CZ	1:A:105:LEU:HB3	2.55	0.41
1:A:53:ILE:HD12	12:L:44:LEU:HD23	2.03	0.41
25:G:1263:PEK:H102	3:P:247:VAL:HG11	2.02	0.41
1:N:98:ASN:HB2	1:N:163:ASN:HD21	1.84	0.41
2:O:16:ILE:HG22	2:O:17:MET:N	2.35	0.41
5:R:36:LEU:O	5:R:39:TYR:HD2	2.04	0.41
12:Y:2:HIS:HB3	12:Y:3:TYR:H	1.66	0.41
1:A:501:PRO:HG2	1:A:504:THR:CG2	2.50	0.41
2:B:151:ARG:NE	2:B:181:GLN:HE21	2.18	0.41
2:B:213:LEU:N	2:B:213:LEU:HD22	2.36	0.41
7:G:2:SER:O	7:G:3:ALA:HB3	2.21	0.41
2:B:222:TRP:HB2	9:I:71:SER:HB2	2.02	0.41
1:N:400:PHE:HB3	22:N:1522:TGL:C28	2.51	0.41
20:P:1525:CHD:H182	20:P:1525:CHD:H111	1.74	0.41
3:P:49:THR:HB	10:W:39:CYS:SG	2.61	0.41
4:Q:86:MET:O	11:X:25:CYS:HB2	2.21	0.41
26:C:270:CDL:H242	26:C:270:CDL:H661	2.03	0.40
10:J:50:LEU:HD22	10:J:50:LEU:O	2.21	0.40
2:O:19:GLU:OE2	2:O:19:GLU:HA	2.21	0.40
26:P:1270:CDL:H641	26:P:1270:CDL:H672	1.77	0.40
7:T:47:PHE:CE2	7:T:77:PRO:HB2	2.56	0.40
1:A:298:ASP:HB3	27:A:2389:HOH:O	2.21	0.40
19:A:524:PGV:O14	19:A:524:PGV:H02	2.21	0.40
2:B:16:ILE:HD13	2:B:16:ILE:HA	1.90	0.40
25:C:265:PEK:H041	6:F:1:ALA:N	2.36	0.40
3:C:50:ASN:OD1	19:C:266:PGV:H91	2.21	0.40
23:O:1230:PSC:H221	23:O:1230:PSC:H251	1.70	0.40
2:O:202:SER:HB2	2:O:203:ASN:HD22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:18:PHE:HD2	7:T:18:PHE:O	2.03	0.40
26:C:270:CDL:H602	26:C:270:CDL:H632	1.78	0.40
19:C:267:PGV:H181	26:C:270:CDL:H812	2.04	0.40
26:C:270:CDL:PA1	26:C:270:CDL:HB22	2.61	0.40
20:C:271:CHD:H12A	20:C:271:CHD:H112	1.60	0.40
3:C:84:ILE:HG12	25:T:263:PEK:H32	2.03	0.40
9:I:21:ILE:HD13	9:I:21:ILE:HA	1.94	0.40
12:L:20:ARG:HH22	22:L:522:TGL:CC3	2.32	0.40
13:M:32:TRP:N	24:M:526:DMU:H1	2.36	0.40
1:N:141:ALA:O	1:N:144:ASP:N	2.54	0.40
3:P:116:TRP:HA	3:P:117:PRO:C	2.40	0.40
3:P:12:ASN:O	3:P:13:PRO:C	2.59	0.40
3:P:49:THR:HA	3:P:52:LEU:HD12	2.04	0.40
22:N:1522:TGL:HB62	12:Y:28:PHE:HZ	1.86	0.40
1:A:34:SER:HB2	18:A:515:HEA:C2B	2.51	0.40
1:A:459:PHE:HB3	4:D:92:THR:HG23	2.02	0.40
10:J:36:MET:HB3	20:J:60:CHD:H181	2.03	0.40
1:N:296:GLY:O	2:O:178:ARG:NH2	2.53	0.40
1:N:478:SER:HA	13:Z:8:THR:O	2.21	0.40
1:N:61:HIS:CE1	18:N:515:HEA:NB	2.87	0.40
3:P:112:LEU:HD13	3:P:118:PRO:HG3	2.03	0.40
3:P:146:TRP:HB2	7:T:16:TRP:HB3	2.03	0.40
3:P:148:HIS:CD2	3:P:235:PHE:HE2	2.40	0.40
22:D:523:TGL:H242	22:D:523:TGL:H212	1.86	0.40
2:B:146:MET:HE1	9:I:56:SER:HB2	2.03	0.40
9:I:67:GLY:HA2	27:I:2310:HOH:O	2.22	0.40
10:J:11:LEU:HD12	10:J:11:LEU:O	2.21	0.40
1:N:373:VAL:HG13	18:N:516:HEA:HBA1	2.04	0.40
2:O:70:ALA:O	2:O:74:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

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%)	488 (95%)	24 (5%)	0	100	100
1	N	512/514 (100%)	484 (94%)	27 (5%)	1 (0%)	47	71
2	B	225/227 (99%)	210 (93%)	10 (4%)	5 (2%)	6	12
2	O	225/227 (99%)	206 (92%)	16 (7%)	3 (1%)	12	24
3	C	257/261 (98%)	249 (97%)	7 (3%)	1 (0%)	34	57
3	P	257/261 (98%)	249 (97%)	7 (3%)	1 (0%)	34	57
4	D	142/147 (97%)	137 (96%)	5 (4%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
5	E	103/109 (94%)	97 (94%)	6 (6%)	0	100	100
5	R	103/109 (94%)	94 (91%)	9 (9%)	0	100	100
6	F	96/98 (98%)	85 (88%)	8 (8%)	3 (3%)	4	6
6	S	96/98 (98%)	85 (88%)	7 (7%)	4 (4%)	3	3
7	G	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	1	0
7	T	81/85 (95%)	65 (80%)	10 (12%)	6 (7%)	1	1
8	H	77/85 (91%)	69 (90%)	7 (9%)	1 (1%)	12	24
8	U	77/85 (91%)	69 (90%)	7 (9%)	1 (1%)	12	24
9	I	71/73 (97%)	66 (93%)	4 (6%)	1 (1%)	11	22
9	V	71/73 (97%)	66 (93%)	4 (6%)	1 (1%)	11	22
10	J	56/59 (95%)	54 (96%)	1 (2%)	1 (2%)	8	16
10	W	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
11	K	47/56 (84%)	44 (94%)	3 (6%)	0	100	100
11	X	47/56 (84%)	45 (96%)	2 (4%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	39 (95%)	2 (5%)	0	100	100
13	Z	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
All	All	3504/3614 (97%)	3279 (94%)	189 (5%)	36 (1%)	15	32

All (36) Ramachandran outliers are listed below:

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

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	413 (97%)	13 (3%)	40	66
1	N	426/426 (100%)	411 (96%)	15 (4%)	36	62
2	B	210/210 (100%)	196 (93%)	14 (7%)	16	33
2	O	210/210 (100%)	200 (95%)	10 (5%)	25	49
3	C	224/226 (99%)	213 (95%)	11 (5%)	25	48
3	P	224/226 (99%)	216 (96%)	8 (4%)	35	61
4	D	128/129 (99%)	125 (98%)	3 (2%)	50	75
4	Q	128/129 (99%)	124 (97%)	4 (3%)	40	66
5	E	92/95 (97%)	89 (97%)	3 (3%)	38	64
5	R	92/95 (97%)	91 (99%)	1 (1%)	73	88
6	F	81/81 (100%)	78 (96%)	3 (4%)	34	60
6	S	81/81 (100%)	75 (93%)	6 (7%)	13	28
7	G	67/68 (98%)	60 (90%)	7 (10%)	7	13
7	T	67/68 (98%)	62 (92%)	5 (8%)	13	27
8	H	71/75 (95%)	67 (94%)	4 (6%)	21	42
8	U	71/75 (95%)	70 (99%)	1 (1%)	67	85
9	I	57/57 (100%)	55 (96%)	2 (4%)	36	62
9	V	57/57 (100%)	56 (98%)	1 (2%)	59	80
10	J	49/50 (98%)	49 (100%)	0	100	100
10	W	49/50 (98%)	48 (98%)	1 (2%)	55	78
11	K	39/46 (85%)	38 (97%)	1 (3%)	46	72
11	X	39/46 (85%)	36 (92%)	3 (8%)	13	25
12	L	39/40 (98%)	37 (95%)	2 (5%)	24	46
12	Y	39/40 (98%)	38 (97%)	1 (3%)	46	72
13	M	37/38 (97%)	30 (81%)	7 (19%)	1	2
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	12
All	All	3040/3082 (99%)	2910 (96%)	130 (4%)	29	54

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	112	LEU

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Mol	Chain	Res	Type
1	A	115	SER
1	A	138	HIS
1	A	180	GLN
1	A	238	PHE
1	A	241	PRO
1	A	338	MET
1	A	369	ASP
1	A	490	THR
1	A	495	LEU
1	A	513	LEU
2	B	16	ILE
2	B	33	LEU
2	B	60	GLU
2	B	65	TRP
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	110	TYR
2	B	113	TYR
2	B	115	ASP
2	B	130	PRO
2	B	167	SER
2	B	185	MET
2	B	205	SER
3	C	17	PRO
3	C	29	SER
3	C	33	MET
3	C	39	SER
3	C	95	THR
3	C	110	PRO
3	C	159	MET
3	C	179	SER
3	C	192	VAL
3	C	214	PHE
3	C	230	ASN
4	D	4	SER
4	D	36	SER
4	D	51	LEU
5	E	7	THR
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU

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Mol	Chain	Res	Type
6	F	53	THR
6	F	95	GLN
7	G	17	ARG
7	G	18	PHE
7	G	35	SER
7	G	36	TRP
7	G	38	HIS
7	G	54	ARG
7	G	84	LYS
8	H	8	ILE
8	H	27	ARG
8	H	29	CYS
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
11	K	54	ARG
12	L	2	HIS
12	L	26	THR
13	M	4	LYS
13	M	5	PRO
13	M	13	LYS
13	M	34	LEU
13	M	37	LEU
13	M	38	ASP
13	M	42	LYS
1	N	109	PHE
1	N	138	HIS
1	N	178	GLN
1	N	180	GLN
1	N	238	PHE
1	N	241	PRO
1	N	264	LYS
1	N	290	HIS
1	N	338	MET
1	N	361	SER
1	N	369	ASP
1	N	380	VAL
1	N	484	THR
1	N	495	LEU
1	N	513	LEU
2	O	16	ILE
2	O	33	LEU

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Mol	Chain	Res	Type
2	O	60	GLU
2	O	65	TRP
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	110	TYR
2	O	203	ASN
2	O	217	LYS
3	P	23	SER
3	P	29	SER
3	P	33	MET
3	P	66	THR
3	P	150	SER
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	51	LEU
4	Q	54	ASP
4	Q	108	PRO
4	Q	121	LYS
5	R	90	ARG
6	S	37	LYS
6	S	48	LEU
6	S	53	THR
6	S	54	ASN
6	S	94	HIS
6	S	96	LEU
7	T	17	ARG
7	T	18	PHE
7	T	35	SER
7	T	43	GLU
7	T	54	ARG
8	U	29	CYS
9	V	8	GLN
10	W	50	LEU
11	X	20	SER
11	X	47	ARG
11	X	54	ARG
12	Y	20	ARG
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP

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Mol	Chain	Res	Type
13	Z	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	151	HIS
1	A	178	GLN
1	A	180	GLN
1	A	413	HIS
2	B	10	GLN
2	B	91	ASN
2	B	102	HIS
2	B	181	GLN
2	B	195	GLN
3	C	3	HIS
3	C	9	HIS
3	C	50	ASN
3	C	68	GLN
3	C	70	HIS
3	C	76	GLN
4	D	32	ASN
4	D	37	GLN
4	D	109	HIS
5	E	94	ASN
7	G	34	ASN
7	G	71	HIS
8	H	31	GLN
11	K	35	GLN
11	K	41	ASN
1	N	151	HIS
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	52	HIS
2	O	203	ASN
3	P	3	HIS
3	P	12	ASN
3	P	50	ASN
3	P	68	GLN
3	P	161	GLN

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Mol	Chain	Res	Type
3	P	243	HIS
4	Q	37	GLN
4	Q	101	HIS
5	R	78	HIS
6	S	54	ASN
6	S	94	HIS
7	T	34	ASN

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
9	SAC	I	1	9	7,8,9	2.53	2 (28%)	8,9,11	2.92	3 (37%)
1	FME	A	1	1	8,9,10	0.76	0	7,9,11	1.25	1 (14%)
7	TPO	T	11	7	8,10,11	1.39	1 (12%)	10,14,16	1.03	0
2	FME	B	1	2	8,9,10	1.01	0	7,9,11	1.66	2 (28%)
1	FME	N	1	1	8,9,10	0.87	0	7,9,11	1.26	1 (14%)
2	FME	O	1	2	8,9,10	0.72	0	7,9,11	2.28	2 (28%)
7	TPO	G	11	7	8,10,11	1.68	2 (25%)	10,14,16	0.95	0
9	SAC	V	1	9	7,8,9	2.86	2 (28%)	8,9,11	3.22	5 (62%)

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
9	SAC	I	1	9	-	3/7/8/10	-
1	FME	A	1	1	-	3/7/9/11	-
7	TPO	T	11	7	-	5/9/11/13	-
2	FME	B	1	2	-	2/7/9/11	-
1	FME	N	1	1	-	3/7/9/11	-
2	FME	O	1	2	-	2/7/9/11	-
7	TPO	G	11	7	-	4/9/11/13	-
9	SAC	V	1	9	-	3/7/8/10	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	OAC-C1A	5.46	1.35	1.23
9	I	1	SAC	OAC-C1A	5.21	1.35	1.23
9	V	1	SAC	CA-N	4.51	1.52	1.46
9	I	1	SAC	CA-N	3.85	1.51	1.46
7	G	11	TPO	CB-CA	3.04	1.60	1.53
7	T	11	TPO	P-O1P	2.47	1.58	1.50
7	G	11	TPO	P-O1P	2.06	1.57	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	1	SAC	CA-N-C1A	-7.18	109.91	123.15
9	I	1	SAC	CA-N-C1A	-6.40	111.34	123.15
2	O	1	FME	C-CA-N	4.73	118.27	109.73
2	O	1	FME	CA-N-CN	-3.50	117.45	122.82
9	I	1	SAC	CB-CA-N	3.19	117.71	110.55
9	V	1	SAC	C2A-C1A-N	2.98	121.15	116.10
9	I	1	SAC	C-CA-N	-2.97	104.38	109.73
9	V	1	SAC	C-CA-N	-2.82	104.65	109.73
2	B	1	FME	CA-N-CN	-2.80	118.51	122.82
2	B	1	FME	C-CA-N	2.76	114.72	109.73
1	N	1	FME	CA-N-CN	-2.51	118.97	122.82
9	V	1	SAC	OAC-C1A-C2A	-2.42	117.57	122.06
9	V	1	SAC	CB-CA-N	2.33	115.79	110.55
1	A	1	FME	CA-N-CN	-2.12	119.57	122.82

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
9	I	1	SAC	CB-CA-N-C1A
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
2	B	1	FME	O1-CN-N-CA
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
1	N	1	FME	C-CA-CB-CG
2	O	1	FME	O1-CN-N-CA
2	O	1	FME	CB-CA-N-CN
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	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
7	T	11	TPO	CB-OG1-P-O2P
2	B	1	FME	CB-CA-N-CN
1	A	1	FME	C-CA-CB-CG
7	T	11	TPO	CB-OG1-P-O3P
7	G	11	TPO	CB-OG1-P-O2P

There are no ring outliers.

3 monomers are involved in 4 short contacts:

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 12 are monoatomic - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
19	PGV	C	267	-	50,50,50	1.04	3 (6%)	53,56,56	1.05	5 (9%)
26	CDL	C	270	-	99,99,99	1.07	8 (8%)	105,111,111	1.09	9 (8%)
20	CHD	J	60	-	29,32,32	1.95	10 (34%)	48,51,51	4.08	28 (58%)
22	TGL	B	521	-	62,62,62	1.08	3 (4%)	65,65,65	1.46	8 (12%)
19	PGV	N	1524	-	50,50,50	1.23	5 (10%)	53,56,56	0.89	1 (1%)
19	PGV	C	266	-	50,50,50	1.17	5 (10%)	53,56,56	0.95	2 (3%)
20	CHD	W	1060	-	29,32,32	2.09	8 (27%)	48,51,51	4.13	28 (58%)
24	DMU	Z	1526	-	34,34,34	3.25	8 (23%)	45,45,45	3.95	20 (44%)
19	PGV	A	524	-	50,50,50	1.26	5 (10%)	53,56,56	0.82	1 (1%)
18	HEA	A	516	1	44,67,67	1.51	7 (15%)	37,103,103	1.37	6 (16%)
25	PEK	C	264	-	52,52,52	1.45	6 (11%)	55,57,57	1.24	3 (5%)
23	PSC	B	230	-	51,51,51	1.40	6 (11%)	57,59,59	1.00	2 (3%)
23	PSC	O	1230	-	51,51,51	1.52	7 (13%)	57,59,59	0.98	1 (1%)
19	PGV	P	1268	-	50,50,50	1.43	5 (10%)	53,56,56	0.87	1 (1%)
22	TGL	O	1521	-	62,62,62	1.11	5 (8%)	65,65,65	1.46	8 (12%)
21	CUA	O	228	2	0,1,1	0.00	-	-		
20	CHD	N	1604	-	29,32,32	0.96	2 (6%)	48,51,51	2.47	17 (35%)
25	PEK	P	1264	-	52,52,52	1.65	8 (15%)	55,57,57	1.37	7 (12%)
24	DMU	P	1272	-	34,34,34	2.70	15 (44%)	45,45,45	3.95	17 (37%)
25	PEK	C	265	-	52,52,52	1.75	11 (21%)	55,57,57	1.21	7 (12%)
18	HEA	N	516	1	44,67,67	1.42	7 (15%)	37,103,103	1.42	6 (16%)
19	PGV	P	1266	-	50,50,50	1.36	6 (12%)	53,56,56	1.04	4 (7%)
19	PGV	C	268	-	50,50,50	1.45	7 (14%)	53,56,56	0.90	0
25	PEK	P	1265	-	52,52,52	1.78	11 (21%)	55,57,57	1.19	7 (12%)
20	CHD	A	525	-	29,32,32	0.95	1 (3%)	48,51,51	2.55	18 (37%)
22	TGL	L	522	-	62,62,62	1.35	5 (8%)	65,65,65	1.68	12 (18%)
18	HEA	A	515	1	44,67,67	2.25	7 (15%)	37,103,103	1.81	12 (32%)
18	HEA	N	515	1	44,67,67	2.00	5 (11%)	37,103,103	1.94	14 (37%)
24	DMU	M	526	-	34,34,34	3.36	9 (26%)	45,45,45	3.94	21 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CHD	P	1525	-	29,32,32	0.98	2 (6%)	48,51,51	2.67	23 (47%)
22	TGL	N	1523	-	62,62,62	0.96	3 (4%)	65,65,65	1.25	7 (10%)
26	CDL	T	1269	-	99,99,99	1.25	11 (11%)	105,111,111	0.99	7 (6%)
25	PEK	G	1263	-	52,52,52	2.08	11 (21%)	55,57,57	1.29	4 (7%)
26	CDL	G	269	-	99,99,99	1.25	9 (9%)	105,111,111	0.98	8 (7%)
25	PEK	T	263	-	52,52,52	2.12	12 (23%)	55,57,57	1.32	4 (7%)
26	CDL	P	1270	-	99,99,99	1.21	9 (9%)	105,111,111	1.09	5 (4%)
24	DMU	C	272	-	34,34,34	2.64	16 (47%)	45,45,45	3.99	18 (40%)
20	CHD	C	271	-	29,32,32	1.38	3 (10%)	48,51,51	3.72	24 (50%)
22	TGL	N	1522	-	62,62,62	1.49	6 (9%)	65,65,65	1.64	10 (15%)
19	PGV	P	1267	-	50,50,50	0.96	3 (6%)	53,56,56	1.02	4 (7%)
20	CHD	B	1086	-	29,32,32	0.82	0	48,51,51	2.52	20 (41%)
22	TGL	D	523	-	62,62,62	1.01	3 (4%)	65,65,65	1.30	9 (13%)
21	CUA	B	228	2	0,1,1	0.00	-	-	-	-
20	CHD	W	1271	-	29,32,32	1.31	4 (13%)	48,51,51	3.63	25 (52%)

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	-
26	CDL	C	270	-	-	68/110/110/110	-
20	CHD	J	60	-	5/5/12/12	6/7/74/74	0/4/4/4
22	TGL	B	521	-	-	14/65/65/65	-
19	PGV	N	1524	-	-	35/55/55/55	-
19	PGV	C	266	-	-	16/55/55/55	-
20	CHD	W	1060	-	5/5/12/12	6/7/74/74	0/4/4/4
24	DMU	Z	1526	-	5/5/10/10	8/19/59/59	0/2/2/2
18	HEA	N	515	1	3/3/7/16	2/24/76/76	-
18	HEA	A	516	1	3/3/7/16	1/24/76/76	-
25	PEK	C	264	-	-	23/56/56/56	-
23	PSC	B	230	-	-	37/55/55/55	-
23	PSC	O	1230	-	-	37/55/55/55	-
19	PGV	P	1268	-	-	35/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	TGL	O	1521	-	-	14/65/65/65	-
20	CHD	N	1604	-	-	1/7/74/74	0/4/4/4
25	PEK	P	1264	-	-	24/56/56/56	-
24	DMU	P	1272	-	6/6/10/10	11/19/59/59	0/2/2/2
25	PEK	C	265	-	-	21/56/56/56	-
18	HEA	N	516	1	3/3/7/16	1/24/76/76	-
19	PGV	P	1266	-	-	15/55/55/55	-
19	PGV	C	268	-	-	34/55/55/55	-
25	PEK	P	1265	-	-	20/56/56/56	-
20	CHD	A	525	-	-	0/7/74/74	0/4/4/4
22	TGL	L	522	-	-	19/65/65/65	-
18	HEA	A	515	1	3/3/7/16	2/24/76/76	-
19	PGV	A	524	-	-	35/55/55/55	-
24	DMU	M	526	-	5/5/10/10	8/19/59/59	0/2/2/2
20	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
22	TGL	N	1523	-	-	15/65/65/65	-
26	CDL	T	1269	-	-	62/110/110/110	-
25	PEK	G	1263	-	-	29/56/56/56	-
26	CDL	G	269	-	-	62/110/110/110	-
25	PEK	T	263	-	-	29/56/56/56	-
26	CDL	P	1270	-	-	69/110/110/110	-
24	DMU	C	272	-	6/6/10/10	10/19/59/59	0/2/2/2
20	CHD	C	271	-	5/5/12/12	6/7/74/74	0/4/4/4
22	TGL	N	1522	-	-	19/65/65/65	-
19	PGV	P	1267	-	-	17/55/55/55	-
20	CHD	B	1086	-	-	0/7/74/74	0/4/4/4
22	TGL	D	523	-	-	15/65/65/65	-
20	CHD	W	1271	-	5/5/12/12	6/7/74/74	0/4/4/4

