



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 08:16 am BST

PDB ID : 2EIK  
Title : Cadmium ion binding structure of bovine heart cytochrome C oxidase in the fully reduced state  
Authors : Muramoto, K.; Hirata, K.; Shinzawa-Itoh, K.; Yoko-O, S.; Yamashita, E.; Aoyama, H.; Tsukihara, T.; Yoshikawa, S.  
Deposited on : 2007-03-13  
Resolution : 2.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

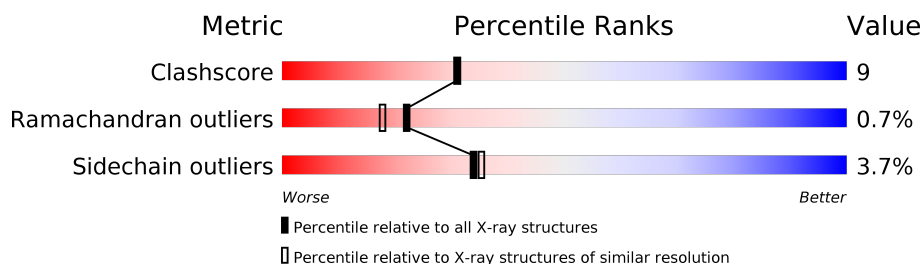
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)





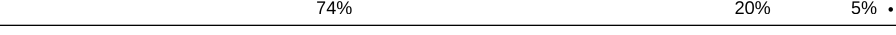
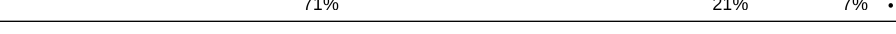
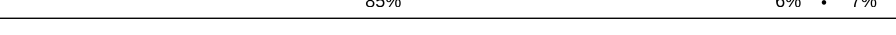
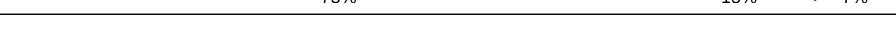










The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	-	-	-
19	TGL	L	522	-	-	X	-
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
23	CHD	P	1271	X	-	-	-
23	CHD	W	1060	X	-	-	-
24	DMU	C	272	X	-	-	-
24	DMU	M	526	X	-	-	-
24	DMU	P	1272	X	-	-	-
24	DMU	Z	1526	X	-	-	-
26	CDL	G	269	-	-	X	-
9	SAC	V	1	-	X	-	-

## 2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 32450 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

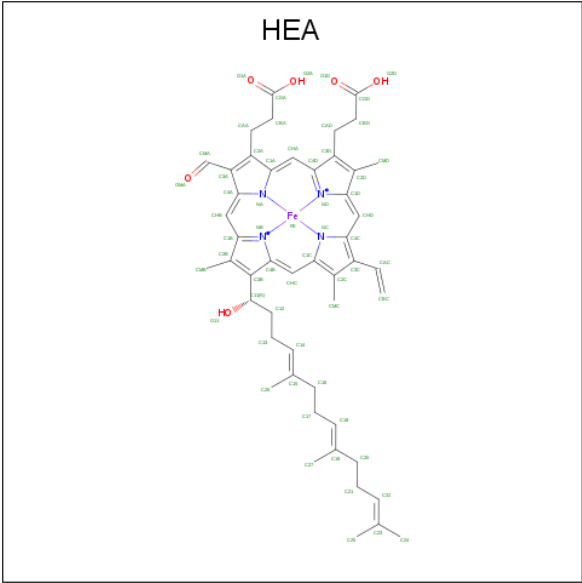
- Molecule 16 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 17 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

- Molecule 18 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



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

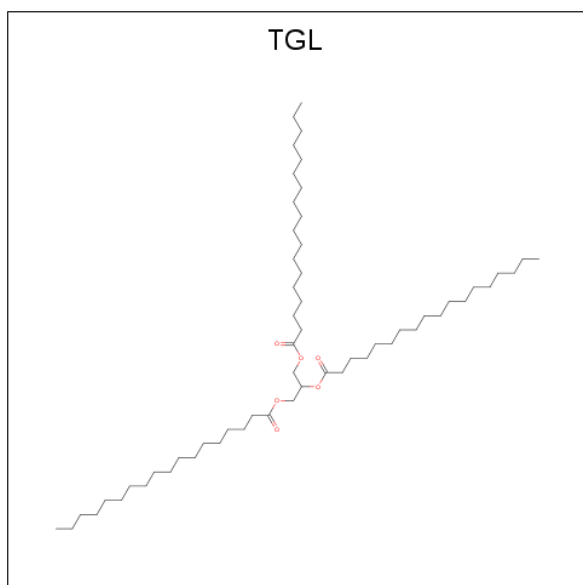
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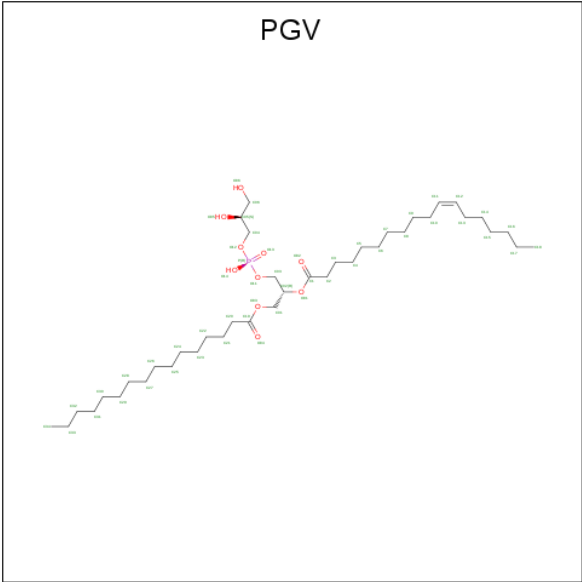
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
18	N	1	Total	C	Fe	N	O	
			60	49	1	4	6	
18	N	1	Total	C	Fe	N	O	
			60	49	1	4	6	

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



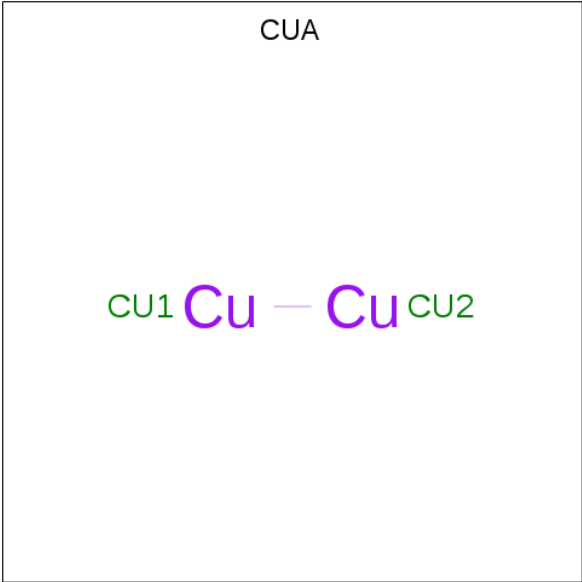
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
19	A	1	Total	C	O		
			63	57	6		
19	A	1	Total	C	O		
			63	57	6		
19	L	1	Total	C	O		
			63	57	6		
19	N	1	Total	C	O		
			63	57	6		
19	Q	1	Total	C	O		
			63	57	6		
19	Y	1	Total	C	O		
			63	57	6		

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



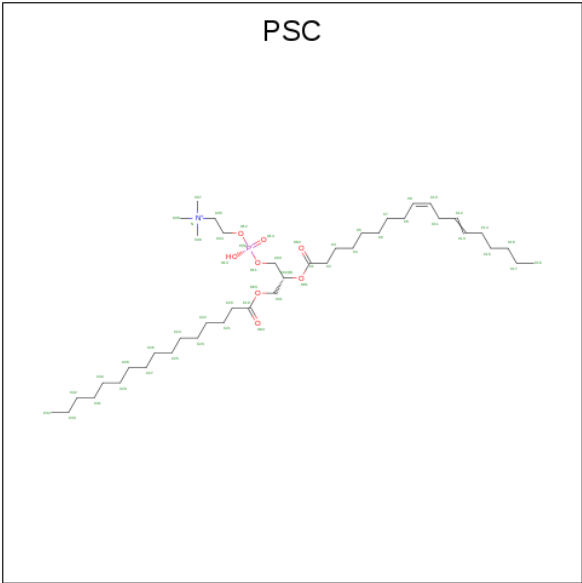
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0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

- Molecule 21 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



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

- Molecule 22 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).



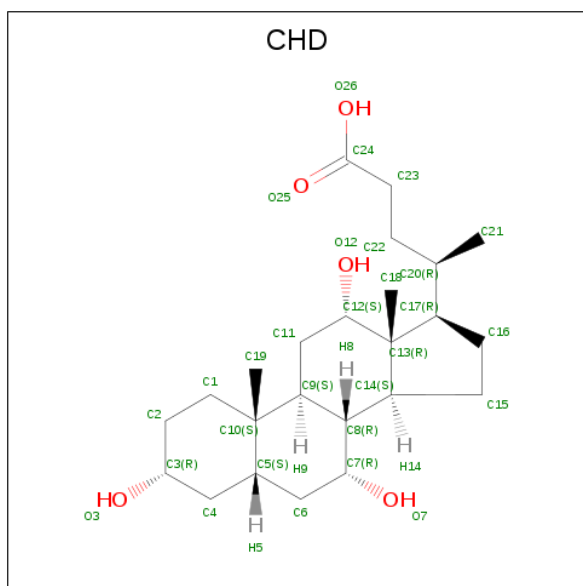
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	B	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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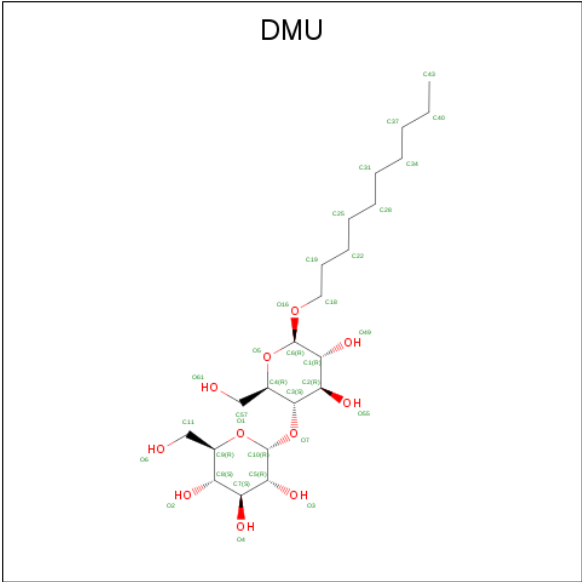
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
22	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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



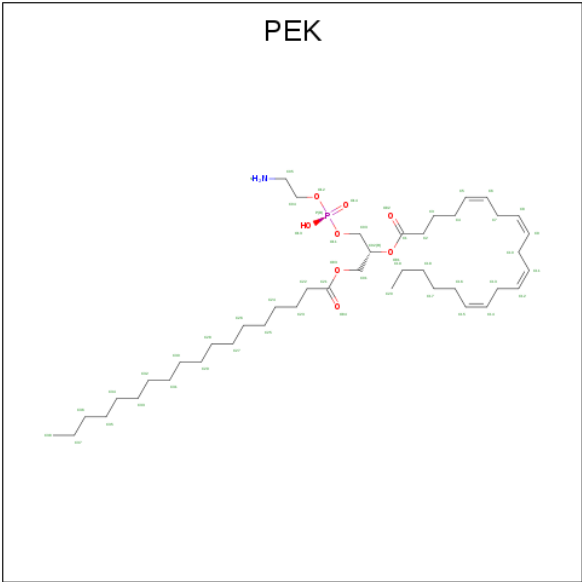
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	B	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		
23	C	1	Total	C	O	0	0
			29	24	5		
23	J	1	Total	C	O	0	0
			29	24	5		
23	O	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	W	1	Total	C	O	0	0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

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



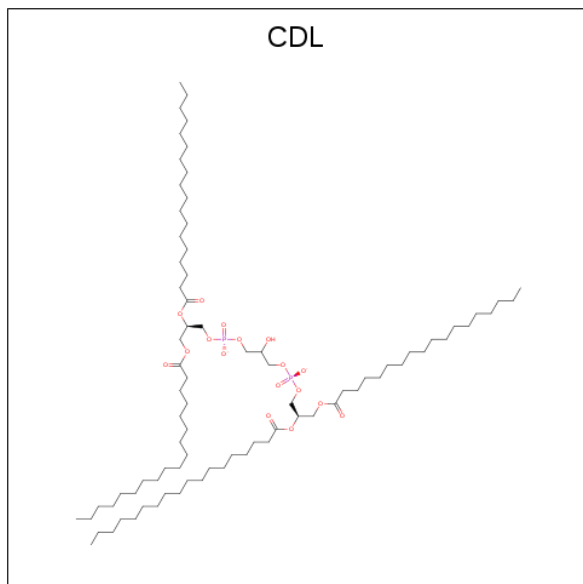
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			33	22	11		
24	M	1	Total	C	O	0	0
			33	22	11		
24	P	1	Total	C	O	0	0
			33	22	11		
24	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 25 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).



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

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



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

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

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

- Molecule 28 is water.

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

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

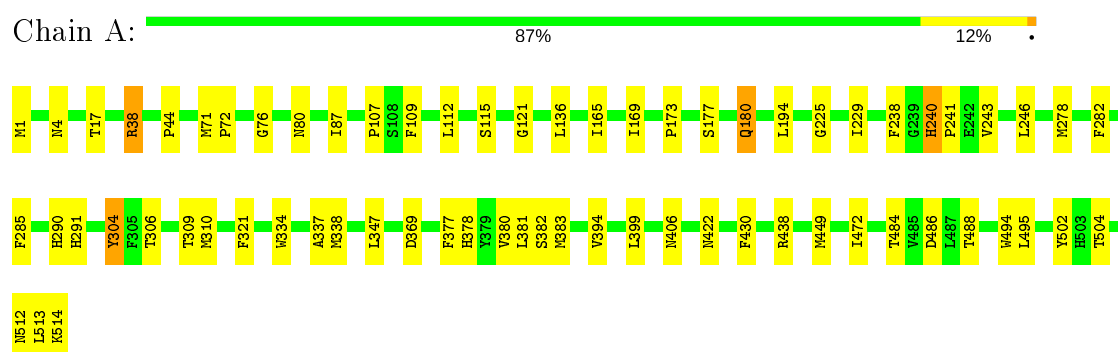


### 3 Residue-property plots

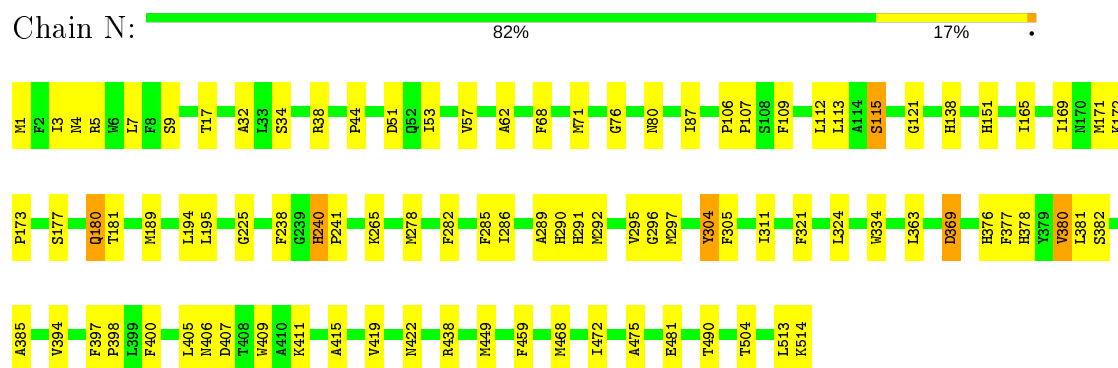
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

Note EDS was not executed.

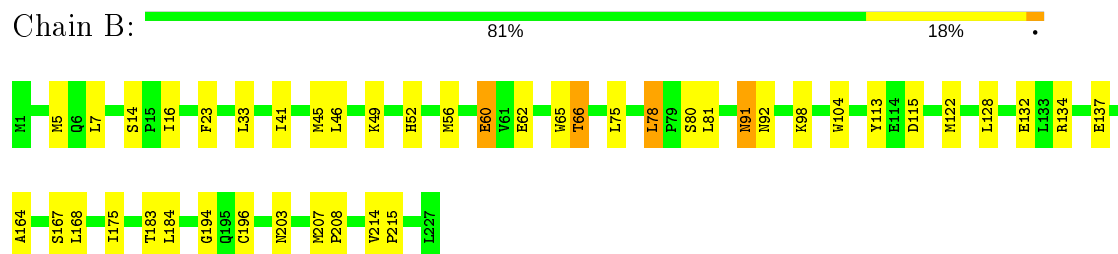
#### • Molecule 1: Cytochrome c oxidase subunit 1



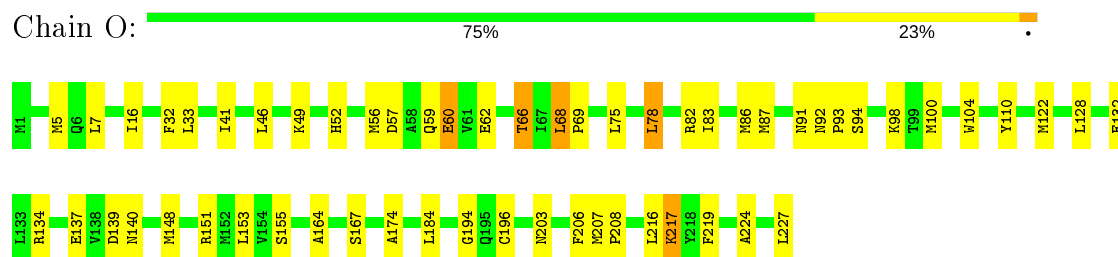
#### • Molecule 1: Cytochrome c oxidase subunit 1



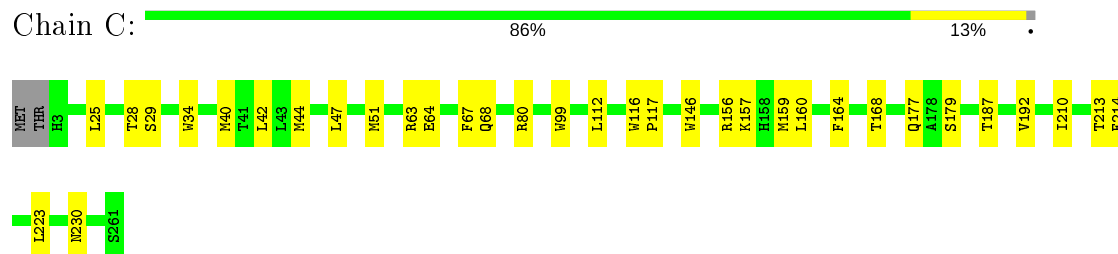
#### • Molecule 2: Cytochrome c oxidase subunit 2



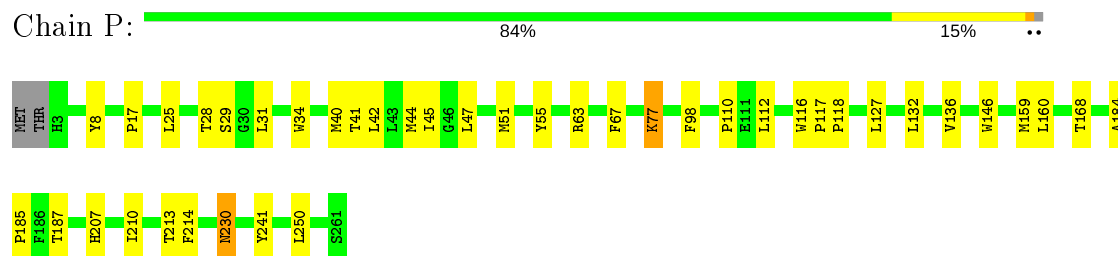
#### • Molecule 2: Cytochrome c oxidase subunit 2



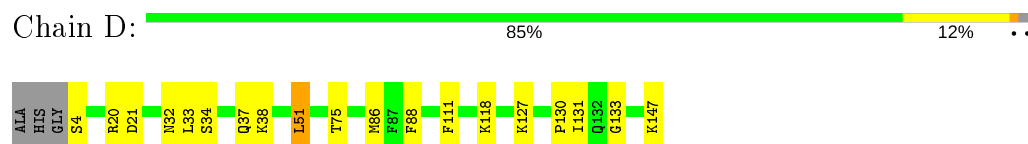
- Molecule 3: Cytochrome c oxidase subunit 3



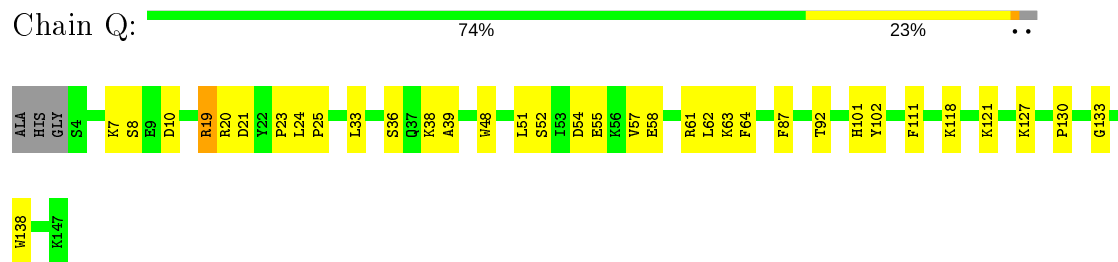
- Molecule 3: Cytochrome c oxidase subunit 3



- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1



- Molecule 5: Cytochrome c oxidase polypeptide Va





- Molecule 5: Cytochrome c oxidase polypeptide Va

Chain R: 68% 28% • •



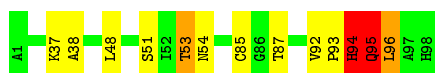
- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F: 83% 15% •



- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S: 87% 9% • •



- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G: 74% 20% 5% •



- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T: 71% 21% 7% •



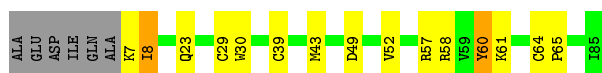
- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

Chain H: 85% 6% 7% • •

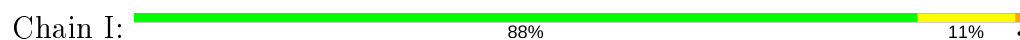


- Molecule 8: Cytochrome c oxidase subunit VIb isoform 1

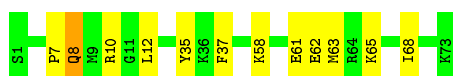
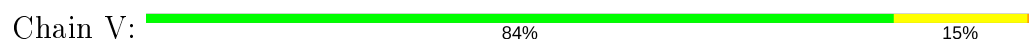
Chain U: 75% 15% 7% • •



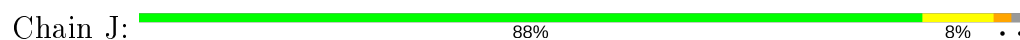
- Molecule 9: Cytochrome c oxidase polypeptide VIc



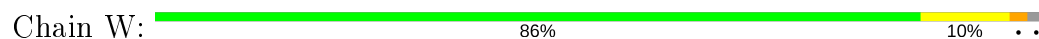
- Molecule 9: Cytochrome c oxidase polypeptide VIc



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



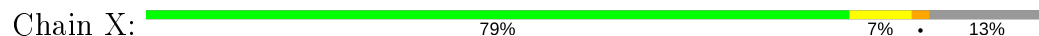
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

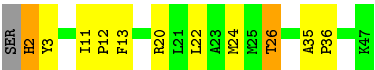


- Molecule 11: Cytochrome c oxidase polypeptide VIIb

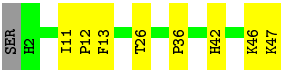
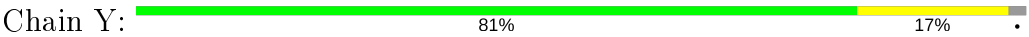


- Molecule 12: Cytochrome c oxidase polypeptide VIIc

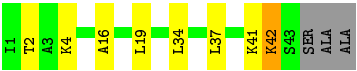




- Molecule 12: Cytochrome c oxidase polypeptide VIIc



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



- Molecule 13: Cytochrome c oxidase polypeptide VIII-heart



## 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, $\alpha$ , $\beta$ , $\gamma$	183.32Å 206.53Å 178.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.199 , 0.228	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32450	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.52	0/4156	0.68	1/5678 (0.0%)
1	N	0.52	0/4156	0.67	0/5678
2	B	0.52	0/1860	0.77	0/2534
2	O	0.53	0/1860	0.78	1/2534 (0.0%)
3	C	0.52	0/2197	0.61	0/3005
3	P	0.50	0/2197	0.62	0/3005
4	D	0.52	0/1229	0.68	2/1658 (0.1%)
4	Q	0.56	0/1229	0.67	1/1658 (0.1%)
5	E	0.52	0/871	0.68	0/1182
5	R	0.56	1/871 (0.1%)	0.73	0/1182
6	F	0.49	0/765	0.81	2/1038 (0.2%)
6	S	0.50	0/765	0.80	2/1038 (0.2%)
7	G	0.53	0/690	0.70	0/937
7	T	0.55	0/690	0.71	1/937 (0.1%)
8	H	0.49	0/682	0.68	0/921
8	U	0.47	0/682	0.65	0/921
9	I	0.53	0/605	0.64	0/802
9	V	0.51	0/605	0.63	0/802
10	J	0.49	0/471	0.64	0/636
10	W	0.50	0/471	0.66	0/636
11	K	0.57	0/398	0.69	0/546
11	X	0.53	0/398	0.68	0/546
12	L	0.54	0/393	0.60	0/526
12	Y	0.57	0/393	0.63	0/526
13	M	0.48	0/345	0.63	0/470
13	Z	0.50	0/345	0.64	0/470
All	All	0.52	1/29324 (0.0%)	0.69	10/39866 (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	2
1	N	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	R	80	GLU	CD-OE2	5.15	1.31	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	94	HIS	N-CA-C	6.57	128.74	111.00
6	F	94	HIS	N-CA-C	6.02	127.25	111.00
4	D	133	GLY	N-CA-C	5.85	127.72	113.10
4	Q	133	GLY	N-CA-C	5.48	126.80	113.10
6	F	93	PRO	N-CA-C	5.47	126.33	112.10
2	O	184	LEU	CA-CB-CG	5.35	127.61	115.30
7	T	33	LEU	CA-CB-CG	5.35	127.60	115.30
4	D	51	LEU	CA-CB-CG	5.26	127.40	115.30
1	A	438	ARG	CB-CA-C	-5.15	100.10	110.40
6	S	93	PRO	N-CA-C	5.10	125.36	112.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
1	A	304	TYR	Sidechain
1	N	240	HIS	Sidechain
1	N	304	TYR	Sidechain

## 5.2 Too-close contacts

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	59	0
1	N	4027	0	4001	76	0
2	B	1824	0	1833	31	0
2	O	1824	0	1833	40	0
3	C	2110	0	2027	30	0
3	P	2110	0	2027	42	0
4	D	1195	0	1183	16	0
4	Q	1195	0	1183	20	0
5	E	852	0	845	4	0
5	R	852	0	845	20	0
6	F	748	0	728	9	0
6	S	748	0	728	9	0
7	G	675	0	644	25	0
7	T	675	0	644	25	0
8	H	662	0	623	5	0
8	U	662	0	623	9	0
9	I	601	0	613	8	0
9	V	601	0	613	12	0
10	J	460	0	459	6	0
10	W	460	0	459	6	0
11	K	384	0	366	5	0
11	X	384	0	366	4	0
12	L	380	0	380	17	0
12	Y	380	0	380	8	0
13	M	335	0	352	8	0
13	Z	335	0	352	5	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	E	1	0	0	0	0
17	N	1	0	0	0	0
17	P	2	0	0	0	0
18	A	120	0	108	5	0
18	N	120	0	108	4	0
19	A	126	0	220	16	0
19	L	63	0	110	23	0
19	N	63	0	110	8	0
19	Q	63	0	110	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Y	63	0	110	17	0
20	A	102	0	152	9	0
20	C	102	0	152	7	0
20	N	102	0	152	10	0
20	P	102	0	152	6	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	14	0
22	O	52	0	80	15	0
23	B	29	0	39	1	0
23	C	58	0	78	7	0
23	J	29	0	39	3	0
23	O	29	0	39	1	0
23	P	58	0	78	1	0
23	W	29	0	39	5	0
24	C	33	0	36	2	0
24	M	33	0	38	0	0
24	P	33	0	36	8	0
24	Z	33	0	38	0	0
25	C	106	0	154	11	0
25	G	53	0	77	9	0
25	P	106	0	154	12	0
25	T	53	0	77	9	0
26	C	100	0	156	16	0
26	G	100	0	156	22	0
26	P	100	0	156	18	0
26	T	100	0	156	19	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	A	223	0	0	2	0
28	B	146	0	0	4	0
28	C	102	0	0	2	0
28	D	98	0	0	4	0
28	E	60	0	0	1	0
28	F	85	0	0	1	0
28	G	41	0	0	1	0
28	H	49	0	0	2	0
28	I	44	0	0	3	0
28	J	26	0	0	2	0
28	K	25	0	0	1	0
28	L	23	0	0	0	0
28	M	22	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	N	213	0	0	3	0
28	O	116	0	0	1	0
28	P	103	0	0	2	0
28	Q	52	0	0	1	0
28	R	41	0	0	0	0
28	S	69	0	0	3	0
28	T	47	0	0	4	0
28	U	43	0	0	1	0
28	V	25	0	0	1	0
28	W	15	0	0	2	0
28	X	17	0	0	0	0
28	Y	15	0	0	1	0
28	Z	14	0	0	1	0
All	All	32450	0	31298	566	0