All (277) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	515	HEA	C3B-C11	-12.57	1.43	1.52
18	N	515	HEA	C3B-C11	-10.46	1.44	1.52
24	M	526	DMU	O7-C3	-8.58	1.21	1.43
24	M	526	DMU	O16-C6	-7.92	1.26	1.40
24	Z	1526	DMU	O7-C3	-7.78	1.23	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Z	1526	DMU	O1-C9	-7.52	1.26	1.44
24	M	526	DMU	O1-C9	-7.50	1.26	1.44
24	Z	1526	DMU	O16-C6	-7.42	1.27	1.40
24	M	526	DMU	O7-C10	-6.66	1.23	1.41
24	Z	1526	DMU	O16-C18	-6.66	1.24	1.43
24	M	526	DMU	O5-C4	-6.61	1.28	1.44
22	N	1522	TGL	OG1-CA1	6.33	1.51	1.33
24	Z	1526	DMU	O7-C10	-6.30	1.24	1.41
24	Z	1526	DMU	O5-C4	-6.24	1.29	1.44
24	M	526	DMU	O16-C18	-6.20	1.25	1.43
20	W	1060	CHD	C13-C17	6.08	1.65	1.55
25	T	263	PEK	O03-C21	5.98	1.50	1.33
24	P	1272	DMU	O16-C18	-5.97	1.26	1.43
20	J	60	CHD	C13-C17	5.76	1.65	1.55
24	C	272	DMU	O16-C18	-5.72	1.27	1.43
24	M	526	DMU	O1-C10	-5.68	1.27	1.41
23	O	1230	PSC	C2-C1	5.50	1.66	1.50
19	P	1266	PGV	O03-C19	5.50	1.49	1.33
25	G	1263	PEK	O03-C21	5.41	1.49	1.33
24	Z	1526	DMU	O1-C10	-5.27	1.28	1.41
24	P	1272	DMU	O16-C6	-5.22	1.31	1.40
25	G	1263	PEK	C01-C02	5.15	1.66	1.50
25	T	263	PEK	C12-C11	5.11	1.61	1.31
25	T	263	PEK	C01-C02	5.11	1.66	1.50
24	C	272	DMU	O1-C9	-4.96	1.32	1.44
19	C	268	PGV	C12-C11	4.93	1.60	1.31
22	L	522	TGL	OG2-CB1	4.87	1.48	1.34
24	C	272	DMU	O16-C6	-4.87	1.31	1.40
25	G	1263	PEK	C12-C11	4.87	1.60	1.31
25	C	264	PEK	C15-C14	4.85	1.59	1.31
22	N	1522	TGL	OG2-CB1	4.84	1.47	1.34
23	O	1230	PSC	C10-C9	4.74	1.59	1.31
19	P	1268	PGV	C12-C11	4.73	1.59	1.31
25	G	1263	PEK	C9-C8	4.71	1.59	1.31
24	C	272	DMU	O7-C3	-4.70	1.31	1.43
24	C	272	DMU	O5-C4	-4.70	1.32	1.44
22	L	522	TGL	OG1-CA1	4.68	1.47	1.33
24	P	1272	DMU	O7-C3	-4.65	1.31	1.43
23	B	230	PSC	C10-C9	4.62	1.58	1.31
24	P	1272	DMU	O1-C9	-4.61	1.33	1.44
25	T	263	PEK	C6-C5	4.61	1.58	1.31
25	C	264	PEK	C12-C11	4.61	1.58	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	1263	PEK	C6-C5	4.60	1.58	1.31
25	C	264	PEK	C6-C5	4.60	1.58	1.31
25	P	1265	PEK	C12-C11	4.58	1.58	1.31
25	T	263	PEK	C9-C8	4.58	1.58	1.31
25	P	1264	PEK	C6-C5	4.57	1.58	1.31
24	P	1272	DMU	C6-C1	4.56	1.65	1.52
24	Z	1526	DMU	O5-C6	-4.51	1.30	1.41
25	P	1265	PEK	C9-C8	4.51	1.57	1.31
24	P	1272	DMU	C8-C7	4.48	1.63	1.52
24	M	526	DMU	O5-C6	-4.47	1.30	1.41
25	P	1264	PEK	C12-C11	4.46	1.57	1.31
25	G	1263	PEK	C03-C02	4.46	1.64	1.50
25	C	265	PEK	C12-C11	4.45	1.57	1.31
19	C	266	PGV	O03-C19	4.43	1.46	1.33
25	C	265	PEK	C15-C14	4.42	1.57	1.31
26	G	269	CDL	OA6-CA5	4.42	1.46	1.34
25	C	265	PEK	C9-C8	4.41	1.57	1.31
25	T	263	PEK	C03-C02	4.39	1.64	1.50
19	N	1524	PGV	C12-C11	4.37	1.57	1.31
25	T	263	PEK	C15-C14	4.36	1.57	1.31
25	P	1264	PEK	C15-C14	4.36	1.57	1.31
25	P	1264	PEK	C9-C8	4.34	1.56	1.31
25	P	1265	PEK	C15-C14	4.33	1.56	1.31
25	G	1263	PEK	C15-C14	4.32	1.56	1.31
26	T	1269	CDL	OA6-CA5	4.23	1.46	1.34
19	A	524	PGV	C12-C11	4.19	1.56	1.31
19	A	524	PGV	O03-C19	4.17	1.45	1.33
18	A	516	HEA	C3B-C11	-4.16	1.49	1.52
25	C	264	PEK	C9-C8	4.16	1.55	1.31
19	P	1268	PGV	O01-C1	4.13	1.45	1.34
24	P	1272	DMU	C3-C4	4.09	1.63	1.52
25	P	1265	PEK	C6-C5	4.06	1.55	1.31
18	N	516	HEA	C3B-C11	-4.03	1.49	1.52
22	D	523	TGL	OG2-CB1	4.02	1.45	1.34
24	C	272	DMU	C6-C1	4.00	1.64	1.52
19	P	1266	PGV	C12-C11	3.95	1.54	1.31
25	C	265	PEK	C6-C5	3.88	1.54	1.31
19	C	266	PGV	C12-C11	3.87	1.54	1.31
26	G	269	CDL	C11-CA5	3.86	1.62	1.50
18	A	515	HEA	C3A-CMA	-3.84	1.37	1.46
22	B	521	TGL	OG2-CB1	3.81	1.45	1.34
19	C	268	PGV	O01-C1	3.79	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	516	HEA	C3A-C2A	-3.79	1.35	1.40
23	B	230	PSC	C13-C12	3.78	1.53	1.31
26	T	1269	CDL	CB6-CB4	3.76	1.62	1.50
18	N	515	HEA	C1C-NC	3.67	1.43	1.36
23	O	1230	PSC	C13-C12	3.65	1.52	1.31
24	P	1272	DMU	O5-C4	-3.57	1.35	1.44
20	W	1060	CHD	C8-C7	3.57	1.59	1.53
24	C	272	DMU	C3-C4	3.56	1.62	1.52
20	W	1060	CHD	C20-C17	3.56	1.60	1.54
19	P	1266	PGV	C01-C02	3.52	1.61	1.50
26	P	1270	CDL	PA1-OA5	3.51	1.73	1.59
26	P	1270	CDL	OA8-CA7	3.46	1.43	1.33
26	T	1269	CDL	C11-CA5	3.45	1.60	1.50
26	G	269	CDL	CB6-CB4	3.44	1.61	1.50
22	L	522	TGL	CG1-CG2	3.42	1.61	1.50
20	C	271	CHD	C13-C14	3.40	1.61	1.55
22	O	1521	TGL	CB2-CB1	3.40	1.60	1.50
26	P	1270	CDL	C31-CA7	3.39	1.60	1.50
25	G	1263	PEK	P-O11	3.38	1.73	1.59
23	B	230	PSC	C2-C1	3.37	1.60	1.50
24	C	272	DMU	O1-C10	-3.37	1.33	1.41
19	C	268	PGV	C04-C05	3.36	1.63	1.51
19	C	267	PGV	O01-C1	3.34	1.43	1.34
20	W	1060	CHD	C10-C5	3.34	1.60	1.55
19	P	1268	PGV	C04-C05	3.33	1.62	1.51
22	O	1521	TGL	OG2-CB1	3.33	1.43	1.34
24	P	1272	DMU	O7-C10	-3.33	1.32	1.41
24	C	272	DMU	O7-C10	-3.32	1.32	1.41
20	J	60	CHD	C10-C5	3.32	1.60	1.55
26	P	1270	CDL	CA3-CA4	3.30	1.60	1.50
25	C	265	PEK	O03-C21	3.29	1.43	1.33
25	P	1265	PEK	O03-C21	3.26	1.42	1.33
22	N	1522	TGL	CG1-CG2	3.26	1.60	1.50
26	P	1270	CDL	C71-CB7	3.26	1.60	1.50
25	P	1264	PEK	O03-C21	3.26	1.42	1.33
20	W	1271	CHD	C13-C17	3.23	1.61	1.55
20	J	60	CHD	C8-C7	3.23	1.59	1.53
19	P	1267	PGV	C12-C11	3.20	1.50	1.31
18	A	516	HEA	C3C-CAC	3.19	1.54	1.47
26	P	1270	CDL	CA6-CA4	3.19	1.60	1.50
25	T	263	PEK	P-O11	3.19	1.72	1.59
25	C	265	PEK	C03-C02	3.18	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	270	CDL	C71-CB7	3.15	1.59	1.50
18	N	516	HEA	C3A-CMA	-3.15	1.39	1.46
20	C	271	CHD	C13-C12	3.15	1.59	1.54
22	L	522	TGL	CG3-CG2	3.14	1.60	1.50
26	C	270	CDL	CA6-CA4	3.13	1.60	1.50
20	C	271	CHD	C13-C17	3.10	1.60	1.55
19	C	267	PGV	C12-C11	3.10	1.49	1.31
23	B	230	PSC	O01-C1	3.08	1.43	1.34
19	C	266	PGV	C03-C02	3.08	1.60	1.50
22	N	1523	TGL	OG2-CB1	3.07	1.43	1.34
25	P	1264	PEK	O01-C1	3.04	1.42	1.34
19	C	267	PGV	O03-C19	3.03	1.42	1.33
25	P	1265	PEK	C03-C02	3.02	1.60	1.50
24	P	1272	DMU	C10-C5	3.02	1.61	1.52
22	N	1522	TGL	CA2-CA1	3.00	1.59	1.50
24	P	1272	DMU	C7-C5	3.00	1.60	1.52
20	J	60	CHD	C8-C9	3.00	1.59	1.53
26	T	1269	CDL	CB2-C1	3.00	1.61	1.51
26	T	1269	CDL	CB3-CB4	2.99	1.59	1.50
24	C	272	DMU	C7-C5	2.98	1.59	1.52
26	G	269	CDL	CB3-CB4	2.97	1.59	1.50
20	W	1060	CHD	C13-C12	2.97	1.59	1.54
24	C	272	DMU	O5-C6	-2.96	1.34	1.41
22	N	1522	TGL	CG3-CG2	2.95	1.59	1.50
22	B	521	TGL	CG3-CG2	2.95	1.59	1.50
26	G	269	CDL	PB2-OB2	2.95	1.71	1.59
25	P	1265	PEK	C01-C02	2.93	1.59	1.50
22	O	1521	TGL	CG3-CG2	2.93	1.59	1.50
26	T	1269	CDL	PB2-OB2	2.90	1.71	1.59
18	N	515	HEA	C3A-CMA	-2.90	1.39	1.46
19	C	268	PGV	P-O12	2.90	1.71	1.59
20	W	1271	CHD	C13-C12	2.89	1.59	1.54
19	P	1268	PGV	P-O12	2.86	1.70	1.59
18	A	516	HEA	C3A-CMA	-2.85	1.39	1.46
24	P	1272	DMU	C8-C9	2.85	1.59	1.53
19	N	1524	PGV	C03-C02	2.85	1.59	1.50
25	P	1265	PEK	P-O11	2.85	1.70	1.59
26	G	269	CDL	OB6-CB5	2.85	1.42	1.34
25	C	265	PEK	P-O11	2.85	1.70	1.59
26	G	269	CDL	CB2-C1	2.80	1.61	1.51
24	C	272	DMU	C8-C7	2.80	1.59	1.52
22	B	521	TGL	CB2-CB1	2.78	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	W	1060	CHD	C10-C9	2.77	1.61	1.56
25	C	265	PEK	C01-C02	2.74	1.59	1.50
18	A	515	HEA	C4D-ND	2.74	1.41	1.36
20	W	1060	CHD	C8-C14	2.73	1.59	1.53
20	W	1271	CHD	C13-C14	2.73	1.60	1.55
24	C	272	DMU	C8-C9	2.71	1.58	1.53
26	P	1270	CDL	OB6-CB5	2.71	1.42	1.34
25	P	1265	PEK	C22-C21	2.70	1.58	1.50
25	G	1263	PEK	O03-C01	2.70	1.51	1.45
25	G	1263	PEK	P-O12	2.69	1.70	1.59
25	P	1264	PEK	C2-C1	2.69	1.58	1.50
24	P	1272	DMU	O5-C6	-2.68	1.35	1.41
20	W	1060	CHD	C8-C9	2.68	1.59	1.53
19	N	1524	PGV	O03-C19	2.66	1.41	1.33
20	J	60	CHD	C13-C12	2.65	1.58	1.54
26	C	270	CDL	CA3-CA4	2.65	1.58	1.50
25	P	1265	PEK	O01-C1	2.65	1.41	1.34
25	T	263	PEK	O03-C01	2.63	1.51	1.45
22	D	523	TGL	CB2-CB1	2.63	1.58	1.50
26	C	270	CDL	C31-CA7	2.63	1.58	1.50
26	P	1270	CDL	C11-CA5	2.63	1.58	1.50
23	O	1230	PSC	P-O12	2.62	1.69	1.59
19	P	1266	PGV	C20-C19	2.62	1.58	1.50
19	P	1267	PGV	O03-C19	2.61	1.41	1.33
19	P	1267	PGV	C01-C02	2.61	1.58	1.50
25	T	263	PEK	C22-C21	2.61	1.58	1.50
19	P	1266	PGV	O01-C1	2.59	1.41	1.34
26	G	269	CDL	CA6-CA4	2.59	1.58	1.50
24	C	272	DMU	C10-C5	2.56	1.59	1.52
19	P	1266	PGV	C03-C02	2.56	1.58	1.50
22	N	1522	TGL	CB2-CB1	2.55	1.58	1.50
19	C	266	PGV	O01-C1	2.54	1.41	1.34
18	N	516	HEA	C3A-C2A	-2.54	1.36	1.40
26	C	270	CDL	OA8-CA7	2.53	1.40	1.33
24	P	1272	DMU	C2-C1	2.53	1.58	1.52
18	N	516	HEA	C1B-CHB	-2.51	1.34	1.41
26	P	1270	CDL	PB2-OB2	2.49	1.69	1.59
26	T	1269	CDL	C31-CA7	2.45	1.57	1.50
18	A	516	HEA	C16-C15	2.45	1.56	1.51
25	P	1265	PEK	P-O12	2.45	1.69	1.59
26	T	1269	CDL	C71-CB7	2.44	1.57	1.50
20	J	60	CHD	C8-C14	2.44	1.58	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	265	PEK	O01-C1	2.43	1.41	1.34
19	A	524	PGV	C03-C02	2.43	1.58	1.50
24	P	1272	DMU	O1-C10	-2.42	1.35	1.41
20	N	1604	CHD	C13-C12	-2.40	1.50	1.54
18	N	516	HEA	C1A-C2A	2.39	1.48	1.42
25	C	265	PEK	C22-C21	2.38	1.57	1.50
22	O	1521	TGL	OG3-CC1	2.37	1.40	1.33
18	A	515	HEA	C4B-C3B	-2.37	1.37	1.42
26	T	1269	CDL	CA6-CA4	2.37	1.58	1.50
26	C	270	CDL	PA1-OA5	2.36	1.68	1.59
19	C	268	PGV	C06-C05	2.34	1.61	1.51
20	P	1525	CHD	C13-C14	2.33	1.59	1.55
25	G	1263	PEK	C22-C21	2.33	1.57	1.50
19	N	1524	PGV	O01-C1	2.33	1.40	1.34
26	C	270	CDL	PB2-OB2	2.32	1.68	1.59
18	N	516	HEA	C17-C18	2.31	1.57	1.50
26	T	1269	CDL	OB6-CB5	2.30	1.40	1.34
18	A	515	HEA	C26-C15	2.30	1.56	1.50
20	J	60	CHD	C1-C10	2.30	1.58	1.54
22	L	522	TGL	CB2-CB1	2.29	1.57	1.50
25	C	265	PEK	P-O12	2.29	1.68	1.59
22	N	1523	TGL	OG3-CC1	2.29	1.40	1.33
20	J	60	CHD	C20-C17	2.28	1.58	1.54
19	A	524	PGV	C20-C19	2.28	1.57	1.50
23	O	1230	PSC	C3-C2	2.28	1.60	1.52
18	A	515	HEA	C1C-NC	2.27	1.40	1.36
25	T	263	PEK	C2-C1	2.25	1.57	1.50
19	C	266	PGV	C20-C19	2.24	1.57	1.50
19	N	1524	PGV	C20-C19	2.23	1.57	1.50
18	N	515	HEA	C3A-C2A	-2.22	1.37	1.40
24	C	272	DMU	C2-C1	2.22	1.58	1.52
23	B	230	PSC	P-O12	2.22	1.68	1.59
18	N	515	HEA	C1C-CHC	-2.21	1.34	1.41
24	C	272	DMU	C2-C3	2.21	1.58	1.52
22	D	523	TGL	OG3-CC1	2.21	1.39	1.33
25	T	263	PEK	P-O12	2.20	1.68	1.59
25	C	264	PEK	O03-C01	-2.20	1.40	1.45
26	T	1269	CDL	C51-CB5	2.18	1.57	1.50
20	J	60	CHD	C10-C9	2.18	1.60	1.56
23	O	1230	PSC	C01-C02	2.16	1.57	1.50
22	N	1523	TGL	CG3-CG2	2.15	1.57	1.50
19	C	268	PGV	P-O11	2.15	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	516	HEA	C20-C19	2.14	1.55	1.51
18	N	516	HEA	C3C-C2C	-2.13	1.37	1.40
23	B	230	PSC	P-O11	2.13	1.67	1.59
22	O	1521	TGL	CA2-CA1	2.10	1.56	1.50
26	C	270	CDL	C11-CA5	2.10	1.56	1.50
20	W	1271	CHD	C1-C10	2.10	1.57	1.54
26	G	269	CDL	C71-CB7	2.08	1.56	1.50
25	P	1264	PEK	C22-C21	2.07	1.56	1.50
19	C	268	PGV	C20-C19	2.06	1.56	1.50
20	P	1525	CHD	C8-C9	2.06	1.57	1.53
19	A	524	PGV	C06-C05	2.05	1.60	1.51
20	A	525	CHD	C10-C9	-2.04	1.52	1.56
20	N	1604	CHD	C19-C10	-2.03	1.50	1.54
18	A	515	HEA	C1C-CHC	-2.02	1.35	1.41
25	C	264	PEK	C4-C5	2.02	1.61	1.50
23	O	1230	PSC	O01-C1	2.01	1.40	1.34
20	J	60	CHD	C13-C14	2.01	1.58	1.55
18	A	516	HEA	C17-C18	2.00	1.57	1.50
24	M	526	DMU	C8-C7	2.00	1.57	1.52
19	P	1268	PGV	C06-C05	2.00	1.59	1.51

All (433) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	1272	DMU	O16-C6-C1	11.86	126.82	108.30
24	C	272	DMU	O16-C6-C1	10.72	125.04	108.30
24	M	526	DMU	C1-C2-C3	9.86	132.19	109.68
24	Z	1526	DMU	C1-C2-C3	9.75	131.95	109.68
20	C	271	CHD	C10-C9-C8	9.68	122.21	111.82
20	B	1086	CHD	C18-C13-C12	-9.56	99.33	109.07
20	W	1060	CHD	C10-C9-C8	9.32	121.82	111.82
20	J	60	CHD	C10-C9-C8	9.13	121.63	111.82
20	W	1271	CHD	C10-C9-C8	9.12	121.62	111.82
24	C	272	DMU	C1-C2-C3	8.87	129.92	109.68
24	C	272	DMU	O1-C9-C11	8.71	128.09	106.44
20	C	271	CHD	C17-C13-C14	8.54	108.70	100.09
20	W	1271	CHD	C19-C10-C9	-8.50	99.47	111.18
20	C	271	CHD	C19-C10-C9	-8.24	99.82	111.18
20	N	1604	CHD	C18-C13-C12	-8.19	100.73	109.07
20	W	1060	CHD	O12-C12-C13	8.16	124.83	111.03
24	P	1272	DMU	O1-C9-C11	8.02	126.37	106.44
20	W	1271	CHD	C17-C13-C14	8.01	108.17	100.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	M	526	DMU	O1-C9-C11	7.95	126.19	106.44
24	P	1272	DMU	C1-C2-C3	7.94	127.81	109.68
24	Z	1526	DMU	C7-C8-C9	7.92	124.37	110.24
24	P	1272	DMU	O5-C4-C3	7.92	126.44	109.75
24	Z	1526	DMU	O1-C9-C11	7.86	125.98	106.44
20	W	1060	CHD	C6-C5-C10	7.79	120.93	112.66
20	W	1271	CHD	C17-C13-C12	-7.73	110.61	117.67
20	J	60	CHD	O12-C12-C13	7.68	124.01	111.03
24	M	526	DMU	C10-C5-C7	7.56	125.75	110.00
24	C	272	DMU	C6-O5-C4	7.55	128.52	113.69
20	W	1060	CHD	C13-C17-C20	7.49	128.43	119.50
20	J	60	CHD	C6-C5-C10	7.45	120.57	112.66
24	P	1272	DMU	O7-C3-C4	7.40	129.74	109.45
24	M	526	DMU	C7-C8-C9	7.32	123.30	110.24
20	W	1060	CHD	C17-C13-C14	7.32	107.47	100.09
24	C	272	DMU	O5-C4-C3	7.29	125.13	109.75
24	Z	1526	DMU	C10-C5-C7	7.28	125.16	110.00
20	C	271	CHD	C17-C13-C12	-7.28	111.02	117.67
20	J	60	CHD	C17-C13-C14	7.27	107.42	100.09
24	Z	1526	DMU	O5-C4-C3	7.25	125.03	109.75
20	J	60	CHD	C13-C17-C20	7.20	128.09	119.50
20	W	1060	CHD	C4-C3-C2	7.19	119.14	110.55
24	M	526	DMU	C6-O5-C4	7.11	127.65	113.69
20	J	60	CHD	C11-C12-C13	7.10	118.54	111.24
20	J	60	CHD	C5-C6-C7	7.06	122.25	114.46
24	M	526	DMU	O5-C4-C3	6.96	124.43	109.75
24	C	272	DMU	O7-C3-C4	6.95	128.48	109.45
24	M	526	DMU	O5-C4-C57	6.92	123.65	106.44
24	Z	1526	DMU	C6-O5-C4	6.90	127.24	113.69
20	W	1060	CHD	C11-C9-C10	6.86	120.81	113.73
24	Z	1526	DMU	O5-C4-C57	6.78	123.28	106.44
20	W	1271	CHD	C14-C13-C12	6.77	113.71	107.40
20	C	271	CHD	C14-C13-C12	6.69	113.63	107.40
20	P	1525	CHD	C10-C9-C8	6.58	118.88	111.82
20	A	525	CHD	C10-C9-C8	6.57	118.87	111.82
20	W	1060	CHD	C5-C6-C7	6.54	121.68	114.46
20	W	1060	CHD	C11-C12-C13	6.43	117.85	111.24
24	M	526	DMU	O1-C9-C8	6.39	121.30	109.69
20	J	60	CHD	C4-C3-C2	6.35	118.14	110.55
24	Z	1526	DMU	O1-C9-C8	6.31	121.16	109.69
20	W	1060	CHD	C18-C13-C14	-6.19	101.52	111.21
20	P	1525	CHD	C11-C12-C13	-6.17	104.91	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	60	CHD	C11-C9-C10	6.11	120.03	113.73
20	C	271	CHD	C9-C8-C7	6.09	119.16	111.88
20	W	1271	CHD	C9-C8-C7	6.08	119.15	111.88
24	P	1272	DMU	O1-C9-C8	6.05	120.68	109.69
24	C	272	DMU	C18-O16-C6	6.00	123.78	113.84
20	C	271	CHD	C4-C3-C2	5.96	117.67	110.55
24	P	1272	DMU	C6-O5-C4	5.96	125.39	113.69
20	W	1271	CHD	C4-C3-C2	5.96	117.66	110.55
24	P	1272	DMU	C18-O16-C6	5.87	123.58	113.84
24	Z	1526	DMU	C8-C7-C5	-5.86	100.59	110.82
24	P	1272	DMU	O5-C6-C1	5.78	122.59	110.35
20	C	271	CHD	C1-C10-C5	5.70	116.19	107.77
24	M	526	DMU	O5-C6-C1	5.69	122.39	110.35
24	C	272	DMU	C8-C7-C5	5.64	120.67	110.82
22	B	521	TGL	CG2-OG2-CB1	5.62	131.63	117.79
20	W	1060	CHD	C14-C8-C9	5.59	117.38	109.71
24	C	272	DMU	O7-C3-C2	5.56	122.08	107.28
24	P	1272	DMU	C8-C7-C5	5.49	120.41	110.82
24	M	526	DMU	C8-C7-C5	-5.48	101.26	110.82
24	C	272	DMU	O5-C4-C57	5.44	119.96	106.44
22	O	1521	TGL	CG2-OG2-CB1	5.41	131.10	117.79
24	P	1272	DMU	O5-C4-C57	5.35	119.74	106.44
20	N	1604	CHD	C10-C9-C8	5.33	117.55	111.82
20	J	60	CHD	C18-C13-C14	-5.32	102.89	111.21
24	Z	1526	DMU	O5-C6-C1	5.30	121.58	110.35
24	Z	1526	DMU	O5-C6-O16	5.22	122.33	109.97
20	P	1525	CHD	C5-C6-C7	5.21	120.21	114.46
24	P	1272	DMU	O7-C3-C2	5.21	121.13	107.28
20	J	60	CHD	C14-C8-C9	5.19	116.83	109.71
24	C	272	DMU	O5-C6-C1	5.17	121.28	110.35
24	C	272	DMU	O7-C10-C5	5.16	121.47	108.10
20	W	1271	CHD	C15-C14-C8	-5.15	111.13	118.33
20	A	525	CHD	C5-C6-C7	5.13	120.12	114.46
24	M	526	DMU	O5-C6-O16	5.11	122.08	109.97
20	A	525	CHD	C4-C3-C2	5.11	116.66	110.55
22	N	1522	TGL	C12-C11-C10	-5.10	88.52	114.42
20	W	1060	CHD	C15-C14-C8	-5.06	111.26	118.33
20	B	1086	CHD	C1-C10-C5	5.05	115.24	107.77
20	A	525	CHD	C13-C17-C20	5.02	125.49	119.50
20	C	271	CHD	C15-C14-C8	-5.01	111.33	118.33
18	A	515	HEA	C26-C15-C16	4.97	123.64	115.27
20	W	1271	CHD	C1-C10-C5	4.97	115.12	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	272	DMU	O1-C9-C8	4.94	118.66	109.69
20	J	60	CHD	C15-C14-C8	-4.94	111.43	118.33
20	W	1060	CHD	C19-C10-C1	-4.93	100.31	108.26
22	L	522	TGL	C12-C11-C10	-4.89	89.60	114.42
20	C	271	CHD	C18-C13-C12	-4.88	104.09	109.07
20	J	60	CHD	C19-C10-C1	-4.85	100.45	108.26
20	J	60	CHD	C13-C14-C8	4.84	120.92	114.74
18	N	515	HEA	C26-C15-C16	4.84	123.41	115.27
20	J	60	CHD	C9-C8-C7	4.82	117.64	111.88
24	Z	1526	DMU	O16-C6-C1	4.81	115.81	108.30
25	T	263	PEK	O03-C01-C02	4.77	122.31	108.43
20	C	271	CHD	C4-C5-C10	4.70	117.65	112.66
24	M	526	DMU	O7-C3-C2	4.69	119.76	107.28
25	G	1263	PEK	O03-C01-C02	4.69	122.09	108.43
20	N	1604	CHD	C1-C10-C5	4.66	114.66	107.77
20	W	1060	CHD	C9-C8-C7	4.64	117.42	111.88
24	P	1272	DMU	O7-C10-C5	4.63	120.09	108.10
24	Z	1526	DMU	O7-C3-C2	4.62	119.57	107.28
20	P	1525	CHD	C1-C10-C5	4.59	114.55	107.77
20	P	1525	CHD	C13-C17-C20	4.59	124.97	119.50
20	W	1060	CHD	C13-C14-C8	4.59	120.59	114.74
20	A	525	CHD	C11-C12-C13	-4.53	106.59	111.24
20	J	60	CHD	C2-C1-C10	4.51	120.52	112.78
24	C	272	DMU	C10-O1-C9	4.51	122.54	113.69
20	W	1060	CHD	C1-C10-C5	4.50	114.42	107.77
24	M	526	DMU	O16-C6-C1	4.48	115.30	108.30
22	N	1522	TGL	CB9-CB8-CB7	-4.48	91.70	114.42
20	W	1060	CHD	C2-C1-C10	4.47	120.45	112.78
20	W	1271	CHD	C4-C5-C10	4.42	117.36	112.66
20	N	1604	CHD	C17-C13-C12	4.38	121.67	117.67
24	Z	1526	DMU	O7-C3-C4	4.37	121.41	109.45
19	P	1266	PGV	O01-C1-C2	-4.21	102.42	111.50
20	C	271	CHD	C6-C5-C10	4.20	117.12	112.66
22	L	522	TGL	CB9-CB8-CB7	-4.17	93.26	114.42
25	T	263	PEK	C02-O01-C1	4.14	127.99	117.79
20	C	271	CHD	C19-C10-C1	-4.14	101.60	108.26
24	Z	1526	DMU	C18-O16-C6	4.13	120.69	113.84
20	J	60	CHD	C1-C10-C5	4.10	113.83	107.77
26	C	270	CDL	PA1-OA5-CA3	4.09	145.67	121.68
20	J	60	CHD	C18-C13-C12	-4.07	104.92	109.07
22	L	522	TGL	C11-C10-CB9	4.07	135.06	114.42
20	W	1060	CHD	C14-C8-C7	4.06	117.20	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	C	271	CHD	C9-C11-C12	4.05	119.65	114.30
19	C	266	PGV	O01-C1-C2	-4.04	102.80	111.50
26	P	1270	CDL	PA1-OA5-CA3	4.03	145.33	121.68
20	A	525	CHD	C1-C10-C5	4.02	113.72	107.77
20	P	1525	CHD	C4-C3-C2	4.02	115.36	110.55
25	T	263	PEK	P-O11-C03	4.02	145.24	121.68
24	Z	1526	DMU	O7-C10-O1	4.00	121.85	110.67
20	P	1525	CHD	C9-C8-C7	4.00	116.66	111.88
18	N	515	HEA	C12-C13-C14	-4.00	101.67	112.23
24	M	526	DMU	O7-C3-C4	3.99	120.39	109.45
20	N	1604	CHD	C15-C14-C13	-3.98	99.65	103.55
22	O	1521	TGL	CG1-OG1-CA1	-3.95	102.48	117.12
24	P	1272	DMU	O1-C10-C5	3.92	118.66	110.35
20	P	1525	CHD	C15-C14-C8	-3.92	112.85	118.33
22	N	1522	TGL	C15-CC9-CC8	3.92	134.31	114.42
20	P	1525	CHD	C6-C5-C10	3.90	116.80	112.66
20	W	1271	CHD	O12-C12-C13	3.89	117.61	111.03
20	B	1086	CHD	C10-C9-C8	3.88	115.99	111.82
24	M	526	DMU	C18-O16-C6	3.86	120.24	113.84
22	L	522	TGL	C15-CC9-CC8	3.84	133.93	114.42
20	J	60	CHD	C1-C2-C3	3.84	115.40	110.47
23	B	230	PSC	C01-O03-C19	-3.81	103.01	117.12
22	L	522	TGL	C16-C15-CC9	3.81	133.75	114.42
25	G	1263	PEK	P-O11-C03	3.80	143.95	121.68
20	N	1604	CHD	C16-C17-C13	-3.79	99.84	103.55
22	N	1522	TGL	C16-C15-CC9	3.74	133.44	114.42
22	N	1522	TGL	C11-C10-CB9	3.74	133.41	114.42
24	C	272	DMU	O7-C10-O1	3.72	121.08	110.67
19	C	267	PGV	O01-C1-C2	-3.70	103.52	111.50
25	P	1264	PEK	O03-C21-C22	-3.67	100.40	111.91
20	W	1271	CHD	C18-C13-C12	-3.66	105.34	109.07
20	B	1086	CHD	C6-C5-C10	3.66	116.54	112.66
20	A	525	CHD	C15-C14-C8	-3.65	113.23	118.33
26	C	270	CDL	CB6-OB8-CB7	-3.64	103.62	117.12
25	G	1263	PEK	C02-O01-C1	3.64	126.74	117.79
20	A	525	CHD	C5-C4-C3	3.63	118.09	112.76
20	J	60	CHD	C14-C8-C7	3.62	116.61	111.81
23	O	1230	PSC	C01-O03-C19	-3.61	103.74	117.12
20	J	60	CHD	C5-C4-C3	3.61	118.06	112.76
20	W	1271	CHD	C5-C4-C3	3.61	118.06	112.76
20	N	1604	CHD	C15-C14-C8	-3.61	113.28	118.33
20	P	1525	CHD	C18-C13-C14	3.59	116.82	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	P	1270	CDL	OB6-CB5-C51	-3.58	103.78	111.50
20	B	1086	CHD	C1-C2-C3	3.55	115.02	110.47
20	N	1604	CHD	C1-C2-C3	3.54	115.00	110.47
22	B	521	TGL	CG1-OG1-CA1	-3.53	104.05	117.12
26	P	1270	CDL	CB6-OB8-CB7	-3.53	104.06	117.12
19	P	1267	PGV	O01-C1-C2	-3.53	103.90	111.50
20	B	1086	CHD	C16-C17-C13	-3.52	100.11	103.55
20	C	271	CHD	O12-C12-C13	3.49	116.94	111.03
25	P	1264	PEK	C3-C2-C1	-3.49	100.92	113.62
18	A	515	HEA	C25-C23-C24	3.49	122.31	114.60
24	P	1272	DMU	C10-O1-C9	3.46	120.49	113.69
20	W	1060	CHD	C1-C2-C3	3.46	114.91	110.47
20	B	1086	CHD	C15-C14-C8	-3.46	113.49	118.33
25	C	265	PEK	C11-C10-C9	3.45	129.03	112.02
20	W	1271	CHD	C9-C11-C12	3.45	118.85	114.30
22	N	1522	TGL	C13-C12-C11	3.43	131.84	114.42
18	N	516	HEA	C27-C19-C20	3.42	121.02	115.27
25	P	1265	PEK	C11-C10-C9	3.41	128.83	112.02
24	M	526	DMU	C10-O7-C3	3.40	126.38	117.96
20	B	1086	CHD	C17-C13-C12	3.40	120.77	117.67
18	N	515	HEA	CMC-C2C-C3C	3.39	131.01	124.68
20	N	1604	CHD	C5-C4-C3	3.38	117.72	112.76
20	P	1525	CHD	C1-C2-C3	3.38	114.80	110.47
24	P	1272	DMU	O7-C10-O1	3.37	120.10	110.67
22	B	521	TGL	CG3-CG2-CG1	3.37	119.77	111.79
22	O	1521	TGL	CG3-CG2-CG1	3.37	119.76	111.79
20	A	525	CHD	C18-C13-C14	3.37	116.48	111.21
20	P	1525	CHD	C4-C5-C10	3.36	116.22	112.66
18	A	516	HEA	C26-C15-C16	3.34	120.89	115.27
20	W	1271	CHD	C5-C6-C7	3.34	118.15	114.46
18	N	515	HEA	C17-C18-C19	-3.32	119.68	127.66
18	A	515	HEA	CMC-C2C-C3C	3.30	130.84	124.68
25	C	264	PEK	C3-C2-C1	-3.29	101.66	113.62
20	A	525	CHD	C6-C5-C10	3.29	116.15	112.66
20	W	1271	CHD	C6-C5-C10	3.28	116.14	112.66
20	P	1525	CHD	C5-C4-C3	3.28	117.58	112.76
20	A	525	CHD	C9-C8-C7	3.27	115.79	111.88
20	W	1271	CHD	C18-C13-C14	-3.27	106.09	111.21
24	M	526	DMU	C10-O1-C9	3.26	120.08	113.69
20	A	525	CHD	C4-C5-C10	3.25	116.10	112.66
18	A	515	HEA	C12-C13-C14	-3.23	103.69	112.23
22	D	523	TGL	CG2-OG2-CB1	3.22	125.72	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	P	1525	CHD	C14-C13-C12	-3.21	104.42	107.40
20	W	1060	CHD	C18-C13-C12	-3.21	105.80	109.07
24	Z	1526	DMU	C2-C3-C4	-3.20	103.59	110.93
24	M	526	DMU	O7-C10-O1	3.20	119.61	110.67
20	B	1086	CHD	C14-C13-C12	3.17	110.35	107.40
20	W	1271	CHD	C19-C10-C1	-3.16	103.17	108.26
20	C	271	CHD	C5-C6-C7	3.16	117.94	114.46
26	C	270	CDL	OB6-CB5-C51	-3.15	104.70	111.50
20	C	271	CHD	C1-C2-C3	3.15	114.51	110.47
20	W	1060	CHD	C5-C4-C3	3.15	117.38	112.76
22	L	522	TGL	C13-C12-C11	3.15	130.40	114.42
20	W	1271	CHD	C2-C1-C10	3.14	118.16	112.78
25	C	265	PEK	P-O11-C03	3.13	140.03	121.68
26	P	1270	CDL	OB6-CB5-OB7	3.13	131.26	123.70
20	W	1060	CHD	C9-C11-C12	3.11	118.41	114.30
22	D	523	TGL	CG1-OG1-CA1	-3.09	105.67	117.12
20	W	1060	CHD	C16-C15-C14	3.08	111.24	105.13
22	N	1523	TGL	CG1-OG1-CA1	-3.08	105.73	117.12
20	C	271	CHD	C5-C4-C3	3.07	117.27	112.76
25	P	1265	PEK	P-O11-C03	3.07	139.67	121.68
25	P	1264	PEK	C23-C22-C21	-3.07	102.47	113.62
19	P	1266	PGV	O03-C01-C02	3.06	117.33	108.43
20	C	271	CHD	C11-C12-C13	3.04	114.36	111.24
22	D	523	TGL	CB3-CB2-CB1	3.02	124.61	113.62
24	M	526	DMU	C2-C3-C4	-3.02	104.01	110.93
20	A	525	CHD	C14-C13-C12	-3.01	104.60	107.40
26	G	269	CDL	C22-C21-C20	2.98	129.56	114.42
20	B	1086	CHD	C9-C8-C7	2.97	115.43	111.88
20	N	1604	CHD	C17-C13-C14	2.96	103.08	100.09
20	J	60	CHD	C15-C16-C17	2.95	110.99	105.13
20	J	60	CHD	C1-C10-C9	2.95	115.99	111.35
20	A	525	CHD	C18-C13-C17	-2.94	106.61	111.21
26	T	1269	CDL	C23-C22-C21	2.94	129.35	114.42
26	T	1269	CDL	C22-C21-C20	2.93	129.31	114.42
20	B	1086	CHD	C5-C6-C7	2.92	117.68	114.46
22	N	1523	TGL	OG2-CG2-CG3	2.92	118.97	108.40
18	N	515	HEA	C1B-C2B-C3B	-2.92	104.97	107.00
20	J	60	CHD	O7-C7-C6	2.92	117.18	109.94
22	L	522	TGL	CC4-CC3-CC2	2.92	123.67	113.19
20	P	1525	CHD	C17-C13-C12	2.90	120.32	117.67
18	A	516	HEA	C1B-C2B-C3B	-2.90	104.98	107.00
18	N	515	HEA	C25-C23-C24	2.90	121.01	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	516	HEA	C3C-C4C-NC	2.90	112.96	109.21
24	M	526	DMU	O7-C10-C5	2.89	115.58	108.10
20	C	271	CHD	C15-C16-C17	2.88	110.85	105.13
20	N	1604	CHD	C5-C6-C7	2.88	117.64	114.46
22	N	1523	TGL	CG2-OG2-CB1	2.88	124.87	117.79
20	A	525	CHD	C17-C13-C12	2.86	120.28	117.67
25	P	1264	PEK	O03-C21-O04	2.86	130.81	123.59
24	C	272	DMU	O1-C10-C5	2.85	116.39	110.35
20	N	1604	CHD	C4-C3-C2	2.84	113.95	110.55
20	J	60	CHD	C16-C15-C14	2.83	110.74	105.13
24	Z	1526	DMU	O1-C10-C5	2.81	116.30	110.35
20	B	1086	CHD	C15-C14-C13	-2.81	100.80	103.55
20	W	1060	CHD	C15-C16-C17	2.81	110.69	105.13
22	L	522	TGL	OG1-CG1-CG2	2.80	116.58	108.43
20	N	1604	CHD	C6-C5-C10	2.79	115.62	112.66
24	C	272	DMU	C10-O7-C3	2.79	124.87	117.96
20	J	60	CHD	C9-C11-C12	2.78	117.98	114.30
20	B	1086	CHD	C5-C4-C3	2.78	116.84	112.76
20	W	1271	CHD	C1-C2-C3	2.77	114.03	110.47
25	C	264	PEK	O03-C21-C22	-2.77	103.21	111.91
20	C	271	CHD	C18-C13-C14	-2.77	106.88	111.21
24	Z	1526	DMU	C10-O7-C3	2.75	124.78	117.96
20	W	1271	CHD	C1-C10-C9	2.74	115.67	111.35
18	N	515	HEA	C16-C15-C14	-2.74	115.57	121.12
20	W	1271	CHD	C11-C12-C13	2.74	114.06	111.24
26	G	269	CDL	C23-C22-C21	2.73	128.27	114.42
26	C	270	CDL	OB6-CB5-OB7	2.71	130.25	123.70
19	C	267	PGV	O01-C1-O02	2.71	130.25	123.70
22	D	523	TGL	CG3-OG3-CC1	2.71	127.14	117.12
20	C	271	CHD	C16-C15-C14	2.69	110.47	105.13
20	B	1086	CHD	C9-C11-C12	2.69	117.86	114.30
25	P	1265	PEK	C24-C23-C22	2.69	122.86	113.19
20	W	1271	CHD	C16-C15-C14	2.68	110.44	105.13
22	D	523	TGL	OG2-CG2-CG3	2.68	118.09	108.40
18	N	516	HEA	C26-C15-C16	2.67	119.76	115.27
18	N	515	HEA	C27-C19-C20	2.66	119.75	115.27
26	T	1269	CDL	OB8-CB7-C71	-2.66	103.57	111.91
20	W	1271	CHD	C15-C16-C17	2.65	110.39	105.13
20	B	1086	CHD	C4-C3-C2	2.65	113.72	110.55
20	B	1086	CHD	O7-C7-C6	-2.65	103.37	109.94
22	B	521	TGL	CG3-OG3-CC1	2.63	126.87	117.12
18	N	516	HEA	CMC-C2C-C1C	-2.63	124.42	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	W	1060	CHD	O7-C7-C6	2.62	116.45	109.94
22	D	523	TGL	OG1-CG1-CG2	2.62	116.07	108.43
22	B	521	TGL	CA8-CA7-CA6	-2.62	101.13	114.42
18	A	515	HEA	C16-C15-C14	-2.62	115.82	121.12
25	C	265	PEK	P-O12-C04	2.60	134.41	121.59
22	O	1521	TGL	CG3-OG3-CC1	2.60	126.77	117.12
25	C	265	PEK	C24-C23-C22	2.60	122.53	113.19
20	J	60	CHD	C17-C13-C12	2.60	120.03	117.67
22	N	1522	TGL	CC4-CC3-CC2	2.59	122.49	113.19
20	W	1060	CHD	C6-C5-C4	2.58	114.17	111.19
20	N	1604	CHD	C18-C13-C14	2.58	115.25	111.21
18	N	515	HEA	CMB-C2B-C3B	2.56	129.71	124.69
20	N	1604	CHD	C19-C10-C1	-2.55	104.15	108.26
25	P	1265	PEK	P-O12-C04	2.55	134.15	121.59
26	T	1269	CDL	OB8-CB6-CB4	2.55	115.86	108.43
20	C	271	CHD	C2-C1-C10	2.55	117.15	112.78
20	B	1086	CHD	O12-C12-C13	-2.55	106.73	111.03
20	C	271	CHD	C1-C10-C9	2.53	115.33	111.35
22	N	1522	TGL	C20-CA9-CA8	2.53	127.25	114.42
22	O	1521	TGL	CA8-CA7-CA6	-2.52	101.61	114.42
22	N	1523	TGL	CB3-CB2-CB1	2.52	122.77	113.62
26	G	269	CDL	OB8-CB7-C71	-2.51	104.04	111.91
25	C	264	PEK	O03-C21-O04	2.50	129.91	123.59
20	A	525	CHD	C2-C1-C10	2.50	117.06	112.78
18	A	516	HEA	C12-C11-C3B	2.49	119.11	112.56
25	P	1265	PEK	C2-C3-C4	2.48	117.66	113.23
22	N	1523	TGL	CG3-OG3-CC1	2.47	126.26	117.12
20	N	1604	CHD	O12-C12-C13	-2.47	106.86	111.03
20	J	60	CHD	C6-C5-C4	2.46	114.02	111.19
19	N	1524	PGV	O01-C02-C03	2.44	117.24	108.40
22	L	522	TGL	C20-CA9-CA8	2.44	126.82	114.42
18	A	515	HEA	C17-C18-C19	-2.44	121.78	127.66
25	C	265	PEK	C23-C22-C21	-2.44	104.76	113.62
18	N	516	HEA	C12-C11-C3B	2.43	118.95	112.56
18	A	516	HEA	C26-C15-C14	-2.43	117.44	123.68
22	L	522	TGL	CC3-CC2-CC1	2.43	122.46	113.62
20	A	525	CHD	C1-C2-C3	2.43	113.58	110.47
19	P	1267	PGV	O03-C19-O04	2.42	129.71	123.59
26	G	269	CDL	OB8-CB6-CB4	2.42	115.48	108.43
22	N	1522	TGL	OG1-CG1-CG2	2.42	115.48	108.43
26	C	270	CDL	C52-C51-CB5	-2.42	104.82	113.62
26	P	1270	CDL	OA8-CA6-CA4	2.42	115.47	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	A	516	HEA	C27-C19-C20	2.42	119.33	115.27
22	L	522	TGL	CG2-OG2-CB1	2.41	123.72	117.79
18	A	515	HEA	C1B-C2B-C3B	-2.40	105.33	107.00
25	C	265	PEK	C03-C02-C01	2.38	117.42	111.79
19	P	1266	PGV	C02-O01-C1	-2.36	111.97	117.79
18	A	515	HEA	C4B-C3B-C2B	2.36	108.52	106.87
25	C	265	PEK	C2-C3-C4	2.35	117.42	113.23
22	O	1521	TGL	CB7-CB6-CB5	-2.35	102.50	114.42
25	P	1264	PEK	C24-C23-C22	-2.35	104.75	113.19
20	P	1525	CHD	C19-C10-C9	-2.34	107.96	111.18
24	M	526	DMU	O1-C10-C5	2.33	115.28	110.35
24	C	272	DMU	C2-C3-C4	-2.33	105.59	110.93
19	C	266	PGV	O03-C01-C02	2.31	115.17	108.43
18	A	515	HEA	C27-C19-C20	2.29	119.13	115.27
25	G	1263	PEK	P-O12-C04	2.29	132.87	121.59
26	C	270	CDL	OA8-CA6-CA4	2.29	115.09	108.43
20	B	1086	CHD	C14-C8-C9	-2.28	106.58	109.71
26	G	269	CDL	C19-C18-C17	2.28	126.00	114.42
20	A	525	CHD	C15-C14-C13	-2.28	101.32	103.55
26	T	1269	CDL	C20-C19-C18	2.27	125.95	114.42
22	N	1523	TGL	OG1-CG1-CG2	2.25	115.00	108.43
18	N	515	HEA	CMC-C2C-C1C	-2.25	125.00	128.46
19	P	1268	PGV	O03-C01-C02	2.24	114.97	108.43
26	T	1269	CDL	C19-C18-C17	2.23	125.77	114.42
19	A	524	PGV	O01-C02-C03	2.22	116.45	108.40
20	P	1525	CHD	C16-C17-C13	-2.22	101.37	103.55
25	P	1265	PEK	C23-C22-C21	-2.22	105.56	113.62
20	P	1525	CHD	C18-C13-C17	-2.22	107.74	111.21
18	N	516	HEA	CMC-C2C-C3C	2.20	128.79	124.68
20	B	1086	CHD	C19-C10-C1	-2.20	104.72	108.26
20	N	1604	CHD	C9-C11-C12	2.19	117.20	114.30
20	B	1086	CHD	C18-C13-C14	2.19	114.64	111.21
20	P	1525	CHD	C15-C14-C13	-2.18	101.42	103.55
22	B	521	TGL	C10-CB9-CB8	2.17	125.46	114.42
25	T	263	PEK	P-O12-C04	2.17	132.29	121.59
22	D	523	TGL	CC3-CC2-CC1	-2.17	105.72	113.62
22	L	522	TGL	CC7-CC6-CC5	2.16	125.40	114.42
26	G	269	CDL	C20-C19-C18	2.16	125.38	114.42
22	O	1521	TGL	C10-CB9-CB8	2.15	125.32	114.42
20	P	1525	CHD	O3-C3-C4	2.14	114.11	109.85
24	Z	1526	DMU	O7-C10-C5	2.14	113.64	108.10
24	P	1272	DMU	O55-C2-C1	2.14	115.29	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	N	1523	TGL	OG2-CG2-CG1	2.13	116.12	108.40
25	P	1265	PEK	C03-C02-C01	2.13	116.82	111.79
22	B	521	TGL	C33-C19-C18	2.12	125.19	114.42
20	W	1060	CHD	C1-C10-C9	2.11	114.68	111.35
22	O	1521	TGL	OG3-CC1-CC2	-2.09	105.33	111.91
23	B	230	PSC	P-O12-C04	2.09	131.90	121.59
22	B	521	TGL	CB7-CB6-CB5	-2.09	103.82	114.42
19	C	267	PGV	C3-C2-C1	-2.08	106.05	113.62
18	A	515	HEA	CMC-C2C-C1C	-2.08	125.26	128.46
19	P	1267	PGV	O01-C1-O02	2.07	128.70	123.70
25	P	1264	PEK	C02-O01-C1	-2.06	112.71	117.79
20	P	1525	CHD	O3-C3-C2	2.06	115.41	110.16
18	A	516	HEA	CMC-C2C-C1C	-2.06	125.30	128.46
26	T	1269	CDL	C83-C82-C81	2.06	124.86	114.42
18	N	515	HEA	CMB-C2B-C1B	-2.06	125.31	128.46
26	C	270	CDL	C79-C78-C77	2.05	124.86	114.42
26	G	269	CDL	O1-C1-CB2	2.05	116.75	109.56
19	P	1267	PGV	C3-C2-C1	-2.05	106.16	113.62
18	N	515	HEA	C27-C19-C18	-2.05	118.42	123.68
18	N	515	HEA	C3C-C4C-NC	2.05	111.86	109.21
18	A	515	HEA	C27-C19-C18	-2.05	118.43	123.68
26	C	270	CDL	C80-C79-C78	2.04	124.79	114.42
18	N	515	HEA	C4B-C3B-C2B	2.04	108.29	106.87
20	W	1271	CHD	C14-C8-C7	2.04	114.51	111.81
22	N	1522	TGL	CC3-CC2-CC1	2.04	121.03	113.62
20	P	1525	CHD	C19-C10-C1	-2.04	104.98	108.26
19	C	267	PGV	C9-C10-C11	-2.04	100.77	112.43
19	C	267	PGV	O03-C19-O04	2.04	128.73	123.59
26	C	270	CDL	CB6-CB4-CB3	-2.03	106.98	111.79
26	G	269	CDL	C83-C82-C81	2.03	124.75	114.42
22	D	523	TGL	C10-CB9-CB8	2.03	124.74	114.42
22	D	523	TGL	CB8-CB7-CB6	2.03	124.71	114.42
25	P	1264	PEK	C25-C24-C23	-2.02	104.15	114.42
20	P	1525	CHD	C11-C9-C10	2.01	115.80	113.73
20	W	1060	CHD	C18-C13-C17	2.01	114.35	111.21
19	P	1266	PGV	O01-C1-O02	2.00	128.54	123.70
18	A	515	HEA	C24-C23-C22	-2.00	116.86	122.65

All (54) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	J	60	CHD	C12

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Mol	Chain	Res	Type	Atom
20	J	60	CHD	C8
20	J	60	CHD	C9
20	J	60	CHD	C14
20	J	60	CHD	C17
20	W	1060	CHD	C12
20	W	1060	CHD	C8
20	W	1060	CHD	C9
20	W	1060	CHD	C14
20	W	1060	CHD	C17
18	A	516	HEA	ND
18	A	516	HEA	NA
18	A	516	HEA	NB
24	P	1272	DMU	C5
24	P	1272	DMU	C6
24	P	1272	DMU	C9
24	P	1272	DMU	C4
24	P	1272	DMU	C2
24	P	1272	DMU	C10
18	N	516	HEA	ND
18	N	516	HEA	NA
18	N	516	HEA	NB
24	Z	1526	DMU	C4
24	Z	1526	DMU	C5
24	Z	1526	DMU	C6
24	Z	1526	DMU	C2
24	Z	1526	DMU	C9
18	A	515	HEA	ND
18	A	515	HEA	NA
18	A	515	HEA	NB
18	N	515	HEA	ND
18	N	515	HEA	NA
18	N	515	HEA	NB
24	M	526	DMU	C4
24	M	526	DMU	C5
24	M	526	DMU	C6
24	M	526	DMU	C2
24	M	526	DMU	C9
24	C	272	DMU	C5
24	C	272	DMU	C6
24	C	272	DMU	C9
24	C	272	DMU	C4
24	C	272	DMU	C2

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Mol	Chain	Res	Type	Atom
24	C	272	DMU	C10
20	C	271	CHD	C12
20	C	271	CHD	C8
20	C	271	CHD	C3
20	C	271	CHD	C9
20	C	271	CHD	C14
20	W	1271	CHD	C12
20	W	1271	CHD	C8
20	W	1271	CHD	C3
20	W	1271	CHD	C9
20	W	1271	CHD	C14

All (849) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	P	1265	PEK	C03-O11-P-O13
25	P	1265	PEK	C04-O12-P-O13
25	P	1265	PEK	C04-O12-P-O14
26	C	270	CDL	CA2-C1-CB2-OB2
26	C	270	CDL	CA2-OA2-PA1-OA3
26	C	270	CDL	CA2-OA2-PA1-OA4
26	C	270	CDL	CA4-CA3-OA5-PA1
26	C	270	CDL	C11-CA5-OA6-CA4
26	C	270	CDL	CB2-OB2-PB2-OB3
26	C	270	CDL	CB2-OB2-PB2-OB4
20	J	60	CHD	C16-C17-C20-C21
20	J	60	CHD	C16-C17-C20-C22
19	N	1524	PGV	C04-O12-P-O11
19	N	1524	PGV	C04-O12-P-O13
19	N	1524	PGV	C04-O12-P-O14
19	N	1524	PGV	C02-C03-O11-P
19	N	1524	PGV	C05-C04-O12-P
19	N	1524	PGV	C04-C05-C06-O06
19	N	1524	PGV	O02-C1-O01-C02
19	N	1524	PGV	C2-C1-O01-C02
19	N	1524	PGV	C20-C19-O03-C01
20	W	1060	CHD	C16-C17-C20-C21
20	W	1060	CHD	C16-C17-C20-C22
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

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Mol	Chain	Res	Type	Atoms
19	A	524	PGV	C05-C04-O12-P
19	A	524	PGV	C04-C05-C06-O06
19	A	524	PGV	O02-C1-O01-C02
19	A	524	PGV	C2-C1-O01-C02
19	A	524	PGV	C20-C19-O03-C01
26	G	269	CDL	CB2-C1-CA2-OA2
26	G	269	CDL	CA2-OA2-PA1-OA3
26	G	269	CDL	C1-CB2-OB2-PB2
26	G	269	CDL	CB3-OB5-PB2-OB3
26	G	269	CDL	CB3-OB5-PB2-OB4
23	B	230	PSC	C04-O12-P-O14
23	O	1230	PSC	C03-O11-P-O14
23	O	1230	PSC	C04-O12-P-O14
19	P	1268	PGV	C04-O12-P-O11
19	P	1268	PGV	C04-O12-P-O13
19	P	1268	PGV	C04-O12-P-O14
19	P	1268	PGV	O05-C05-C06-O06
22	O	1521	TGL	CB2-CB1-OG2-CG2
25	C	265	PEK	C03-O11-P-O13
25	C	265	PEK	C04-O12-P-O13
19	C	268	PGV	C04-O12-P-O11
19	C	268	PGV	C04-O12-P-O13
19	C	268	PGV	C04-O12-P-O14
19	C	268	PGV	O05-C05-C06-O06
24	Z	1526	DMU	O5-C6-O16-C18
18	A	515	HEA	C14-C15-C16-C17
18	A	515	HEA	C26-C15-C16-C17
18	N	515	HEA	C14-C15-C16-C17
18	N	515	HEA	C26-C15-C16-C17
24	M	526	DMU	O5-C6-O16-C18
19	C	266	PGV	C04-O12-P-O13
25	G	1263	PEK	C03-O11-P-O13
25	G	1263	PEK	C03-O11-P-O14
25	G	1263	PEK	O12-C04-C05-N
25	T	263	PEK	C03-O11-P-O14
25	T	263	PEK	O12-C04-C05-N
26	P	1270	CDL	CA2-C1-CB2-OB2
26	P	1270	CDL	CA2-OA2-PA1-OA3
26	P	1270	CDL	CA2-OA2-PA1-OA4
26	P	1270	CDL	CA4-CA3-OA5-PA1
26	P	1270	CDL	C11-CA5-OA6-CA4
26	P	1270	CDL	CB2-OB2-PB2-OB3

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Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	CB2-OB2-PB2-OB4
26	T	1269	CDL	CB2-C1-CA2-OA2
26	T	1269	CDL	CA2-OA2-PA1-OA3
26	T	1269	CDL	C1-CB2-OB2-PB2
26	T	1269	CDL	CB3-OB5-PB2-OB3
26	T	1269	CDL	CB3-OB5-PB2-OB4
19	N	1524	PGV	O04-C19-O03-C01
19	A	524	PGV	O04-C19-O03-C01
22	N	1523	TGL	OC1-CC1-OG3-CG3
22	D	523	TGL	OC1-CC1-OG3-CG3
22	B	521	TGL	OB1-CB1-OG2-CG2
23	B	230	PSC	O02-C1-O01-C02
23	O	1230	PSC	O02-C1-O01-C02
22	O	1521	TGL	OB1-CB1-OG2-CG2
22	B	521	TGL	CB2-CB1-OG2-CG2
22	O	1521	TGL	OA1-CA1-OG1-CG1
26	C	270	CDL	C40-C41-C42-C43
26	C	270	CDL	C60-C61-C62-C63
26	C	270	CDL	C77-C78-C79-C80
26	C	270	CDL	C80-C81-C82-C83
26	G	269	CDL	C20-C21-C22-C23
26	G	269	CDL	C40-C41-C42-C43
26	G	269	CDL	C57-C58-C59-C60
22	O	1521	TGL	C16-C15-CC9-CC8
26	P	1270	CDL	C40-C41-C42-C43
26	P	1270	CDL	C57-C58-C59-C60
26	P	1270	CDL	C80-C81-C82-C83
26	T	1269	CDL	C37-C38-C39-C40
26	T	1269	CDL	C40-C41-C42-C43
26	T	1269	CDL	C57-C58-C59-C60
22	B	521	TGL	CA2-CA1-OG1-CG1
26	G	269	CDL	C31-CA7-OA8-CA6
26	T	1269	CDL	C31-CA7-OA8-CA6
26	C	270	CDL	C20-C21-C22-C23
26	C	270	CDL	C57-C58-C59-C60
26	G	269	CDL	C37-C38-C39-C40
26	G	269	CDL	C77-C78-C79-C80
26	P	1270	CDL	C60-C61-C62-C63
22	N	1522	TGL	C21-C20-CA9-CA8
26	T	1269	CDL	C17-C18-C19-C20
26	T	1269	CDL	C20-C21-C22-C23
26	T	1269	CDL	C60-C61-C62-C63

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Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	C77-C78-C79-C80
22	B	521	TGL	C16-C15-CC9-CC8
26	G	269	CDL	C17-C18-C19-C20
22	L	522	TGL	C21-C20-CA9-CA8
26	P	1270	CDL	C20-C21-C22-C23
26	P	1270	CDL	C77-C78-C79-C80
22	D	523	TGL	C21-C20-CA9-CA8
26	C	270	CDL	OA7-CA5-OA6-CA4
26	P	1270	CDL	OA7-CA5-OA6-CA4
22	B	521	TGL	OA1-CA1-OG1-CG1
26	G	269	CDL	OA9-CA7-OA8-CA6
26	T	1269	CDL	OA9-CA7-OA8-CA6
26	C	270	CDL	C37-C38-C39-C40
26	G	269	CDL	C60-C61-C62-C63
26	P	1270	CDL	C17-C18-C19-C20
26	C	270	CDL	C17-C18-C19-C20
26	G	269	CDL	C80-C81-C82-C83
22	N	1523	TGL	C21-C20-CA9-CA8
26	P	1270	CDL	C37-C38-C39-C40
22	D	523	TGL	C11-C10-CB9-CB8
19	A	524	PGV	O12-C04-C05-O05
26	G	269	CDL	O1-C1-CA2-OA2
26	T	1269	CDL	O1-C1-CA2-OA2
22	O	1521	TGL	CA2-CA1-OG1-CG1
22	N	1523	TGL	CC2-CC1-OG3-CG3
22	D	523	TGL	CC2-CC1-OG3-CG3
22	N	1523	TGL	C11-C10-CB9-CB8
26	T	1269	CDL	C80-C81-C82-C83
23	B	230	PSC	C2-C1-O01-C02
23	O	1230	PSC	C2-C1-O01-C02
24	C	272	DMU	O6-C11-C9-O1
22	L	522	TGL	C16-C15-CC9-CC8
22	N	1522	TGL	C11-C10-CB9-CB8
22	N	1522	TGL	C16-C15-CC9-CC8
22	D	523	TGL	C16-C15-CC9-CC8
22	L	522	TGL	OA1-CA1-OG1-CG1
22	B	521	TGL	C21-C20-CA9-CA8
22	B	521	TGL	C11-C10-CB9-CB8
22	O	1521	TGL	C21-C20-CA9-CA8
22	O	1521	TGL	C11-C10-CB9-CB8
22	L	522	TGL	C11-C10-CB9-CB8
22	N	1523	TGL	C16-C15-CC9-CC8

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Mol	Chain	Res	Type	Atoms
23	B	230	PSC	C20-C19-O03-C01
23	O	1230	PSC	C20-C19-O03-C01
24	P	1272	DMU	O6-C11-C9-O1
24	M	526	DMU	O6-C11-C9-C8
24	Z	1526	DMU	O6-C11-C9-C8
23	B	230	PSC	O04-C19-O03-C01
22	N	1522	TGL	OA1-CA1-OG1-CG1
24	M	526	DMU	O5-C4-C57-O61
20	J	60	CHD	C17-C20-C22-C23
20	W	1060	CHD	C17-C20-C22-C23
19	N	1524	PGV	O12-C04-C05-C06
19	A	524	PGV	O12-C04-C05-C06
20	J	60	CHD	C21-C20-C22-C23
23	O	1230	PSC	O04-C19-O03-C01
22	L	522	TGL	CA2-CA1-OG1-CG1
22	N	1523	TGL	CA2-CA1-OG1-CG1
22	N	1522	TGL	CA2-CA1-OG1-CG1
22	D	523	TGL	CA2-CA1-OG1-CG1
20	J	60	CHD	C13-C17-C20-C22
20	W	1060	CHD	C13-C17-C20-C22
24	P	1272	DMU	C3-C4-C57-O61
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
20	W	1060	CHD	C21-C20-C22-C23
24	P	1272	DMU	C1-C6-O16-C18
24	C	272	DMU	C1-C6-O16-C18
26	G	269	CDL	OB6-CB4-CB6-OB8
26	T	1269	CDL	OB6-CB4-CB6-OB8
24	C	272	DMU	C3-C4-C57-O61
24	Z	1526	DMU	O5-C4-C57-O61
26	T	1269	CDL	C11-CA5-OA6-CA4
23	B	230	PSC	C20-C21-C22-C23
22	L	522	TGL	CC3-CC4-CC5-CC6
19	N	1524	PGV	C19-C20-C21-C22
19	A	524	PGV	C19-C20-C21-C22
25	G	1263	PEK	C28-C29-C30-C31
25	T	263	PEK	C28-C29-C30-C31
23	O	1230	PSC	C20-C21-C22-C23
19	N	1524	PGV	O05-C05-C06-O06
20	C	271	CHD	C13-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
23	B	230	PSC	C1-C2-C3-C4
25	G	1263	PEK	C1-C2-C3-C4
25	T	263	PEK	C1-C2-C3-C4
22	N	1522	TGL	CC3-CC4-CC5-CC6
23	B	230	PSC	C22-C23-C24-C25
20	W	1060	CHD	C13-C17-C20-C21
22	N	1523	TGL	OA1-CA1-OG1-CG1
23	O	1230	PSC	C22-C23-C24-C25
19	N	1524	PGV	O12-C04-C05-O05
19	P	1268	PGV	O12-C04-C05-O05
19	C	268	PGV	O12-C04-C05-O05
20	J	60	CHD	C13-C17-C20-C21
22	D	523	TGL	OA1-CA1-OG1-CG1
20	W	1271	CHD	C13-C17-C20-C22
26	C	270	CDL	CB7-C71-C72-C73
22	O	1521	TGL	OC1-CC1-OG3-CG3
26	G	269	CDL	C11-CA5-OA6-CA4
19	C	268	PGV	C2-C1-O01-C02
25	P	1265	PEK	C04-O12-P-O11
26	C	270	CDL	CA2-OA2-PA1-OA5
26	C	270	CDL	CB2-OB2-PB2-OB5
26	G	269	CDL	CB3-OB5-PB2-OB2
25	C	265	PEK	C04-O12-P-O11
25	G	1263	PEK	C03-O11-P-O12
25	T	263	PEK	C03-O11-P-O12
26	P	1270	CDL	CA2-OA2-PA1-OA5
26	P	1270	CDL	CB2-OB2-PB2-OB5
26	T	1269	CDL	CB3-OB5-PB2-OB2
23	O	1230	PSC	C1-C2-C3-C4
22	B	521	TGL	OC1-CC1-OG3-CG3
26	G	269	CDL	CA5-C11-C12-C13
26	G	269	CDL	CA2-C1-CB2-OB2
19	P	1268	PGV	O12-C04-C05-C06
19	C	268	PGV	O12-C04-C05-C06
26	T	1269	CDL	CA2-C1-CB2-OB2
26	G	269	CDL	OA7-CA5-OA6-CA4
26	T	1269	CDL	OA7-CA5-OA6-CA4
22	B	521	TGL	CB6-CB7-CB8-CB9
26	T	1269	CDL	C73-C74-C75-C76
19	N	1524	PGV	C4-C5-C6-C7
23	O	1230	PSC	C2-C3-C4-C5
19	P	1268	PGV	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
20	C	271	CHD	C17-C20-C22-C23
26	C	270	CDL	C55-C56-C57-C58
19	C	267	PGV	C7-C8-C9-C10
19	A	524	PGV	C4-C5-C6-C7
19	P	1268	PGV	C13-C14-C15-C16
19	P	1266	PGV	C29-C30-C31-C32
19	C	268	PGV	C13-C14-C15-C16
19	C	268	PGV	C22-C23-C24-C25
19	C	266	PGV	C6-C7-C8-C9
26	P	1270	CDL	C51-C52-C53-C54
26	P	1270	CDL	C55-C56-C57-C58
19	P	1267	PGV	C7-C8-C9-C10
25	P	1265	PEK	C25-C26-C27-C28
26	C	270	CDL	C16-C17-C18-C19
19	C	267	PGV	C22-C23-C24-C25
26	G	269	CDL	C72-C73-C74-C75
23	B	230	PSC	C2-C3-C4-C5
19	P	1268	PGV	C22-C23-C24-C25
25	C	265	PEK	C25-C26-C27-C28
24	M	526	DMU	C25-C28-C31-C34
26	P	1270	CDL	C16-C17-C18-C19
19	P	1267	PGV	C22-C23-C24-C25
19	P	1268	PGV	O02-C1-O01-C02
19	C	268	PGV	O02-C1-O01-C02
26	C	270	CDL	C51-C52-C53-C54
24	Z	1526	DMU	C25-C28-C31-C34
19	C	266	PGV	C29-C30-C31-C32
26	T	1269	CDL	C72-C73-C74-C75
19	P	1266	PGV	C6-C7-C8-C9
26	T	1269	CDL	C58-C59-C60-C61
22	O	1521	TGL	CB6-CB7-CB8-CB9
25	G	1263	PEK	C27-C28-C29-C30
25	T	263	PEK	C27-C28-C29-C30
26	P	1270	CDL	C72-C73-C74-C75
25	P	1265	PEK	C21-C22-C23-C24
25	G	1263	PEK	O03-C01-C02-O01
26	G	269	CDL	C13-C14-C15-C16
26	G	269	CDL	C58-C59-C60-C61
19	C	268	PGV	C3-C4-C5-C6
24	Z	1526	DMU	O16-C18-C19-C22
25	T	263	PEK	C29-C30-C31-C32
26	G	269	CDL	C56-C57-C58-C59