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

All (566) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:33:ARG:HG2	23:W:1060:CHD:H152	1.31	1.11
22:O:1230:PSC:H142	22:O:1230:PSC:H343	1.39	1.02
7:T:5:LYS:HB2	25:T:263:PEK:H362	1.42	1.00
10:J:33:ARG:HG2	23:J:60:CHD:H152	1.40	0.99
22:B:230:PSC:H343	22:B:230:PSC:H142	1.40	0.99
7:G:84:LYS:HD2	7:G:84:LYS:H	1.24	0.99
7:T:84:LYS:H	7:T:84:LYS:HD2	1.25	0.96
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.30	0.95
4:D:34:SER:H	4:D:37:GLN:HE21	1.14	0.94
3:P:63:ARG:HE	26:P:1270:CDL:HA22	1.33	0.91
25:C:264:PEK:H102	25:C:264:PEK:H161	1.52	0.91
26:G:269:CDL:H541	26:G:269:CDL:H231	1.52	0.90
6:S:94:HIS:CD2	6:S:95:GLN:H	1.89	0.89
26:T:1269:CDL:H541	26:T:1269:CDL:H231	1.55	0.89
7:G:5:LYS:HB2	25:G:1263:PEK:H362	1.56	0.88
26:P:1270:CDL:H642	26:P:1270:CDL:H191	1.55	0.88
2:O:41:ILE:HD13	22:O:1230:PSC:H342	1.54	0.88
12:L:20:ARG:HH22	19:L:522:TGL:HC61	1.39	0.87
26:C:270:CDL:H642	26:C:270:CDL:H191	1.56	0.86
25:P:1264:PEK:H102	25:P:1264:PEK:H161	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:31:CYS:SG	26:G:269:CDL:H532	2.16	0.86
19:A:521:TGL:H281	19:A:521:TGL:H102	1.57	0.86
28:C:4303:HOH:O	6:F:1:ALA:HB2	1.74	0.86
7:T:31:CYS:SG	26:T:1269:CDL:H532	2.15	0.86
19:N:1521:TGL:H102	19:N:1521:TGL:H281	1.58	0.84
1:A:278:MET:SD	7:T:5:LYS:HB3	2.18	0.83
7:T:5:LYS:HG3	25:T:263:PEK:H383	1.61	0.82
19:Y:1522:TGL:HC22	19:Y:1522:TGL:HC62	1.62	0.82
19:L:522:TGL:HC62	19:L:522:TGL:HC22	1.61	0.82
19:N:1521:TGL:H102	19:N:1521:TGL:C28	2.11	0.81
12:L:24:MET:SD	19:L:522:TGL:H162	2.22	0.80
3:C:67:PHE:HE1	26:C:270:CDL:H1	1.46	0.80
3:P:67:PHE:HE1	26:P:1270:CDL:H1	1.47	0.80
19:A:521:TGL:H102	19:A:521:TGL:C28	2.12	0.80
4:D:147:LYS:HG2	28:D:4622:HOH:O	1.81	0.79
1:N:514:LYS:HE2	28:S:3395:HOH:O	1.82	0.79
7:G:5:LYS:HB3	1:N:278:MET:SD	2.24	0.78
1:N:1:FME:HCN	1:N:4:ASN:H	1.49	0.78
13:M:42:LYS:HA	13:M:42:LYS:HE3	1.65	0.78
1:A:472:ILE:HG21	19:L:522:TGL:HA92	1.65	0.77
26:G:269:CDL:H622	20:P:1268:PGV:H152	1.65	0.77
1:N:472:ILE:HG21	19:Y:1522:TGL:HA92	1.65	0.76
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.69	0.75
7:T:5:LYS:HD2	25:T:263:PEK:H371	1.67	0.75
19:A:521:TGL:H201	19:A:521:TGL:H241	1.70	0.74
26:G:269:CDL:H522	26:G:269:CDL:H202	1.69	0.74
7:G:5:LYS:HG3	25:G:1263:PEK:H383	1.67	0.74
19:N:1521:TGL:H201	19:N:1521:TGL:H241	1.69	0.73
19:Y:1522:TGL:HC41	28:Y:4411:HOH:O	1.88	0.73
6:F:8:THR:OG1	6:F:11:GLU:HG3	1.88	0.72
26:T:1269:CDL:H522	26:T:1269:CDL:H202	1.72	0.72
12:Y:13:PHE:HA	19:Y:1522:TGL:HC31	1.70	0.72
3:C:160:LEU:HD13	23:C:271:CHD:H181	1.69	0.72
5:R:89:LEU:O	5:R:93:LEU:HG	1.90	0.72
7:G:84:LYS:H	7:G:84:LYS:CD	1.97	0.72
22:O:1230:PSC:H071	9:V:10:ARG:HE	1.54	0.72
3:P:160:LEU:HD13	23:P:1271:CHD:H181	1.71	0.71
12:L:13:PHE:HA	19:L:522:TGL:HC31	1.72	0.71
6:S:94:HIS:CG	6:S:95:GLN:H	2.09	0.70
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.74	0.70
12:L:20:ARG:NH2	19:L:522:TGL:HC61	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:3:ALA:HB1	25:T:263:PEK:H382	1.73	0.70
28:B:4845:HOH:O	4:D:21:ASP:HB2	1.91	0.69
26:G:269:CDL:C23	26:G:269:CDL:H541	2.23	0.69
1:N:334:TRP:CZ3	19:Q:1523:TGL:HA51	2.28	0.69
6:F:85:CYS:SG	6:F:87:THR:HG23	2.33	0.69
6:F:92:VAL:O	6:F:92:VAL:HG23	1.94	0.68
19:Y:1522:TGL:H242	19:Y:1522:TGL:H202	1.76	0.68
19:L:522:TGL:H242	19:L:522:TGL:H202	1.76	0.67
3:P:34:TRP:CZ2	24:P:1272:DMU:H29	2.29	0.67
5:R:81:ILE:HG12	9:V:7:PRO:HG2	1.77	0.67
26:P:1270:CDL:H391	28:P:4551:HOH:O	1.95	0.67
26:T:1269:CDL:H172	26:T:1269:CDL:H511	1.77	0.67
7:T:38:HIS:NE2	26:T:1269:CDL:H111	2.10	0.66
20:C:267:PGV:H172	26:C:270:CDL:H662	1.76	0.66
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.78	0.65
1:N:296:GLY:HA2	8:U:23:GLN:OE1	1.96	0.65
26:T:1269:CDL:H541	26:T:1269:CDL:C23	2.26	0.65
20:C:268:PGV:H152	26:T:1269:CDL:H622	1.79	0.65
26:G:269:CDL:HB32	1:N:304:TYR:HD1	1.60	0.65
8:H:8:ILE:HG21	28:H:4749:HOH:O	1.97	0.65
3:P:168:THR:HG22	25:P:1265:PEK:H14	1.79	0.64
11:K:24:PHE:O	11:K:28:VAL:HG12	1.96	0.64
6:S:94:HIS:CD2	6:S:95:GLN:N	2.64	0.64
26:G:269:CDL:H172	26:G:269:CDL:H511	1.78	0.64
3:C:168:THR:HG22	25:C:265:PEK:H14	1.80	0.64
3:C:40:MET:O	3:C:44:MET:HG2	1.98	0.64
1:N:53:ILE:O	1:N:57:VAL:HG23	1.98	0.64
3:P:168:THR:CG2	25:P:1265:PEK:H14	2.27	0.64
1:A:177:SER:H	1:A:180:GLN:HE21	1.46	0.63
12:L:20:ARG:HH22	19:L:522:TGL:CC6	2.10	0.63
20:N:1524:PGV:H152	20:N:1524:PGV:H321	1.79	0.63
19:N:1521:TGL:H161	2:O:7:LEU:HD11	1.81	0.63
2:B:56:MET:HG2	22:B:230:PSC:H211	1.80	0.63
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.63	0.63
22:B:230:PSC:C07	9:I:10:ARG:HH21	2.12	0.63
10:J:7:GLU:HG3	28:J:4635:HOH:O	1.98	0.63
1:N:378:HIS:O	1:N:382:SER:HB2	1.99	0.62
3:P:210:ILE:HG23	20:P:1267:PGV:H102	1.80	0.62
1:A:321:PHE:CD2	22:B:230:PSC:H341	2.34	0.62
12:L:20:ARG:HH12	19:L:522:TGL:HC61	1.65	0.62
3:C:168:THR:CG2	25:C:265:PEK:H14	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.82	0.62
22:O:1230:PSC:H222	22:O:1230:PSC:H21	1.80	0.62
1:N:76:GLY:O	1:N:80:ASN:HB2	1.98	0.62
19:Q:1523:TGL:HG11	19:Q:1523:TGL:HC21	1.80	0.62
20:A:524:PGV:H152	20:A:524:PGV:H321	1.82	0.62
1:N:151:HIS:CD2	25:P:1264:PEK:H382	2.34	0.62
4:D:34:SER:H	4:D:37:GLN:NE2	1.93	0.61
20:P:1267:PGV:H12	20:P:1267:PGV:H161	1.82	0.61
6:S:53:THR:HG22	28:S:4719:HOH:O	1.99	0.61
19:A:523:TGL:HG11	19:A:523:TGL:HC21	1.83	0.61
6:F:64:GLU:O	6:F:65:ASP:HB2	2.00	0.61
1:N:169:ILE:HD11	1:N:189:MET:SD	2.40	0.61
20:C:267:PGV:H12	20:C:267:PGV:H161	1.81	0.61
1:N:472:ILE:HG21	19:Y:1522:TGL:CA9	2.31	0.60
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.83	0.60
22:B:230:PSC:H21	22:B:230:PSC:H222	1.83	0.60
3:C:34:TRP:CZ2	24:C:272:DMU:H29	2.36	0.60
1:N:321:PHE:CD2	22:O:1230:PSC:H341	2.36	0.60
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.83	0.60
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.37	0.60
20:P:1268:PGV:H062	28:U:4194:HOH:O	2.01	0.60
3:P:40:MET:O	3:P:44:MET:HG2	2.01	0.60
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.83	0.60
2:B:91:ASN:HD21	2:B:183:THR:HG21	1.65	0.59
20:A:604:PGV:H182	3:C:28:THR:HG22	1.85	0.59
7:G:3:ALA:HB1	25:G:1263:PEK:H382	1.85	0.59
1:A:484:THR:HB	13:M:2:THR:OG1	2.03	0.59
2:B:41:ILE:HD13	22:B:230:PSC:H342	1.84	0.59
3:C:210:ILE:HG23	20:C:267:PGV:H102	1.83	0.59
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.68	0.59
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.68	0.59
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.33	0.59
18:N:515:HEA:HMC1	18:N:515:HEA:HBC1	1.85	0.59
1:A:177:SER:H	1:A:180:GLN:NE2	2.01	0.58
5:R:78:HIS:CD2	9:V:12:LEU:HD13	2.38	0.58
5:R:48:ILE:O	5:R:52:LEU:HG	2.03	0.58
19:A:521:TGL:HA82	19:A:521:TGL:H222	1.85	0.58
7:G:2:SER:O	25:G:1263:PEK:H322	2.03	0.58
3:P:51:MET:HB3	26:P:1270:CDL:H622	1.85	0.58
22:O:1230:PSC:C07	9:V:10:ARG:HE	2.17	0.58
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:PHE:CD1	18:A:516:HEA:HAD1	2.39	0.58
1:N:51:ASP:OD1	2:O:206:PHE:HE1	1.86	0.57
2:B:62:GLU:O	2:B:66:THR:HB	2.04	0.57
1:A:282:PHE:HA	7:T:4:ALA:CB	2.34	0.57
1:N:449:MET:SD	2:O:5:MET:HG2	2.44	0.57
1:N:481:GLU:HB2	13:Z:4:LYS:HE2	1.85	0.57
26:P:1270:CDL:H642	26:P:1270:CDL:C19	2.31	0.57
19:A:521:TGL:HC22	28:I:2383:HOH:O	2.04	0.57
6:F:90:LYS:HD2	28:F:4237:HOH:O	2.05	0.57
2:B:49:LYS:HE2	28:E:4310:HOH:O	2.03	0.57
4:D:34:SER:O	4:D:38:LYS:HG3	2.05	0.57
25:C:265:PEK:H231	7:G:21:PHE:CD2	2.40	0.57
1:N:71:MET:HE1	1:N:195:LEU:HD21	1.87	0.57
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.87	0.57
1:A:282:PHE:HZ	26:T:1269:CDL:H761	1.70	0.57
28:B:4901:HOH:O	25:P:1265:PEK:H031	2.04	0.56
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.87	0.56
2:O:224:ALA:O	2:O:227:LEU:HG	2.05	0.56
24:P:1272:DMU:H25	25:P:1264:PEK:H341	1.87	0.56
20:P:1267:PGV:H172	26:P:1270:CDL:H662	1.88	0.56
12:Y:12:PRO:HB2	19:Y:1522:TGL:HG2	1.87	0.56
22:B:230:PSC:H072	9:I:10:ARG:HH21	1.69	0.56
26:C:270:CDL:C19	26:C:270:CDL:H642	2.31	0.56
1:N:44:PRO:HG2	4:Q:111:PHE:CZ	2.40	0.56
19:N:1521:TGL:H222	19:N:1521:TGL:HA82	1.87	0.56
5:E:84:TYR:O	5:E:88:GLU:HG2	2.06	0.55
11:X:24:PHE:O	11:X:28:VAL:HG12	2.06	0.55
20:N:1524:PGV:H311	13:Z:16:ALA:HA	1.89	0.55
18:A:515:HEA:HMC1	18:A:515:HEA:HBC1	1.88	0.55
1:N:171:MET:HG2	3:P:8:TYR:CE1	2.42	0.55
1:A:1:FME:HCN	1:A:4:ASN:H	1.71	0.55
1:A:304:TYR:HD1	26:T:1269:CDL:HB32	1.72	0.55
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.89	0.55
10:W:40:LEU:HD12	23:W:1060:CHD:H183	1.87	0.55
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.40	0.55
1:A:378:HIS:O	1:A:382:SER:HB2	2.07	0.54
1:A:17:THR:OG1	19:L:522:TGL:H281	2.07	0.54
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.90	0.54
20:A:524:PGV:H062	28:M:2160:HOH:O	2.08	0.54
22:O:1230:PSC:C34	22:O:1230:PSC:H142	2.27	0.54
2:B:78:LEU:HD12	26:T:1269:CDL:H351	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:524:PGV:H311	13:M:16:ALA:HA	1.89	0.54
3:C:34:TRP:HZ2	24:C:272:DMU:H29	1.71	0.54
8:U:49:ASP:O	8:U:52:VAL:HG22	2.08	0.54
4:Q:33:LEU:HB2	4:Q:38:LYS:HG2	1.89	0.54
4:D:20:ARG:HG3	28:D:4203:HOH:O	2.06	0.53
1:A:240:HIS:O	1:A:243:VAL:HG22	2.08	0.53
3:P:34:TRP:HZ2	24:P:1272:DMU:H29	1.73	0.53
4:D:86:MET:HE3	28:K:4855:HOH:O	2.08	0.53
19:Q:1523:TGL:H363	28:V:4756:HOH:O	2.09	0.53
8:U:7:LYS:O	8:U:8:ILE:HG22	2.08	0.53
1:N:165:ILE:O	1:N:169:ILE:HG12	2.08	0.53
9:V:65:LYS:O	11:X:54:ARG:NH1	2.41	0.53
22:B:230:PSC:C34	22:B:230:PSC:H142	2.28	0.53
2:O:83:ILE:O	2:O:87:MET:HG3	2.09	0.53
7:T:3:ALA:O	7:T:4:ALA:HB2	2.09	0.53
7:G:84:LYS:N	7:G:84:LYS:HD2	2.09	0.53
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.91	0.53
7:G:3:ALA:O	7:G:4:ALA:HB2	2.09	0.53
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.44	0.53
3:P:67:PHE:CE1	26:P:1270:CDL:H1	2.35	0.52
3:C:156:ARG:HE	23:C:271:CHD:H232	1.74	0.52
25:P:1264:PEK:H102	25:P:1264:PEK:C16	2.34	0.52
7:T:2:SER:O	25:T:263:PEK:H322	2.09	0.52
1:A:472:ILE:HG21	19:L:522:TGL:CA9	2.35	0.52
1:A:406:ASN:HD21	20:A:524:PGV:C2	2.23	0.52
1:A:502:TYR:CD1	12:L:2:HIS:HD2	2.28	0.52
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.90	0.52
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.44	0.52
2:O:56:MET:HA	22:O:1230:PSC:H202	1.91	0.52
10:W:2:GLU:HA	28:W:4707:HOH:O	2.08	0.52
12:L:20:ARG:NH1	19:L:522:TGL:HC61	2.24	0.52
19:A:521:TGL:H161	2:B:7:LEU:HD11	1.92	0.52
1:A:1:FME:HE2	1:A:1:FME:HA	1.93	0.51
1:A:377:PHE:O	1:A:381:LEU:HB3	2.10	0.51
3:C:63:ARG:NE	26:C:270:CDL:HA22	2.13	0.51
7:T:84:LYS:H	7:T:84:LYS:CD	2.05	0.51
22:B:230:PSC:H12	22:B:230:PSC:H322	1.93	0.51
1:N:112:LEU:HG	28:N:3073:HOH:O	2.11	0.51
25:C:265:PEK:C38	26:G:269:CDL:H273	2.41	0.51
7:G:5:LYS:HD2	25:G:1263:PEK:H371	1.93	0.51
2:B:23:PHE:CZ	2:B:80:SER:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:422:ASN:HB3	19:N:1521:TGL:H242	1.93	0.51
1:A:472:ILE:HD13	19:L:522:TGL:HA91	1.93	0.51
20:C:267:PGV:H182	26:C:270:CDL:H673	1.92	0.51
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.93	0.51
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.92	0.51
19:L:522:TGL:HC21	19:L:522:TGL:OA1	2.10	0.51
3:C:80:ARG:NH1	25:T:263:PEK:H032	2.25	0.51
1:N:472:ILE:HD13	19:Y:1522:TGL:HA91	1.93	0.51
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.46	0.50
1:N:406:ASN:HD21	20:N:1524:PGV:C2	2.24	0.50
1:N:87:ILE:O	1:N:173:PRO:HD3	2.11	0.50
22:O:1230:PSC:H322	22:O:1230:PSC:H12	1.94	0.50
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.94	0.50
2:O:82:ARG:HG2	2:O:86:MET:HE3	1.92	0.50
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.47	0.50
4:D:130:PRO:HG2	4:D:131:ILE:HD12	1.94	0.50
1:A:290:HIS:CD2	1:A:291:HIS:CD2	2.99	0.50
5:R:78:HIS:HD2	9:V:12:LEU:HD13	1.76	0.50
4:Q:58:GLU:O	4:Q:62:LEU:HG	2.12	0.50
1:N:369:ASP:C	1:N:438:ARG:HG3	2.33	0.49
19:N:1521:TGL:HC22	28:Q:3383:HOH:O	2.12	0.49
2:B:41:ILE:O	2:B:45:MET:HG2	2.12	0.49
10:W:50:LEU:HD22	10:W:50:LEU:O	2.12	0.49
1:A:334:TRP:CZ3	19:A:523:TGL:HA51	2.47	0.49
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.95	0.49
20:N:1524:PGV:H062	28:Z:3160:HOH:O	2.12	0.49
25:G:1263:PEK:H042	3:P:77:LYS:NZ	2.26	0.49
1:N:177:SER:H	1:N:180:GLN:NE2	2.11	0.49
26:T:1269:CDL:C54	26:T:1269:CDL:H231	2.35	0.49
2:B:91:ASN:ND2	2:B:183:THR:HG21	2.28	0.49
3:P:207:HIS:HD2	3:P:241:TYR:OH	1.95	0.49
3:C:51:MET:HB3	26:C:270:CDL:H622	1.94	0.49
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.94	0.49
7:G:2:SER:OG	25:G:1263:PEK:H301	2.13	0.49
3:C:177:GLN:OE1	3:C:177:GLN:HA	2.13	0.49
12:L:20:ARG:HH22	19:L:522:TGL:HC32	1.78	0.49
1:N:177:SER:H	1:N:180:GLN:HE21	1.60	0.49
2:O:57:ASP:H	22:O:1230:PSC:H201	1.78	0.49
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.77	0.49
3:C:157:LYS:NZ	25:C:265:PEK:H052	2.27	0.48
23:C:271:CHD:H161	28:C:4708:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:N:1266:PGV:H182	3:P:28:THR:HG22	1.95	0.48
1:N:405:LEU:HD23	1:N:475:ALA:HB2	1.93	0.48
7:T:84:LYS:N	7:T:84:LYS:HD2	2.10	0.48
4:D:127:LYS:HD2	28:I:2391:HOH:O	2.14	0.48
1:N:449:MET:SD	2:O:5:MET:CG	3.01	0.48
19:L:522:TGL:H231	19:L:522:TGL:H272	1.96	0.48
2:O:68:LEU:CB	2:O:69:PRO:HD3	2.44	0.48
3:P:250:LEU:HD22	26:T:1269:CDL:C67	2.43	0.48
1:A:76:GLY:O	1:A:80:ASN:HB2	2.13	0.48
5:R:37:VAL:HG11	5:R:70:VAL:HG21	1.95	0.48
4:D:33:LEU:HD22	4:D:37:GLN:HB3	1.94	0.48
3:P:34:TRP:CE2	24:P:1272:DMU:H29	2.49	0.48
26:G:269:CDL:HB32	1:N:304:TYR:CD1	2.45	0.48
5:R:105:GLY:O	5:R:108:LYS:HG2	2.13	0.48
6:S:51:SER:O	6:S:94:HIS:N	2.46	0.48
7:T:45:PRO:HD2	28:T:3152:HOH:O	2.13	0.48
25:P:1265:PEK:C38	26:T:1269:CDL:H273	2.43	0.48
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.14	0.48
26:C:270:CDL:H602	26:C:270:CDL:H632	1.59	0.48
2:O:203:ASN:HD22	2:O:203:ASN:N	2.12	0.48
3:P:34:TRP:NE1	24:P:1272:DMU:H29	2.29	0.48
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.96	0.48
4:Q:57:VAL:O	4:Q:61:ARG:HG2	2.14	0.48
19:Y:1522:TGL:C24	19:Y:1522:TGL:H202	2.43	0.48
1:A:422:ASN:HB3	19:A:521:TGL:H242	1.96	0.48
26:G:269:CDL:H761	1:N:282:PHE:HZ	1.78	0.48
2:O:139:ASP:OD2	2:O:140:ASN:N	2.46	0.48
6:S:85:CYS:SG	6:S:87:THR:HG23	2.54	0.48
26:T:1269:CDL:HA62	26:T:1269:CDL:H322	1.96	0.48
1:N:377:PHE:CD1	18:N:516:HEA:HAD1	2.49	0.48
7:G:17:ARG:HD2	28:G:2309:HOH:O	2.14	0.47
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.78	0.47
20:A:524:PGV:H302	13:M:19:LEU:HD23	1.95	0.47
1:A:87:ILE:O	1:A:173:PRO:HD3	2.14	0.47
19:Y:1522:TGL:H231	19:Y:1522:TGL:H272	1.95	0.47
1:A:44:PRO:HG2	4:D:111:PHE:CZ	2.50	0.47
1:A:321:PHE:CZ	22:B:230:PSC:H171	2.50	0.47
6:F:92:VAL:O	6:F:92:VAL:CG2	2.61	0.47
19:L:522:TGL:C24	19:L:522:TGL:H202	2.41	0.47
23:C:271:CHD:H12A	23:C:271:CHD:H112	1.78	0.47
11:K:42:PRO:HG2	11:K:47:ARG:HE	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:41:ILE:CD1	22:O:1230:PSC:H342	2.35	0.47
19:Y:1522:TGL:H361	19:Y:1522:TGL:HB91	1.96	0.47
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.96	0.47
28:O:4280:HOH:O	8:U:61:LYS:HD2	2.14	0.47
26:G:269:CDL:H351	2:O:78:LEU:HD12	1.96	0.47
4:Q:101:HIS:HD2	4:Q:102:TYR:CD2	2.33	0.47
4:Q:127:LYS:O	4:Q:130:PRO:HD3	2.15	0.47
5:R:8:ASP:HB3	9:V:10:ARG:CZ	2.44	0.47
1:N:68:PHE:HE2	1:N:112:LEU:CD1	2.28	0.47
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.50	0.47
2:B:214:VAL:HB	2:B:215:PRO:CD	2.44	0.47
1:A:225:GLY:HA3	3:C:112:LEU:HD21	1.96	0.47
3:C:156:ARG:HE	23:C:271:CHD:C23	2.28	0.47
3:P:187:THR:HG22	25:P:1264:PEK:H052	1.97	0.47
7:T:2:SER:O	7:T:3:ALA:HB3	2.15	0.47
1:A:306:THR:O	1:A:310:MET:HG3	2.15	0.47
3:C:63:ARG:HE	26:C:270:CDL:CA2	2.15	0.47
2:O:98:LYS:HG2	2:O:153:LEU:HB2	1.97	0.47
12:L:20:ARG:NH2	19:L:522:TGL:HC32	2.30	0.47
1:N:321:PHE:CZ	22:O:1230:PSC:H171	2.50	0.47
7:T:2:SER:OG	25:T:263:PEK:H301	2.14	0.47
3:P:132:LEU:O	3:P:136:VAL:HG23	2.16	0.46
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.97	0.46
22:O:1230:PSC:C07	9:V:10:ARG:HH21	2.28	0.46
7:T:33:LEU:HD12	28:T:4821:HOH:O	2.14	0.46
2:B:164:ALA:O	2:B:194:GLY:HA3	2.14	0.46
26:G:269:CDL:C54	26:G:269:CDL:H231	2.32	0.46
8:H:27:ARG:NH1	28:H:2303:HOH:O	2.47	0.46
1:N:34:SER:HB2	18:N:515:HEA:C2B	2.46	0.46
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.15	0.46
1:N:115:SER:O	1:N:121:GLY:HA2	2.16	0.46
19:N:1521:TGL:HB91	2:O:32:PHE:HE2	1.79	0.46
5:R:7:THR:HB	5:R:9:GLU:OE2	2.16	0.46
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.97	0.46
3:P:34:TRP:HE1	24:P:1272:DMU:H29	1.80	0.46
6:S:92:VAL:HG23	6:S:92:VAL:O	2.16	0.46
19:A:521:TGL:HC92	28:B:4798:HOH:O	2.14	0.46
12:L:12:PRO:HB2	19:L:522:TGL:HG2	1.97	0.46
4:D:34:SER:N	4:D:37:GLN:HE21	1.96	0.46
7:G:37:LEU:HD21	26:G:269:CDL:H361	1.97	0.46
4:Q:101:HIS:HD2	4:Q:102:TYR:CE2	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.51	0.46
2:O:164:ALA:O	2:O:194:GLY:HA3	2.15	0.46
2:O:62:GLU:O	2:O:66:THR:HB	2.16	0.46
26:P:1270:CDL:H672	26:P:1270:CDL:H641	1.84	0.46
2:O:155:SER:O	2:O:174:ALA:HB1	2.15	0.46
3:P:47:LEU:O	3:P:51:MET:HG2	2.16	0.46
4:Q:63:LYS:HG2	4:Q:64:PHE:CE1	2.51	0.46
20:N:1524:PGV:H12	4:Q:87:PHE:CD2	2.51	0.46
1:A:406:ASN:HD21	20:A:524:PGV:H22	1.81	0.45
1:N:415:ALA:O	1:N:419:VAL:HG23	2.16	0.45
26:C:270:CDL:H202	26:C:270:CDL:H171	1.79	0.45
8:H:43:MET:HE3	8:H:49:ASP:N	2.30	0.45
19:Y:1522:TGL:OA1	19:Y:1522:TGL:HC21	2.15	0.45
4:D:32:ASN:ND2	28:D:4451:HOH:O	2.45	0.45
23:O:229:CHD:H212	23:O:229:CHD:H12	1.98	0.45
4:Q:24:LEU:HD12	5:R:30:ARG:HA	1.98	0.45
5:R:12:ASP:HA	5:R:47:ILE:HD11	1.98	0.45
19:L:522:TGL:HB91	19:L:522:TGL:H361	1.98	0.45
4:D:88:PHE:HZ	13:M:19:LEU:HD21	1.80	0.45
26:G:269:CDL:H322	26:G:269:CDL:HA62	1.97	0.45
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.17	0.45
7:G:4:ALA:CB	1:N:282:PHE:HA	2.47	0.45
12:L:22:LEU:O	12:L:26:THR:HB	2.17	0.45
2:O:93:PRO:HG3	2:O:151:ARG:HB2	1.98	0.45
3:C:47:LEU:O	3:C:51:MET:HG2	2.17	0.45
1:N:240:HIS:HB3	1:N:241:PRO:HD3	1.99	0.45
1:N:400:PHE:HB3	19:Y:1522:TGL:H283	1.98	0.45
1:A:1:FME:HA	1:A:1:FME:CE	2.46	0.45
1:A:240:HIS:HB3	1:A:241:PRO:HD3	1.99	0.45
2:B:128:LEU:HD11	2:B:134:ARG:HA	1.98	0.45
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.98	0.45
3:P:55:TYR:CE1	26:P:1270:CDL:H161	2.52	0.45
7:T:7:ASP:HB2	28:T:4278:HOH:O	2.16	0.45
12:Y:11:ILE:HD12	12:Y:13:PHE:CE1	2.51	0.45
1:A:309:THR:HG22	18:A:516:HEA:HMB2	1.99	0.45
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.99	0.45
3:P:168:THR:HG21	25:P:1265:PEK:H14	1.99	0.45
26:P:1270:CDL:H602	26:P:1270:CDL:H632	1.59	0.45
19:L:522:TGL:CC2	19:L:522:TGL:HC62	2.33	0.45
3:P:110:PRO:HB3	8:U:30:TRP:CE3	2.51	0.45
26:T:1269:CDL:H571	26:T:1269:CDL:H771	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:C:267:PGV:C16	20:C:267:PGV:H12	2.45	0.44
26:G:269:CDL:H571	26:G:269:CDL:H601	1.57	0.44
9:I:2:THR:HG22	9:I:3:ALA:N	2.32	0.44
26:P:1270:CDL:H171	26:P:1270:CDL:H202	1.77	0.44
19:Q:1523:TGL:H212	19:Q:1523:TGL:H242	1.78	0.44
19:Y:1522:TGL:HB61	19:Y:1522:TGL:HB31	1.81	0.44
3:P:34:TRP:HE1	24:P:1272:DMU:C57	2.30	0.44
3:C:213:THR:HG23	26:C:270:CDL:H762	1.98	0.44
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.17	0.44
12:L:20:ARG:CZ	19:L:522:TGL:HC61	2.47	0.44
1:N:62:ALA:HB2	18:N:515:HEA:HBD1	1.98	0.44
2:O:100:MET:SD	2:O:155:SER:HB3	2.57	0.44
1:A:115:SER:O	1:A:121:GLY:HA2	2.17	0.44
4:Q:118:LYS:HB3	11:X:53:TRP:HB3	1.98	0.44
19:A:523:TGL:HC51	19:A:523:TGL:HC22	1.89	0.44
3:P:213:THR:HG23	26:P:1270:CDL:H762	2.00	0.44
12:Y:42:HIS:NE2	12:Y:46:LYS:HD2	2.33	0.44
1:N:407:ASP:O	1:N:411:LYS:HG3	2.18	0.44
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.99	0.44
2:O:56:MET:HA	22:O:1230:PSC:C20	2.47	0.44
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.17	0.44
1:A:347:LEU:HD13	1:A:383:MET:SD	2.57	0.44
1:A:449:MET:SD	2:B:5:MET:HG2	2.57	0.44
7:G:50:TYR:HB3	7:G:52:HIS:CE1	2.52	0.44
7:G:5:LYS:HD3	1:N:278:MET:HB3	2.00	0.44
1:A:165:ILE:O	1:A:169:ILE:HG12	2.17	0.44
20:A:524:PGV:C15	20:A:524:PGV:H321	2.48	0.44
3:P:67:PHE:HE1	26:P:1270:CDL:C1	2.25	0.44
5:R:5:HIS:HB3	5:R:6:GLU:H	1.58	0.44
28:N:3339:HOH:O	6:S:87:THR:HG21	2.17	0.44
7:G:2:SER:O	7:G:3:ALA:HB3	2.18	0.43
8:H:60:TYR:C	8:H:60:TYR:CD1	2.91	0.43
2:O:216:LEU:O	2:O:219:PHE:HB3	2.18	0.43
4:D:75:THR:HB	28:D:2332:HOH:O	2.18	0.43
7:G:31:CYS:HG	26:G:269:CDL:H532	1.79	0.43
1:N:400:PHE:HB3	19:Y:1522:TGL:C28	2.48	0.43
5:R:63:SER:O	5:R:67:ILE:HG13	2.19	0.43
26:T:1269:CDL:H571	26:T:1269:CDL:H601	1.56	0.43
7:T:5:LYS:HD2	25:T:263:PEK:C37	2.44	0.43
8:U:58:ARG:HA	8:U:58:ARG:HD2	1.80	0.43
2:B:52:HIS:HE1	22:B:230:PSC:H02	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:C:270:CDL:H641	26:C:270:CDL:H672	1.84	0.43
1:N:5:ARG:O	1:N:9:SER:HB2	2.18	0.43
1:N:376:HIS:O	1:N:380:VAL:HG22	2.19	0.43
2:O:52:HIS:HE1	22:O:1230:PSC:H212	1.83	0.43
5:R:57:ARG:HH11	5:R:57:ARG:HG3	1.84	0.43
4:Q:138:TRP:CH2	11:X:50:PRO:HG2	2.54	0.43
9:I:35:TYR:C	9:I:37:PHE:H	2.22	0.43
1:N:409:TRP:CE2	20:N:1524:PGV:H61	2.53	0.43
5:R:86:ILE:HA	5:R:86:ILE:HD13	1.76	0.43
2:B:14:SER:HB3	2:B:168:LEU:HD23	2.01	0.43
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.79	0.43
13:M:42:LYS:CE	13:M:42:LYS:HA	2.39	0.43
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.06	0.43
26:G:269:CDL:H212	1:N:311:ILE:HD12	2.01	0.43
3:P:112:LEU:HD13	3:P:118:PRO:HG3	2.01	0.43
3:P:41:THR:O	3:P:45:ILE:HG13	2.18	0.43
8:U:39:CYS:O	8:U:43:MET:HG2	2.18	0.43
10:W:36:MET:HB3	23:W:1060:CHD:H181	2.01	0.43
26:C:270:CDL:H242	26:C:270:CDL:H661	2.01	0.43
26:P:1270:CDL:H273	28:P:4551:HOH:O	2.17	0.43
3:P:187:THR:HB	7:T:68:THR:HG21	2.01	0.43
1:A:229:ILE:HD11	2:B:175:ILE:CD1	2.48	0.43
20:N:1524:PGV:C15	20:N:1524:PGV:H321	2.46	0.43
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.92	0.43
1:A:488:THR:HB	1:A:495:LEU:HD13	2.01	0.42
2:O:59:GLN:O	2:O:59:GLN:HG3	2.19	0.42
23:B:1086:CHD:H212	23:B:1086:CHD:H12	2.01	0.42
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.19	0.42
25:C:265:PEK:H371	26:G:269:CDL:H261	2.00	0.42
5:R:82:TYR:N	5:R:83:PRO:CD	2.82	0.42
1:A:430:PHE:HE1	19:A:521:TGL:HB21	1.84	0.42
1:A:377:PHE:CE2	1:A:378:HIS:CE1	3.07	0.42
1:N:113:LEU:CD1	19:Y:1522:TGL:H292	2.49	0.42
1:N:406:ASN:HD21	20:N:1524:PGV:H21	1.84	0.42
26:P:1270:CDL:H242	26:P:1270:CDL:H661	2.02	0.42
7:T:5:LYS:CB	25:T:263:PEK:H362	2.32	0.42
3:C:187:THR:HG22	25:C:264:PEK:H052	2.01	0.42
3:P:207:HIS:CD2	3:P:241:TYR:OH	2.72	0.42
1:N:459:PHE:HB3	4:Q:92:THR:HG23	2.01	0.42
5:R:99:SER:HB2	5:R:104:LEU:HD21	2.01	0.42
9:V:35:TYR:C	9:V:37:PHE:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:LEU:HD11	28:B:4860:HOH:O	2.20	0.42
2:B:56:MET:HA	22:B:230:PSC:H202	2.02	0.42
26:G:269:CDL:H771	26:G:269:CDL:H571	2.02	0.42
1:N:292:MET:O	1:N:295:VAL:HG22	2.20	0.42
25:P:1265:PEK:H371	26:T:1269:CDL:H261	2.02	0.42
19:Q:1523:TGL:CC2	19:Q:1523:TGL:HG11	2.48	0.42
10:W:30:ILE:O	10:W:34:VAL:HG23	2.20	0.42
3:C:164:PHE:CD1	23:C:271:CHD:H192	2.54	0.42
1:N:289:ALA:HB3	1:N:305:PHE:CD2	2.53	0.42
1:N:3:ILE:HG23	1:N:7:LEU:HD22	2.02	0.42
2:B:81:LEU:HD13	26:T:1269:CDL:H122	2.01	0.42
5:E:105:GLY:O	5:E:108:LYS:HG2	2.19	0.42
9:I:2:THR:CG2	9:I:3:ALA:N	2.82	0.42
28:A:4044:HOH:O	12:L:3:TYR:HB3	2.19	0.42
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.50	0.42
1:N:225:GLY:HA3	3:P:112:LEU:HD21	2.02	0.42
3:C:116:TRP:HA	3:C:117:PRO:C	2.40	0.42
3:P:116:TRP:HA	3:P:117:PRO:C	2.39	0.42
19:A:523:TGL:H242	19:A:523:TGL:H212	1.77	0.42
12:L:35:ALA:HB3	12:L:36:PRO:HD3	2.01	0.42
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.49	0.42
19:Q:1523:TGL:HB81	19:Q:1523:TGL:H122	2.01	0.42
10:J:50:LEU:HD22	10:J:50:LEU:O	2.20	0.41
2:O:217:LYS:HA	2:O:217:LYS:HE2	2.01	0.41
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.91	0.41
12:L:11:ILE:CG2	19:L:522:TGL:H271	2.49	0.41
1:A:136:LEU:HD12	28:A:4243:HOH:O	2.19	0.41
26:G:269:CDL:H152	26:G:269:CDL:H181	1.94	0.41
18:A:515:HEA:H11	18:A:515:HEA:HHC	1.87	0.41
25:C:265:PEK:H383	26:G:269:CDL:H273	2.01	0.41
26:G:269:CDL:H221	1:N:286:ILE:CD1	2.51	0.41
9:I:1:SAC:OAC	9:I:1:SAC:HB2	2.20	0.41
1:N:297:MET:HB2	28:N:4474:HOH:O	2.21	0.41
3:C:223:LEU:HD21	23:C:271:CHD:C18	2.50	0.41
26:C:270:CDL:H532	26:C:270:CDL:H561	1.74	0.41
1:A:304:TYR:CD1	26:T:1269:CDL:HB32	2.53	0.41
8:U:64:CYS:HA	8:U:65:PRO:HD3	1.97	0.41
1:N:17:THR:OG1	19:Y:1522:TGL:H281	2.20	0.41
19:A:521:TGL:H201	19:A:521:TGL:C24	2.46	0.41
2:B:65:TRP:CZ3	22:B:230:PSC:H331	2.55	0.41
10:J:40:LEU:HD12	23:J:60:CHD:H183	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:381:LEU:O	1:N:385:ALA:HB3	2.20	0.41
9:V:58:LYS:O	9:V:62:GLU:HG3	2.19	0.41
2:B:78:LEU:HA	2:B:78:LEU:HD12	1.88	0.41
2:B:98:LYS:HB2	2:B:98:LYS:HE3	1.90	0.41
10:J:14:GLU:HG3	28:J:4760:HOH:O	2.21	0.41
1:N:468:MET:O	1:N:472:ILE:HG13	2.20	0.41
25:P:1265:PEK:H201	28:T:4510:HOH:O	2.19	0.41
4:Q:52:SER:OG	4:Q:55:GLU:HG3	2.21	0.41
8:U:57:ARG:HA	8:U:60:TYR:CE2	2.56	0.41
23:W:1060:CHD:H161	23:W:1060:CHD:H212	1.73	0.41
19:A:523:TGL:HB81	19:A:523:TGL:H122	2.03	0.41
1:A:334:TRP:CZ2	2:B:46:LEU:HB3	2.56	0.41
1:A:334:TRP:HH2	2:B:46:LEU:HD13	1.84	0.41
11:K:42:PRO:HG2	11:K:47:ARG:NE	2.35	0.41
12:L:2:HIS:HB3	12:L:3:TYR:H	1.55	0.41
9:I:5:ALA:HB3	28:I:4611:HOH:O	2.21	0.41
20:P:1267:PGV:H182	26:P:1270:CDL:H673	2.01	0.41
2:B:168:LEU:HD13	2:B:184:LEU:HG	2.03	0.41
25:C:264:PEK:H102	25:C:264:PEK:C16	2.36	0.41
7:G:2:SER:OG	25:G:1263:PEK:H291	2.20	0.41
25:C:264:PEK:H041	7:G:70:PHE:HB2	2.03	0.41
23:J:60:CHD:H161	23:J:60:CHD:H212	1.74	0.41
1:N:363:LEU:HA	1:N:363:LEU:HD23	1.87	0.41
26:P:1270:CDL:H162	26:P:1270:CDL:H352	2.03	0.41
24:P:1272:DMU:H30	24:P:1272:DMU:O1	2.21	0.41
4:Q:48:TRP:CH2	5:R:56:ARG:HA	2.56	0.41
7:T:21:PHE:HD2	7:T:25:LEU:HD12	1.85	0.41
22:B:230:PSC:C07	9:I:10:ARG:HE	2.34	0.41
11:K:43:SER:HA	11:K:44:PRO:HD3	1.97	0.41
3:P:184:ALA:HA	3:P:185:PRO:HD2	1.94	0.41
4:Q:36:SER:O	4:Q:39:ALA:HB3	2.20	0.41
23:W:1060:CHD:H211	28:W:4516:HOH:O	2.20	0.41
1:A:38:ARG:HD2	18:A:515:HEA:OMA	2.22	0.40
1:A:406:ASN:HD21	20:A:524:PGV:H21	1.86	0.40
25:G:1263:PEK:H182	3:P:98:PHE:CD2	2.56	0.40
13:M:37:LEU:O	13:M:41:LYS:HG3	2.21	0.40
2:O:46:LEU:HD12	19:Q:1523:TGL:H271	2.03	0.40
3:P:230:ASN:HB2	28:S:3287:HOH:O	2.21	0.40
1:A:246:LEU:HD13	1:A:381:LEU:HD11	2.03	0.40
19:A:523:TGL:HG11	19:A:523:TGL:CC2	2.49	0.40
26:C:270:CDL:H162	26:C:270:CDL:H352	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:82:CYS:HA	6:F:83:PRO:HD3	1.95	0.40
2:O:122:MET:SD	2:O:206:PHE:HB3	2.62	0.40
2:O:217:LYS:CA	2:O:217:LYS:HE2	2.52	0.40
3:P:42:LEU:HA	3:P:42:LEU:HD23	1.94	0.40
1:A:399:LEU:HB2	1:A:494:TRP:CZ3	2.55	0.40
4:D:118:LYS:HB3	11:K:53:TRP:HB3	2.02	0.40
7:G:11:TPO:CG2	7:G:11:TPO:O	2.68	0.40
10:J:29:ASN:H	10:J:29:ASN:HD22	1.68	0.40
3:C:99:TRP:CE2	20:C:268:PGV:H232	2.57	0.40
8:H:49:ASP:O	8:H:52:VAL:HG22	2.21	0.40
20:N:1524:PGV:H011	20:N:1524:PGV:H202	1.94	0.40
3:P:31:LEU:HA	3:P:31:LEU:HD23	1.86	0.40
5:R:81:ILE:HD11	9:V:8:GLN:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	499 (98%)	13 (2%)	0	100	100
1	N	512/514 (100%)	500 (98%)	12 (2%)	0	100	100
2	B	225/227 (99%)	212 (94%)	11 (5%)	2 (1%)	17	12
2	O	225/227 (99%)	211 (94%)	13 (6%)	1 (0%)	34	32
3	C	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
3	P	257/261 (98%)	251 (98%)	6 (2%)	0	100	100
4	D	142/147 (97%)	139 (98%)	3 (2%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
5	E	103/109 (94%)	100 (97%)	3 (3%)	0	100	100
5	R	103/109 (94%)	101 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	96/98 (98%)	88 (92%)	5 (5%)	3 (3%)	4	1
6	S	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	4	1
7	G	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	1	0
7	T	81/85 (95%)	66 (82%)	8 (10%)	7 (9%)	1	0
8	H	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	12	7
8	U	77/85 (91%)	70 (91%)	6 (8%)	1 (1%)	12	7
9	I	71/73 (97%)	68 (96%)	3 (4%)	0	100	100
9	V	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
10	J	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
10	W	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
11	K	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
12	Y	44/47 (94%)	43 (98%)	1 (2%)	0	100	100
13	M	41/46 (89%)	41 (100%)	0	0	100	100
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3504/3614 (97%)	3354 (96%)	125 (4%)	25 (1%)	22	18