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Mol	Chain	Res	Type	Atoms
19	P	1268	PGV	C3-C4-C5-C6
19	P	1268	PGV	C24-C25-C26-C27
19	C	268	PGV	C24-C25-C26-C27
25	G	1263	PEK	C29-C30-C31-C32
26	T	1269	CDL	C13-C14-C15-C16
26	P	1270	CDL	CB7-C71-C72-C73
26	T	1269	CDL	CA5-C11-C12-C13
19	N	1524	PGV	C5-C6-C7-C8
26	P	1270	CDL	C13-C14-C15-C16
24	P	1272	DMU	O5-C4-C57-O61
26	C	270	CDL	C13-C14-C15-C16
19	A	524	PGV	C5-C6-C7-C8
19	A	524	PGV	C28-C29-C30-C31
26	T	1269	CDL	C56-C57-C58-C59
19	P	1268	PGV	C04-C05-C06-O06
19	C	268	PGV	C04-C05-C06-O06
25	P	1265	PEK	C16-C17-C18-C19
19	N	1524	PGV	C28-C29-C30-C31
23	B	230	PSC	C29-C30-C31-C32
24	P	1272	DMU	C25-C28-C31-C34
19	P	1266	PGV	C23-C24-C25-C26
23	O	1230	PSC	C13-C14-C15-C16
26	C	270	CDL	CA5-C11-C12-C13
26	P	1270	CDL	CA5-C11-C12-C13
25	P	1265	PEK	C29-C30-C31-C32
19	A	524	PGV	C22-C23-C24-C25
26	G	269	CDL	C73-C74-C75-C76
25	C	264	PEK	C23-C24-C25-C26
25	C	264	PEK	C31-C32-C33-C34
19	P	1268	PGV	C27-C28-C29-C30
25	C	265	PEK	C16-C17-C18-C19
19	C	266	PGV	C23-C24-C25-C26
24	P	1272	DMU	O5-C6-O16-C18
20	W	1271	CHD	C17-C20-C22-C23
19	N	1524	PGV	C22-C23-C24-C25
23	O	1230	PSC	C29-C30-C31-C32
25	P	1264	PEK	C23-C24-C25-C26
25	C	265	PEK	C29-C30-C31-C32
22	L	522	TGL	CB4-CB5-CB6-CB7
19	C	266	PGV	C5-C6-C7-C8
24	C	272	DMU	C25-C28-C31-C34
22	N	1522	TGL	CC2-CC3-CC4-CC5

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Mol	Chain	Res	Type	Atoms
25	P	1264	PEK	O12-C04-C05-N
25	P	1265	PEK	C31-C32-C33-C34
26	C	270	CDL	C72-C73-C74-C75
19	N	1524	PGV	C24-C25-C26-C27
19	A	524	PGV	C24-C25-C26-C27
26	G	269	CDL	C79-C80-C81-C82
25	C	265	PEK	C31-C32-C33-C34
19	P	1266	PGV	C5-C6-C7-C8
24	Z	1526	DMU	C22-C25-C28-C31
24	M	526	DMU	C22-C25-C28-C31
26	T	1269	CDL	C43-C44-C45-C46
26	T	1269	CDL	C79-C80-C81-C82
19	C	268	PGV	C27-C28-C29-C30
22	L	522	TGL	CC2-CC3-CC4-CC5
26	C	270	CDL	C74-C75-C76-C77
25	P	1264	PEK	C31-C32-C33-C34
24	M	526	DMU	O16-C18-C19-C22
25	G	1263	PEK	C25-C26-C27-C28
25	T	263	PEK	C25-C26-C27-C28
22	N	1522	TGL	CB4-CB5-CB6-CB7
26	C	270	CDL	C32-C33-C34-C35
26	C	270	CDL	C59-C60-C61-C62
26	C	270	CDL	C73-C74-C75-C76
22	B	521	TGL	C12-C13-C14-C29
26	G	269	CDL	C43-C44-C45-C46
19	P	1267	PGV	C20-C21-C22-C23
25	C	264	PEK	C1-C2-C3-C4
26	P	1270	CDL	C75-C76-C77-C78
19	A	524	PGV	O05-C05-C06-O06
19	C	267	PGV	C20-C21-C22-C23
19	P	1266	PGV	C7-C8-C9-C10
19	C	267	PGV	C11-C10-C9-C8
23	B	230	PSC	C13-C14-C15-C16
19	P	1267	PGV	C11-C10-C9-C8
25	C	265	PEK	C21-C22-C23-C24
26	P	1270	CDL	C32-C33-C34-C35
26	P	1270	CDL	C73-C74-C75-C76
26	P	1270	CDL	C74-C75-C76-C77
25	P	1264	PEK	C1-C2-C3-C4
25	P	1264	PEK	C16-C17-C18-C19
26	P	1270	CDL	C18-C19-C20-C21
24	Z	1526	DMU	C3-C4-C57-O61

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Mol	Chain	Res	Type	Atoms
19	C	266	PGV	C7-C8-C9-C10
26	P	1270	CDL	C59-C60-C61-C62
26	C	270	CDL	C18-C19-C20-C21
19	P	1267	PGV	C23-C24-C25-C26
26	T	1269	CDL	CB5-C51-C52-C53
25	G	1263	PEK	C16-C17-C18-C19
26	G	269	CDL	CB5-C51-C52-C53
19	P	1268	PGV	C25-C26-C27-C28
19	C	268	PGV	C25-C26-C27-C28
25	G	1263	PEK	C26-C27-C28-C29
20	C	271	CHD	C16-C17-C20-C22
19	C	268	PGV	C11-C10-C9-C8
19	P	1268	PGV	C1-C2-C3-C4
22	B	521	TGL	CC2-CC1-OG3-CG3
25	C	264	PEK	C22-C21-O03-C01
22	O	1521	TGL	CC2-CC1-OG3-CG3
22	N	1522	TGL	CC2-CC1-OG3-CG3
26	C	270	CDL	C63-C64-C65-C66
26	C	270	CDL	C75-C76-C77-C78
25	T	263	PEK	C34-C35-C36-C37
26	P	1270	CDL	C63-C64-C65-C66
25	C	264	PEK	C22-C23-C24-C25
19	P	1268	PGV	C30-C31-C32-C33
25	T	263	PEK	C16-C17-C18-C19
19	C	268	PGV	C1-C2-C3-C4
20	C	271	CHD	C21-C20-C22-C23
19	C	267	PGV	C13-C14-C15-C16
26	G	269	CDL	C82-C83-C84-C85
19	C	268	PGV	C30-C31-C32-C33
25	G	1263	PEK	C34-C35-C36-C37
26	T	1269	CDL	C82-C83-C84-C85
19	P	1267	PGV	C13-C14-C15-C16
25	P	1264	PEK	C22-C21-O03-C01
20	W	1271	CHD	C16-C17-C20-C22
25	C	264	PEK	C16-C17-C18-C19
19	C	266	PGV	C4-C5-C6-C7
25	T	263	PEK	C26-C27-C28-C29
26	P	1270	CDL	C51-CB5-OB6-CB4
26	C	270	CDL	C71-C72-C73-C74
26	P	1270	CDL	C36-C37-C38-C39
26	P	1270	CDL	C71-C72-C73-C74
25	C	264	PEK	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
26	C	270	CDL	OB7-CB5-OB6-CB4
22	L	522	TGL	OB1-CB1-OG2-CG2
25	P	1264	PEK	C22-C23-C24-C25
25	T	263	PEK	O03-C01-C02-O01
19	C	267	PGV	C23-C24-C25-C26
19	N	1524	PGV	C12-C13-C14-C15
19	A	524	PGV	C12-C13-C14-C15
19	P	1268	PGV	C11-C10-C9-C8
19	P	1268	PGV	C12-C13-C14-C15
26	T	1269	CDL	C33-C34-C35-C36
26	T	1269	CDL	C53-C54-C55-C56
26	C	270	CDL	C64-C65-C66-C67
26	G	269	CDL	C33-C34-C35-C36
23	O	1230	PSC	C27-C28-C29-C30
22	L	522	TGL	CC2-CC1-OG3-CG3
23	B	230	PSC	C27-C28-C29-C30
26	P	1270	CDL	OB7-CB5-OB6-CB4
22	N	1522	TGL	OB1-CB1-OG2-CG2
26	G	269	CDL	C53-C54-C55-C56
23	O	1230	PSC	C04-O12-P-O11
26	G	269	CDL	C21-C22-C23-C24
23	B	230	PSC	C23-C24-C25-C26
23	O	1230	PSC	C23-C24-C25-C26
26	P	1270	CDL	C64-C65-C66-C67
26	C	270	CDL	OB5-CB3-CB4-CB6
25	T	263	PEK	C01-C02-C03-O11
26	C	270	CDL	C36-C37-C38-C39
19	P	1266	PGV	C19-C20-C21-C22
19	P	1268	PGV	C28-C29-C30-C31
19	C	268	PGV	C28-C29-C30-C31
19	C	268	PGV	C12-C13-C14-C15
26	P	1270	CDL	C42-C43-C44-C45
19	A	524	PGV	C26-C27-C28-C29
26	T	1269	CDL	C21-C22-C23-C24
26	T	1269	CDL	C14-C15-C16-C17
25	C	264	PEK	C2-C1-O01-C02
26	G	269	CDL	C71-C72-C73-C74
26	T	1269	CDL	C71-C72-C73-C74
20	C	271	CHD	C13-C17-C20-C21
26	C	270	CDL	CB3-CB4-CB6-OB8
26	G	269	CDL	CB3-CB4-CB6-OB8
23	B	230	PSC	O03-C01-C02-C03

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Mol	Chain	Res	Type	Atoms
23	O	1230	PSC	O03-C01-C02-C03
25	P	1264	PEK	O03-C01-C02-C03
19	P	1266	PGV	C4-C5-C6-C7
25	G	1263	PEK	O03-C01-C02-C03
25	T	263	PEK	O03-C01-C02-C03
26	P	1270	CDL	CB3-CB4-CB6-OB8
26	T	1269	CDL	CB3-CB4-CB6-OB8
19	C	267	PGV	C15-C16-C17-C18
19	P	1267	PGV	C15-C16-C17-C18
25	P	1264	PEK	C26-C27-C28-C29
26	P	1270	CDL	C61-C62-C63-C64
25	C	264	PEK	O04-C21-O03-C01
26	C	270	CDL	C44-C45-C46-C47
22	L	522	TGL	CC7-CC8-CC9-C15
26	P	1270	CDL	C44-C45-C46-C47
20	W	1271	CHD	C16-C17-C20-C21
22	N	1522	TGL	CC7-CC8-CC9-C15
26	G	269	CDL	C14-C15-C16-C17
19	C	268	PGV	C23-C24-C25-C26
26	C	270	CDL	C42-C43-C44-C45
25	P	1264	PEK	C25-C26-C27-C28
26	C	270	CDL	C61-C62-C63-C64
26	C	270	CDL	C84-C85-C86-C87
26	G	269	CDL	C41-C42-C43-C44
20	C	271	CHD	C16-C17-C20-C21
19	N	1524	PGV	C03-C02-O01-C1
19	A	524	PGV	C03-C02-O01-C1
19	N	1524	PGV	C26-C27-C28-C29
26	C	270	CDL	C11-C12-C13-C14
25	G	1263	PEK	C30-C31-C32-C33
19	P	1268	PGV	C23-C24-C25-C26
26	P	1270	CDL	C38-C39-C40-C41
26	P	1270	CDL	C84-C85-C86-C87
26	T	1269	CDL	C31-C32-C33-C34
26	C	270	CDL	OA5-CA3-CA4-OA6
26	P	1270	CDL	OA5-CA3-CA4-OA6
26	P	1270	CDL	C11-C12-C13-C14
20	W	1271	CHD	C13-C17-C20-C21
19	C	268	PGV	C31-C32-C33-C34
19	C	266	PGV	C30-C31-C32-C33
19	C	266	PGV	C19-C20-C21-C22
25	C	265	PEK	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
25	T	263	PEK	C30-C31-C32-C33
19	P	1267	PGV	C24-C25-C26-C27
19	C	268	PGV	C14-C15-C16-C17
19	P	1268	PGV	C14-C15-C16-C17
19	P	1266	PGV	C30-C31-C32-C33
26	T	1269	CDL	C35-C36-C37-C38
20	W	1271	CHD	C21-C20-C22-C23
26	G	269	CDL	C35-C36-C37-C38
26	G	269	CDL	C31-C32-C33-C34
26	P	1270	CDL	C34-C35-C36-C37
19	P	1268	PGV	C31-C32-C33-C34
19	P	1268	PGV	C4-C5-C6-C7
26	C	270	CDL	C51-CB5-OB6-CB4
26	C	270	CDL	C34-C35-C36-C37
23	B	230	PSC	C24-C25-C26-C27
25	C	264	PEK	C26-C27-C28-C29
25	P	1265	PEK	C32-C33-C34-C35
24	M	526	DMU	C34-C37-C40-C43
26	P	1270	CDL	OB5-CB3-CB4-CB6
22	O	1521	TGL	C12-C13-C14-C29
19	P	1267	PGV	C1-C2-C3-C4
26	C	270	CDL	C38-C39-C40-C41
24	Z	1526	DMU	C34-C37-C40-C43
26	T	1269	CDL	C41-C42-C43-C44
26	G	269	CDL	C15-C16-C17-C18
19	C	267	PGV	C25-C26-C27-C28
23	O	1230	PSC	C24-C25-C26-C27
26	G	269	CDL	C44-C45-C46-C47
23	B	230	PSC	C3-C4-C5-C6
26	T	1269	CDL	C44-C45-C46-C47
22	N	1522	TGL	CC5-CC6-CC7-CC8
26	G	269	CDL	CA3-CA4-CA6-OA8
25	C	264	PEK	O03-C01-C02-C03
23	O	1230	PSC	C3-C4-C5-C6
25	P	1264	PEK	C35-C36-C37-C38
26	T	1269	CDL	C15-C16-C17-C18
25	C	264	PEK	C17-C18-C19-C20
25	C	264	PEK	C27-C28-C29-C30
19	C	268	PGV	C4-C5-C6-C7
26	C	270	CDL	C39-C40-C41-C42
26	P	1270	CDL	C39-C40-C41-C42
19	P	1267	PGV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
22	D	523	TGL	CA9-C20-C21-C22
24	P	1272	DMU	C34-C37-C40-C43
26	C	270	CDL	C43-C44-C45-C46
25	C	264	PEK	C24-C25-C26-C27
23	O	1230	PSC	C14-C15-C16-C17
26	P	1270	CDL	C78-C79-C80-C81
25	P	1265	PEK	C11-C12-C13-C14
25	C	264	PEK	C5-C6-C7-C8
25	C	264	PEK	C9-C10-C11-C12
25	P	1264	PEK	C5-C6-C7-C8
25	P	1264	PEK	C9-C10-C11-C12
25	C	265	PEK	C11-C12-C13-C14
25	G	1263	PEK	C6-C7-C8-C9
25	T	263	PEK	C6-C7-C8-C9
25	P	1264	PEK	O04-C21-O03-C01
25	P	1264	PEK	C17-C18-C19-C20
24	C	272	DMU	C22-C25-C28-C31
23	B	230	PSC	C14-C15-C16-C17
26	C	270	CDL	OB5-CB3-CB4-OB6
26	P	1270	CDL	OB5-CB3-CB4-OB6
19	C	268	PGV	C20-C19-O03-C01
25	C	264	PEK	C32-C33-C34-C35
23	O	1230	PSC	C31-C32-C33-C34
19	C	267	PGV	C1-C2-C3-C4
19	P	1268	PGV	C26-C27-C28-C29
19	C	268	PGV	C15-C16-C17-C18
19	A	524	PGV	C7-C8-C9-C10
23	B	230	PSC	C31-C32-C33-C34
25	P	1264	PEK	C24-C25-C26-C27
22	N	1523	TGL	CA9-C20-C21-C22
26	P	1270	CDL	C43-C44-C45-C46
19	C	267	PGV	C02-C03-O11-P
19	C	267	PGV	C24-C25-C26-C27
25	C	264	PEK	C35-C36-C37-C38
22	N	1522	TGL	CB5-CB6-CB7-CB8
19	P	1267	PGV	C31-C32-C33-C34
19	C	268	PGV	C5-C6-C7-C8
19	P	1268	PGV	C15-C16-C17-C18
19	C	267	PGV	C31-C32-C33-C34
26	G	269	CDL	OA5-CA3-CA4-CA6
25	G	1263	PEK	C01-C02-C03-O11
26	T	1269	CDL	OA5-CA3-CA4-CA6

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Mol	Chain	Res	Type	Atoms
25	P	1264	PEK	C27-C28-C29-C30
26	C	270	CDL	C78-C79-C80-C81
24	C	272	DMU	O5-C4-C57-O61
19	P	1268	PGV	C5-C6-C7-C8
19	N	1524	PGV	O03-C01-C02-C03
19	A	524	PGV	O03-C01-C02-C03
26	T	1269	CDL	CA3-CA4-CA6-OA8
22	L	522	TGL	CC5-CC6-CC7-CC8
19	P	1266	PGV	C26-C27-C28-C29
25	C	265	PEK	C35-C36-C37-C38
24	P	1272	DMU	O6-C11-C9-C8
19	P	1268	PGV	O04-C19-O03-C01
19	C	268	PGV	O04-C19-O03-C01
22	N	1522	TGL	OC1-CC1-OG3-CG3
26	C	270	CDL	OB6-CB4-CB6-OB8
26	G	269	CDL	OA6-CA4-CA6-OA8
26	P	1270	CDL	OB6-CB4-CB6-OB8
26	T	1269	CDL	OA6-CA4-CA6-OA8
25	T	263	PEK	O04-C21-O03-C01
19	N	1524	PGV	C7-C8-C9-C10
26	G	269	CDL	C19-C20-C21-C22
25	G	1263	PEK	C15-C16-C17-C18
26	T	1269	CDL	C19-C20-C21-C22
25	G	1263	PEK	O04-C21-O03-C01
22	L	522	TGL	CB5-CB6-CB7-CB8
26	C	270	CDL	C24-C25-C26-C27
19	C	268	PGV	C26-C27-C28-C29
26	P	1270	CDL	C24-C25-C26-C27
25	P	1265	PEK	C35-C36-C37-C38
26	G	269	CDL	CB2-OB2-PB2-OB5
23	B	230	PSC	C04-O12-P-O11
26	T	1269	CDL	CB2-OB2-PB2-OB5
25	G	1263	PEK	C32-C33-C34-C35
26	P	1270	CDL	C83-C84-C85-C86
26	G	269	CDL	CB4-CB3-OB5-PB2
25	G	1263	PEK	C02-C03-O11-P
26	T	1269	CDL	CB4-CB3-OB5-PB2
19	P	1267	PGV	C02-C03-O11-P
23	B	230	PSC	C4-C5-C6-C7
22	L	522	TGL	OC1-CC1-OG3-CG3
25	P	1265	PEK	C03-O11-P-O14
23	B	230	PSC	C03-O11-P-O14

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Mol	Chain	Res	Type	Atoms
23	B	230	PSC	C04-O12-P-O13
23	O	1230	PSC	C04-O12-P-O13
25	C	265	PEK	C03-O11-P-O14
25	C	265	PEK	C04-O12-P-O14
25	T	263	PEK	C03-O11-P-O13
26	T	1269	CDL	CB7-C71-C72-C73
22	B	521	TGL	CG2-CG3-OG3-CC1
19	P	1268	PGV	C20-C19-O03-C01
26	C	270	CDL	OA5-CA3-CA4-CA6
19	N	1524	PGV	C01-C02-C03-O11
19	A	524	PGV	C01-C02-C03-O11
24	M	526	DMU	C3-C4-C57-O61
26	G	269	CDL	CB7-C71-C72-C73
25	G	1263	PEK	C21-C22-C23-C24
22	O	1521	TGL	CG2-CG3-OG3-CC1
22	N	1522	TGL	CA5-CA6-CA7-CA8
25	G	1263	PEK	C22-C21-O03-C01
25	T	263	PEK	C22-C21-O03-C01
25	G	1263	PEK	O01-C02-C03-O11
25	T	263	PEK	C21-C22-C23-C24
25	T	263	PEK	C32-C33-C34-C35
26	T	1269	CDL	C64-C65-C66-C67
18	A	516	HEA	C4D-C3D-CAD-CBD
18	N	516	HEA	C4D-C3D-CAD-CBD
19	N	1524	PGV	O03-C01-C02-O01
19	A	524	PGV	O03-C01-C02-O01
25	C	264	PEK	O03-C01-C02-O01
23	B	230	PSC	O03-C01-C02-O01
23	O	1230	PSC	O03-C01-C02-O01
25	P	1264	PEK	O03-C01-C02-O01
25	T	263	PEK	C02-C03-O11-P
25	P	1264	PEK	C32-C33-C34-C35
19	A	524	PGV	C20-C21-C22-C23
23	O	1230	PSC	C4-C5-C6-C7
24	C	272	DMU	O5-C6-O16-C18
19	N	1524	PGV	C20-C21-C22-C23
23	B	230	PSC	C04-C05-N-C08
23	O	1230	PSC	C04-C05-N-C08
22	O	1521	TGL	C13-C14-C29-C30
19	C	266	PGV	C26-C27-C28-C29
25	T	263	PEK	O01-C02-C03-O11
19	A	524	PGV	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	C76-C77-C78-C79
25	P	1265	PEK	C03-O11-P-O12
26	C	270	CDL	CA3-OA5-PA1-OA2
19	N	1524	PGV	C03-O11-P-O12
19	A	524	PGV	C03-O11-P-O12
26	G	269	CDL	CA2-OA2-PA1-OA5
25	C	265	PEK	C03-O11-P-O12
26	P	1270	CDL	CA3-OA5-PA1-OA2
26	T	1269	CDL	CA2-OA2-PA1-OA5
26	C	270	CDL	C23-C24-C25-C26
26	G	269	CDL	C12-C13-C14-C15
19	C	266	PGV	C25-C26-C27-C28
26	P	1270	CDL	C23-C24-C25-C26
26	G	269	CDL	C24-C25-C26-C27
22	L	522	TGL	CA5-CA6-CA7-CA8
26	G	269	CDL	C64-C65-C66-C67
25	P	1265	PEK	C30-C31-C32-C33
26	T	1269	CDL	C24-C25-C26-C27
26	C	270	CDL	C1-CA2-OA2-PA1
26	P	1270	CDL	C1-CA2-OA2-PA1
25	G	1263	PEK	C31-C32-C33-C34
26	C	270	CDL	C83-C84-C85-C86
19	A	524	PGV	C21-C22-C23-C24
19	A	524	PGV	C11-C10-C9-C8
23	B	230	PSC	C11-C12-C13-C14
26	T	1269	CDL	C54-C55-C56-C57
23	B	230	PSC	C04-C05-N-C07
26	G	269	CDL	C54-C55-C56-C57
25	T	263	PEK	C31-C32-C33-C34
26	T	1269	CDL	C12-C13-C14-C15
19	C	266	PGV	C02-C01-O03-C19
26	T	1269	CDL	C38-C39-C40-C41
26	C	270	CDL	C52-C53-C54-C55
19	P	1268	PGV	O03-C01-C02-O01
19	P	1268	PGV	C02-C03-O11-P
19	C	268	PGV	C02-C03-O11-P
25	P	1265	PEK	C3-C4-C5-C6
25	C	265	PEK	C3-C4-C5-C6
19	P	1266	PGV	C9-C10-C11-C12
19	P	1266	PGV	O03-C19-C20-C21
19	N	1524	PGV	C11-C10-C9-C8
19	N	1524	PGV	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
25	C	265	PEK	C30-C31-C32-C33
26	C	270	CDL	C76-C77-C78-C79
19	N	1524	PGV	C25-C26-C27-C28
24	P	1272	DMU	C22-C25-C28-C31
26	G	269	CDL	C38-C39-C40-C41
25	C	265	PEK	C26-C27-C28-C29
23	B	230	PSC	C03-C02-O01-C1
23	O	1230	PSC	C03-C02-O01-C1
25	C	264	PEK	O02-C1-O01-C02
26	G	269	CDL	C36-C37-C38-C39
25	P	1265	PEK	C12-C13-C14-C15
23	B	230	PSC	C9-C10-C11-C12
23	O	1230	PSC	C9-C10-C11-C12
25	C	265	PEK	C12-C13-C14-C15
26	P	1270	CDL	C52-C53-C54-C55
25	P	1265	PEK	C17-C18-C19-C20
19	P	1266	PGV	C25-C26-C27-C28
26	G	269	CDL	C39-C40-C41-C42
26	P	1270	CDL	C56-C57-C58-C59
19	C	268	PGV	O01-C02-C03-O11
25	C	265	PEK	C17-C18-C19-C20
23	B	230	PSC	C01-C02-C03-O11
24	C	272	DMU	C28-C31-C34-C37
26	C	270	CDL	C41-C42-C43-C44
19	C	268	PGV	O03-C01-C02-O01
26	C	270	CDL	C56-C57-C58-C59
23	O	1230	PSC	C11-C12-C13-C14
19	C	267	PGV	C14-C15-C16-C17
22	N	1522	TGL	CB2-CB1-OG2-CG2
22	L	522	TGL	OG2-CB1-CB2-CB3
19	C	266	PGV	O03-C19-C20-C21
25	T	263	PEK	C33-C34-C35-C36
26	T	1269	CDL	C36-C37-C38-C39
26	T	1269	CDL	C39-C40-C41-C42
26	T	1269	CDL	C52-C53-C54-C55
23	O	1230	PSC	C04-C05-N-C07
24	C	272	DMU	C34-C37-C40-C43
19	C	266	PGV	C9-C10-C11-C12
19	C	267	PGV	C29-C30-C31-C32
22	N	1522	TGL	OG2-CB1-CB2-CB3
26	G	269	CDL	C52-C53-C54-C55
22	B	521	TGL	C13-C14-C29-C30

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Mol	Chain	Res	Type	Atoms
19	C	267	PGV	C9-C10-C11-C12
25	C	264	PEK	C3-C4-C5-C6
23	O	1230	PSC	C04-C05-N-C06
19	P	1268	PGV	C01-C02-C03-O11
26	P	1270	CDL	OA5-CA3-CA4-CA6
26	P	1270	CDL	C41-C42-C43-C44
19	A	524	PGV	C9-C10-C11-C12
25	P	1264	PEK	C3-C4-C5-C6
19	P	1267	PGV	C9-C10-C11-C12
23	B	230	PSC	O03-C19-C20-C21
19	C	267	PGV	C05-C04-O12-P
22	N	1523	TGL	OG2-CG2-CG3-OG3
24	P	1272	DMU	C18-C19-C22-C25
22	L	522	TGL	OG3-CC1-CC2-CC3
23	O	1230	PSC	C7-C8-C9-C10
19	C	266	PGV	C11-C12-C13-C14
23	O	1230	PSC	O03-C19-C20-C21
20	N	1604	CHD	C17-C20-C22-C23
19	P	1267	PGV	C14-C15-C16-C17
22	D	523	TGL	C21-C22-C23-C24
22	N	1523	TGL	OG2-CB1-CB2-CB3
26	P	1270	CDL	C32-C31-CA7-OA8
22	N	1522	TGL	OG3-CC1-CC2-CC3
19	N	1524	PGV	C9-C10-C11-C12
23	B	230	PSC	C7-C8-C9-C10
22	B	521	TGL	CG1-CG2-OG2-CB1
19	P	1266	PGV	C20-C21-C22-C23
22	N	1523	TGL	CC3-CC4-CC5-CC6
25	P	1264	PEK	O01-C1-C2-C3
19	C	266	PGV	C20-C21-C22-C23
19	C	267	PGV	C11-C12-C13-C14
25	T	263	PEK	C15-C16-C17-C18
19	P	1267	PGV	C29-C30-C31-C32
19	P	1268	PGV	O01-C02-C03-O11
26	C	270	CDL	C32-C31-CA7-OA8
25	C	264	PEK	O01-C1-C2-C3
26	P	1270	CDL	C22-C23-C24-C25
25	G	1263	PEK	C33-C34-C35-C36
25	P	1265	PEK	C26-C27-C28-C29
22	D	523	TGL	OG2-CB1-CB2-CB3
24	P	1272	DMU	C4-C3-O7-C10
26	G	269	CDL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	O	1230	PSC	C01-C02-C03-O11
19	C	268	PGV	C01-C02-C03-O11
26	T	1269	CDL	C55-C56-C57-C58
25	C	265	PEK	O03-C01-C02-O01
22	D	523	TGL	OG2-CG2-CG3-OG3
19	P	1266	PGV	C11-C12-C13-C14
25	G	1263	PEK	C14-C15-C16-C17
22	L	522	TGL	CB2-CB1-OG2-CG2
26	C	270	CDL	C12-C11-CA5-OA6
26	C	270	CDL	C22-C23-C24-C25
19	C	268	PGV	C05-C04-O12-P
25	T	263	PEK	C14-C15-C16-C17
19	P	1267	PGV	C11-C12-C13-C14
26	P	1270	CDL	C12-C11-CA5-OA6
22	N	1523	TGL	C21-C22-C23-C24
26	P	1270	CDL	C52-C51-CB5-OB6
26	T	1269	CDL	C11-C12-C13-C14
26	T	1269	CDL	C59-C60-C61-C62
25	T	263	PEK	C3-C4-C5-C6
26	G	269	CDL	C78-C79-C80-C81
23	B	230	PSC	C15-C16-C17-C18
26	P	1270	CDL	C32-C31-CA7-OA9
25	P	1264	PEK	O02-C1-O01-C02
25	P	1264	PEK	C2-C1-O01-C02
25	P	1265	PEK	C34-C35-C36-C37
25	G	1263	PEK	C3-C4-C5-C6
26	C	270	CDL	C32-C31-CA7-OA9
19	N	1524	PGV	O02-C1-C2-C3
23	O	1230	PSC	O04-C19-C20-C21
22	D	523	TGL	OB1-CB1-CB2-CB3
22	D	523	TGL	OC1-CC1-CC2-CC3
23	B	230	PSC	O04-C19-C20-C21
22	D	523	TGL	CC3-CC4-CC5-CC6
19	N	1524	PGV	O01-C1-C2-C3
19	P	1268	PGV	C05-C04-O12-P
19	N	1524	PGV	C03-O11-P-O13
19	A	524	PGV	C03-O11-P-O13
23	B	230	PSC	C04-C05-N-C06
23	O	1230	PSC	C03-O11-P-O13
19	P	1266	PGV	C04-O12-P-O13
25	G	1263	PEK	C24-C25-C26-C27
25	C	264	PEK	O02-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
22	N	1523	TGL	OC1-CC1-CC2-CC3
19	A	524	PGV	O02-C1-C2-C3
22	N	1523	TGL	OB1-CB1-CB2-CB3
26	P	1270	CDL	C15-C16-C17-C18
25	P	1264	PEK	O02-C1-C2-C3
26	C	270	CDL	C52-C51-CB5-OB6
23	B	230	PSC	O02-C1-C2-C3
23	O	1230	PSC	C15-C16-C17-C18
23	B	230	PSC	C05-C04-O12-P
22	O	1521	TGL	CG1-CG2-OG2-CB1
22	N	1523	TGL	CG1-CG2-OG2-CB1
22	D	523	TGL	CG1-CG2-OG2-CB1
23	O	1230	PSC	O02-C1-C2-C3
23	B	230	PSC	O01-C1-C2-C3
23	O	1230	PSC	O01-C1-C2-C3
19	P	1268	PGV	C7-C8-C9-C10
19	P	1267	PGV	C05-C04-O12-P
19	A	524	PGV	O01-C1-C2-C3
26	G	269	CDL	C55-C56-C57-C58
22	L	522	TGL	OC1-CC1-CC2-CC3
22	N	1522	TGL	OC1-CC1-CC2-CC3
24	C	272	DMU	C4-C3-O7-C10
25	T	263	PEK	C24-C25-C26-C27
25	C	265	PEK	O03-C21-C22-C23

There are no ring outliers.

41 monomers are involved in 312 short contacts:

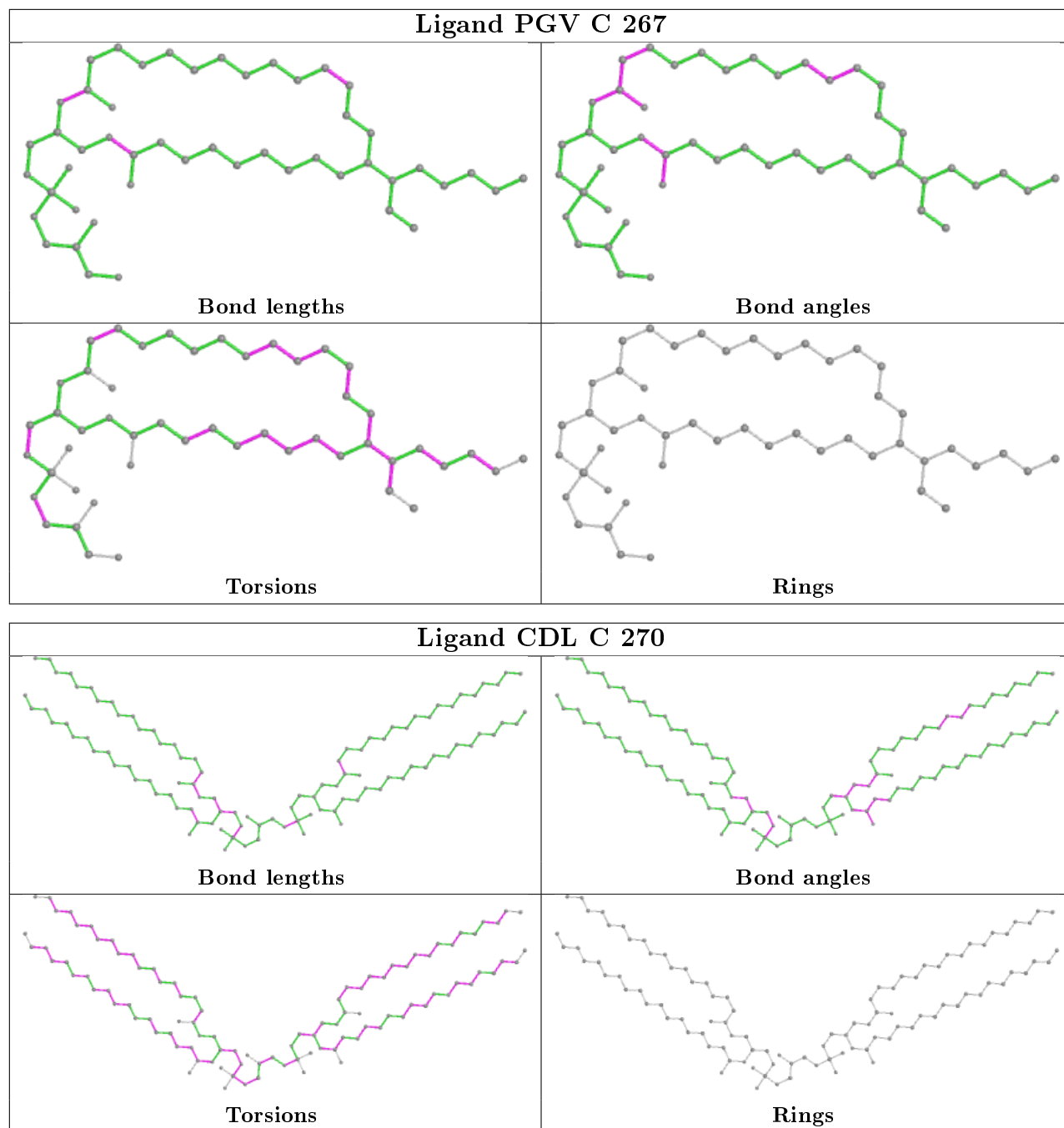
Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	C	267	PGV	7	0
26	C	270	CDL	19	0
20	J	60	CHD	5	0
22	B	521	TGL	6	0
19	N	1524	PGV	10	0
19	C	266	PGV	3	0
20	W	1060	CHD	3	0
19	A	524	PGV	7	0
18	A	516	HEA	5	0
25	C	264	PEK	6	0
23	B	230	PSC	19	0
23	O	1230	PSC	18	0
19	P	1268	PGV	1	0

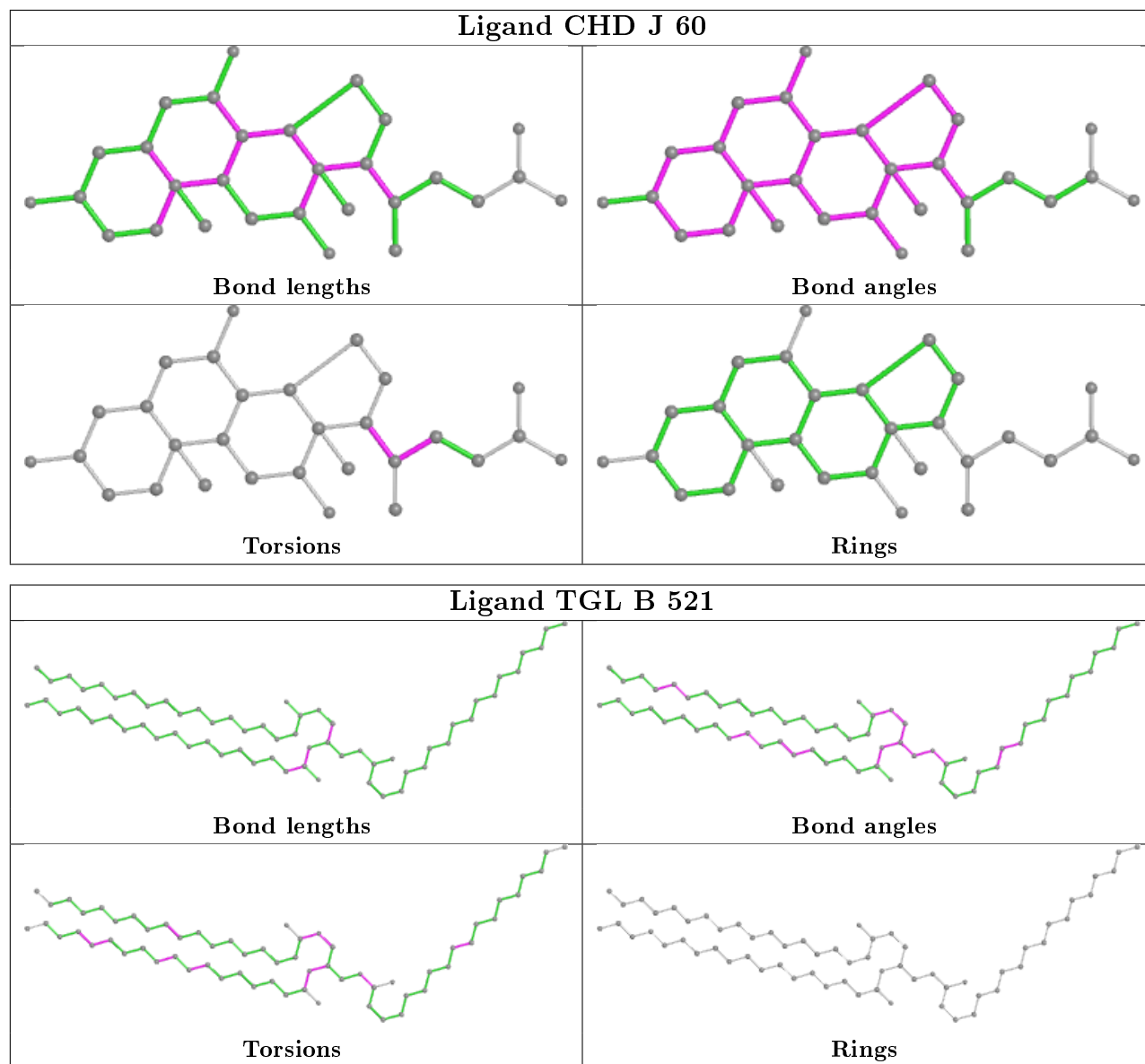
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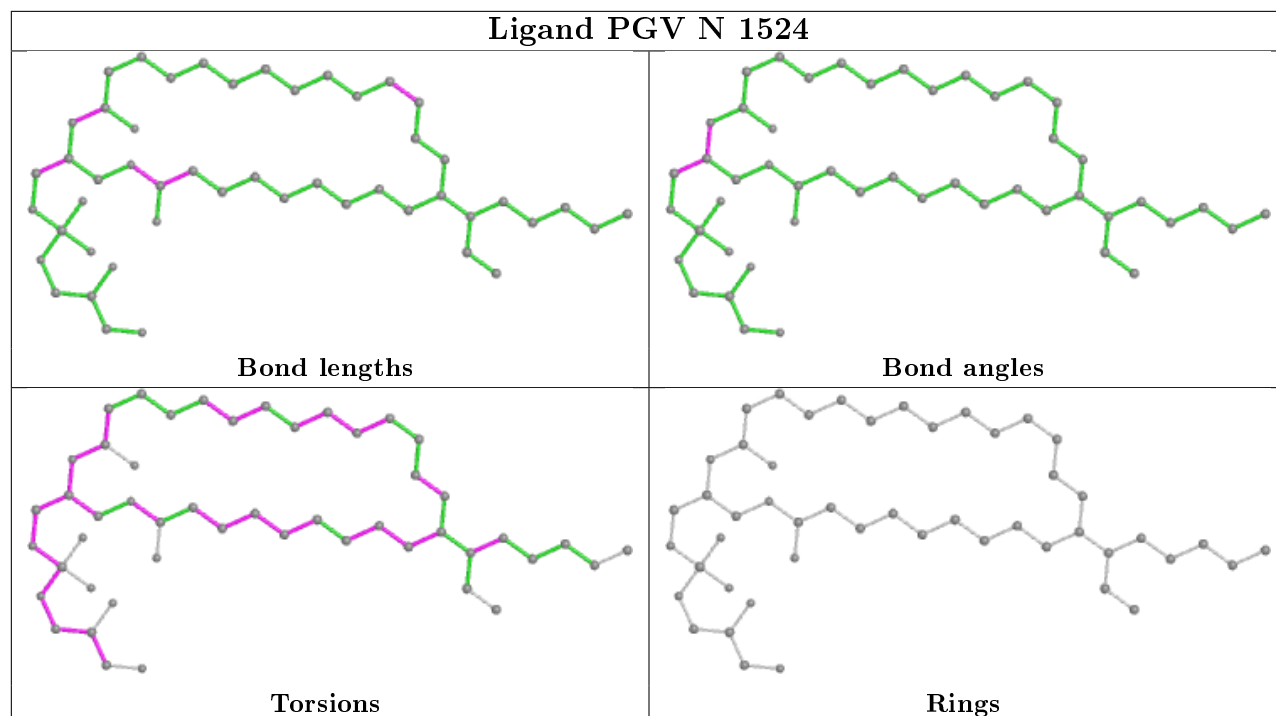
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	O	1521	TGL	8	0
20	N	1604	CHD	2	0
25	P	1264	PEK	9	0
24	P	1272	DMU	4	0
25	C	265	PEK	11	0
18	N	516	HEA	8	0
19	P	1266	PGV	2	0
19	C	268	PGV	2	0
25	P	1265	PEK	9	0
20	A	525	CHD	1	0
22	L	522	TGL	27	0
18	A	515	HEA	4	0
18	N	515	HEA	4	0
24	M	526	DMU	1	0
20	P	1525	CHD	2	0
22	N	1523	TGL	7	0
26	T	1269	CDL	23	0
25	G	1263	PEK	9	0
26	G	269	CDL	22	0
25	T	263	PEK	14	0
26	P	1270	CDL	13	0
24	C	272	DMU	3	0
20	C	271	CHD	2	0
22	N	1522	TGL	15	0
19	P	1267	PGV	8	0
20	B	1086	CHD	1	0
22	D	523	TGL	5	0
20	W	1271	CHD	2	0

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

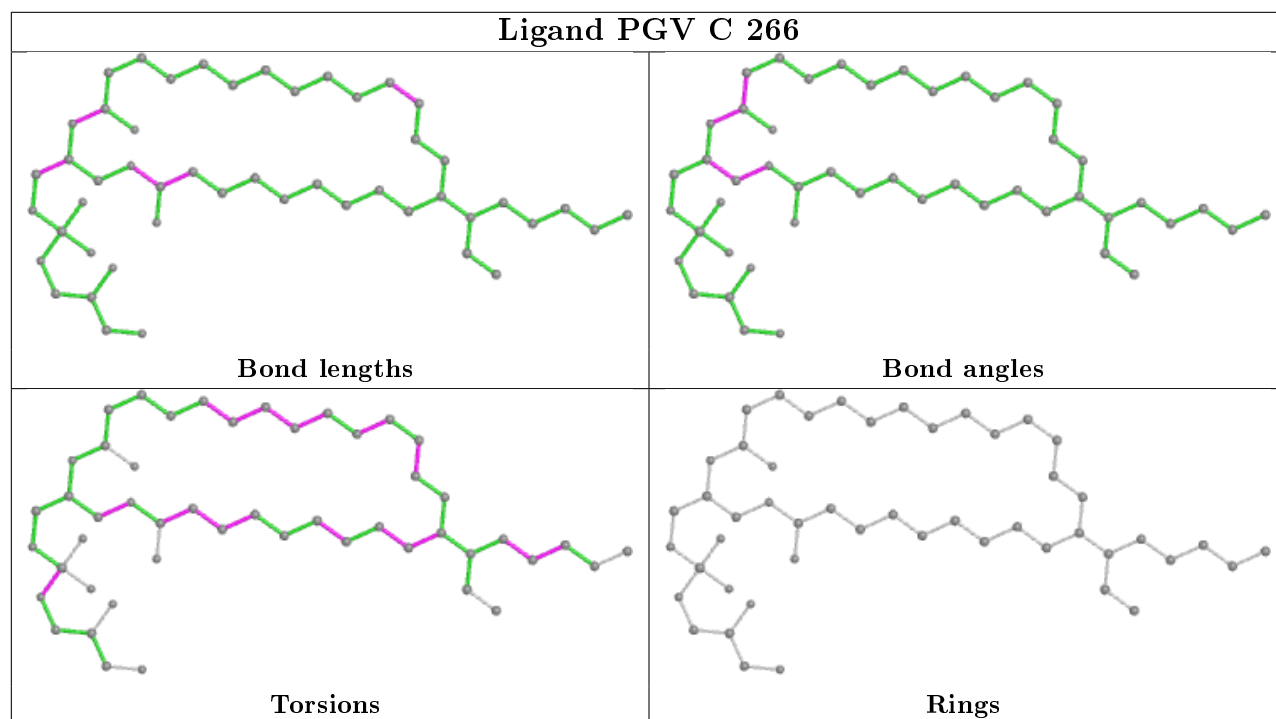




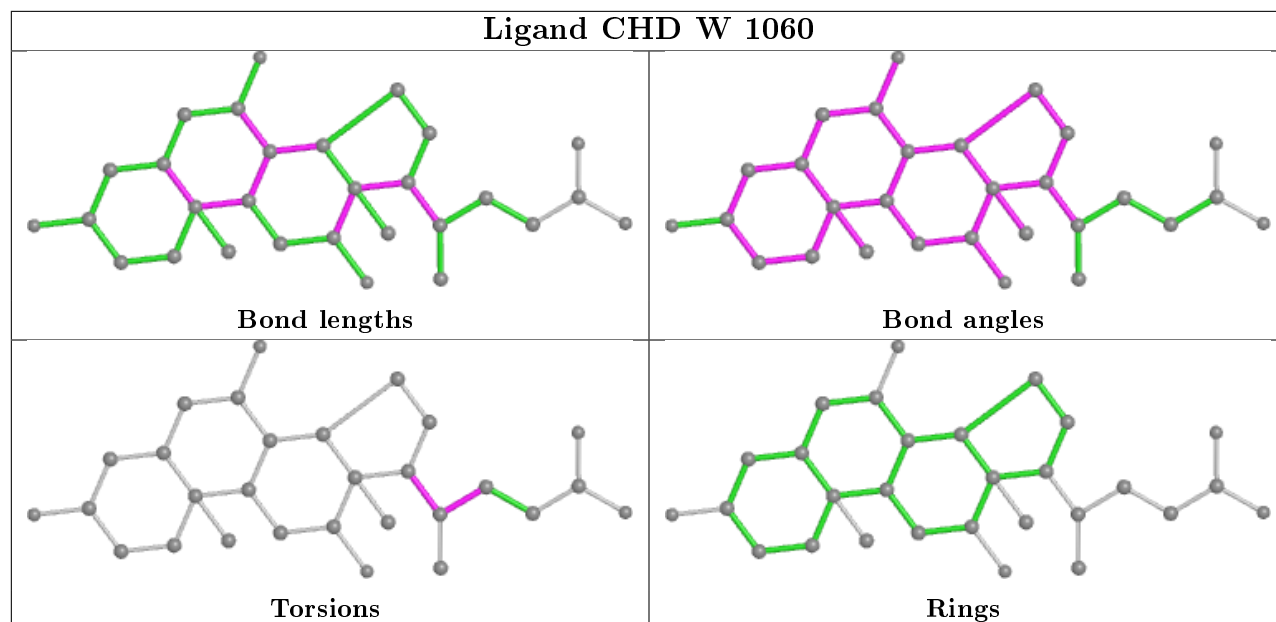
Ligand PGV N 1524



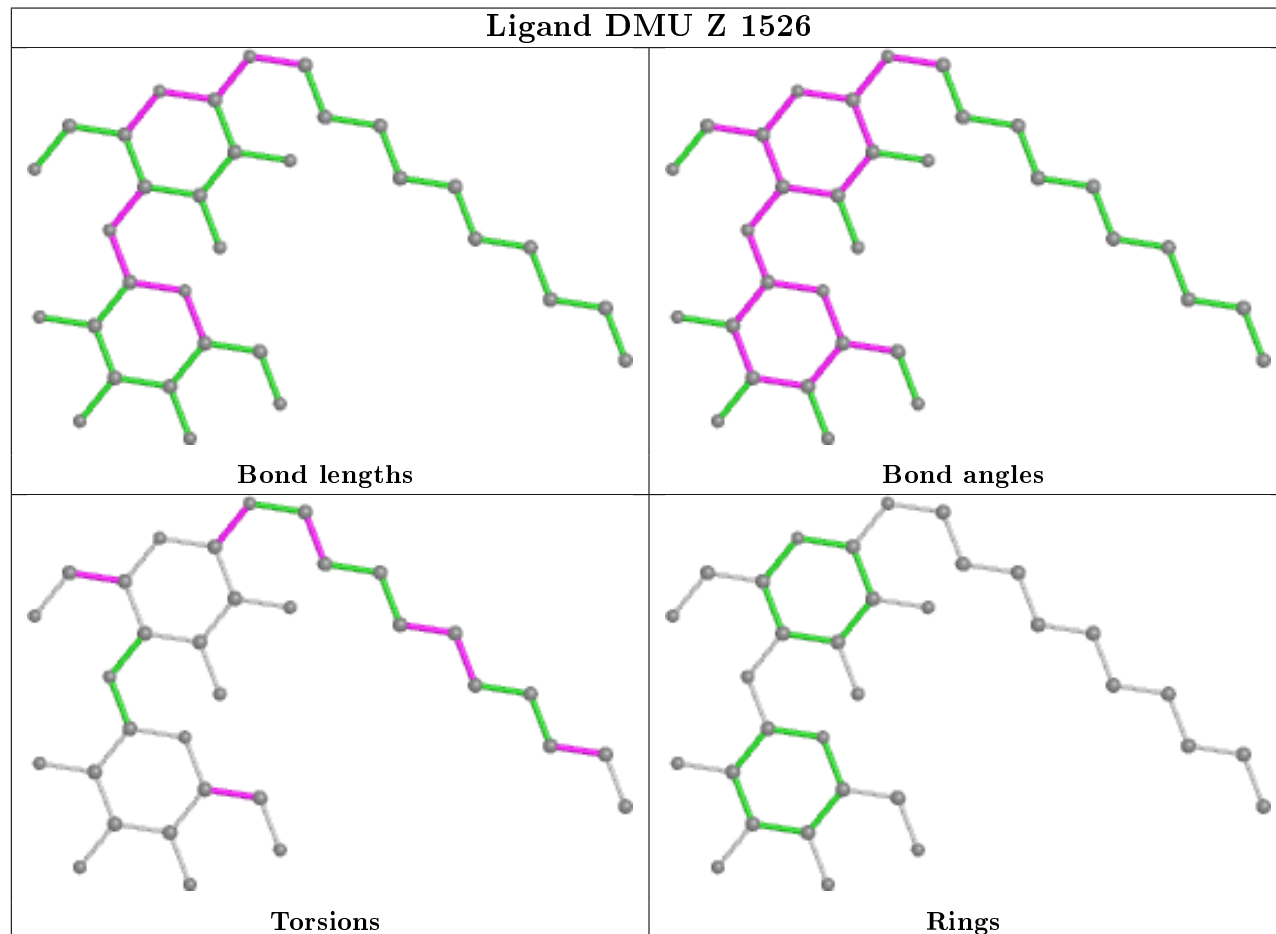
Ligand PGV C 266

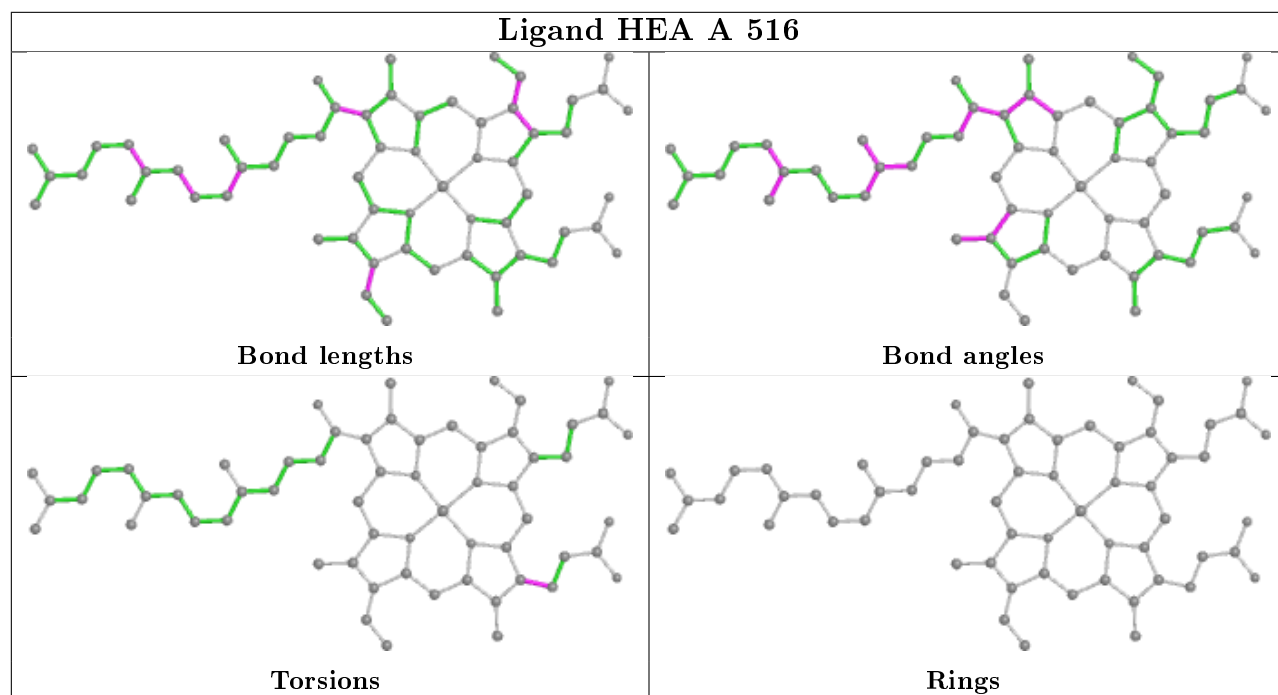
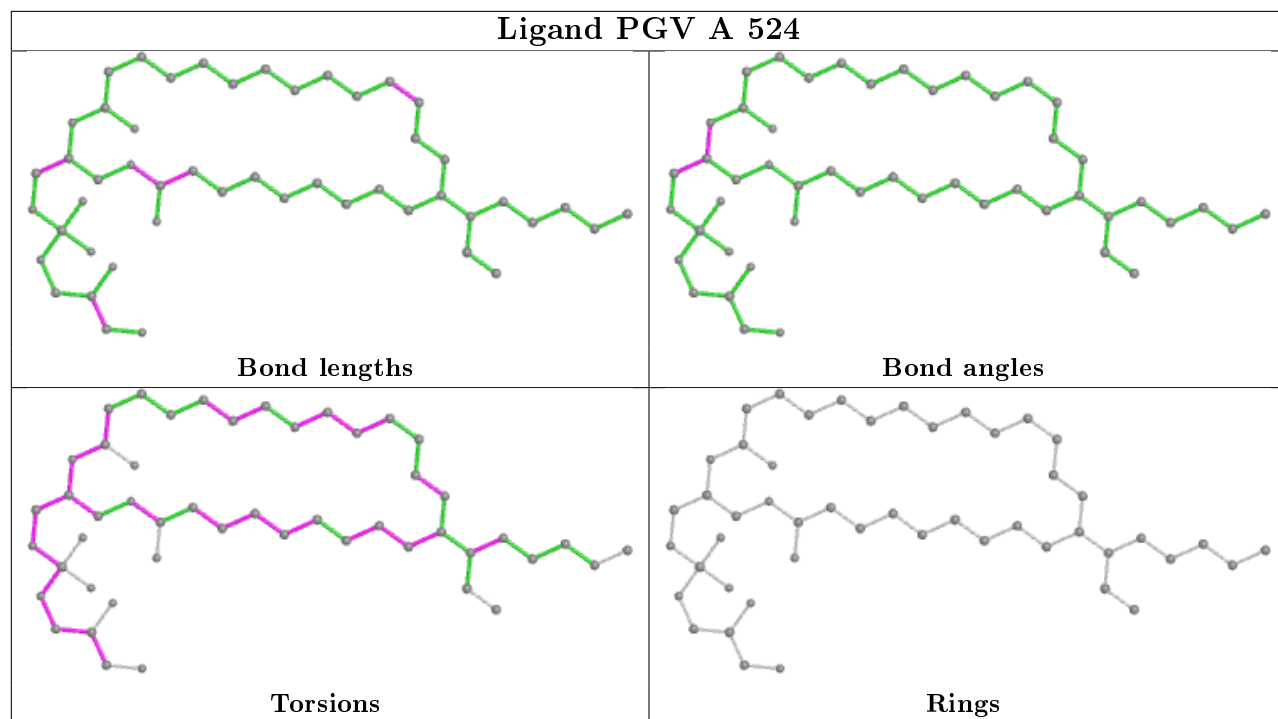