All (25) Ramachandran outliers are listed below:

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

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

### 5.3.2 Protein sidechains [i](#)

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%)	414 (97%)	12 (3%)	43	47
1	N	426/426 (100%)	415 (97%)	11 (3%)	46	50
2	B	210/210 (100%)	200 (95%)	10 (5%)	25	24
2	O	210/210 (100%)	198 (94%)	12 (6%)	20	18
3	C	224/226 (99%)	219 (98%)	5 (2%)	52	57
3	P	224/226 (99%)	218 (97%)	6 (3%)	44	48
4	D	128/129 (99%)	126 (98%)	2 (2%)	62	69
4	Q	128/129 (99%)	123 (96%)	5 (4%)	32	33
5	E	92/95 (97%)	89 (97%)	3 (3%)	38	40
5	R	92/95 (97%)	89 (97%)	3 (3%)	38	40
6	F	81/81 (100%)	79 (98%)	2 (2%)	47	52
6	S	81/81 (100%)	74 (91%)	7 (9%)	10	7
7	G	67/68 (98%)	62 (92%)	5 (8%)	13	10
7	T	67/68 (98%)	61 (91%)	6 (9%)	9	6
8	H	71/75 (95%)	69 (97%)	2 (3%)	43	47
8	U	71/75 (95%)	69 (97%)	2 (3%)	43	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	57/57 (100%)	54 (95%)	3 (5%)	22	20
9	V	57/57 (100%)	55 (96%)	2 (4%)	36	38
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	60
10	W	49/50 (98%)	48 (98%)	1 (2%)	55	60
11	K	39/46 (85%)	38 (97%)	1 (3%)	46	50
11	X	39/46 (85%)	38 (97%)	1 (3%)	46	50
12	L	39/40 (98%)	37 (95%)	2 (5%)	24	22
12	Y	39/40 (98%)	39 (100%)	0	100	100
13	M	37/38 (97%)	34 (92%)	3 (8%)	11	8
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	3
All	All	3040/3082 (99%)	2929 (96%)	111 (4%)	34	35

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

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	112	LEU
1	A	180	GLN
1	A	238	PHE
1	A	338	MET
1	A	369	ASP
1	A	380	VAL
1	A	486	ASP
1	A	504	THR
1	A	512	ASN
1	A	513	LEU
2	B	16	ILE
2	B	33	LEU
2	B	60	GLU
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	113	TYR
2	B	115	ASP
2	B	167	SER
3	C	159	MET

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Mol	Chain	Res	Type
3	C	179	SER
3	C	192	VAL
3	C	214	PHE
3	C	230	ASN
4	D	4	SER
4	D	51	LEU
5	E	70	VAL
5	E	80	GLU
5	E	90	ARG
6	F	48	LEU
6	F	96	LEU
7	G	17	ARG
7	G	18	PHE
7	G	36	TRP
7	G	54	ARG
7	G	84	LYS
8	H	29	CYS
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
9	I	37	PHE
10	J	50	LEU
11	K	54	ARG
12	L	2	HIS
12	L	26	THR
13	M	4	LYS
13	M	34	LEU
13	M	42	LYS
1	N	38	ARG
1	N	109	PHE
1	N	115	SER
1	N	138	HIS
1	N	180	GLN
1	N	238	PHE
1	N	369	ASP
1	N	380	VAL
1	N	394	VAL
1	N	504	THR
1	N	513	LEU
2	O	33	LEU
2	O	60	GLU
2	O	66	THR

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Mol	Chain	Res	Type
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	110	TYR
2	O	148	MET
2	O	167	SER
2	O	217	LYS
3	P	17	PRO
3	P	77	LYS
3	P	127	LEU
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	8	SER
4	Q	19	ARG
4	Q	51	LEU
4	Q	54	ASP
4	Q	121	LYS
5	R	77	PRO
5	R	80	GLU
5	R	90	ARG
6	S	37	LYS
6	S	48	LEU
6	S	53	THR
6	S	54	ASN
6	S	94	HIS
6	S	95	GLN
6	S	96	LEU
7	T	18	PHE
7	T	26	PRO
7	T	38	HIS
7	T	43	GLU
7	T	54	ARG
7	T	84	LYS
8	U	29	CYS
8	U	60	TYR
9	V	8	GLN
9	V	61	GLU
10	W	50	LEU
11	X	54	ARG

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Mol	Chain	Res	Type
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS

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

Mol	Chain	Res	Type
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	10	GLN
2	B	52	HIS
2	B	91	ASN
2	B	181	GLN
3	C	3	HIS
3	C	50	ASN
3	C	68	GLN
3	C	149	HIS
4	D	32	ASN
4	D	37	GLN
4	D	101	HIS
4	D	109	HIS
5	E	94	ASN
9	I	8	GLN
10	J	29	ASN
11	K	35	GLN
11	K	41	ASN
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	52	HIS
2	O	91	ASN
2	O	181	GLN
2	O	203	ASN
3	P	50	ASN
3	P	68	GLN
3	P	207	HIS
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN

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Mol	Chain	Res	Type
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
10	W	57	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
9	SAC	I	1	9	7,8,9	2.96	2 (28%)	8,9,11	2.75	3 (37%)
2	FME	O	1	2	8,9,10	0.69	0	7,9,11	2.54	2 (28%)
1	FME	N	1	1	8,9,10	0.77	0	7,9,11	1.59	1 (14%)
2	FME	B	1	2	8,9,10	0.69	0	7,9,11	1.89	2 (28%)
1	FME	A	1	1	8,9,10	0.63	0	7,9,11	1.07	0
7	TPO	G	11	7	8,10,11	1.58	1 (12%)	10,14,16	1.02	0
9	SAC	V	1	9	7,8,9	2.93	2 (28%)	8,9,11	3.05	5 (62%)
7	TPO	T	11	7	8,10,11	1.44	1 (12%)	10,14,16	0.94	0

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	-
2	FME	O	1	2	-	2/7/9/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	N	1	1	-	4/7/9/11	-
2	FME	B	1	2	-	1/7/9/11	-
1	FME	A	1	1	-	3/7/9/11	-
7	TPO	G	11	7	-	5/9/11/13	-
9	SAC	V	1	9	-	3/7/8/10	-
7	TPO	T	11	7	-	5/9/11/13	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	I	1	SAC	OAC-C1A	5.60	1.35	1.23
9	V	1	SAC	CA-N	5.51	1.54	1.46
9	I	1	SAC	CA-N	5.27	1.53	1.46
9	V	1	SAC	OAC-C1A	4.90	1.34	1.23
7	G	11	TPO	CB-CA	3.06	1.60	1.53
7	T	11	TPO	CB-CA	2.14	1.58	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	1	SAC	CA-N-C1A	-6.38	111.38	123.15
9	I	1	SAC	CA-N-C1A	-5.48	113.05	123.15
2	O	1	FME	C-CA-N	5.30	119.29	109.73
2	O	1	FME	CA-N-CN	-3.98	116.71	122.82
2	B	1	FME	C-CA-N	3.87	116.72	109.73
1	N	1	FME	CA-N-CN	-3.51	117.42	122.82
9	I	1	SAC	CB-CA-N	3.49	118.38	110.55
9	V	1	SAC	C2A-C1A-N	3.24	121.59	116.10
9	I	1	SAC	C-CA-N	-2.98	104.36	109.73
9	V	1	SAC	CB-CA-N	2.79	116.80	110.55
2	B	1	FME	CA-N-CN	-2.76	118.58	122.82
9	V	1	SAC	C-CA-N	-2.66	104.93	109.73
9	V	1	SAC	OAC-C1A-C2A	-2.29	117.80	122.06

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	I	1	SAC	CB-CA-N-C1A
2	O	1	FME	O1-CN-N-CA

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

There are no ring outliers.