Ligand CHD W 1060

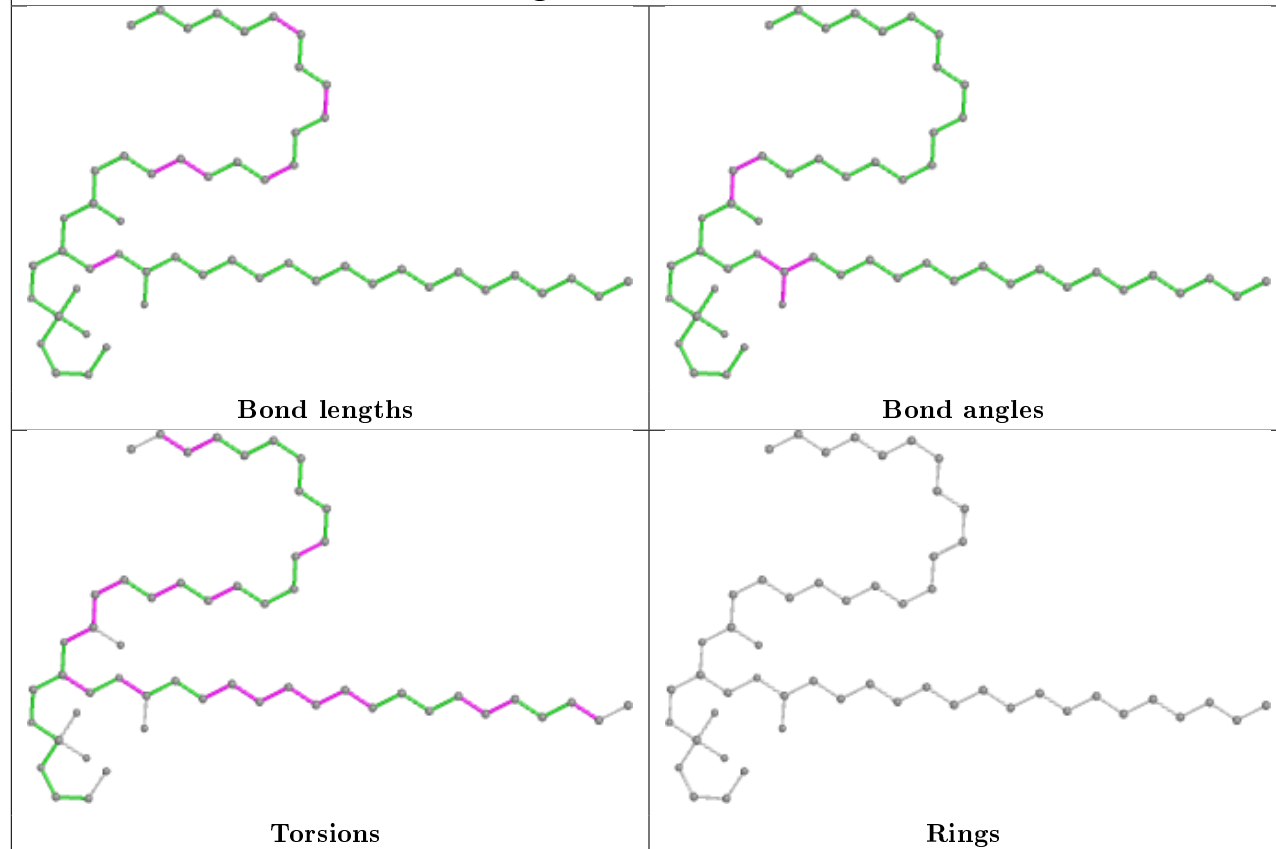


Ligand DMU Z 1526

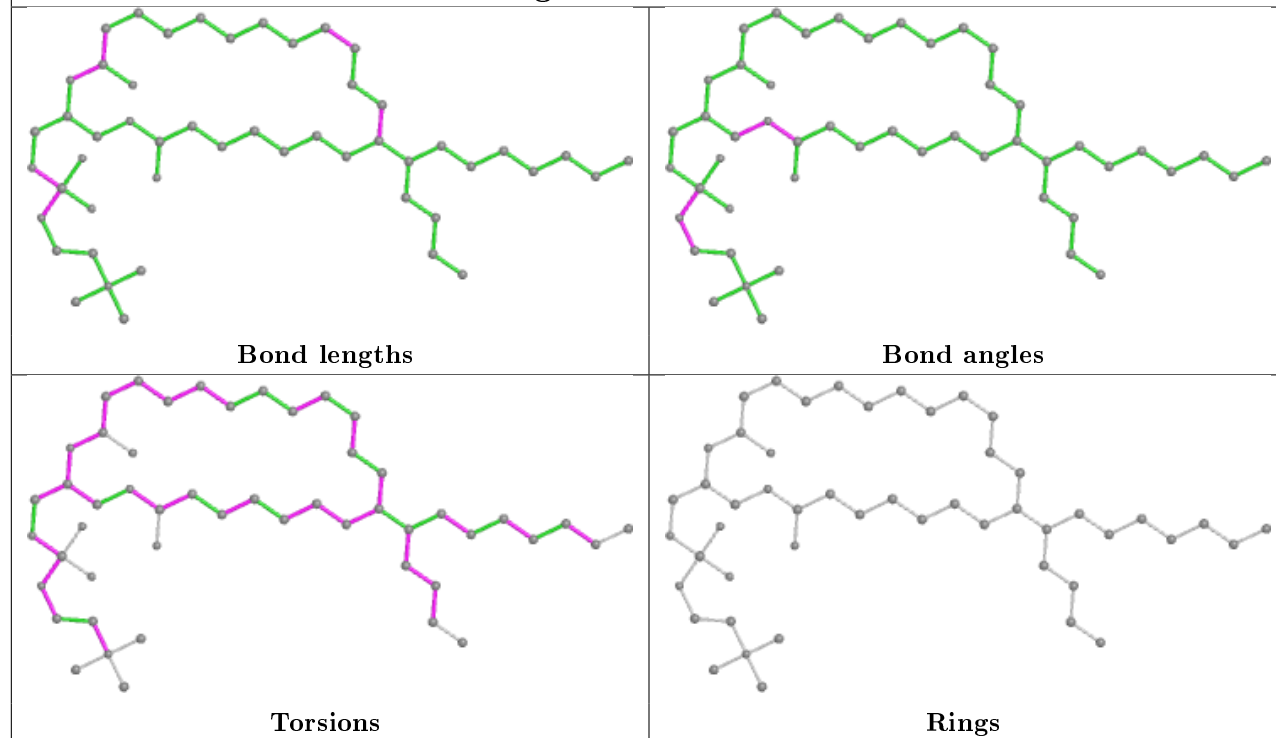


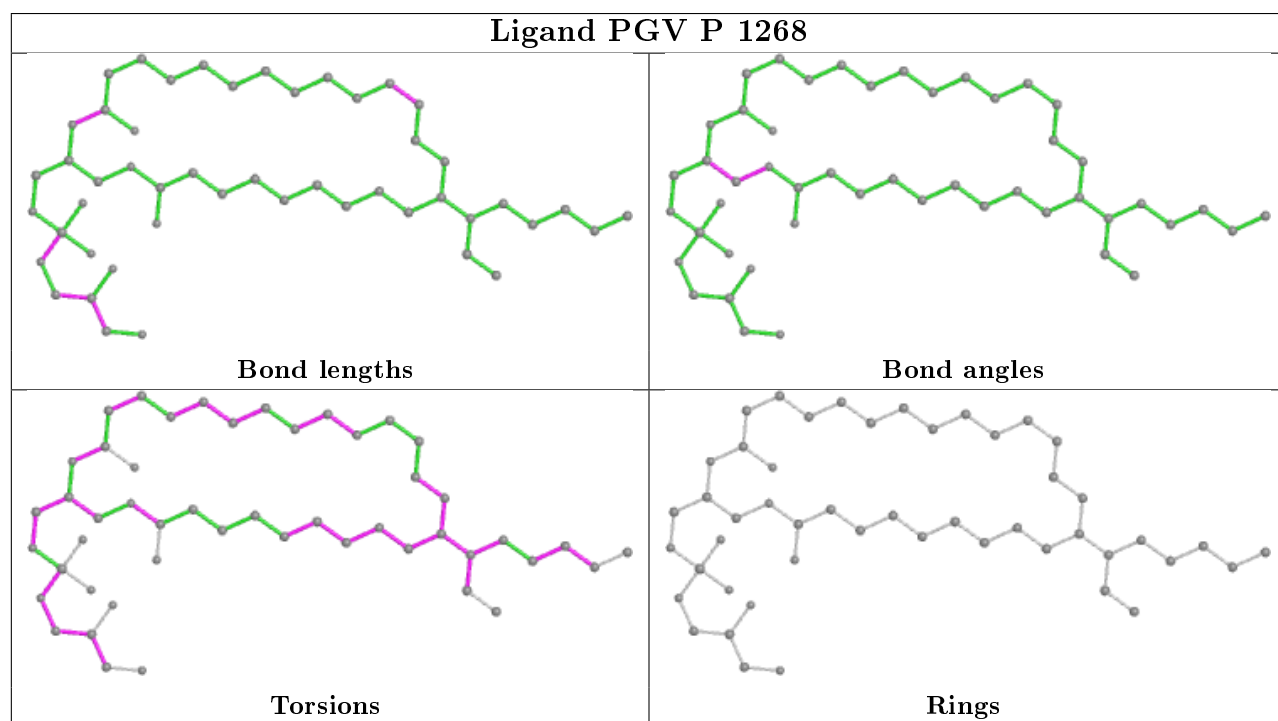
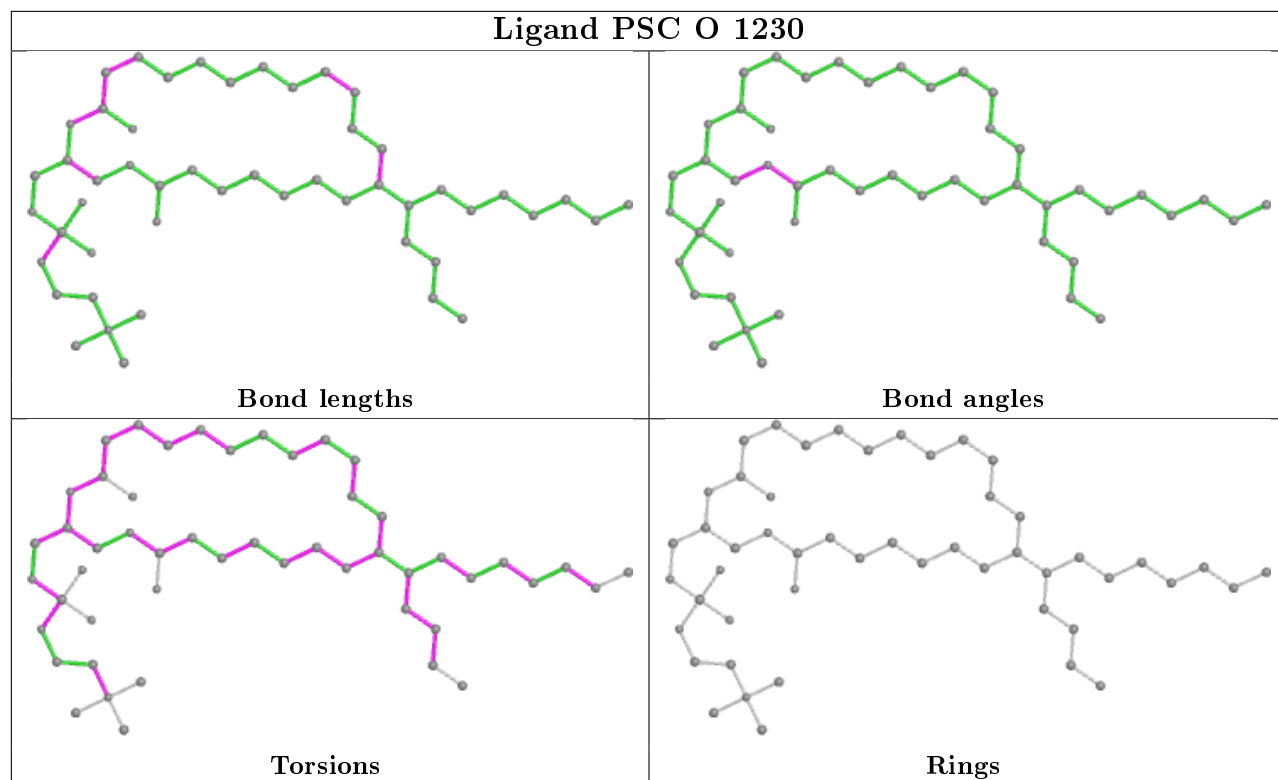


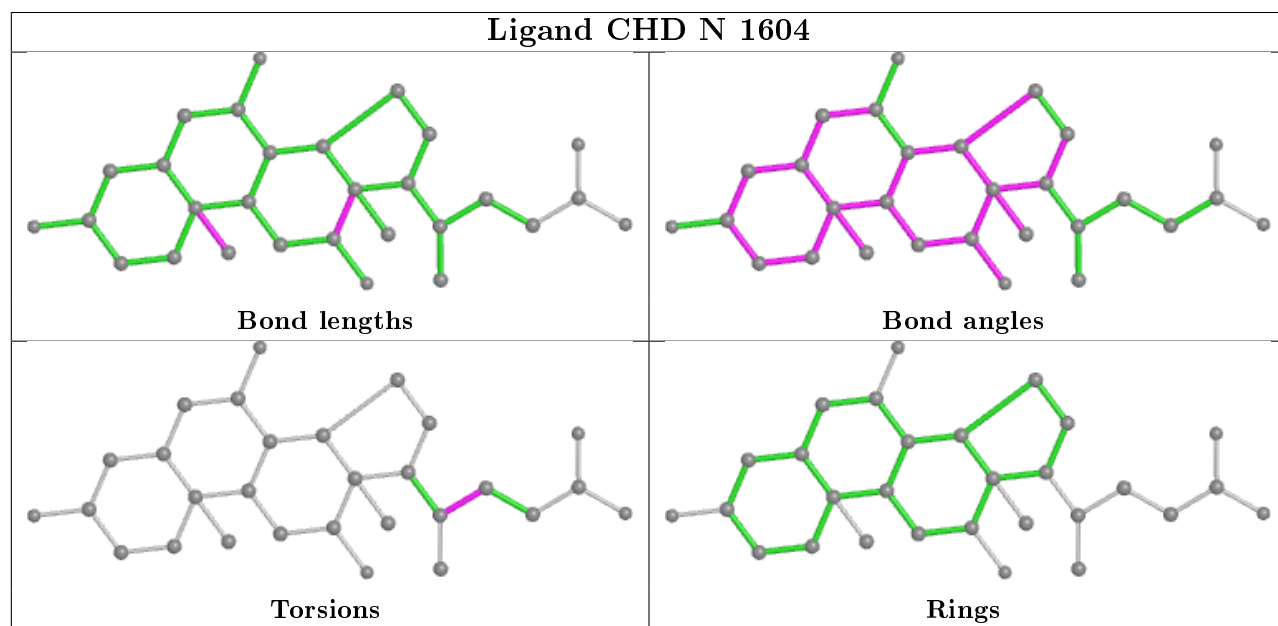
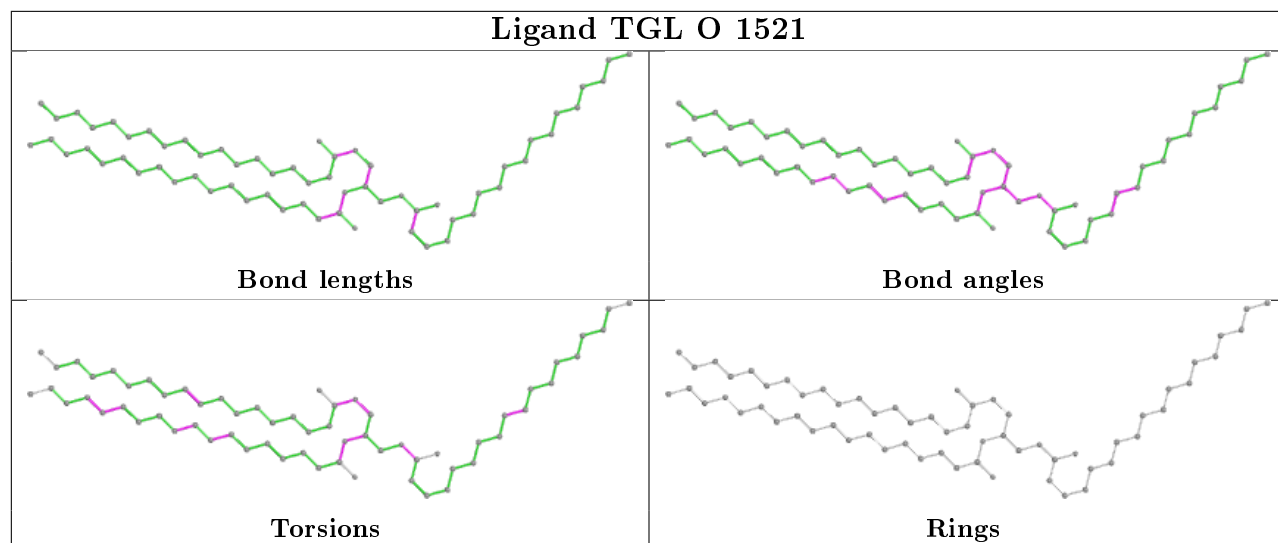
Ligand PEK C 264