5 monomers are involved in 7 short contacts:

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

Of 58 ligands modelled in this entry, 14 are monoatomic - leaving 44 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	PGV	A	524	-	50,50,50	1.05	3 (6%)	53,56,56	0.94	3 (5%)
25	PEK	T	263	-	52,52,52	1.80	10 (19%)	55,57,57	1.16	6 (10%)
26	CDL	C	270	-	99,99,99	0.84	3 (3%)	105,111,111	1.01	6 (5%)
23	CHD	C	525	-	29,32,32	0.86	1 (3%)	48,51,51	1.92	14 (29%)
19	TGL	A	523	-	62,62,62	0.76	1 (1%)	65,65,65	1.28	11 (16%)
19	TGL	N	1521	-	62,62,62	0.71	1 (1%)	65,65,65	1.42	9 (13%)
19	TGL	L	522	-	62,62,62	1.12	6 (9%)	65,65,65	1.72	13 (20%)
25	PEK	P	1264	-	52,52,52	1.45	5 (9%)	55,57,57	1.17	6 (10%)
23	CHD	B	1086	-	29,32,32	0.67	0	48,51,51	1.80	12 (25%)
19	TGL	A	521	-	62,62,62	0.71	1 (1%)	65,65,65	1.43	9 (13%)
18	HEA	N	515	1	44,67,67	1.62	5 (11%)	37,103,103	1.40	7 (18%)
19	TGL	Y	1522	-	62,62,62	1.15	5 (8%)	65,65,65	1.70	13 (20%)
26	CDL	P	1270	-	99,99,99	0.89	5 (5%)	105,111,111	1.00	7 (6%)
26	CDL	G	269	-	99,99,99	0.98	7 (7%)	105,111,111	0.96	6 (5%)
22	PSC	O	1230	-	51,51,51	1.21	3 (5%)	57,59,59	0.91	1 (1%)
20	PGV	P	1268	-	50,50,50	1.14	2 (4%)	53,56,56	0.84	0
18	HEA	A	516	1	44,67,67	1.29	6 (13%)	37,103,103	1.39	5 (13%)
23	CHD	J	60	-	29,32,32	1.35	3 (10%)	48,51,51	3.64	28 (58%)
18	HEA	A	515	1	44,67,67	1.24	2 (4%)	37,103,103	1.43	7 (18%)
23	CHD	O	229	-	29,32,32	0.65	0	48,51,51	1.78	12 (25%)
25	PEK	C	265	-	52,52,52	1.60	10 (19%)	55,57,57	1.14	7 (12%)
20	PGV	N	1524	-	50,50,50	1.04	4 (8%)	53,56,56	0.92	3 (5%)
23	CHD	P	1525	-	29,32,32	0.84	1 (3%)	48,51,51	1.83	12 (25%)
19	TGL	Q	1523	-	62,62,62	0.80	1 (1%)	65,65,65	1.25	6 (9%)
24	DMU	Z	1526	-	34,34,34	3.23	9 (26%)	45,45,45	3.95	20 (44%)
21	CUA	O	228	2	0,1,1	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	PGV	C	267	-	50,50,50	0.81	1 (2%)	53,56,56	0.96	3 (5%)
24	DMU	C	272	-	34,34,34	2.82	13 (38%)	45,45,45	4.13	19 (42%)
22	PSC	B	230	-	51,51,51	1.20	3 (5%)	57,59,59	0.90	1 (1%)
23	CHD	P	1271	-	29,32,32	0.90	1 (3%)	48,51,51	3.72	26 (54%)
18	HEA	N	516	1	44,67,67	1.28	5 (11%)	37,103,103	1.37	6 (16%)
20	PGV	P	1267	-	50,50,50	0.80	1 (2%)	53,56,56	0.86	1 (1%)
20	PGV	C	268	-	50,50,50	1.16	3 (6%)	53,56,56	0.80	0
26	CDL	T	1269	-	99,99,99	0.96	7 (7%)	105,111,111	0.97	6 (5%)
20	PGV	N	1266	-	50,50,50	0.89	2 (4%)	53,56,56	0.82	3 (5%)
23	CHD	W	1060	-	29,32,32	1.41	3 (10%)	48,51,51	3.67	26 (54%)
20	PGV	A	604	-	50,50,50	0.86	1 (2%)	53,56,56	0.74	1 (1%)
23	CHD	C	271	-	29,32,32	0.96	1 (3%)	48,51,51	3.80	25 (52%)
25	PEK	C	264	-	52,52,52	1.37	4 (7%)	55,57,57	1.21	5 (9%)
24	DMU	M	526	-	34,34,34	3.31	8 (23%)	45,45,45	4.02	20 (44%)
25	PEK	G	1263	-	52,52,52	1.76	10 (19%)	55,57,57	1.15	5 (9%)
21	CUA	B	228	2	0,1,1	0.00	-	-	-	-
25	PEK	P	1265	-	52,52,52	1.61	10 (19%)	55,57,57	1.14	7 (12%)
24	DMU	P	1272	-	34,34,34	2.86	12 (35%)	45,45,45	4.00	19 (42%)

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
20	PGV	A	524	-	-	34/55/55/55	-
25	PEK	T	263	-	-	29/56/56/56	-
26	CDL	C	270	-	-	69/110/110/110	-
23	CHD	C	525	-	-	0/7/74/74	0/4/4/4
19	TGL	A	523	-	-	14/65/65/65	-
19	TGL	N	1521	-	-	14/65/65/65	-
19	TGL	L	522	-	-	16/65/65/65	-
25	PEK	P	1264	-	-	24/56/56/56	-
23	CHD	B	1086	-	-	0/7/74/74	0/4/4/4
19	TGL	A	521	-	-	14/65/65/65	-
18	HEA	N	515	1	3/3/7/16	1/24/76/76	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	TGL	Y	1522	-	-	16/65/65/65	-
26	CDL	P	1270	-	-	69/110/110/110	-
26	CDL	G	269	-	-	62/110/110/110	-
22	PSC	O	1230	-	-	40/55/55/55	-
20	PGV	P	1268	-	-	35/55/55/55	-
18	HEA	A	516	1	3/3/7/16	3/24/76/76	-
23	CHD	J	60	-	5/5/12/12	6/7/74/74	0/4/4/4
18	HEA	A	515	1	3/3/7/16	1/24/76/76	-
23	CHD	O	229	-	-	0/7/74/74	0/4/4/4
25	PEK	C	265	-	-	19/56/56/56	-
20	PGV	N	1524	-	-	34/55/55/55	-
23	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
19	TGL	Q	1523	-	-	14/65/65/65	-
24	DMU	Z	1526	-	5/5/10/10	10/19/59/59	0/2/2/2
23	CHD	W	1060	-	5/5/12/12	6/7/74/74	0/4/4/4
20	PGV	C	267	-	-	17/55/55/55	-
24	DMU	C	272	-	6/6/10/10	8/19/59/59	0/2/2/2
22	PSC	B	230	-	-	40/55/55/55	-
26	CDL	T	1269	-	-	62/110/110/110	-
23	CHD	P	1271	-	5/5/12/12	6/7/74/74	0/4/4/4
20	PGV	P	1267	-	-	16/55/55/55	-
20	PGV	C	268	-	-	35/55/55/55	-
18	HEA	N	516	1	3/3/7/16	2/24/76/76	-
20	PGV	N	1266	-	-	14/55/55/55	-
20	PGV	A	604	-	-	13/55/55/55	-
23	CHD	C	271	-	5/5/12/12	6/7/74/74	0/4/4/4
25	PEK	C	264	-	-	26/56/56/56	-
24	DMU	M	526	-	5/5/10/10	10/19/59/59	0/2/2/2
25	PEK	G	1263	-	-	29/56/56/56	-
25	PEK	P	1265	-	-	20/56/56/56	-
24	DMU	P	1272	-	6/6/10/10	9/19/59/59	0/2/2/2

All (179) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M	526	DMU	O7-C3	-8.35	1.22	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Z	1526	DMU	O7-C3	-7.91	1.23	1.43
24	M	526	DMU	O16-C6	-7.68	1.27	1.40
24	Z	1526	DMU	O16-C6	-7.52	1.27	1.40
18	N	515	HEA	C3B-C11	-7.42	1.47	1.52
24	M	526	DMU	O5-C4	-6.84	1.27	1.44
24	M	526	DMU	O1-C9	-6.73	1.28	1.44
24	Z	1526	DMU	O5-C4	-6.52	1.28	1.44
24	M	526	DMU	O16-C18	-6.52	1.24	1.43
24	Z	1526	DMU	O1-C9	-6.46	1.28	1.44
24	P	1272	DMU	O1-C9	-6.44	1.28	1.44
24	M	526	DMU	O7-C10	-6.37	1.23	1.41
24	Z	1526	DMU	O16-C18	-6.34	1.25	1.43
24	P	1272	DMU	O16-C6	-6.28	1.29	1.40
24	Z	1526	DMU	O7-C10	-6.28	1.24	1.41
24	P	1272	DMU	O7-C3	-6.17	1.27	1.43
24	C	272	DMU	O1-C9	-6.10	1.29	1.44
24	C	272	DMU	O16-C6	-6.03	1.29	1.40
24	P	1272	DMU	O16-C18	-5.98	1.26	1.43
24	C	272	DMU	O7-C3	-5.92	1.28	1.43
24	C	272	DMU	O16-C18	-5.85	1.26	1.43
24	M	526	DMU	O1-C10	-5.72	1.27	1.41
18	A	515	HEA	C3B-C11	-5.31	1.48	1.52
24	Z	1526	DMU	O1-C10	-5.28	1.28	1.41
24	C	272	DMU	O5-C4	-5.26	1.31	1.44
24	Z	1526	DMU	O5-C6	-5.02	1.29	1.41
24	M	526	DMU	O5-C6	-4.96	1.29	1.41
19	Y	1522	TGL	OG2-CB1	4.94	1.48	1.34
25	P	1264	PEK	C15-C14	4.89	1.60	1.31
25	G	1263	PEK	C12-C11	4.82	1.59	1.31
25	C	264	PEK	C15-C14	4.79	1.59	1.31
24	P	1272	DMU	O5-C4	-4.73	1.32	1.44
24	P	1272	DMU	O7-C10	-4.71	1.28	1.41
25	T	263	PEK	C12-C11	4.68	1.58	1.31
19	L	522	TGL	OG2-CB1	4.66	1.47	1.34
24	P	1272	DMU	O1-C10	-4.60	1.30	1.41
23	W	1060	CHD	C13-C17	4.56	1.63	1.55
25	T	263	PEK	C6-C5	4.55	1.58	1.31
24	C	272	DMU	O7-C10	-4.49	1.29	1.41
20	P	1268	PGV	C12-C11	4.48	1.57	1.31
25	C	264	PEK	C12-C11	4.44	1.57	1.31
25	G	1263	PEK	C6-C5	4.42	1.57	1.31
20	C	268	PGV	C12-C11	4.39	1.57	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	C	272	DMU	O1-C10	-4.39	1.30	1.41
25	P	1265	PEK	C12-C11	4.38	1.57	1.31
25	P	1264	PEK	C12-C11	4.37	1.57	1.31
25	C	265	PEK	C12-C11	4.34	1.56	1.31
25	C	265	PEK	C15-C14	4.33	1.56	1.31
25	C	265	PEK	C9-C8	4.27	1.56	1.31
23	J	60	CHD	C13-C17	4.25	1.62	1.55
22	O	1230	PSC	C10-C9	4.25	1.56	1.31
22	B	230	PSC	C10-C9	4.23	1.56	1.31
22	O	1230	PSC	C13-C12	4.22	1.56	1.31
25	G	1263	PEK	C9-C8	4.21	1.56	1.31
25	P	1265	PEK	C9-C8	4.19	1.56	1.31
25	P	1265	PEK	C15-C14	4.16	1.55	1.31
24	C	272	DMU	O5-C6	-4.16	1.31	1.41
25	T	263	PEK	C9-C8	4.14	1.55	1.31
25	P	1265	PEK	C6-C5	4.08	1.55	1.31
25	C	265	PEK	C6-C5	4.07	1.55	1.31
25	P	1264	PEK	C9-C8	4.06	1.55	1.31
25	T	263	PEK	C15-C14	4.05	1.55	1.31
20	N	1266	PGV	C12-C11	4.04	1.55	1.31
25	G	1263	PEK	C15-C14	4.04	1.55	1.31
18	A	516	HEA	C4D-ND	4.00	1.44	1.36
25	C	264	PEK	C6-C5	3.99	1.54	1.31
24	P	1272	DMU	O5-C6	-3.98	1.31	1.41
22	B	230	PSC	C13-C12	3.98	1.54	1.31
20	N	1524	PGV	C12-C11	3.96	1.54	1.31
20	A	604	PGV	C12-C11	3.93	1.54	1.31
25	T	263	PEK	O03-C21	3.85	1.44	1.33
18	N	516	HEA	C4D-ND	3.83	1.44	1.36
19	Y	1522	TGL	OG1-CA1	3.82	1.44	1.33
20	A	524	PGV	C12-C11	3.80	1.53	1.31
25	C	264	PEK	C9-C8	3.78	1.53	1.31
25	P	1264	PEK	C6-C5	3.74	1.53	1.31
25	T	263	PEK	C03-C02	3.73	1.62	1.50
25	G	1263	PEK	C03-C02	3.67	1.61	1.50
25	G	1263	PEK	O03-C21	3.56	1.43	1.33
26	T	1269	CDL	CB6-CB4	3.43	1.61	1.50
25	G	1263	PEK	C01-C02	3.42	1.61	1.50
25	T	263	PEK	C01-C02	3.32	1.60	1.50
18	N	516	HEA	C3B-C11	-3.30	1.50	1.52
26	G	269	CDL	CB6-CB4	3.25	1.60	1.50
19	L	522	TGL	OG1-CA1	3.23	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	P	1267	PGV	C12-C11	3.22	1.50	1.31
18	A	516	HEA	C3A-C2A	-3.11	1.36	1.40
20	C	267	PGV	C12-C11	3.08	1.49	1.31
25	P	1264	PEK	C2-C1	3.03	1.59	1.50
18	N	516	HEA	C3A-CMA	-2.97	1.39	1.46
20	P	1268	PGV	O01-C1	2.96	1.42	1.34
20	A	524	PGV	O03-C19	2.94	1.41	1.33
19	L	522	TGL	CG1-CG2	2.94	1.59	1.50
19	Y	1522	TGL	CG1-CG2	2.86	1.59	1.50
25	T	263	PEK	C2-C1	2.85	1.59	1.50
26	G	269	CDL	C11-CA5	2.82	1.59	1.50
23	W	1060	CHD	C8-C7	2.82	1.58	1.53
25	C	265	PEK	C03-C02	2.82	1.59	1.50
25	T	263	PEK	P-O11	2.81	1.70	1.59
18	N	515	HEA	C3A-CMA	-2.81	1.39	1.46
25	P	1265	PEK	O03-C21	2.80	1.41	1.33
26	P	1270	CDL	CA6-CA4	2.79	1.59	1.50
18	A	516	HEA	C3A-CMA	-2.78	1.39	1.46
20	C	268	PGV	O01-C1	2.77	1.42	1.34
18	N	515	HEA	C3A-C2A	-2.75	1.36	1.40
20	N	1524	PGV	O03-C19	2.69	1.41	1.33
24	P	1272	DMU	C6-C1	2.67	1.60	1.52
24	C	272	DMU	C3-C4	2.67	1.60	1.52
24	P	1272	DMU	C3-C4	2.66	1.60	1.52
25	P	1265	PEK	C01-C02	2.66	1.58	1.50
26	C	270	CDL	CA6-CA4	2.64	1.58	1.50
24	C	272	DMU	C6-C1	2.63	1.60	1.52
25	G	1263	PEK	P-O11	2.60	1.69	1.59
26	G	269	CDL	OA6-CA5	2.60	1.41	1.34
25	C	265	PEK	O03-C21	2.59	1.40	1.33
19	N	1521	TGL	OG2-CB1	2.56	1.41	1.34
25	P	1265	PEK	C03-C02	2.56	1.58	1.50
23	C	271	CHD	C13-C14	2.54	1.59	1.55
22	O	1230	PSC	C2-C1	2.54	1.58	1.50
22	B	230	PSC	C2-C1	2.53	1.58	1.50
26	T	1269	CDL	CA6-CA4	2.52	1.58	1.50
18	A	515	HEA	C3A-CMA	-2.51	1.40	1.46
20	N	1266	PGV	C01-C02	2.50	1.58	1.50
25	C	265	PEK	C01-C02	2.49	1.58	1.50
26	T	1269	CDL	C11-CA5	2.49	1.58	1.50
23	W	1060	CHD	C20-C17	2.49	1.58	1.54
18	A	516	HEA	C3C-C2C	-2.49	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P	1270	CDL	OA8-CA7	2.47	1.40	1.33
18	N	515	HEA	C4C-NC	2.46	1.41	1.36
26	T	1269	CDL	CB2-C1	2.46	1.59	1.51
25	P	1265	PEK	P-O11	2.45	1.69	1.59
26	P	1270	CDL	C31-CA7	2.43	1.57	1.50
26	G	269	CDL	CA6-CA4	2.41	1.58	1.50
23	J	60	CHD	C20-C17	2.40	1.58	1.54
26	T	1269	CDL	OA6-CA5	2.40	1.41	1.34
23	J	60	CHD	C8-C7	2.39	1.57	1.53
26	P	1270	CDL	CA3-CA4	2.39	1.58	1.50
18	N	516	HEA	C1B-NB	2.39	1.41	1.36
26	C	270	CDL	CA3-CA4	2.39	1.58	1.50
26	T	1269	CDL	CB3-CB4	2.38	1.58	1.50
24	Z	1526	DMU	C8-C9	2.37	1.58	1.53
18	N	516	HEA	C3A-C2A	-2.36	1.37	1.40
26	G	269	CDL	CB3-CB4	2.35	1.57	1.50
25	C	265	PEK	P-O11	2.32	1.68	1.59
20	N	1524	PGV	C20-C19	2.31	1.57	1.50
23	P	1271	CHD	C13-C14	2.30	1.59	1.55
20	A	524	PGV	C20-C19	2.28	1.57	1.50
25	G	1263	PEK	P-O12	2.25	1.68	1.59
24	C	272	DMU	C7-C5	2.23	1.58	1.52
19	A	521	TGL	OG2-CB1	2.22	1.40	1.34
26	G	269	CDL	CB2-C1	2.21	1.59	1.51
19	Y	1522	TGL	CG3-CG2	2.21	1.57	1.50
26	C	270	CDL	OA8-CA7	2.18	1.39	1.33
19	Q	1523	TGL	CG3-CG2	2.18	1.57	1.50
25	C	265	PEK	C22-C21	2.17	1.57	1.50
25	C	265	PEK	P-O12	2.16	1.68	1.59
23	C	525	CHD	C13-C12	-2.16	1.51	1.54
18	A	516	HEA	C3B-C11	-2.16	1.51	1.52
19	L	522	TGL	CG3-CG2	2.15	1.57	1.50
18	A	516	HEA	C20-C19	2.14	1.55	1.51
26	P	1270	CDL	CB2-C1	2.13	1.58	1.51
19	Y	1522	TGL	CC2-CC1	2.13	1.56	1.50
20	N	1524	PGV	C03-C02	2.13	1.57	1.50
24	C	272	DMU	C2-C3	2.11	1.58	1.52
20	C	268	PGV	C04-C05	2.10	1.58	1.51
19	A	523	TGL	OG3-CC1	2.09	1.39	1.33
25	P	1265	PEK	C22-C21	2.08	1.56	1.50
24	P	1272	DMU	C8-C9	2.07	1.57	1.53
25	G	1263	PEK	C2-C1	2.07	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	P	1265	PEK	P-O12	2.07	1.67	1.59
24	P	1272	DMU	C8-C7	2.06	1.57	1.52
25	T	263	PEK	P-O12	2.06	1.67	1.59
26	G	269	CDL	C71-CB7	2.05	1.56	1.50
19	L	522	TGL	CC2-CC1	2.04	1.56	1.50
24	C	272	DMU	C8-C7	2.03	1.57	1.52
26	T	1269	CDL	C71-CB7	2.03	1.56	1.50
23	P	1525	CHD	C8-C9	2.02	1.57	1.53
19	L	522	TGL	CC3-CC2	2.01	1.59	1.52
18	N	515	HEA	C1C-NC	2.01	1.40	1.36

All (396) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	272	DMU	O16-C6-C1	11.36	126.04	108.30
24	M	526	DMU	C10-C5-C7	10.35	131.56	110.00
24	Z	1526	DMU	C10-C5-C7	10.21	131.26	110.00
23	P	1271	CHD	C10-C9-C8	10.14	122.71	111.82
23	C	271	CHD	C10-C9-C8	9.85	122.40	111.82
23	C	271	CHD	C17-C13-C14	9.83	110.00	100.09
23	W	1060	CHD	C17-C13-C14	9.81	109.98	100.09
23	J	60	CHD	C17-C13-C14	9.80	109.97	100.09
24	P	1272	DMU	O16-C6-C1	9.52	123.17	108.30
23	P	1271	CHD	C17-C13-C14	9.47	109.64	100.09
24	C	272	DMU	C1-C2-C3	9.24	130.78	109.68
24	P	1272	DMU	C1-C2-C3	9.14	130.54	109.68
23	C	271	CHD	C19-C10-C9	-8.85	98.99	111.18
24	C	272	DMU	C6-O5-C4	8.76	130.89	113.69
24	C	272	DMU	O1-C9-C11	8.68	128.01	106.44
24	P	1272	DMU	C6-O5-C4	8.37	130.11	113.69
23	P	1271	CHD	C17-C13-C12	-8.16	110.22	117.67
23	P	1271	CHD	C19-C10-C9	-8.13	99.98	111.18
24	P	1272	DMU	O1-C9-C11	8.06	126.48	106.44
23	W	1060	CHD	C13-C17-C20	8.04	129.09	119.50
23	J	60	CHD	C13-C17-C20	7.92	128.95	119.50
23	C	271	CHD	C17-C13-C12	-7.91	110.44	117.67
24	M	526	DMU	C8-C7-C5	-7.85	97.13	110.82
24	Z	1526	DMU	C8-C7-C5	-7.73	97.33	110.82
24	M	526	DMU	O1-C9-C8	7.63	123.54	109.69
24	M	526	DMU	O5-C4-C57	7.41	124.86	106.44
24	C	272	DMU	O5-C4-C3	7.40	125.35	109.75
24	Z	1526	DMU	O1-C9-C8	7.36	123.06	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Z	1526	DMU	O5-C4-C57	7.36	124.73	106.44
24	M	526	DMU	C7-C8-C9	7.25	123.17	110.24
24	M	526	DMU	C6-O5-C4	7.24	127.89	113.69
24	Z	1526	DMU	C7-C8-C9	7.22	123.11	110.24
24	M	526	DMU	O1-C9-C11	7.22	124.38	106.44
24	P	1272	DMU	C18-O16-C6	7.21	125.80	113.84
24	Z	1526	DMU	O1-C9-C11	7.20	124.35	106.44
24	P	1272	DMU	O7-C3-C4	7.04	128.75	109.45
24	Z	1526	DMU	O5-C6-O16	6.98	126.52	109.97
24	Z	1526	DMU	C6-O5-C4	6.96	127.35	113.69
24	M	526	DMU	O5-C6-O16	6.73	125.91	109.97
23	W	1060	CHD	C6-C5-C10	6.70	119.77	112.66
24	Z	1526	DMU	O5-C4-C3	6.62	123.71	109.75
23	J	60	CHD	C10-C9-C8	6.60	118.90	111.82
24	P	1272	DMU	O5-C4-C57	6.55	122.72	106.44
24	P	1272	DMU	O5-C4-C3	6.53	123.52	109.75
24	M	526	DMU	O5-C4-C3	6.49	123.44	109.75
24	C	272	DMU	C18-O16-C6	6.42	124.49	113.84
23	W	1060	CHD	C10-C9-C8	6.40	118.69	111.82
23	C	271	CHD	C4-C3-C2	6.37	118.16	110.55
24	C	272	DMU	O7-C3-C4	6.30	126.71	109.45
23	C	271	CHD	C1-C10-C5	6.26	117.02	107.77
23	J	60	CHD	C4-C3-C2	6.24	118.00	110.55
23	W	1060	CHD	C4-C3-C2	6.23	118.00	110.55
23	C	271	CHD	C4-C5-C10	6.10	119.14	112.66
23	W	1060	CHD	C18-C13-C14	-6.02	101.79	111.21
23	P	1271	CHD	C1-C10-C5	5.96	116.58	107.77
23	J	60	CHD	C6-C5-C10	5.87	118.89	112.66
23	C	271	CHD	C14-C13-C12	5.86	112.86	107.40
23	P	1271	CHD	C4-C5-C10	5.83	118.84	112.66
23	W	1060	CHD	C11-C9-C10	5.80	119.71	113.73
23	P	1271	CHD	C4-C3-C2	5.79	117.47	110.55
24	C	272	DMU	O7-C3-C2	5.79	122.69	107.28
24	M	526	DMU	C18-O16-C6	5.77	123.41	113.84
23	P	1271	CHD	C14-C13-C12	5.74	112.75	107.40
24	M	526	DMU	O7-C3-C2	5.72	122.50	107.28
24	C	272	DMU	O5-C4-C57	5.70	120.61	106.44
23	J	60	CHD	C18-C13-C14	-5.67	102.34	111.21
24	P	1272	DMU	O1-C9-C8	5.56	119.79	109.69
23	J	60	CHD	C15-C14-C8	-5.55	110.57	118.33
23	W	1060	CHD	C15-C14-C8	-5.55	110.58	118.33
24	C	272	DMU	C10-O1-C9	5.54	124.57	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	1272	DMU	O7-C3-C2	5.52	121.97	107.28
23	C	271	CHD	C9-C8-C7	5.52	118.47	111.88
23	P	1271	CHD	C9-C8-C7	5.44	118.38	111.88
24	C	272	DMU	O7-C10-C5	5.42	122.16	108.10
23	J	60	CHD	C11-C9-C10	5.41	119.30	113.73
24	C	272	DMU	C8-C7-C5	5.40	120.25	110.82
23	C	525	CHD	C13-C17-C20	5.39	125.92	119.50
24	Z	1526	DMU	C18-O16-C6	5.34	122.70	113.84
24	P	1272	DMU	C10-O1-C9	5.31	124.11	113.69
24	Z	1526	DMU	O7-C3-C2	5.29	121.35	107.28
23	P	1525	CHD	C13-C17-C20	5.25	125.76	119.50
24	P	1272	DMU	O5-C6-C1	5.21	121.39	110.35
23	C	525	CHD	C14-C13-C12	-5.19	102.57	107.40
24	M	526	DMU	O16-C6-C1	5.17	116.37	108.30
23	P	1271	CHD	C15-C14-C8	-5.16	111.11	118.33
24	P	1272	DMU	O7-C10-C5	5.05	121.17	108.10
23	C	271	CHD	C15-C14-C8	-5.04	111.29	118.33
24	C	272	DMU	O1-C9-C8	4.98	118.74	109.69
19	A	521	TGL	CG2-OG2-CB1	4.96	130.00	117.79
24	Z	1526	DMU	O16-C6-C1	4.92	115.99	108.30
23	J	60	CHD	C5-C6-C7	4.90	119.87	114.46
23	W	1060	CHD	C1-C10-C5	4.82	114.89	107.77
19	N	1521	TGL	CG2-OG2-CB1	4.78	129.56	117.79
19	L	522	TGL	C12-C11-C10	-4.77	90.22	114.42
19	Y	1522	TGL	C12-C11-C10	-4.75	90.31	114.42
23	B	1086	CHD	C15-C14-C13	-4.66	98.99	103.55
19	Y	1522	TGL	CB9-CB8-CB7	-4.61	91.02	114.42
24	Z	1526	DMU	C6-C1-C2	4.56	119.49	110.00
19	L	522	TGL	CB9-CB8-CB7	-4.51	91.51	114.42
23	J	60	CHD	C1-C10-C5	4.49	114.41	107.77
23	B	1086	CHD	C16-C17-C13	-4.46	99.18	103.55
23	J	60	CHD	C2-C1-C10	4.46	120.42	112.78
23	O	229	CHD	C16-C17-C13	-4.40	99.24	103.55
23	W	1060	CHD	C9-C8-C7	4.39	117.13	111.88
23	W	1060	CHD	C5-C6-C7	4.37	119.29	114.46
23	P	1525	CHD	C14-C13-C12	-4.36	103.35	107.40
23	J	60	CHD	O12-C12-C13	4.34	118.36	111.03
24	M	526	DMU	C6-C1-C2	4.34	119.03	110.00
23	W	1060	CHD	O12-C12-C13	4.30	118.30	111.03
23	W	1060	CHD	C2-C1-C10	4.27	120.10	112.78
23	J	60	CHD	C9-C8-C7	4.25	116.96	111.88
23	C	271	CHD	C19-C10-C1	-4.21	101.47	108.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	60	CHD	C14-C8-C7	4.12	117.27	111.81
23	J	60	CHD	C13-C14-C8	4.08	119.95	114.74
23	O	229	CHD	C10-C9-C8	4.08	116.20	111.82
19	A	521	TGL	CG1-OG1-CA1	-4.08	102.02	117.12
23	W	1060	CHD	C13-C14-C8	4.08	119.94	114.74
19	N	1521	TGL	CG1-OG1-CA1	-4.06	102.09	117.12
19	Y	1522	TGL	C15-CC9-CC8	4.04	134.94	114.42
24	P	1272	DMU	C8-C7-C5	4.04	117.87	110.82
23	J	60	CHD	C5-C4-C3	4.02	118.66	112.76
23	W	1060	CHD	C5-C4-C3	4.00	118.64	112.76
19	L	522	TGL	C15-CC9-CC8	4.00	134.73	114.42
23	W	1060	CHD	C14-C8-C7	3.99	117.10	111.81
23	C	271	CHD	C18-C13-C12	-3.98	105.01	109.07
23	C	525	CHD	C15-C14-C8	-3.97	112.78	118.33
24	C	272	DMU	O5-C6-C1	3.95	118.72	110.35
24	Z	1526	DMU	O7-C10-O1	3.86	121.45	110.67
18	A	516	HEA	CMC-C2C-C3C	3.84	131.87	124.68
24	P	1272	DMU	O7-C10-O1	3.83	121.37	110.67
24	C	272	DMU	O7-C10-O1	3.81	121.33	110.67
19	Y	1522	TGL	C16-C15-CC9	3.79	133.67	114.42
23	P	1525	CHD	C15-C14-C8	-3.78	113.04	118.33
19	L	522	TGL	C16-C15-CC9	3.78	133.59	114.42
23	C	271	CHD	C9-C11-C12	3.77	119.28	114.30
25	T	263	PEK	P-O11-C03	3.71	143.45	121.68
23	P	1525	CHD	C1-C10-C5	3.69	113.23	107.77
19	L	522	TGL	CC3-CC2-CC1	3.67	126.97	113.62
24	M	526	DMU	C10-O7-C3	3.65	127.00	117.96
24	M	526	DMU	O7-C10-C5	3.64	117.53	108.10
19	A	523	TGL	CG3-OG3-CC1	3.64	130.58	117.12
25	G	1263	PEK	P-O11-C03	3.61	142.85	121.68
25	G	1263	PEK	O03-C01-C02	3.58	118.84	108.43
23	P	1271	CHD	C19-C10-C1	-3.55	102.54	108.26
23	J	60	CHD	C11-C12-C13	3.54	114.88	111.24
23	B	1086	CHD	C15-C14-C8	-3.54	113.39	118.33
19	Q	1523	TGL	CG3-OG3-CC1	3.53	130.20	117.12
25	T	263	PEK	O03-C01-C02	3.52	118.68	108.43
23	J	60	CHD	C6-C5-C4	3.52	115.24	111.19
23	P	1271	CHD	C9-C11-C12	3.50	118.92	114.30
23	O	229	CHD	C15-C14-C13	-3.50	100.12	103.55
23	P	1271	CHD	C14-C8-C7	3.49	116.44	111.81
19	L	522	TGL	C11-C10-CB9	3.47	132.06	114.42
23	O	229	CHD	C5-C6-C7	3.47	118.29	114.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Z	1526	DMU	O7-C3-C4	3.44	118.89	109.45
19	Y	1522	TGL	CC3-CC2-CC1	3.44	126.13	113.62
23	C	525	CHD	C10-C9-C8	3.43	115.50	111.82
23	J	60	CHD	C1-C2-C3	3.42	114.86	110.47
19	L	522	TGL	CG2-OG2-CB1	3.42	126.21	117.79
24	C	272	DMU	C2-C3-C4	-3.41	103.10	110.93
19	Y	1522	TGL	C11-C10-CB9	3.41	131.74	114.42
23	O	229	CHD	C15-C14-C8	-3.38	113.60	118.33
26	P	1270	CDL	PA1-OA5-CA3	3.38	141.49	121.68
18	N	515	HEA	CMD-C2D-C3D	3.37	131.30	124.94
23	C	271	CHD	C14-C8-C7	3.36	116.26	111.81
23	P	1525	CHD	C14-C8-C9	-3.36	105.10	109.71
24	M	526	DMU	O5-C6-C1	3.35	117.45	110.35
23	W	1060	CHD	C16-C15-C14	3.33	111.72	105.13
23	W	1060	CHD	C1-C2-C3	3.32	114.72	110.47
20	A	524	PGV	C02-O01-C1	3.31	125.94	117.79
23	P	1525	CHD	C11-C12-C13	-3.31	107.85	111.24
25	C	264	PEK	O03-C21-C22	-3.29	101.57	111.91
18	A	516	HEA	CMC-C2C-C1C	-3.29	123.40	128.46
26	C	270	CDL	PA1-OA5-CA3	3.28	140.94	121.68
23	P	1271	CHD	C5-C6-C7	3.28	118.08	114.46
24	Z	1526	DMU	O5-C6-C1	3.28	117.29	110.35
23	O	229	CHD	C5-C4-C3	3.28	117.57	112.76
23	B	1086	CHD	C10-C9-C8	3.26	115.32	111.82
23	W	1060	CHD	C6-C5-C4	3.24	114.92	111.19
24	C	272	DMU	C10-O7-C3	3.23	125.95	117.96
23	J	60	CHD	C14-C8-C9	3.22	114.13	109.71
19	Y	1522	TGL	CG2-OG2-CB1	3.22	125.71	117.79
23	P	1271	CHD	C5-C4-C3	3.21	117.47	112.76
23	P	1525	CHD	C10-C9-C8	3.19	115.25	111.82
20	N	1524	PGV	C02-O01-C1	3.19	125.63	117.79
23	W	1060	CHD	C11-C12-C13	3.18	114.51	111.24
18	N	516	HEA	C27-C19-C20	3.17	120.61	115.27
24	P	1272	DMU	C10-O7-C3	3.17	125.81	117.96
26	C	270	CDL	OB6-CB5-C51	-3.17	104.67	111.50
23	B	1086	CHD	C1-C2-C3	3.15	114.50	110.47
18	A	515	HEA	C26-C15-C16	3.14	120.56	115.27
23	J	60	CHD	C16-C15-C14	3.14	111.35	105.13
23	W	1060	CHD	C18-C13-C12	-3.13	105.88	109.07
23	P	1271	CHD	C18-C13-C12	-3.13	105.88	109.07
25	C	265	PEK	P-O11-C03	3.11	139.91	121.68
19	L	522	TGL	CC4-CC3-CC2	3.10	124.34	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	M	526	DMU	O7-C10-O1	3.10	119.33	110.67
23	W	1060	CHD	C14-C8-C9	3.09	113.95	109.71
24	Z	1526	DMU	C10-O7-C3	3.08	125.59	117.96
24	M	526	DMU	O7-C3-C4	3.08	117.89	109.45
23	C	525	CHD	C14-C8-C9	-3.04	105.54	109.71
23	J	60	CHD	C15-C16-C17	3.04	111.15	105.13
19	Y	1522	TGL	CC4-CC3-CC2	3.03	124.09	113.19
18	N	515	HEA	C26-C15-C16	3.03	120.36	115.27
22	O	1230	PSC	C01-O03-C19	-3.02	105.92	117.12
26	P	1270	CDL	CB6-OB8-CB7	-3.02	105.96	117.12
25	P	1265	PEK	P-O11-C03	3.01	139.36	121.68
18	N	516	HEA	CMC-C2C-C3C	3.01	130.30	124.68
19	A	521	TGL	CG3-OG3-CC1	2.99	128.19	117.12
23	W	1060	CHD	C15-C16-C17	2.99	111.05	105.13
23	P	1271	CHD	C1-C2-C3	2.99	114.30	110.47
23	B	1086	CHD	C1-C10-C5	2.98	112.18	107.77
23	B	1086	CHD	C5-C4-C3	2.97	117.12	112.76
23	C	271	CHD	C1-C2-C3	2.97	114.28	110.47
24	M	526	DMU	C10-O1-C9	2.97	119.52	113.69
19	Q	1523	TGL	CG1-OG1-CA1	-2.97	106.13	117.12
25	P	1264	PEK	C3-C2-C1	-2.95	102.89	113.62
25	C	264	PEK	C3-C2-C1	-2.95	102.90	113.62
23	C	271	CHD	C15-C16-C17	2.94	110.96	105.13
19	A	523	TGL	CB3-CB2-CB1	2.94	124.31	113.62
26	C	270	CDL	CB6-OB8-CB7	-2.94	106.24	117.12
19	Q	1523	TGL	OG2-CG2-CG3	2.92	118.96	108.40
18	A	515	HEA	CMC-C2C-C3C	2.90	130.11	124.68
23	C	271	CHD	C5-C6-C7	2.88	117.64	114.46
20	C	267	PGV	O01-C1-C2	-2.88	105.29	111.50
26	T	1269	CDL	C23-C22-C21	2.88	129.05	114.42
19	N	1521	TGL	CG3-OG3-CC1	2.88	127.79	117.12
23	O	229	CHD	C1-C10-C5	2.87	112.01	107.77
23	J	60	CHD	C18-C13-C12	-2.87	106.15	109.07
22	B	230	PSC	C01-O03-C19	-2.86	106.52	117.12
26	P	1270	CDL	OB6-CB5-C51	-2.86	105.34	111.50
23	C	525	CHD	C5-C6-C7	2.85	117.61	114.46
25	P	1265	PEK	C11-C10-C9	2.84	126.00	112.02
18	A	515	HEA	CMD-C2D-C3D	2.84	130.29	124.94
23	B	1086	CHD	C17-C13-C14	2.84	102.95	100.09
23	P	1525	CHD	C1-C2-C3	2.84	114.11	110.47
23	C	271	CHD	C1-C10-C9	2.83	115.81	111.35
23	C	525	CHD	C1-C10-C5	2.83	111.95	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	1060	CHD	C9-C11-C12	2.82	118.03	114.30
26	T	1269	CDL	C22-C21-C20	2.81	128.70	114.42
19	A	523	TGL	OG1-CG1-CG2	2.81	116.61	108.43
23	B	1086	CHD	C9-C11-C12	2.81	118.01	114.30
19	A	523	TGL	CG1-OG1-CA1	-2.80	106.76	117.12
18	N	515	HEA	CMB-C2B-C1B	-2.80	124.16	128.46
26	G	269	CDL	C22-C21-C20	2.79	128.60	114.42
26	G	269	CDL	C23-C22-C21	2.79	128.56	114.42
25	C	265	PEK	C11-C10-C9	2.78	125.72	112.02
25	G	1263	PEK	C02-O01-C1	2.78	124.63	117.79
23	O	229	CHD	C1-C2-C3	2.76	114.01	110.47
18	N	516	HEA	CMC-C2C-C1C	-2.73	124.27	128.46
23	P	1271	CHD	C15-C16-C17	2.72	110.53	105.13
18	A	515	HEA	CMB-C2B-C1B	-2.70	124.32	128.46
19	A	523	TGL	OG2-CG2-CG3	2.70	118.17	108.40
25	T	263	PEK	C02-O01-C1	2.69	124.40	117.79
25	C	264	PEK	C23-C22-C21	-2.68	103.87	113.62
24	Z	1526	DMU	O7-C10-C5	2.68	115.04	108.10
19	L	522	TGL	C20-CA9-CA8	2.68	128.01	114.42
23	P	1271	CHD	C9-C10-C5	2.67	112.33	108.58
25	P	1264	PEK	O03-C01-C02	-2.67	100.66	108.43
23	J	60	CHD	C19-C10-C1	-2.67	103.97	108.26
19	Q	1523	TGL	CB3-CB2-CB1	2.66	123.30	113.62
23	P	1271	CHD	C2-C1-C10	2.66	117.34	112.78
23	C	271	CHD	C16-C15-C14	2.64	110.36	105.13
19	Y	1522	TGL	C13-C12-C11	2.63	127.77	114.42
26	C	270	CDL	OB6-CB5-OB7	2.62	130.04	123.70
23	P	1271	CHD	C16-C15-C14	2.62	110.32	105.13
23	W	1060	CHD	C19-C10-C1	-2.61	104.05	108.26
23	C	271	CHD	C5-C4-C3	2.61	116.59	112.76
24	C	272	DMU	O1-C10-C5	2.60	115.86	110.35
18	N	516	HEA	C3C-C4C-NC	2.59	112.56	109.21
23	P	1525	CHD	C5-C6-C7	2.59	117.32	114.46
23	O	229	CHD	C17-C13-C14	2.58	102.70	100.09
23	P	1271	CHD	C11-C9-C10	2.58	116.39	113.73
25	P	1265	PEK	P-O12-C04	2.58	134.28	121.59
25	P	1264	PEK	O03-C21-C22	-2.56	103.88	111.91
24	M	526	DMU	C1-C2-C3	2.55	115.52	109.68
24	P	1272	DMU	O1-C10-C5	2.54	115.72	110.35
26	G	269	CDL	C20-C19-C18	2.54	127.30	114.42
25	C	265	PEK	P-O12-C04	2.53	134.07	121.59
19	L	522	TGL	C13-C12-C11	2.52	127.24	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	515	HEA	CMC-C2C-C3C	2.52	129.39	124.68
23	P	1271	CHD	C1-C10-C9	2.52	115.31	111.35
20	N	1266	PGV	O01-C1-C2	-2.51	106.09	111.50
18	A	515	HEA	CMB-C2B-C3B	2.51	129.60	124.69
23	P	1271	CHD	C11-C12-C13	2.51	113.82	111.24
18	A	515	HEA	C26-C15-C14	-2.51	117.25	123.68
26	T	1269	CDL	C20-C19-C18	2.50	127.13	114.42
23	B	1086	CHD	C14-C8-C9	-2.50	106.28	109.71
23	C	271	CHD	C11-C9-C10	2.50	116.31	113.73
20	P	1267	PGV	C9-C10-C11	-2.50	98.10	112.43
19	Y	1522	TGL	C20-CA9-CA8	2.49	127.06	114.42
19	Y	1522	TGL	C10-CB9-CB8	2.49	127.06	114.42
19	A	521	TGL	CA8-CA7-CA6	-2.47	101.86	114.42
25	C	265	PEK	C24-C23-C22	2.47	122.08	113.19
23	O	229	CHD	C9-C11-C12	2.47	117.56	114.30
19	N	1521	TGL	CA8-CA7-CA6	-2.46	101.92	114.42
18	A	516	HEA	C21-C20-C19	2.46	121.07	112.98
25	P	1264	PEK	C23-C22-C21	-2.46	104.69	113.62
19	L	522	TGL	OG1-CG1-CG2	2.46	115.58	108.43
20	N	1524	PGV	C3-C2-C1	-2.46	104.69	113.62
23	C	271	CHD	C9-C10-C5	2.45	112.02	108.58
19	A	521	TGL	CG3-CG2-CG1	2.45	117.57	111.79
24	Z	1526	DMU	C10-O1-C9	2.44	118.49	113.69
26	P	1270	CDL	OB6-CB5-OB7	2.44	129.60	123.70
18	N	515	HEA	CMB-C2B-C3B	2.44	129.47	124.69
26	C	270	CDL	OA8-CA6-CA4	2.44	115.54	108.43
25	P	1265	PEK	C2-C3-C4	2.44	117.57	113.23
19	N	1521	TGL	OG2-CG2-CG3	2.44	117.22	108.40
23	C	271	CHD	C2-C1-C10	2.42	116.93	112.78
23	J	60	CHD	C9-C11-C12	2.42	117.49	114.30
19	L	522	TGL	C10-CB9-CB8	2.40	126.63	114.42
24	Z	1526	DMU	C1-C2-C3	2.40	115.16	109.68
19	Y	1522	TGL	OG1-CG1-CG2	2.39	115.39	108.43
23	O	229	CHD	C14-C8-C9	-2.39	106.44	109.71
23	O	229	CHD	C19-C10-C1	-2.38	104.43	108.26
18	A	516	HEA	C27-C19-C20	2.38	119.27	115.27
25	C	264	PEK	O03-C21-O04	2.37	129.57	123.59
25	P	1265	PEK	C03-C02-C01	2.36	117.37	111.79
26	C	270	CDL	C52-C51-CB5	-2.36	105.05	113.62
23	C	525	CHD	C11-C12-C13	-2.36	108.83	111.24
20	N	1266	PGV	C01-O03-C19	-2.35	108.41	117.12
19	A	521	TGL	OG2-CG2-CG3	2.35	116.90	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	525	CHD	C9-C11-C12	2.35	117.40	114.30
23	W	1060	CHD	C19-C10-C5	-2.34	106.39	110.36
20	A	524	PGV	C3-C2-C1	-2.34	105.11	113.62
25	C	265	PEK	C2-C3-C4	2.33	117.38	113.23
19	Q	1523	TGL	OG1-CG1-CG2	2.32	115.20	108.43
19	N	1521	TGL	C10-CB9-CB8	2.32	126.22	114.42
26	P	1270	CDL	OA8-CA6-CA4	2.32	115.19	108.43
23	P	1525	CHD	C19-C10-C9	-2.32	107.98	111.18
19	A	523	TGL	OG2-CG2-CG1	2.32	116.80	108.40
20	C	267	PGV	C9-C10-C11	-2.31	99.18	112.43
20	A	524	PGV	O01-C02-C03	2.31	116.75	108.40
24	P	1272	DMU	O5-C6-O16	2.30	115.43	109.97
23	J	60	CHD	C19-C10-C5	-2.30	106.46	110.36
19	L	522	TGL	CC7-CC6-CC5	2.29	126.06	114.42
19	Q	1523	TGL	OG2-CG2-CG1	2.29	116.68	108.40
23	P	1525	CHD	C11-C9-C10	2.27	116.07	113.73
26	T	1269	CDL	C19-C18-C17	2.27	125.97	114.42
23	J	60	CHD	C4-C5-C10	2.27	115.07	112.66
26	P	1270	CDL	C52-C51-CB5	-2.26	105.39	113.62
26	G	269	CDL	C19-C18-C17	2.26	125.92	114.42
25	C	265	PEK	C03-C02-C01	2.26	117.14	111.79
25	P	1265	PEK	C24-C23-C22	2.26	121.31	113.19
25	C	265	PEK	O03-C01-C02	2.26	115.00	108.43
20	N	1524	PGV	O01-C02-C03	2.25	116.56	108.40
23	B	1086	CHD	C14-C13-C12	-2.25	105.31	107.40
19	N	1521	TGL	CG3-CG2-CG1	2.25	117.11	111.79
23	P	1271	CHD	C6-C5-C4	2.25	113.78	111.19
25	C	264	PEK	O01-C1-C2	-2.25	106.66	111.50
25	T	263	PEK	P-O12-C04	2.25	132.65	121.59
24	P	1272	DMU	C2-C3-C4	-2.24	105.78	110.93
23	C	271	CHD	C11-C12-C13	2.24	113.54	111.24
19	A	521	TGL	C10-CB9-CB8	2.23	125.75	114.42
25	P	1265	PEK	O03-C01-C02	2.23	114.92	108.43
24	C	272	DMU	O5-C6-O16	2.23	115.24	109.97
25	G	1263	PEK	P-O12-C04	2.22	132.53	121.59
18	N	516	HEA	C21-C20-C19	2.21	120.24	112.98
23	C	271	CHD	C6-C5-C10	2.20	114.99	112.66
25	P	1264	PEK	O03-C21-O04	2.19	129.12	123.59
20	A	604	PGV	O01-C1-C2	-2.19	106.79	111.50
25	T	263	PEK	C03-C02-C01	2.18	116.95	111.79
18	N	516	HEA	C17-C18-C19	2.16	132.86	127.66
23	C	525	CHD	C19-C10-C9	-2.14	108.23	111.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	T	1269	CDL	OB8-CB6-CB4	2.13	114.64	108.43
25	G	1263	PEK	C03-C02-C01	2.12	116.81	111.79
23	C	525	CHD	C6-C5-C10	2.12	114.91	112.66
25	P	1264	PEK	C24-C23-C22	-2.12	105.58	113.19
20	C	267	PGV	C3-C2-C1	-2.12	105.92	113.62
18	A	516	HEA	C26-C15-C16	2.12	118.83	115.27
19	Y	1522	TGL	CC7-CC6-CC5	2.11	125.16	114.42
23	C	525	CHD	C18-C13-C12	2.11	111.22	109.07
23	J	60	CHD	C1-C10-C9	2.11	114.67	111.35
19	N	1521	TGL	CA6-CA5-CA4	-2.10	103.76	114.42
26	T	1269	CDL	OB8-CB7-C71	-2.09	105.34	111.91
23	C	525	CHD	C11-C9-C10	2.09	115.88	113.73
23	C	525	CHD	C1-C2-C3	2.09	113.15	110.47
20	N	1266	PGV	O03-C01-C02	2.07	114.47	108.43
19	A	521	TGL	OG1-CG1-CG2	2.07	114.46	108.43
26	G	269	CDL	OB8-CB7-C71	-2.07	105.41	111.91
19	A	523	TGL	CB4-CB3-CB2	2.07	120.63	113.19
19	A	523	TGL	CC3-CC2-CC1	-2.07	106.10	113.62
18	N	515	HEA	C26-C15-C14	-2.07	118.38	123.68
19	N	1521	TGL	OG1-CG1-CG2	2.06	114.42	108.43
18	A	515	HEA	C20-C21-C22	-2.06	105.12	111.88
26	G	269	CDL	OB8-CB6-CB4	2.05	114.40	108.43
18	N	515	HEA	C3C-C4C-NC	2.05	111.86	109.21
26	P	1270	CDL	C82-C81-C80	2.04	124.78	114.42
19	A	521	TGL	CA6-CA5-CA4	-2.04	104.08	114.42
23	P	1271	CHD	C18-C13-C14	-2.03	108.03	111.21
25	T	263	PEK	C2-C3-C4	2.03	116.84	113.23
23	B	1086	CHD	C5-C6-C7	2.02	116.69	114.46
23	P	1525	CHD	C9-C11-C12	2.02	116.97	114.30
19	A	523	TGL	CA3-CA2-CA1	-2.02	106.28	113.62
19	A	523	TGL	CB8-CB7-CB6	2.02	124.67	114.42
19	A	523	TGL	CG2-OG2-CB1	2.00	122.72	117.79