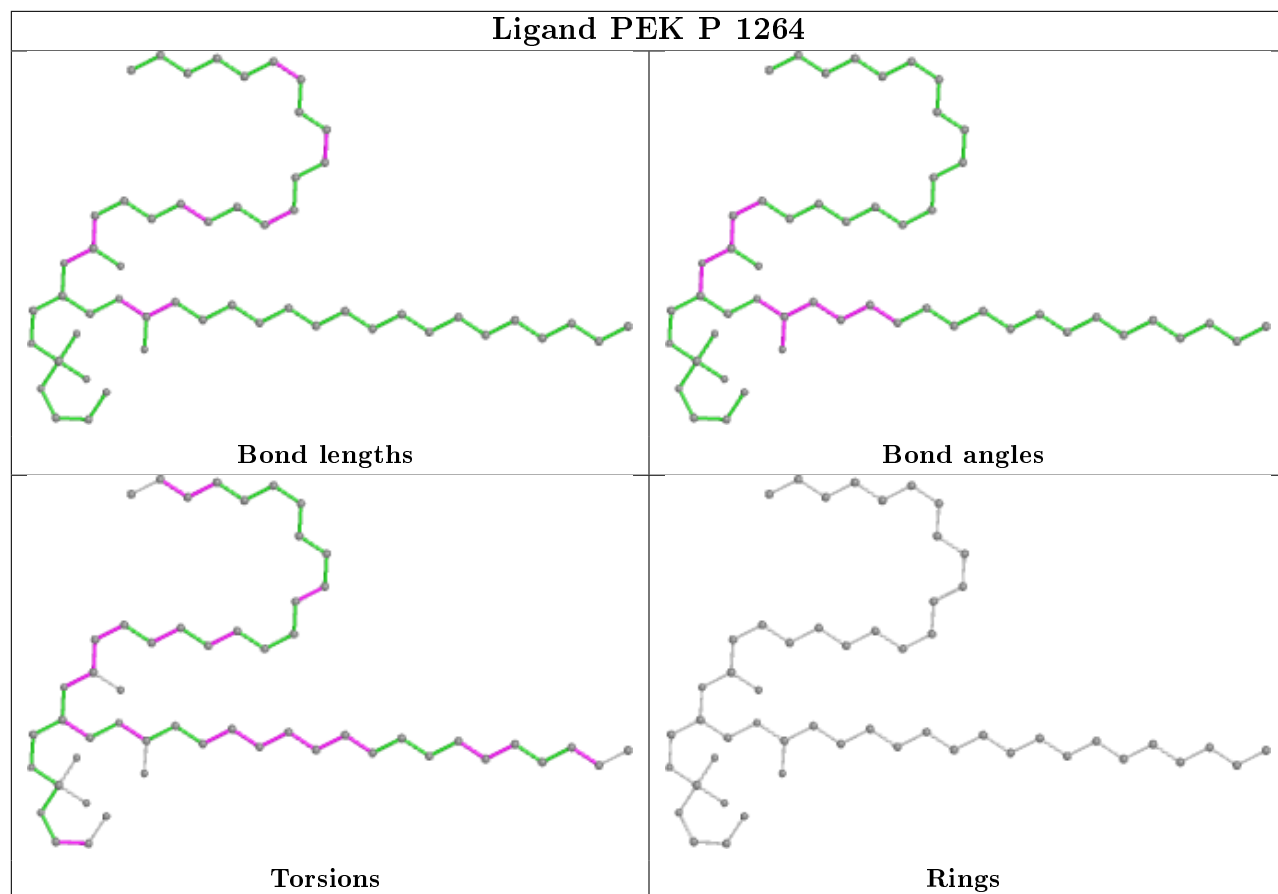


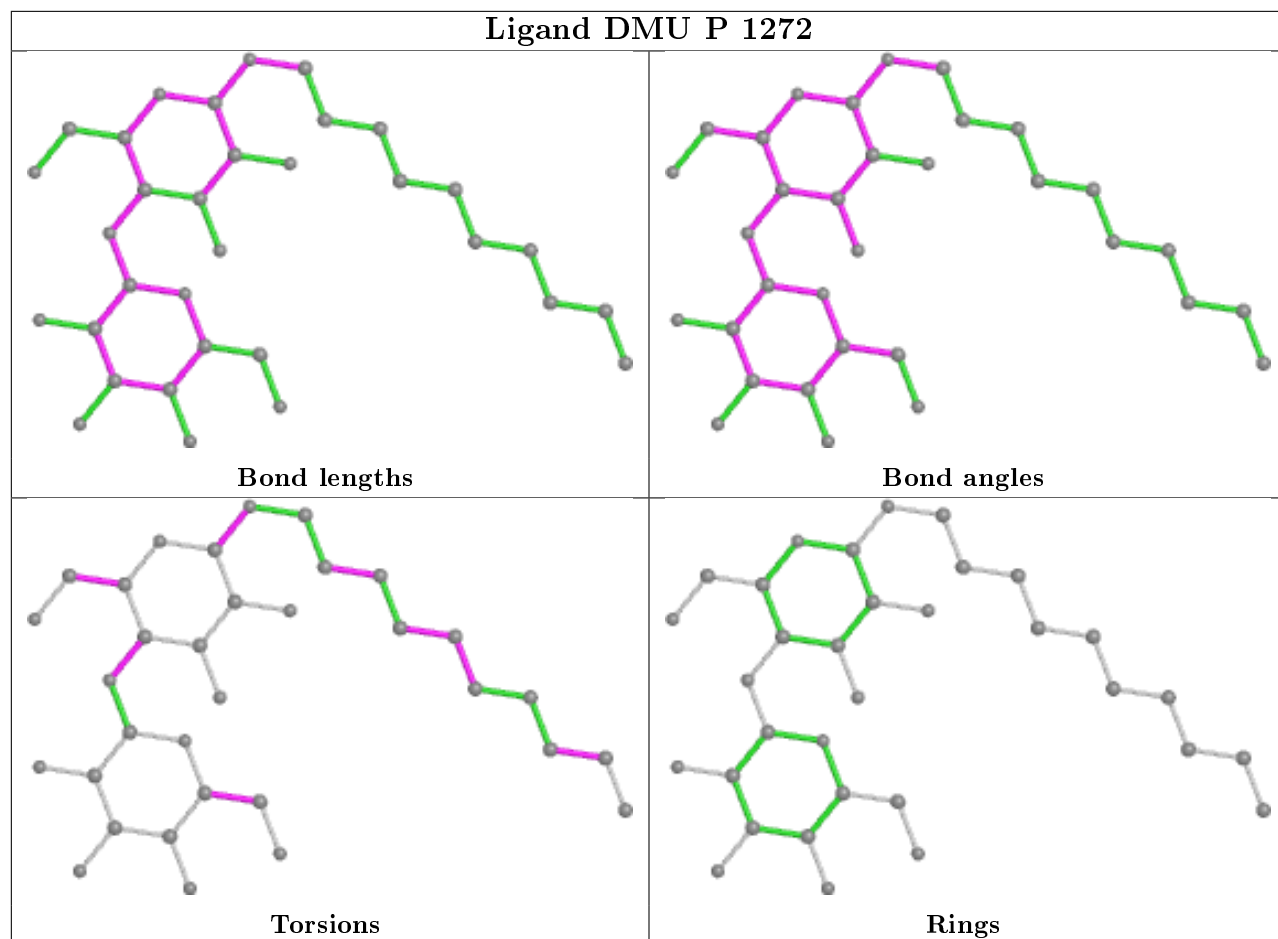
Ligand PSC B 230



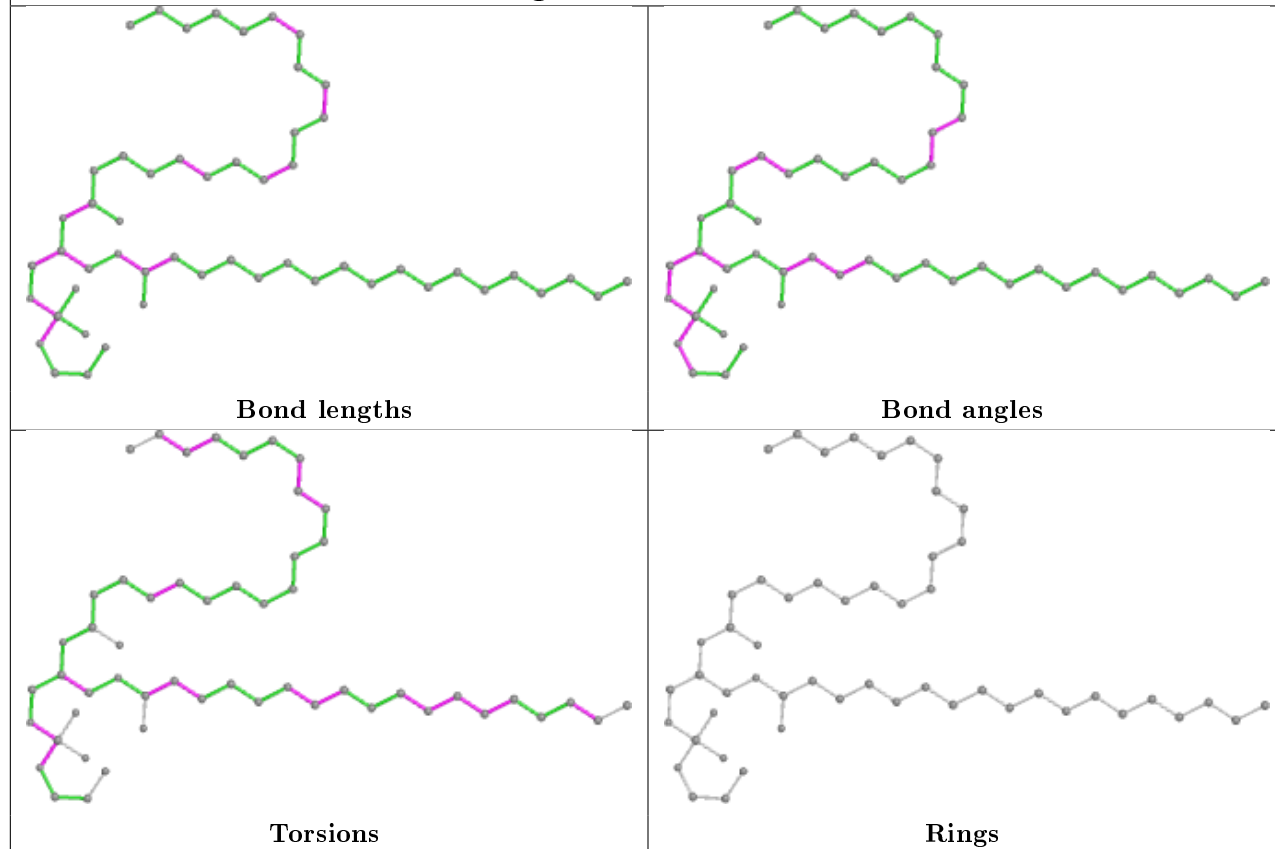




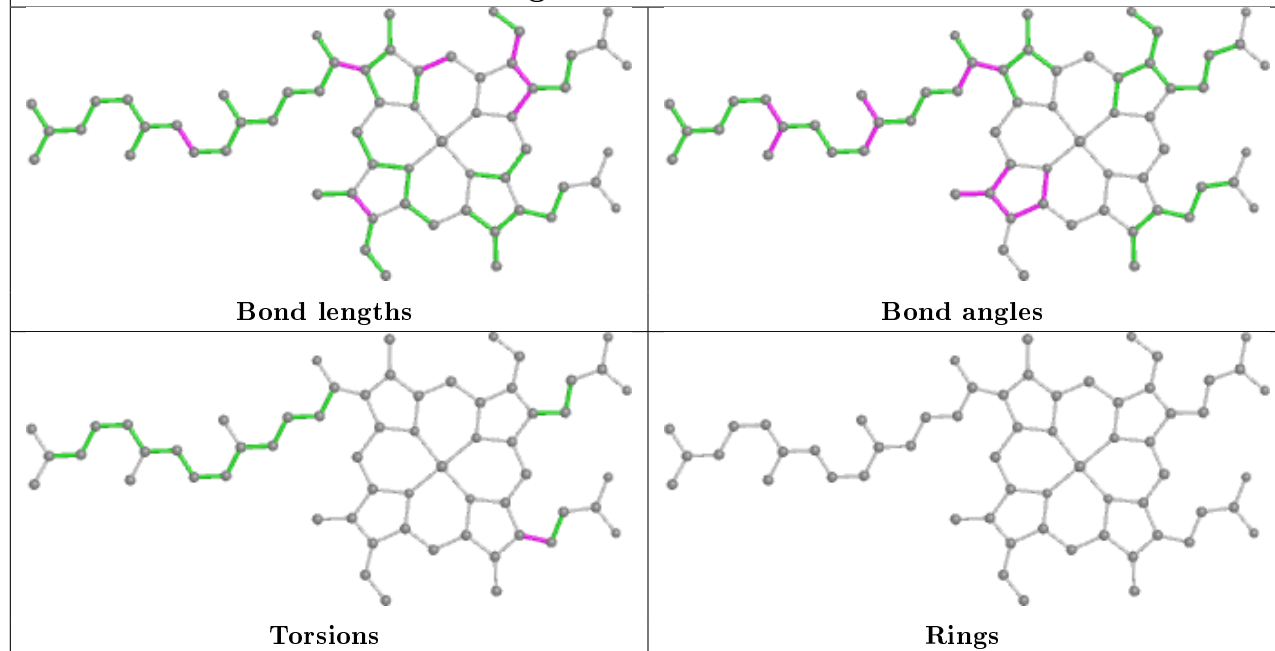


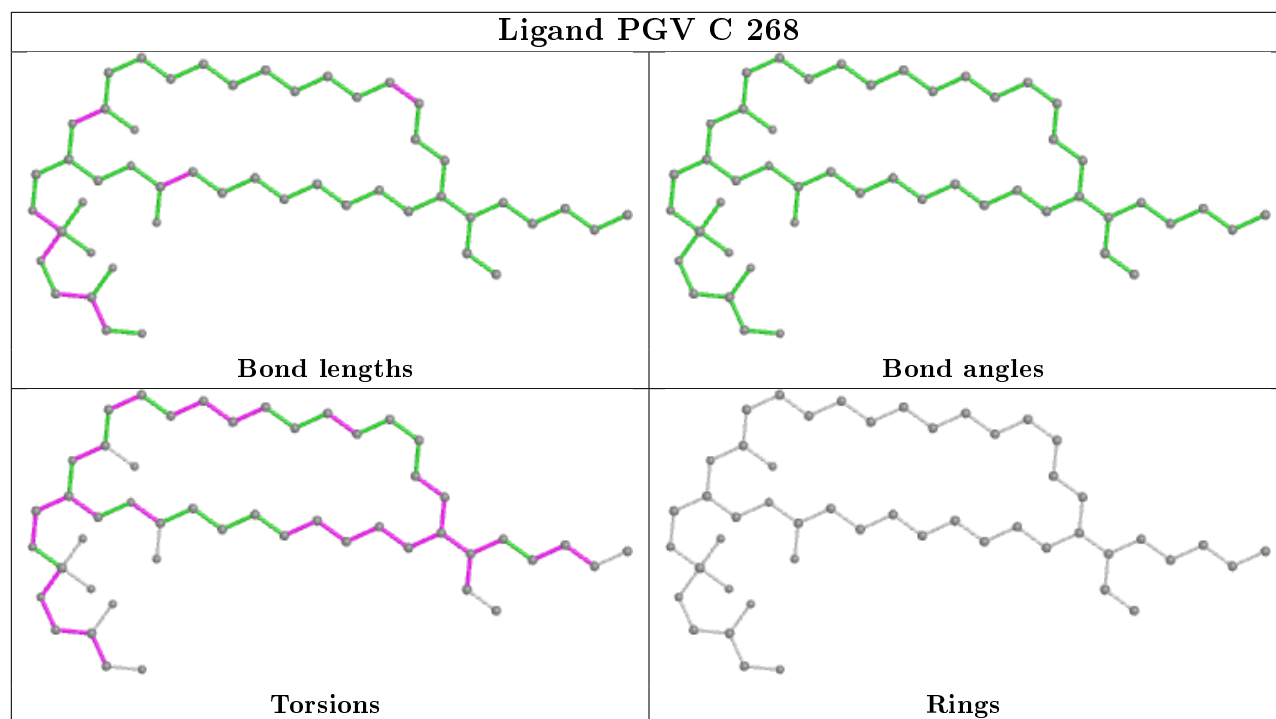
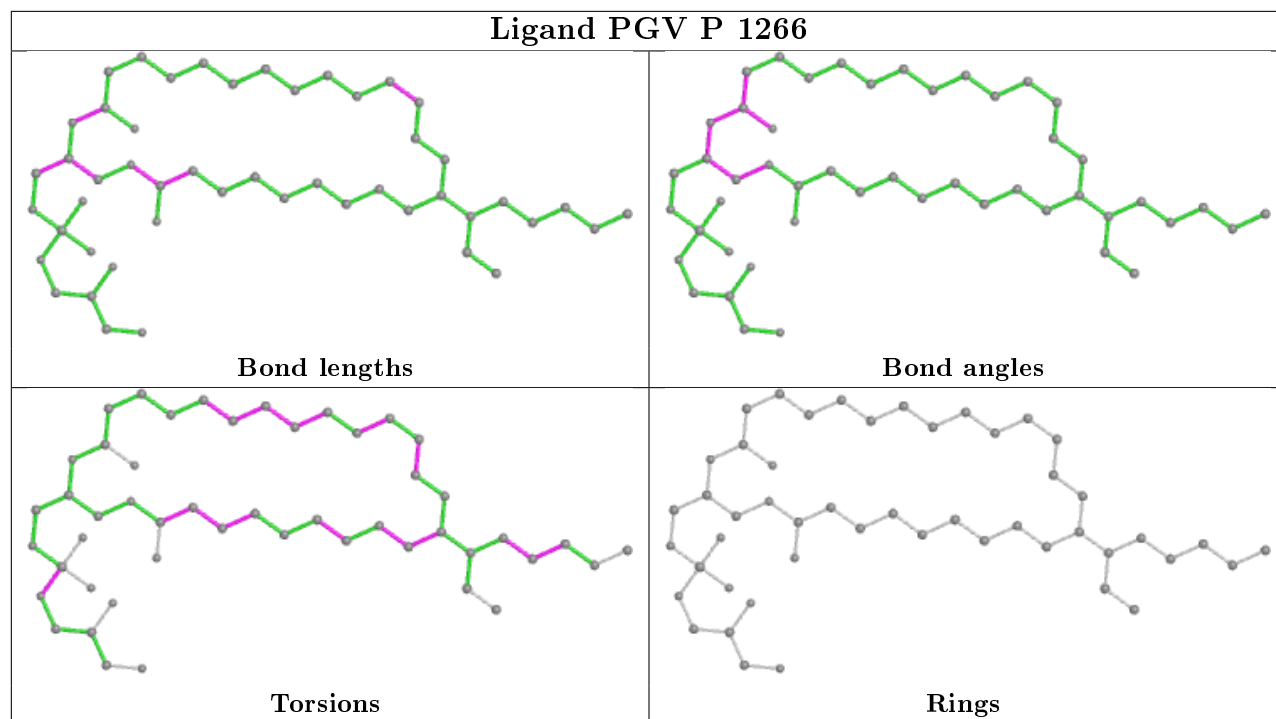


Ligand PEK C 265

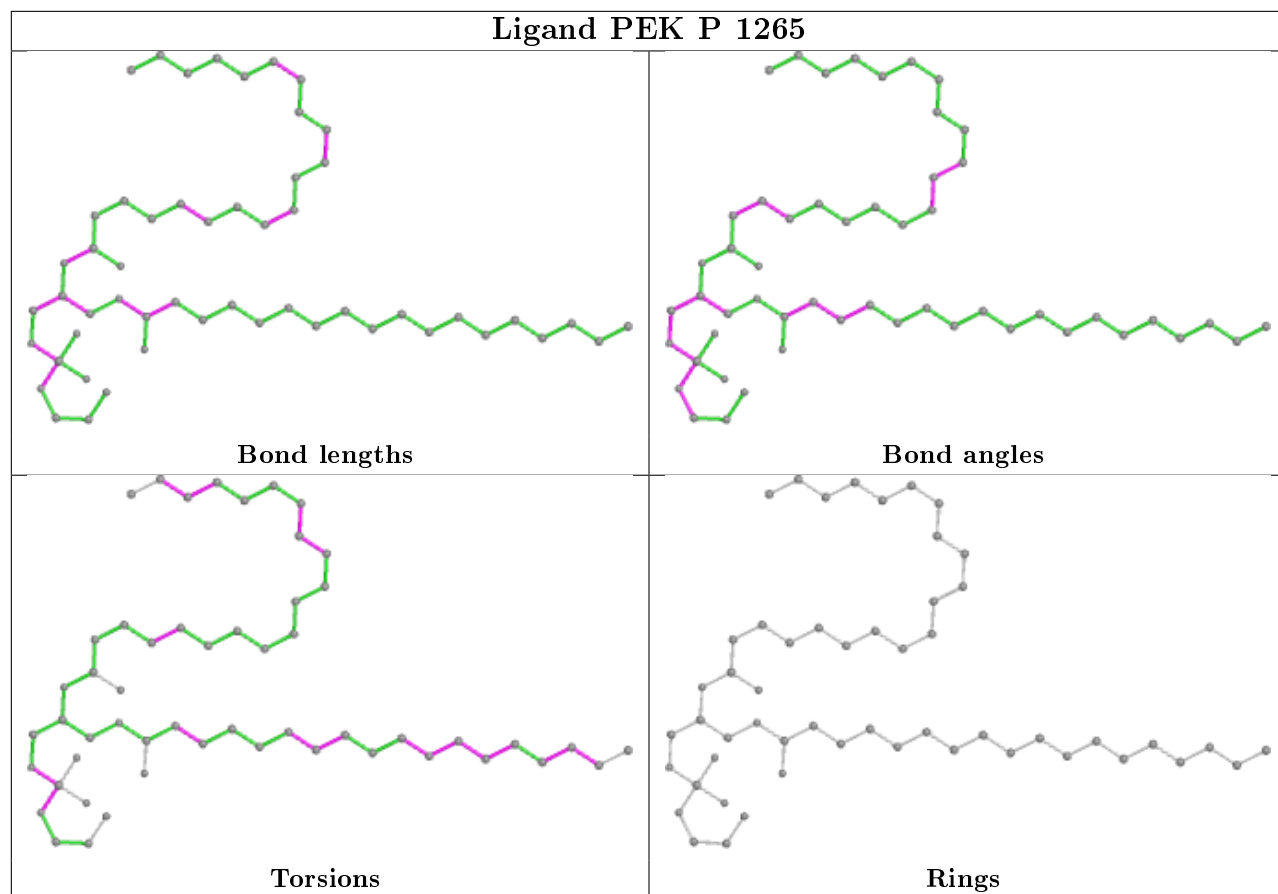


Ligand HEA N 516

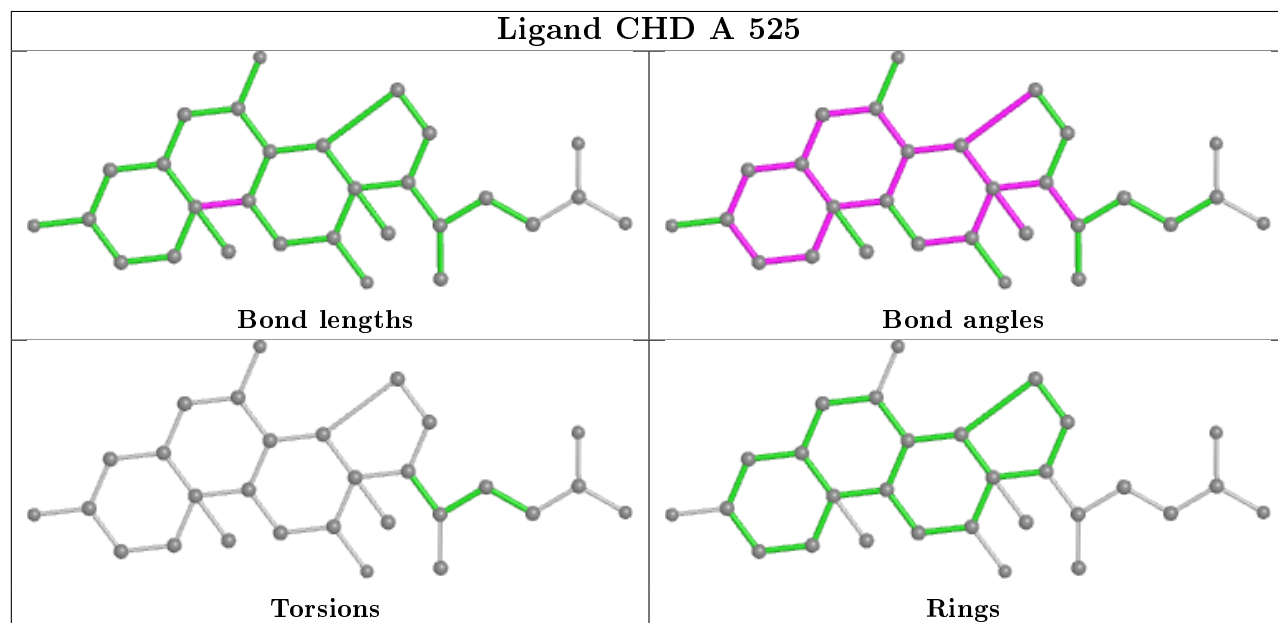


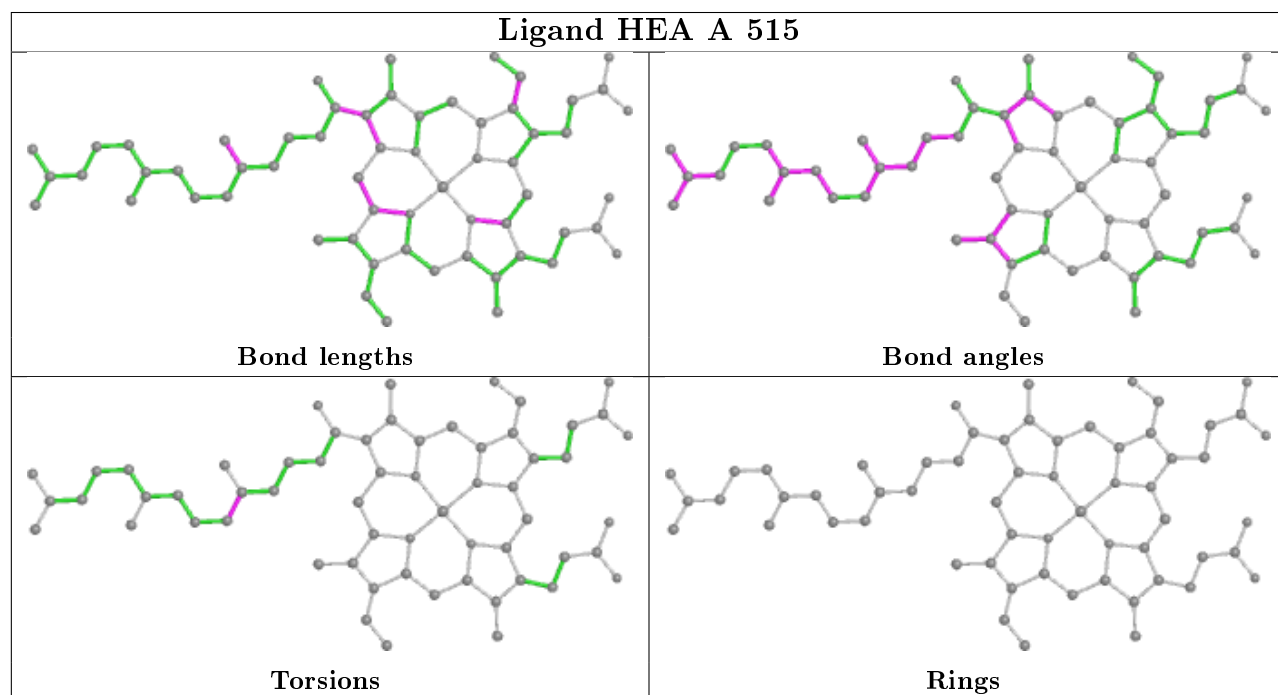
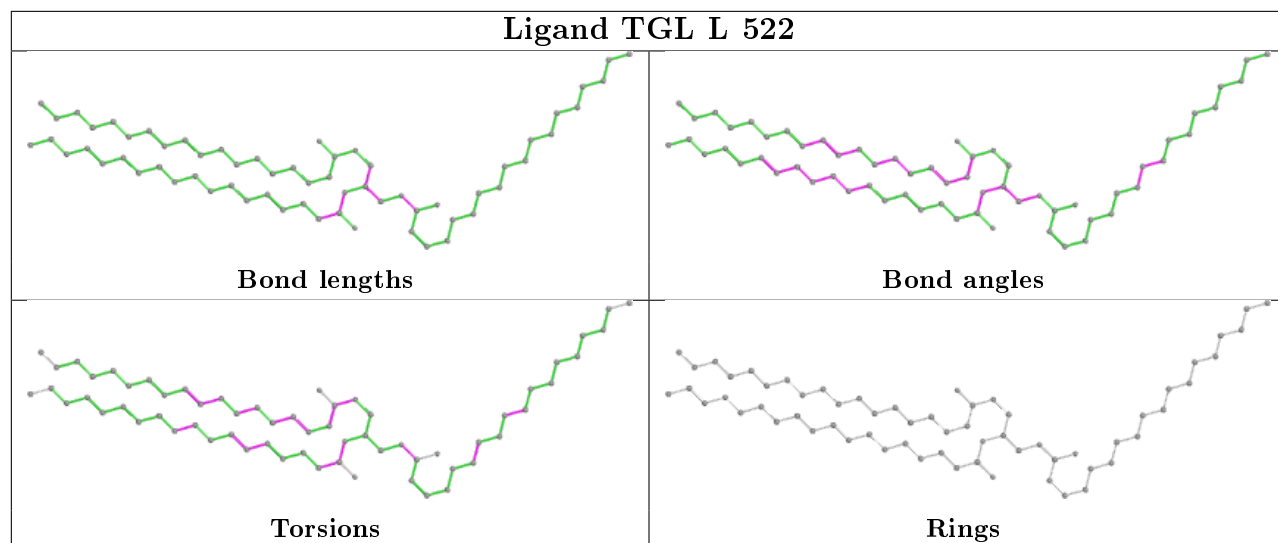


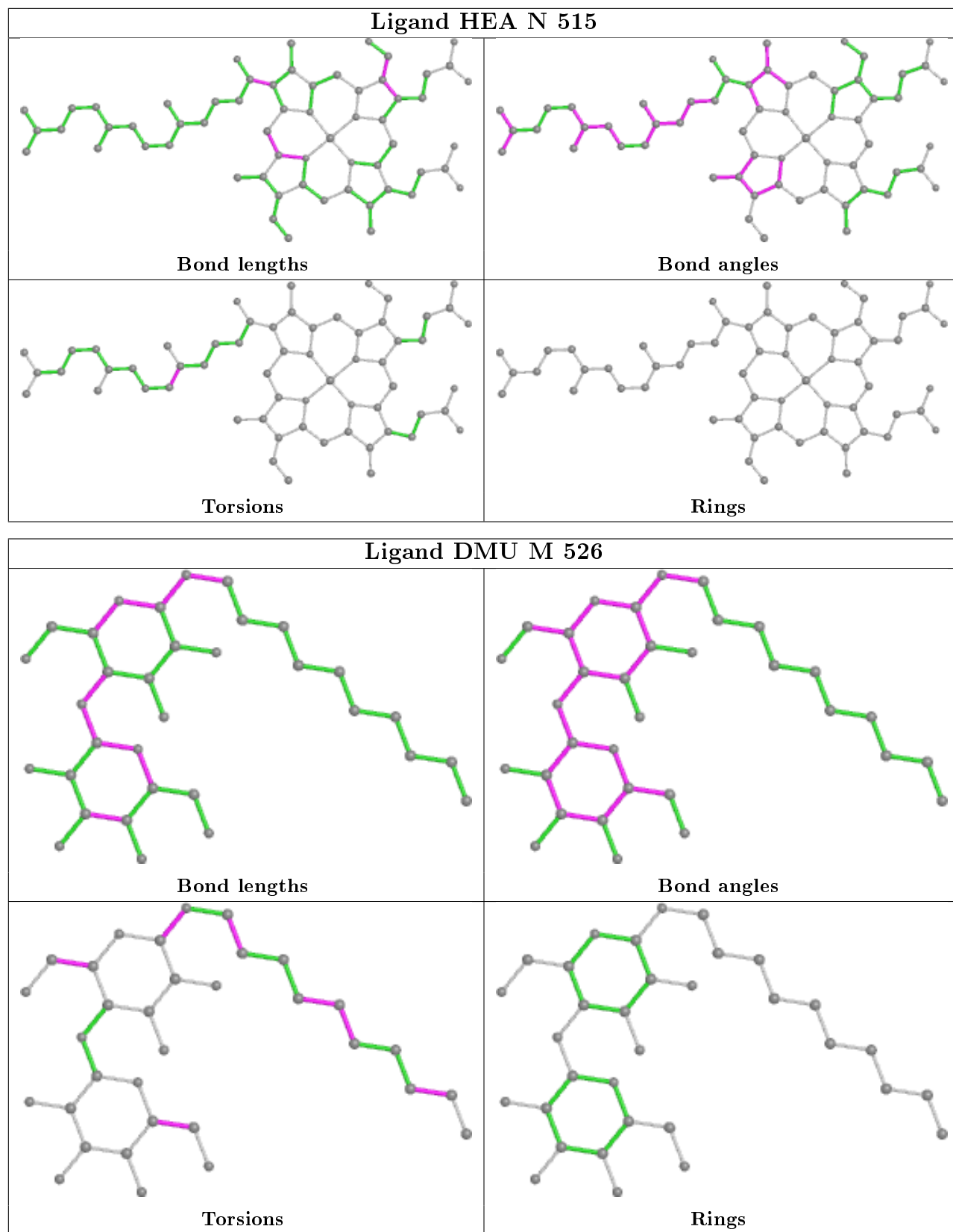
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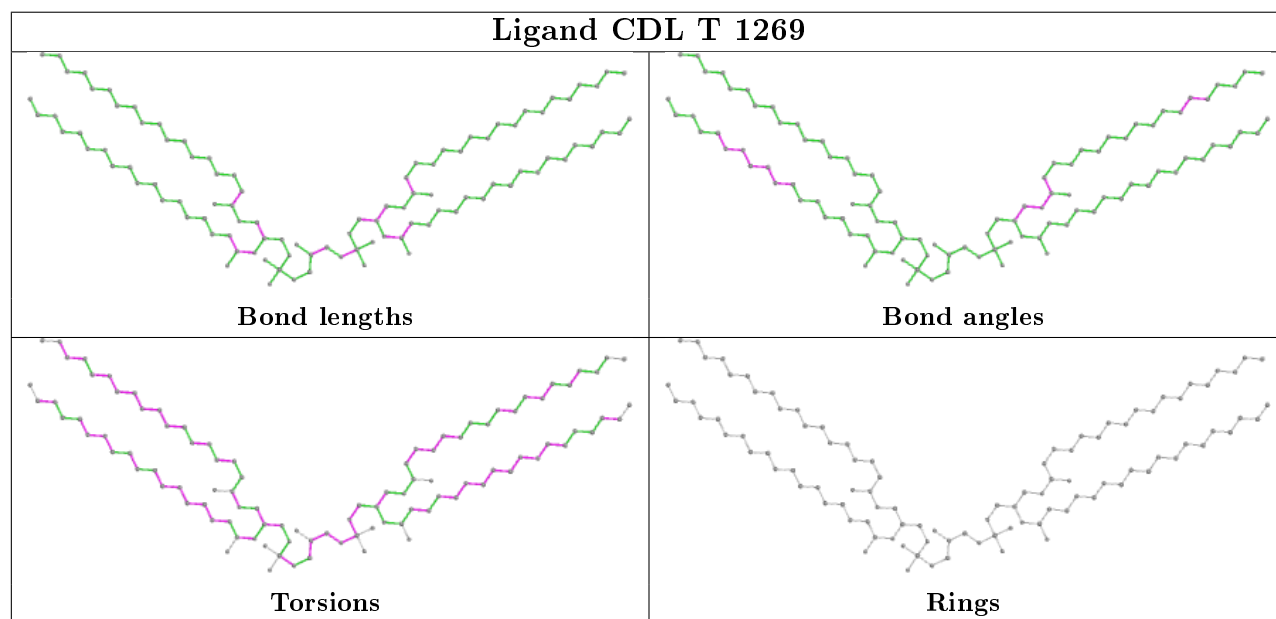
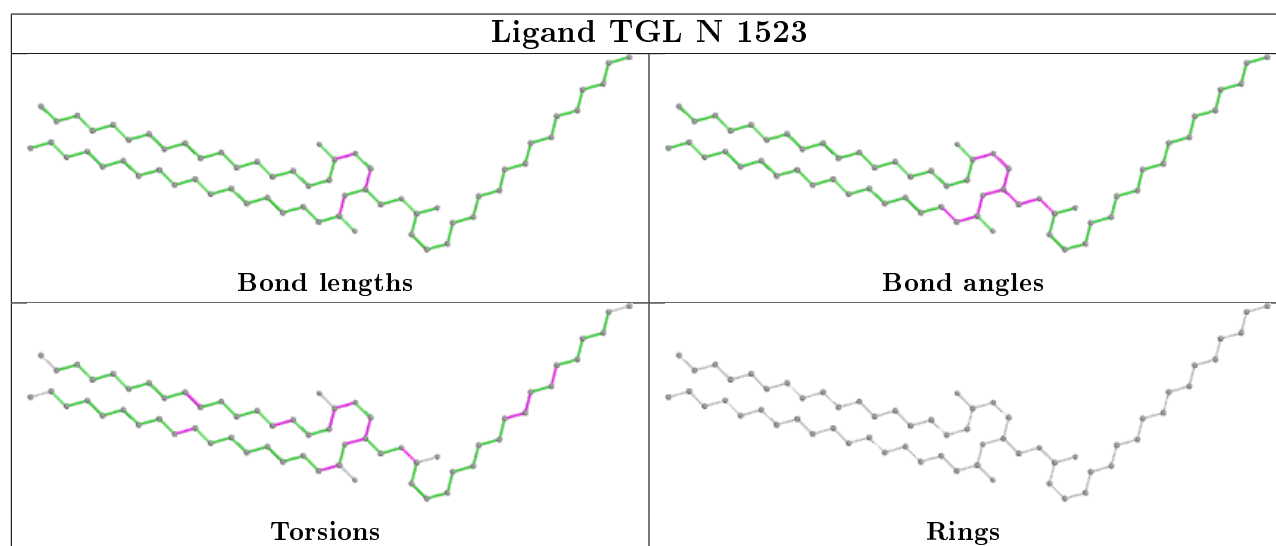
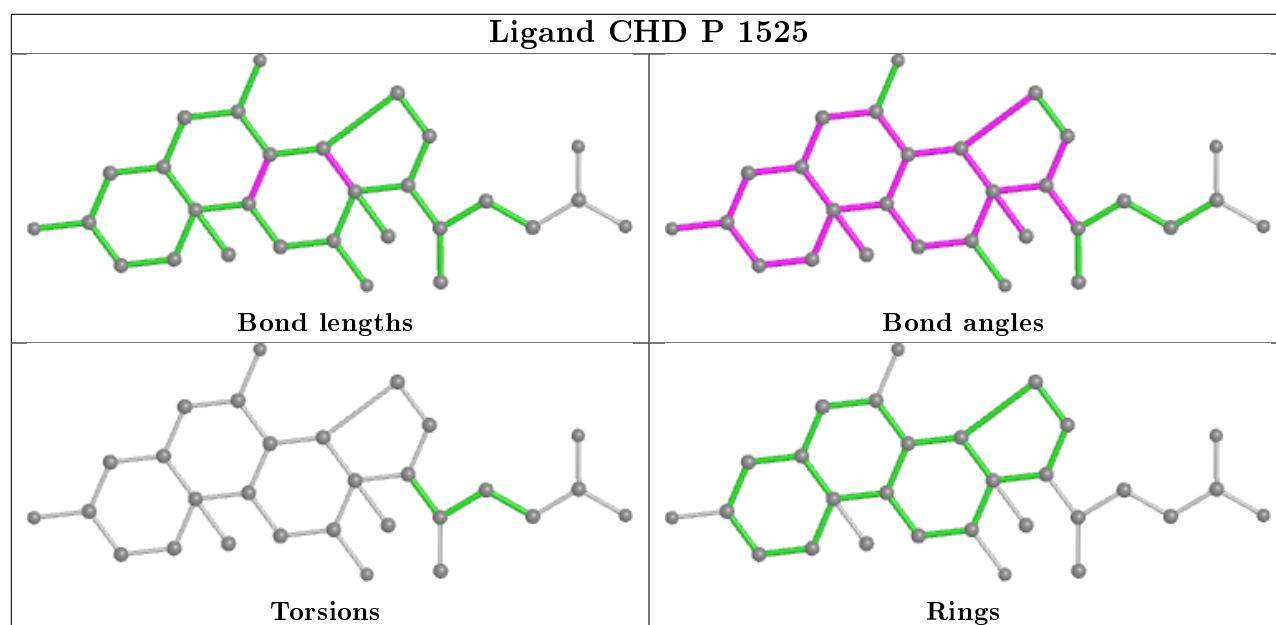