All (54) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	N	515	HEA	ND
18	N	515	HEA	NA
18	N	515	HEA	NB
18	A	516	HEA	ND
18	A	516	HEA	NA
18	A	516	HEA	NB

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Mol	Chain	Res	Type	Atom
23	J	60	CHD	C12
23	J	60	CHD	C8
23	J	60	CHD	C9
23	J	60	CHD	C14
23	J	60	CHD	C17
18	A	515	HEA	ND
18	A	515	HEA	NA
18	A	515	HEA	NB
24	Z	1526	DMU	C2
24	Z	1526	DMU	C4
24	Z	1526	DMU	C6
24	Z	1526	DMU	C5
24	Z	1526	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
24	C	272	DMU	C10
23	P	1271	CHD	C12
23	P	1271	CHD	C8
23	P	1271	CHD	C3
23	P	1271	CHD	C9
23	P	1271	CHD	C14
18	N	516	HEA	ND
18	N	516	HEA	NA
18	N	516	HEA	NB
23	C	271	CHD	C12
23	C	271	CHD	C8
23	C	271	CHD	C3
23	C	271	CHD	C9
23	C	271	CHD	C14
24	M	526	DMU	C2
24	M	526	DMU	C4
24	M	526	DMU	C6
24	M	526	DMU	C5
24	M	526	DMU	C9
23	W	1060	CHD	C12
23	W	1060	CHD	C8
23	W	1060	CHD	C9
23	W	1060	CHD	C14
23	W	1060	CHD	C17

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Mol	Chain	Res	Type	Atom
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

All (843) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	A	524	PGV	C04-O12-P-O11
20	A	524	PGV	C04-O12-P-O13
20	A	524	PGV	C04-O12-P-O14
20	A	524	PGV	C02-C03-O11-P
20	A	524	PGV	C05-C04-O12-P
20	A	524	PGV	C04-C05-C06-O06
20	A	524	PGV	O02-C1-O01-C02
20	A	524	PGV	C20-C19-O03-C01
25	T	263	PEK	C03-O11-P-O14
25	T	263	PEK	O12-C04-C05-N
26	C	270	CDL	CA2-C1-CB2-OB2
26	C	270	CDL	CA2-OA2-PA1-OA3
26	C	270	CDL	CA2-OA2-PA1-OA4
26	C	270	CDL	CA2-OA2-PA1-OA5
26	C	270	CDL	CA4-CA3-OA5-PA1
26	C	270	CDL	C11-CA5-OA6-CA4
26	C	270	CDL	CB2-OB2-PB2-OB3
26	C	270	CDL	CB2-OB2-PB2-OB4
26	P	1270	CDL	CA2-C1-CB2-OB2
26	P	1270	CDL	CA2-OA2-PA1-OA3
26	P	1270	CDL	CA2-OA2-PA1-OA4
26	P	1270	CDL	CA4-CA3-OA5-PA1
26	P	1270	CDL	C11-CA5-OA6-CA4
26	P	1270	CDL	CB2-OB2-PB2-OB3
26	P	1270	CDL	CB2-OB2-PB2-OB4
26	G	269	CDL	CB2-C1-CA2-OA2
26	G	269	CDL	CA2-OA2-PA1-OA3
26	G	269	CDL	C1-CB2-OB2-PB2
26	G	269	CDL	CB3-OB5-PB2-OB3
26	G	269	CDL	CB3-OB5-PB2-OB4
26	G	269	CDL	OB6-CB4-CB6-OB8
22	O	1230	PSC	C03-O11-P-O14

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Mol	Chain	Res	Type	Atoms
22	O	1230	PSC	C04-O12-P-O14
20	P	1268	PGV	C04-O12-P-O11
20	P	1268	PGV	C04-O12-P-O13
20	P	1268	PGV	C04-O12-P-O14
23	J	60	CHD	C16-C17-C20-C21
23	J	60	CHD	C16-C17-C20-C22
24	Z	1526	DMU	O5-C6-O16-C18
25	C	265	PEK	C04-O12-P-O11
25	C	265	PEK	C04-O12-P-O13
25	C	265	PEK	C04-O12-P-O14
22	B	230	PSC	C03-O11-P-O14
22	B	230	PSC	C04-O12-P-O14
26	T	1269	CDL	CB2-C1-CA2-OA2
26	T	1269	CDL	CA2-OA2-PA1-OA3
26	T	1269	CDL	C1-CB2-OB2-PB2
26	T	1269	CDL	CB3-OB5-PB2-OB3
26	T	1269	CDL	CB3-OB5-PB2-OB4
26	T	1269	CDL	OB6-CB4-CB6-OB8
20	C	268	PGV	C04-O12-P-O11
20	C	268	PGV	C04-O12-P-O13
20	C	268	PGV	C04-O12-P-O14
20	C	268	PGV	O05-C05-C06-O06
25	P	1265	PEK	C04-O12-P-O11
25	P	1265	PEK	C04-O12-P-O13
25	P	1265	PEK	C04-O12-P-O14
20	N	1524	PGV	C04-O12-P-O11
20	N	1524	PGV	C04-O12-P-O13
20	N	1524	PGV	C04-O12-P-O14
20	N	1524	PGV	C02-C03-O11-P
20	N	1524	PGV	C05-C04-O12-P
20	N	1524	PGV	C04-C05-C06-O06
20	N	1524	PGV	O02-C1-O01-C02
20	N	1524	PGV	C20-C19-O03-C01
24	M	526	DMU	O5-C6-O16-C18
25	G	1263	PEK	C03-O11-P-O14
25	G	1263	PEK	O12-C04-C05-N
23	W	1060	CHD	C16-C17-C20-C21
23	W	1060	CHD	C16-C17-C20-C22
20	A	524	PGV	O04-C19-O03-C01
20	N	1524	PGV	O04-C19-O03-C01
19	A	523	TGL	OC1-CC1-OG3-CG3
19	Q	1523	TGL	OC1-CC1-OG3-CG3

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Mol	Chain	Res	Type	Atoms
26	C	270	CDL	OA7-CA5-OA6-CA4
19	A	521	TGL	OB1-CB1-OG2-CG2
26	P	1270	CDL	OA7-CA5-OA6-CA4
22	O	1230	PSC	O02-C1-O01-C02
22	B	230	PSC	O02-C1-O01-C02
19	N	1521	TGL	OB1-CB1-OG2-CG2
20	A	524	PGV	C2-C1-O01-C02
19	A	521	TGL	CB2-CB1-OG2-CG2
20	N	1524	PGV	C2-C1-O01-C02
19	N	1521	TGL	CB2-CB1-OG2-CG2
26	C	270	CDL	C40-C41-C42-C43
26	C	270	CDL	C80-C81-C82-C83
26	P	1270	CDL	C40-C41-C42-C43
26	P	1270	CDL	C57-C58-C59-C60
26	P	1270	CDL	C60-C61-C62-C63
26	P	1270	CDL	C80-C81-C82-C83
26	G	269	CDL	C17-C18-C19-C20
26	G	269	CDL	C20-C21-C22-C23
26	G	269	CDL	C57-C58-C59-C60
26	G	269	CDL	C77-C78-C79-C80
26	T	1269	CDL	C17-C18-C19-C20
26	T	1269	CDL	C20-C21-C22-C23
26	T	1269	CDL	C40-C41-C42-C43
26	T	1269	CDL	C77-C78-C79-C80
19	A	523	TGL	CC2-CC1-OG3-CG3
26	G	269	CDL	C31-CA7-OA8-CA6
19	Q	1523	TGL	CC2-CC1-OG3-CG3
26	T	1269	CDL	C31-CA7-OA8-CA6
24	C	272	DMU	O6-C11-C9-O1
24	P	1272	DMU	O6-C11-C9-O1
26	C	270	CDL	C20-C21-C22-C23
26	C	270	CDL	C57-C58-C59-C60
26	C	270	CDL	C60-C61-C62-C63
26	C	270	CDL	C77-C78-C79-C80
19	A	521	TGL	C16-C15-CC9-CC8
26	P	1270	CDL	C37-C38-C39-C40
26	G	269	CDL	C40-C41-C42-C43
26	G	269	CDL	C80-C81-C82-C83
26	T	1269	CDL	C57-C58-C59-C60
19	N	1521	TGL	C16-C15-CC9-CC8
26	C	270	CDL	C37-C38-C39-C40
26	P	1270	CDL	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	C77-C78-C79-C80
26	G	269	CDL	C37-C38-C39-C40
26	T	1269	CDL	C37-C38-C39-C40
26	T	1269	CDL	C60-C61-C62-C63
26	T	1269	CDL	C80-C81-C82-C83
19	L	522	TGL	OA1-CA1-OG1-CG1
19	A	521	TGL	OA1-CA1-OG1-CG1
26	G	269	CDL	OA9-CA7-OA8-CA6
26	T	1269	CDL	OA9-CA7-OA8-CA6
19	Y	1522	TGL	OA1-CA1-OG1-CG1
19	N	1521	TGL	OA1-CA1-OG1-CG1
26	C	270	CDL	C17-C18-C19-C20
26	P	1270	CDL	C17-C18-C19-C20
26	G	269	CDL	C60-C61-C62-C63
19	Y	1522	TGL	C21-C20-CA9-CA8
19	L	522	TGL	C21-C20-CA9-CA8
26	G	269	CDL	O1-C1-CA2-OA2
26	T	1269	CDL	O1-C1-CA2-OA2
19	A	521	TGL	CA2-CA1-OG1-CG1
19	N	1521	TGL	CA2-CA1-OG1-CG1
19	A	523	TGL	C21-C20-CA9-CA8
19	Q	1523	TGL	C21-C20-CA9-CA8
22	O	1230	PSC	C2-C1-O01-C02
22	B	230	PSC	C2-C1-O01-C02
19	A	523	TGL	C11-C10-CB9-CB8
19	Q	1523	TGL	C11-C10-CB9-CB8
19	N	1521	TGL	C11-C10-CB9-CB8
19	A	523	TGL	C16-C15-CC9-CC8
19	L	522	TGL	C11-C10-CB9-CB8
19	L	522	TGL	C16-C15-CC9-CC8
19	A	521	TGL	C21-C20-CA9-CA8
19	A	521	TGL	C11-C10-CB9-CB8
19	Q	1523	TGL	C16-C15-CC9-CC8
19	Y	1522	TGL	C11-C10-CB9-CB8
19	N	1521	TGL	C21-C20-CA9-CA8
23	W	1060	CHD	C13-C17-C20-C22
19	Y	1522	TGL	C16-C15-CC9-CC8
23	W	1060	CHD	C17-C20-C22-C23
19	Y	1522	TGL	CA2-CA1-OG1-CG1
23	W	1060	CHD	C13-C17-C20-C21
23	J	60	CHD	C13-C17-C20-C22
20	A	524	PGV	O12-C04-C05-C06