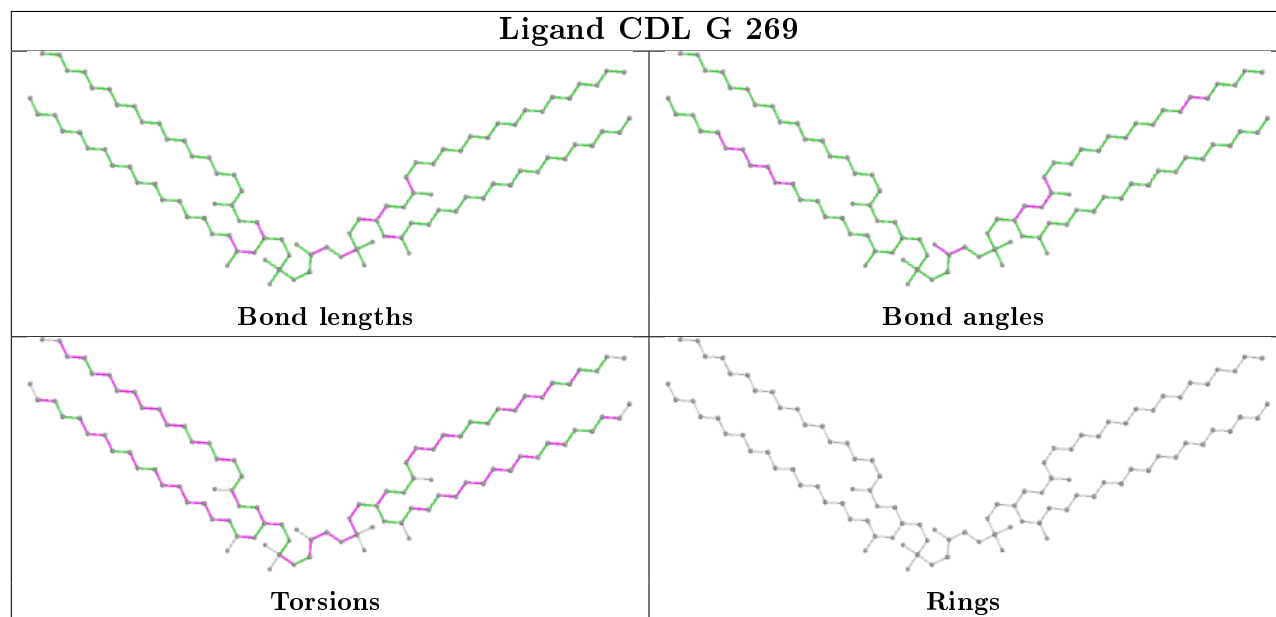
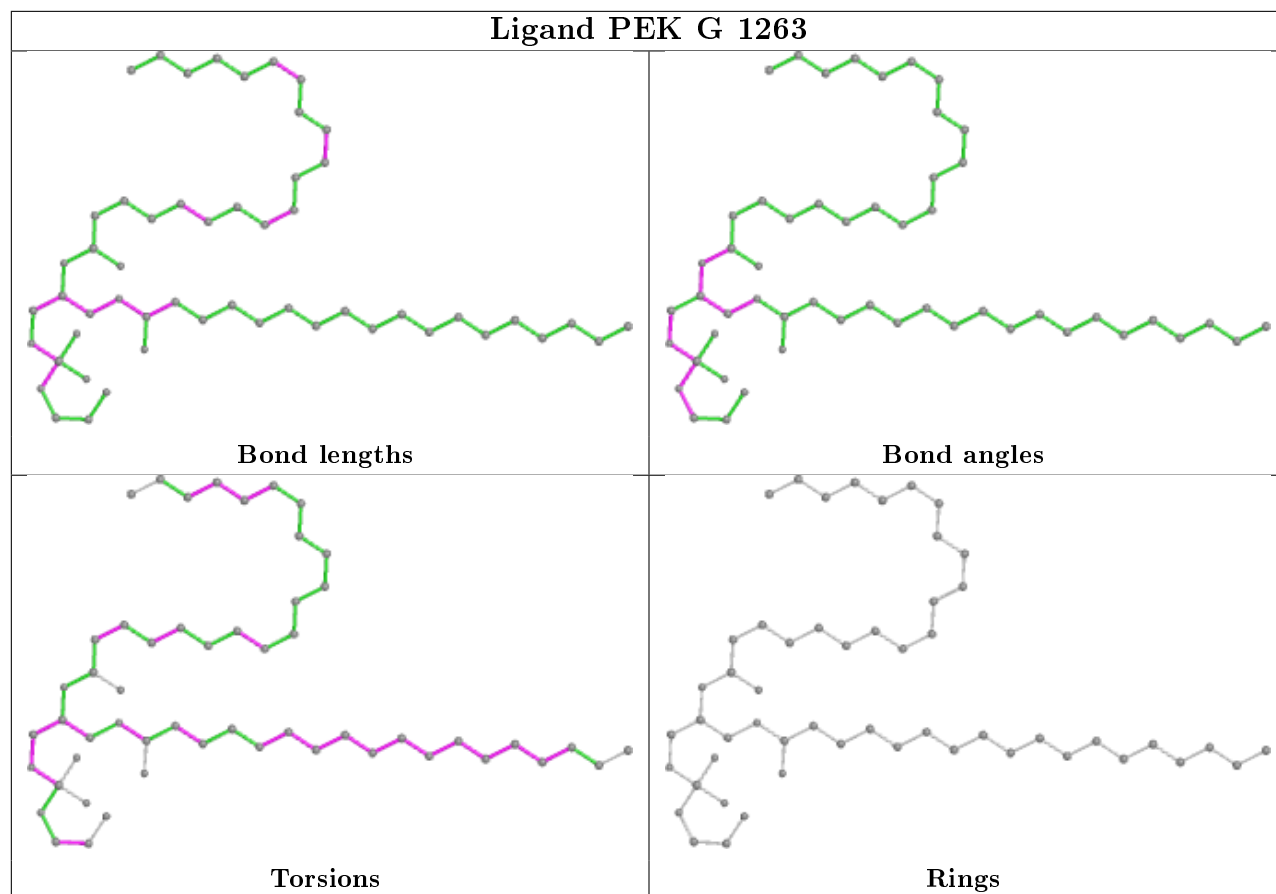
Ligand CHD A 525

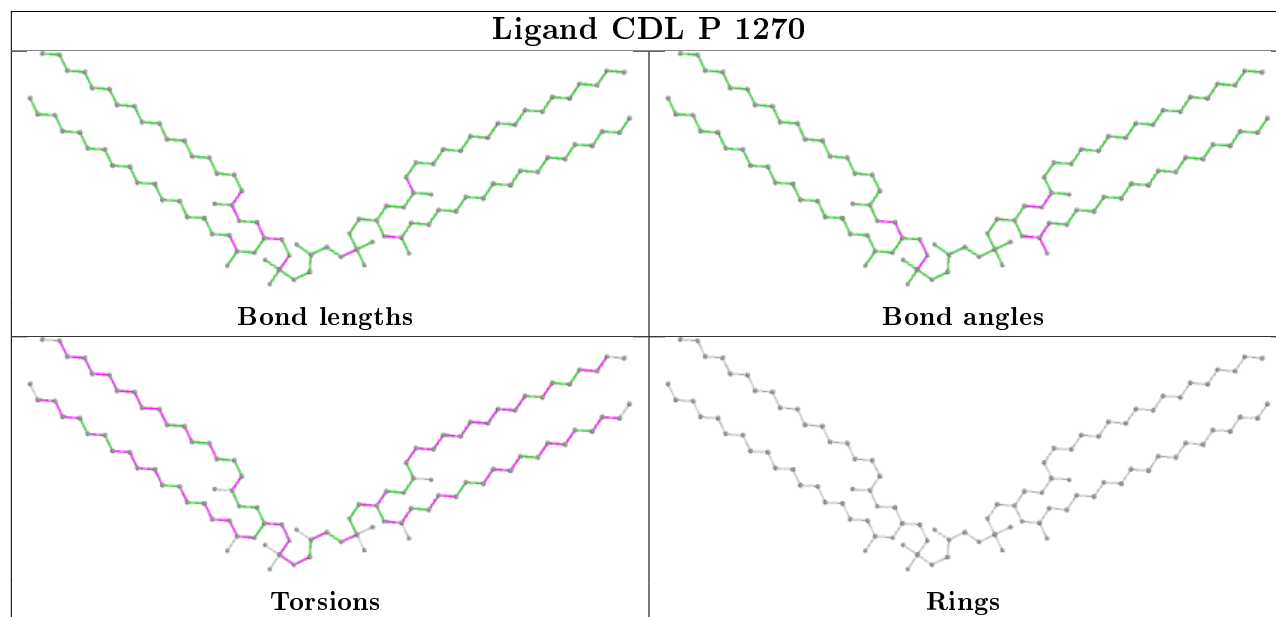
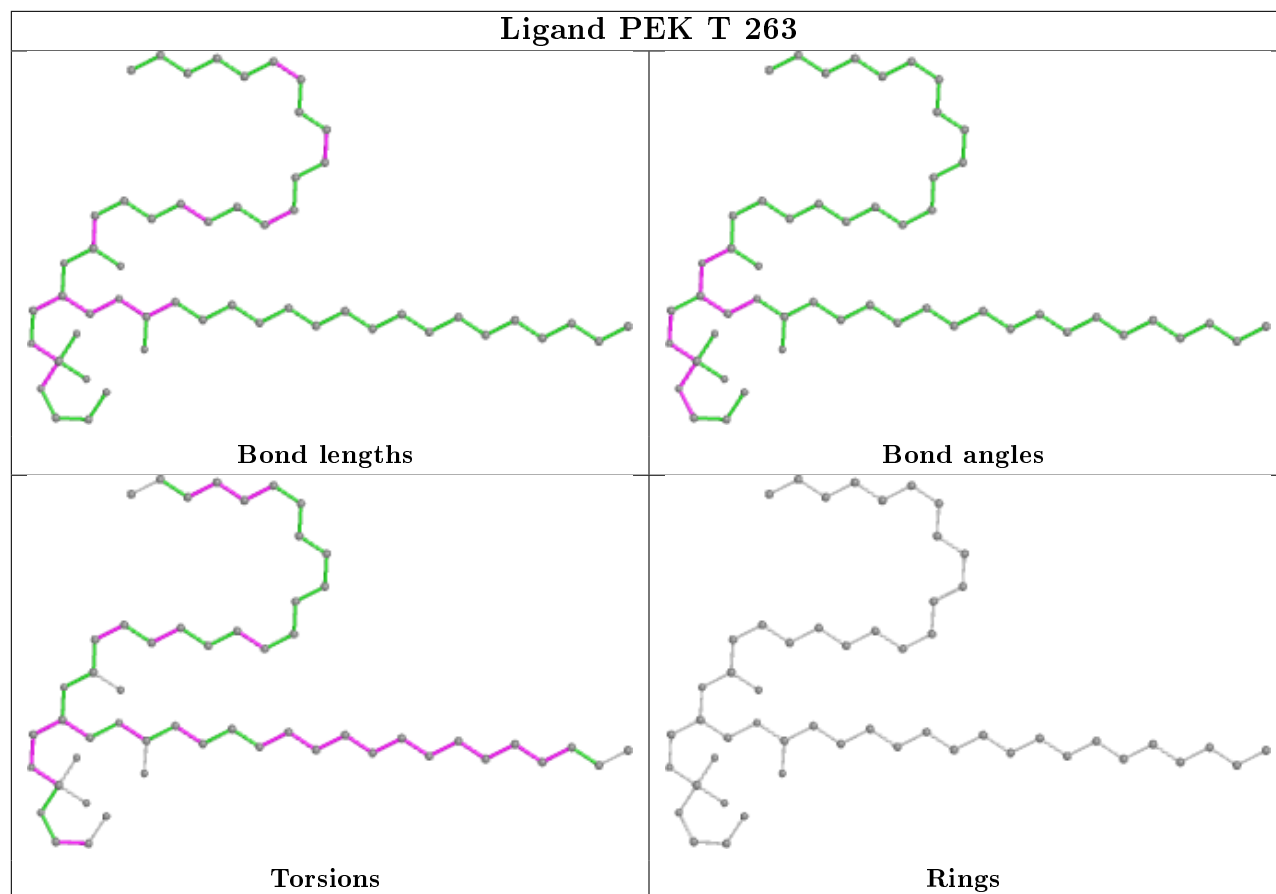




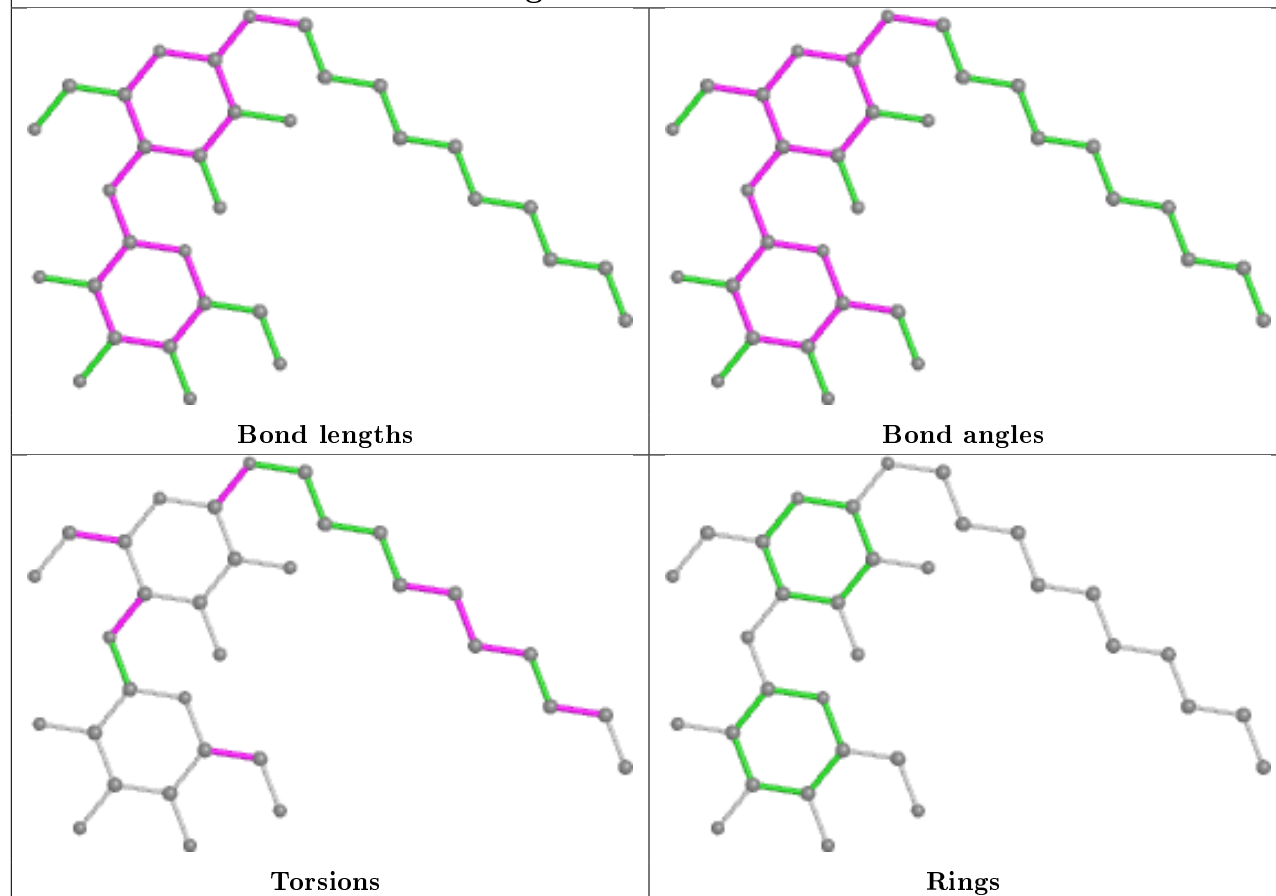




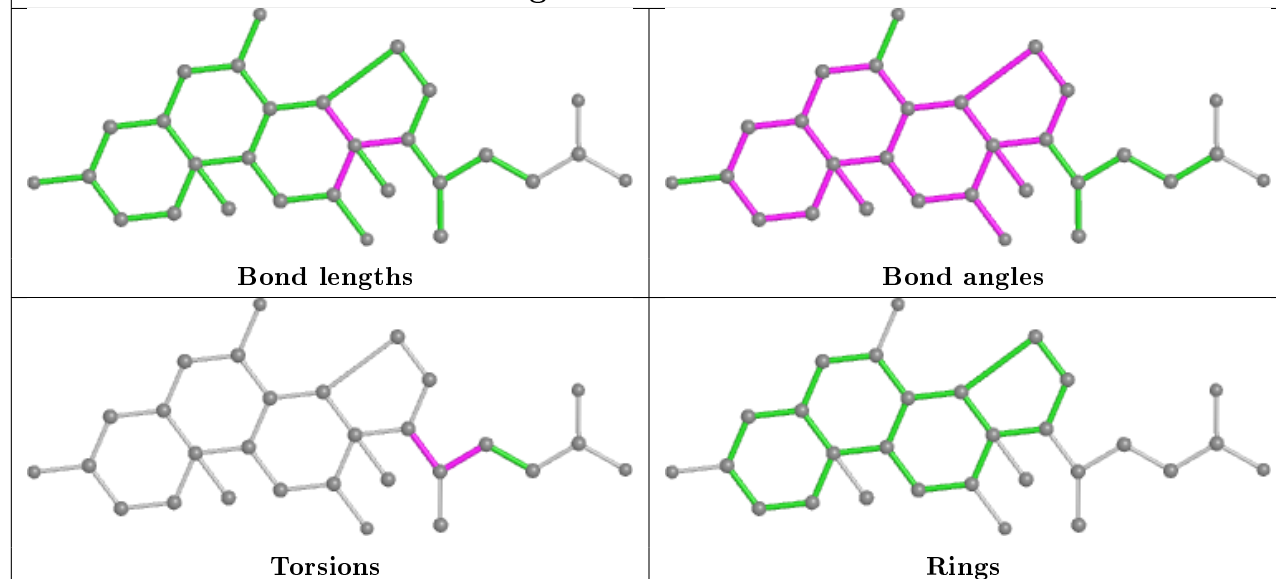


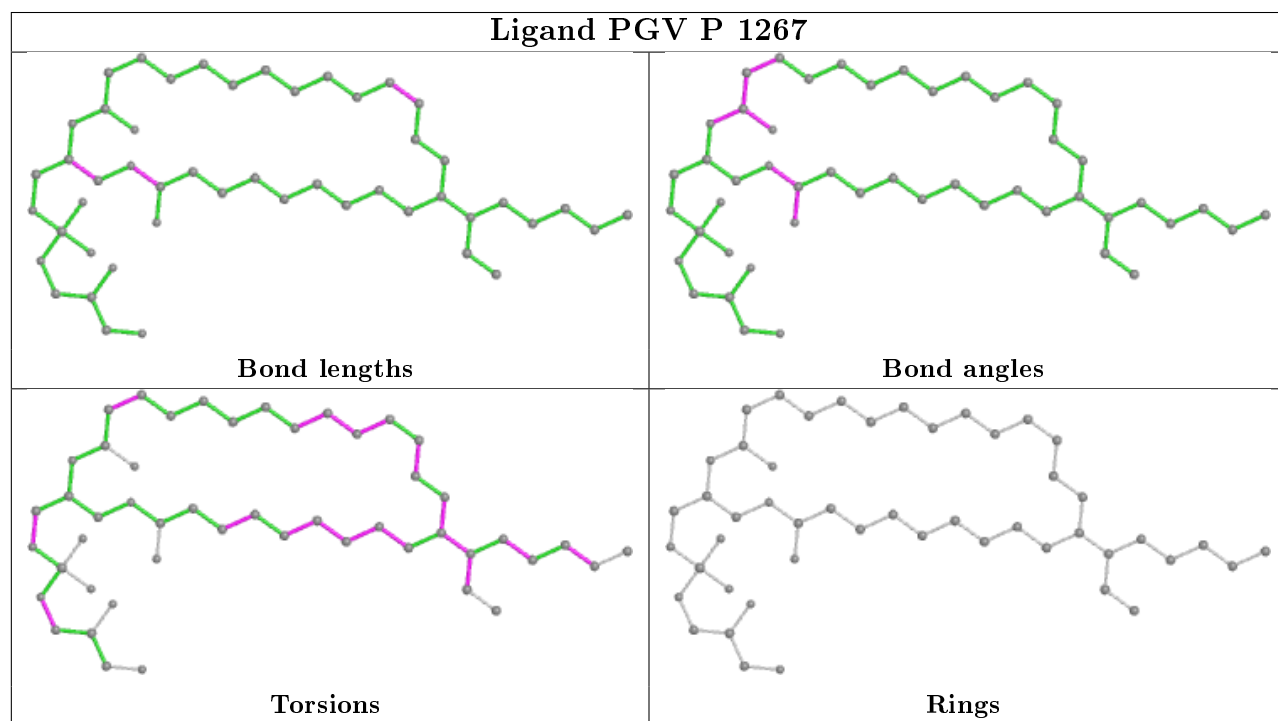
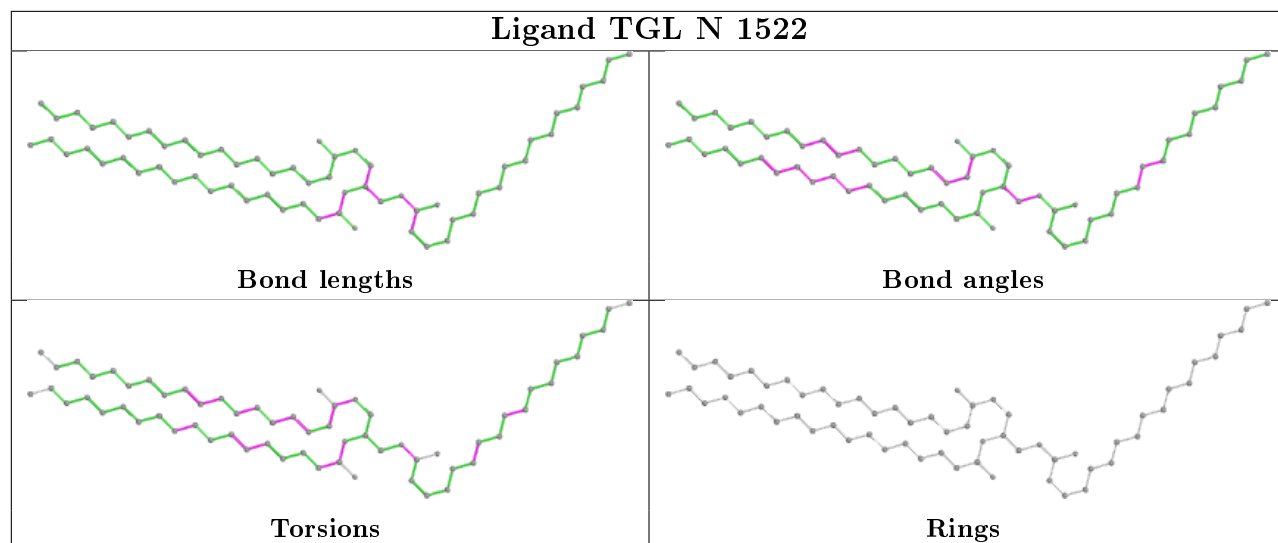


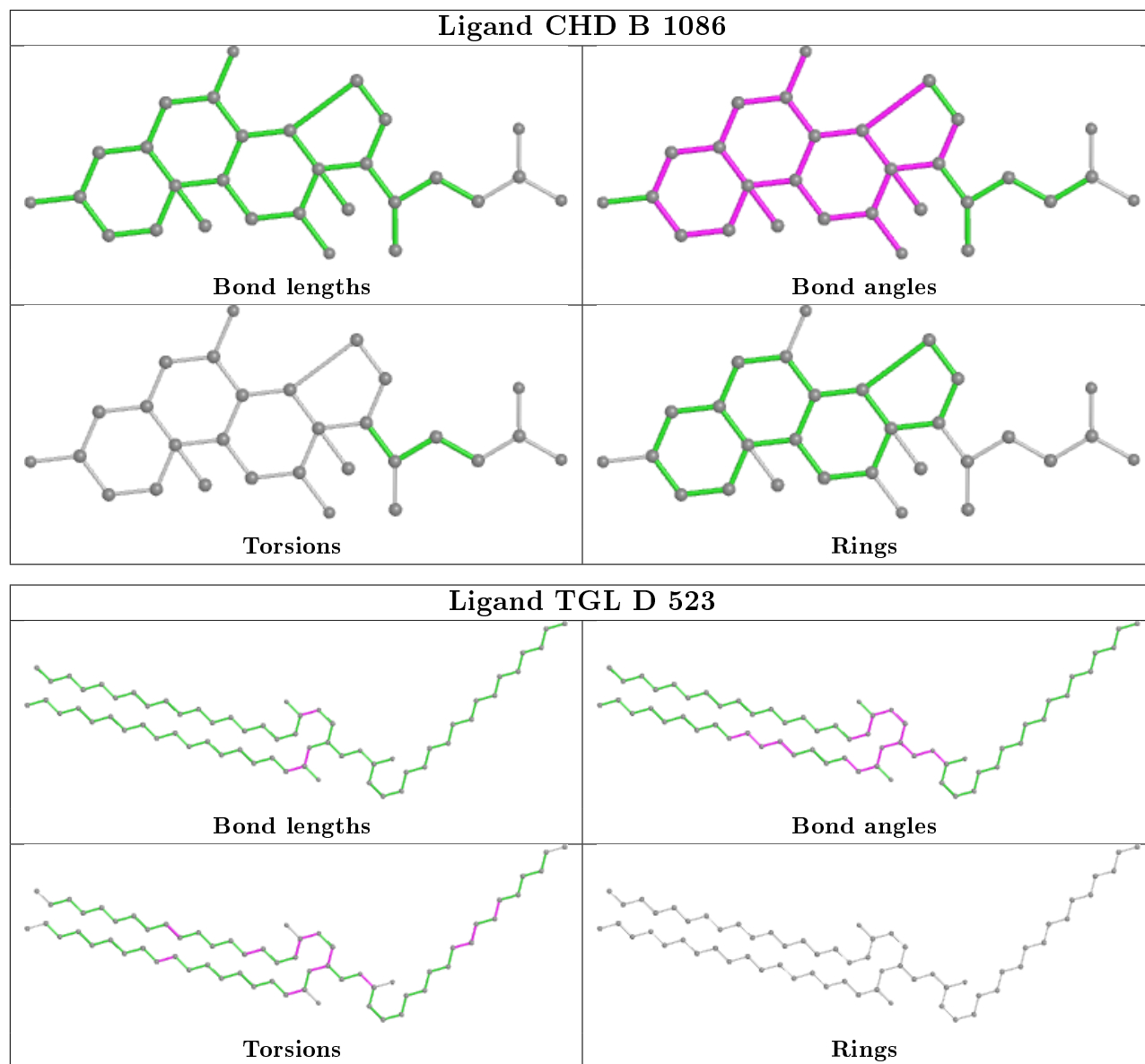
Ligand DMU C 272

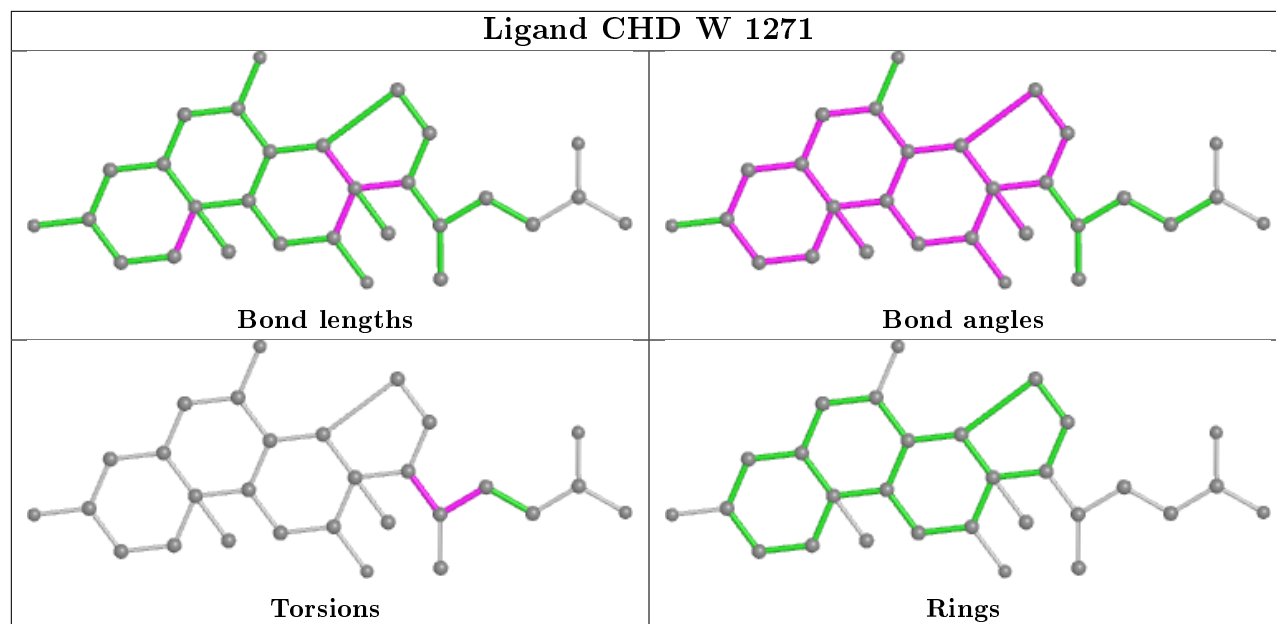


Ligand CHD C 271









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.