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Mol	Chain	Res	Type	Atoms
20	N	1524	PGV	O12-C04-C05-C06
19	L	522	TGL	CA2-CA1-OG1-CG1
22	O	1230	PSC	C20-C19-O03-C01
22	B	230	PSC	C20-C19-O03-C01
23	J	60	CHD	C13-C17-C20-C21
23	J	60	CHD	C17-C20-C22-C23
20	A	524	PGV	O12-C04-C05-O05
26	C	270	CDL	O1-C1-CB2-OB2
26	P	1270	CDL	O1-C1-CB2-OB2
26	G	269	CDL	O1-C1-CB2-OB2
26	T	1269	CDL	O1-C1-CB2-OB2
20	N	1524	PGV	O12-C04-C05-O05
23	W	1060	CHD	C21-C20-C22-C23
24	C	272	DMU	C1-C6-O16-C18
24	P	1272	DMU	C1-C6-O16-C18
22	O	1230	PSC	O04-C19-O03-C01
22	B	230	PSC	O04-C19-O03-C01
24	M	526	DMU	O5-C4-C57-O61
24	M	526	DMU	O6-C11-C9-C8
24	P	1272	DMU	C3-C4-C57-O61
24	Z	1526	DMU	O6-C11-C9-C8
20	A	524	PGV	C19-C20-C21-C22
22	O	1230	PSC	C1-C2-C3-C4
22	B	230	PSC	C1-C2-C3-C4
20	N	1524	PGV	C19-C20-C21-C22
24	Z	1526	DMU	O5-C4-C57-O61
24	C	272	DMU	C3-C4-C57-O61
23	J	60	CHD	C21-C20-C22-C23
19	L	522	TGL	CC3-CC4-CC5-CC6
25	T	263	PEK	C28-C29-C30-C31
25	G	1263	PEK	C28-C29-C30-C31
20	P	1268	PGV	O05-C05-C06-O06
22	B	230	PSC	C20-C21-C22-C23
22	O	1230	PSC	C20-C21-C22-C23
19	Y	1522	TGL	CC3-CC4-CC5-CC6
24	Z	1526	DMU	O16-C18-C19-C22
24	M	526	DMU	O16-C18-C19-C22
20	P	1268	PGV	O12-C04-C05-O05
20	C	268	PGV	O12-C04-C05-O05
19	A	523	TGL	CA2-CA1-OG1-CG1
26	C	270	CDL	CB7-C71-C72-C73
26	P	1270	CDL	CB7-C71-C72-C73

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Mol	Chain	Res	Type	Atoms
26	G	269	CDL	CA5-C11-C12-C13
26	T	1269	CDL	CA5-C11-C12-C13
23	C	271	CHD	C17-C20-C22-C23
20	P	1268	PGV	C2-C1-O01-C02
26	T	1269	CDL	C11-CA5-OA6-CA4
25	T	263	PEK	C03-O11-P-O12
26	C	270	CDL	CB2-OB2-PB2-OB5
26	P	1270	CDL	CA2-OA2-PA1-OA5
26	P	1270	CDL	CB2-OB2-PB2-OB5
26	G	269	CDL	CB3-OB5-PB2-OB2
26	T	1269	CDL	CB3-OB5-PB2-OB2
25	G	1263	PEK	C03-O11-P-O12
19	Q	1523	TGL	CA2-CA1-OG1-CG1
19	A	523	TGL	OA1-CA1-OG1-CG1
19	Q	1523	TGL	OA1-CA1-OG1-CG1
26	G	269	CDL	CA2-C1-CB2-OB2
20	P	1268	PGV	O12-C04-C05-C06
26	T	1269	CDL	CA2-C1-CB2-OB2
20	C	268	PGV	O12-C04-C05-C06
26	G	269	CDL	OA7-CA5-OA6-CA4
26	T	1269	CDL	OA7-CA5-OA6-CA4
24	Z	1526	DMU	C3-C4-C57-O61
26	G	269	CDL	C11-CA5-OA6-CA4
20	C	268	PGV	C2-C1-O01-C02
23	P	1271	CHD	C17-C20-C22-C23
26	C	270	CDL	C51-C52-C53-C54
26	P	1270	CDL	C59-C60-C61-C62
26	G	269	CDL	C58-C59-C60-C61
22	O	1230	PSC	C2-C3-C4-C5
22	O	1230	PSC	C29-C30-C31-C32
20	P	1268	PGV	C22-C23-C24-C25
22	B	230	PSC	C2-C3-C4-C5
22	B	230	PSC	C29-C30-C31-C32
26	T	1269	CDL	C58-C59-C60-C61
20	C	268	PGV	C13-C14-C15-C16
20	C	268	PGV	C22-C23-C24-C25
20	N	1266	PGV	C6-C7-C8-C9
20	N	1524	PGV	C4-C5-C6-C7
26	C	270	CDL	C16-C17-C18-C19
26	C	270	CDL	C59-C60-C61-C62
26	P	1270	CDL	C16-C17-C18-C19
20	P	1268	PGV	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
20	A	604	PGV	C6-C7-C8-C9
20	P	1268	PGV	O02-C1-O01-C02
20	C	268	PGV	O02-C1-O01-C02
20	A	524	PGV	C4-C5-C6-C7
26	P	1270	CDL	C13-C14-C15-C16
26	P	1270	CDL	C51-C52-C53-C54
25	C	265	PEK	C25-C26-C27-C28
26	T	1269	CDL	C73-C74-C75-C76
25	P	1265	PEK	C25-C26-C27-C28
26	C	270	CDL	C13-C14-C15-C16
26	T	1269	CDL	C56-C57-C58-C59
26	G	269	CDL	C56-C57-C58-C59
26	G	269	CDL	C72-C73-C74-C75
26	G	269	CDL	C73-C74-C75-C76
20	P	1268	PGV	C24-C25-C26-C27
26	T	1269	CDL	C72-C73-C74-C75
20	C	268	PGV	C24-C25-C26-C27
23	C	271	CHD	C21-C20-C22-C23
24	P	1272	DMU	O5-C4-C57-O61
25	T	263	PEK	C1-C2-C3-C4
25	G	1263	PEK	O03-C01-C02-O01
26	T	1269	CDL	C13-C14-C15-C16
19	A	521	TGL	OC1-CC1-OG3-CG3
25	T	263	PEK	C29-C30-C31-C32
26	G	269	CDL	C13-C14-C15-C16
24	Z	1526	DMU	C25-C28-C31-C34
24	M	526	DMU	C25-C28-C31-C34
25	G	1263	PEK	C29-C30-C31-C32
25	T	263	PEK	C27-C28-C29-C30
20	P	1268	PGV	C3-C4-C5-C6
19	Y	1522	TGL	CC2-CC3-CC4-CC5
20	C	268	PGV	C3-C4-C5-C6
20	N	1266	PGV	C23-C24-C25-C26
20	N	1266	PGV	C29-C30-C31-C32
20	A	604	PGV	C23-C24-C25-C26
20	A	604	PGV	C29-C30-C31-C32
25	G	1263	PEK	C27-C28-C29-C30
20	A	524	PGV	C28-C29-C30-C31
20	P	1268	PGV	C04-C05-C06-O06
20	C	268	PGV	C04-C05-C06-O06
20	N	1524	PGV	C28-C29-C30-C31
19	L	522	TGL	CB4-CB5-CB6-CB7

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Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	C75-C76-C77-C78
20	C	267	PGV	C22-C23-C24-C25
25	C	264	PEK	C31-C32-C33-C34
20	P	1267	PGV	C22-C23-C24-C25
20	A	524	PGV	C24-C25-C26-C27
25	P	1264	PEK	C31-C32-C33-C34
26	G	269	CDL	C79-C80-C81-C82
20	P	1268	PGV	C27-C28-C29-C30
26	T	1269	CDL	C79-C80-C81-C82
19	Y	1522	TGL	CB4-CB5-CB6-CB7
20	C	268	PGV	C27-C28-C29-C30
20	N	1524	PGV	C24-C25-C26-C27
20	A	524	PGV	C22-C23-C24-C25
25	C	265	PEK	C31-C32-C33-C34
20	P	1267	PGV	C7-C8-C9-C10
20	N	1524	PGV	C22-C23-C24-C25
26	C	270	CDL	CA5-C11-C12-C13
26	P	1270	CDL	CA5-C11-C12-C13
20	P	1268	PGV	C1-C2-C3-C4
19	N	1521	TGL	OC1-CC1-OG3-CG3
26	C	270	CDL	C75-C76-C77-C78
19	A	521	TGL	CB6-CB7-CB8-CB9
20	C	267	PGV	C7-C8-C9-C10
24	C	272	DMU	C25-C28-C31-C34
25	P	1265	PEK	C16-C17-C18-C19
25	P	1265	PEK	C31-C32-C33-C34
24	P	1272	DMU	C25-C28-C31-C34
23	P	1271	CHD	C21-C20-C22-C23
26	C	270	CDL	C73-C74-C75-C76
26	P	1270	CDL	C73-C74-C75-C76
26	C	270	CDL	C55-C56-C57-C58
26	C	270	CDL	C74-C75-C76-C77
26	P	1270	CDL	C55-C56-C57-C58
25	C	265	PEK	C29-C30-C31-C32
25	C	265	PEK	C21-C22-C23-C24
20	C	268	PGV	C1-C2-C3-C4
25	P	1265	PEK	C21-C22-C23-C24
25	G	1263	PEK	C1-C2-C3-C4
25	C	264	PEK	C23-C24-C25-C26
25	P	1264	PEK	C23-C24-C25-C26
20	A	524	PGV	O05-C05-C06-O06
20	N	1524	PGV	O05-C05-C06-O06

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Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	C74-C75-C76-C77
25	P	1265	PEK	C29-C30-C31-C32
20	N	1266	PGV	C7-C8-C9-C10
22	O	1230	PSC	C13-C14-C15-C16
20	C	267	PGV	C11-C10-C9-C8
22	B	230	PSC	C13-C14-C15-C16
20	P	1267	PGV	C11-C10-C9-C8
25	C	265	PEK	C16-C17-C18-C19
20	N	1266	PGV	C5-C6-C7-C8
25	T	263	PEK	C25-C26-C27-C28
20	P	1268	PGV	C25-C26-C27-C28
25	C	264	PEK	C25-C26-C27-C28
26	C	270	CDL	OB7-CB5-OB6-CB4
26	P	1270	CDL	OB7-CB5-OB6-CB4
26	P	1270	CDL	C72-C73-C74-C75
20	C	268	PGV	C25-C26-C27-C28
20	A	604	PGV	C5-C6-C7-C8
19	N	1521	TGL	CB6-CB7-CB8-CB9
25	G	1263	PEK	C25-C26-C27-C28
26	C	270	CDL	C72-C73-C74-C75
20	P	1267	PGV	C25-C26-C27-C28
25	P	1264	PEK	C16-C17-C18-C19
20	A	604	PGV	C7-C8-C9-C10
26	C	270	CDL	C18-C19-C20-C21
22	B	230	PSC	C22-C23-C24-C25
20	P	1268	PGV	C28-C29-C30-C31
26	T	1269	CDL	C43-C44-C45-C46
25	C	264	PEK	C22-C23-C24-C25
26	P	1270	CDL	C18-C19-C20-C21
20	C	268	PGV	C28-C29-C30-C31
20	P	1268	PGV	C11-C10-C9-C8
25	P	1264	PEK	C22-C21-O03-C01
19	Y	1522	TGL	CC2-CC1-OG3-CG3
25	C	264	PEK	C22-C21-O03-C01
26	G	269	CDL	C21-C22-C23-C24
26	G	269	CDL	C43-C44-C45-C46
25	T	263	PEK	C26-C27-C28-C29
20	C	267	PGV	C25-C26-C27-C28
26	T	1269	CDL	C21-C22-C23-C24
25	G	1263	PEK	C26-C27-C28-C29
20	C	267	PGV	C13-C14-C15-C16
25	P	1264	PEK	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
19	L	522	TGL	CC2-CC3-CC4-CC5
20	P	1267	PGV	C13-C14-C15-C16
25	G	1263	PEK	C34-C35-C36-C37
25	T	263	PEK	C34-C35-C36-C37
26	C	270	CDL	C71-C72-C73-C74
26	P	1270	CDL	C71-C72-C73-C74
25	C	264	PEK	C16-C17-C18-C19
26	C	270	CDL	C51-CB5-OB6-CB4
26	P	1270	CDL	C51-CB5-OB6-CB4
26	C	270	CDL	C32-C33-C34-C35
25	P	1264	PEK	C25-C26-C27-C28
26	T	1269	CDL	CB5-C51-C52-C53
26	C	270	CDL	C61-C62-C63-C64
26	P	1270	CDL	C61-C62-C63-C64
25	T	263	PEK	O03-C01-C02-O01
26	P	1270	CDL	C32-C33-C34-C35
22	O	1230	PSC	C22-C23-C24-C25
22	O	1230	PSC	C04-C05-N-C08
22	B	230	PSC	C04-C05-N-C08
26	P	1270	CDL	C11-C12-C13-C14
20	P	1268	PGV	C12-C13-C14-C15
20	C	268	PGV	C11-C10-C9-C8
25	G	1263	PEK	C15-C16-C17-C18
26	T	1269	CDL	C33-C34-C35-C36
26	P	1270	CDL	C63-C64-C65-C66
26	G	269	CDL	C33-C34-C35-C36
26	G	269	CDL	C82-C83-C84-C85
24	M	526	DMU	C3-C4-C57-O61
26	C	270	CDL	C11-C12-C13-C14
26	C	270	CDL	C63-C64-C65-C66
20	C	268	PGV	C30-C31-C32-C33
26	P	1270	CDL	C42-C43-C44-C45
26	G	269	CDL	C41-C42-C43-C44
20	P	1268	PGV	C30-C31-C32-C33
26	C	270	CDL	C36-C37-C38-C39
26	C	270	CDL	C42-C43-C44-C45
26	G	269	CDL	C53-C54-C55-C56
22	O	1230	PSC	C14-C15-C16-C17
22	B	230	PSC	C14-C15-C16-C17
26	T	1269	CDL	C53-C54-C55-C56
22	O	1230	PSC	C03-O11-P-O12
22	O	1230	PSC	C04-O12-P-O11

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Mol	Chain	Res	Type	Atoms
22	B	230	PSC	C03-O11-P-O12
22	B	230	PSC	C04-O12-P-O11
25	T	263	PEK	C01-C02-C03-O11
26	C	270	CDL	OB5-CB3-CB4-CB6
26	P	1270	CDL	OB5-CB3-CB4-CB6
26	G	269	CDL	OA5-CA3-CA4-CA6
25	G	1263	PEK	C01-C02-C03-O11
26	T	1269	CDL	C82-C83-C84-C85
26	G	269	CDL	CB5-C51-C52-C53
20	A	524	PGV	C5-C6-C7-C8
26	T	1269	CDL	C41-C42-C43-C44
24	Z	1526	DMU	C22-C25-C28-C31
22	B	230	PSC	C23-C24-C25-C26
20	A	524	PGV	C12-C13-C14-C15
20	C	268	PGV	C12-C13-C14-C15
22	O	1230	PSC	C23-C24-C25-C26
20	N	1266	PGV	C30-C31-C32-C33
24	M	526	DMU	C22-C25-C28-C31
24	Z	1526	DMU	O6-C11-C9-O1
25	P	1264	PEK	C35-C36-C37-C38
22	O	1230	PSC	C27-C28-C29-C30
25	T	263	PEK	O03-C01-C02-C03
26	C	270	CDL	CB3-CB4-CB6-OB8
26	C	270	CDL	C64-C65-C66-C67
25	P	1264	PEK	O03-C01-C02-C03
26	P	1270	CDL	C36-C37-C38-C39
26	P	1270	CDL	CB3-CB4-CB6-OB8
26	P	1270	CDL	C64-C65-C66-C67
26	G	269	CDL	CB3-CB4-CB6-OB8
22	O	1230	PSC	O03-C01-C02-C03
22	B	230	PSC	O03-C01-C02-C03
26	T	1269	CDL	CB3-CB4-CB6-OB8
25	C	264	PEK	O03-C01-C02-C03
25	G	1263	PEK	O03-C01-C02-C03
20	N	1524	PGV	C5-C6-C7-C8
20	A	604	PGV	C30-C31-C32-C33
22	B	230	PSC	C27-C28-C29-C30
26	C	270	CDL	C44-C45-C46-C47
26	P	1270	CDL	C44-C45-C46-C47
20	N	1524	PGV	C12-C13-C14-C15
25	G	1263	PEK	C2-C3-C4-C5
25	P	1264	PEK	O04-C21-O03-C01

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Mol	Chain	Res	Type	Atoms
25	P	1265	PEK	C32-C33-C34-C35
24	M	526	DMU	C34-C37-C40-C43
26	P	1270	CDL	C78-C79-C80-C81
26	G	269	CDL	C31-C32-C33-C34
25	C	264	PEK	C27-C28-C29-C30
20	C	268	PGV	C31-C32-C33-C34
25	P	1264	PEK	C1-C2-C3-C4
19	A	521	TGL	CC2-CC1-OG3-CG3
26	G	269	CDL	C15-C16-C17-C18
24	Z	1526	DMU	C34-C37-C40-C43
20	C	267	PGV	C15-C16-C17-C18
26	T	1269	CDL	C71-C72-C73-C74
20	P	1267	PGV	C15-C16-C17-C18
25	G	1263	PEK	C30-C31-C32-C33
20	A	524	PGV	C03-C02-O01-C1
20	N	1524	PGV	C03-C02-O01-C1
20	A	524	PGV	C26-C27-C28-C29
25	C	265	PEK	C32-C33-C34-C35
22	B	230	PSC	C3-C4-C5-C6
20	N	1524	PGV	C26-C27-C28-C29
25	T	263	PEK	C30-C31-C32-C33
26	P	1270	CDL	C39-C40-C41-C42
26	G	269	CDL	C35-C36-C37-C38
22	O	1230	PSC	C3-C4-C5-C6
20	P	1268	PGV	C31-C32-C33-C34
26	T	1269	CDL	C31-C32-C33-C34
25	C	264	PEK	C35-C36-C37-C38
20	C	268	PGV	C14-C15-C16-C17
19	L	522	TGL	CC2-CC1-OG3-CG3
26	C	270	CDL	C78-C79-C80-C81
25	P	1264	PEK	C24-C25-C26-C27
26	C	270	CDL	C84-C85-C86-C87
26	T	1269	CDL	C35-C36-C37-C38
26	P	1270	CDL	C84-C85-C86-C87
19	L	522	TGL	OB1-CB1-OG2-CG2
26	C	270	CDL	C39-C40-C41-C42
26	G	269	CDL	C71-C72-C73-C74
20	C	268	PGV	C23-C24-C25-C26
20	P	1268	PGV	C23-C24-C25-C26
20	P	1268	PGV	C14-C15-C16-C17
22	O	1230	PSC	C24-C25-C26-C27
22	B	230	PSC	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
25	C	264	PEK	O04-C21-O03-C01
25	C	264	PEK	C24-C25-C26-C27
25	P	1264	PEK	C17-C18-C19-C20
26	G	269	CDL	C14-C15-C16-C17
26	T	1269	CDL	C44-C45-C46-C47
26	G	269	CDL	C44-C45-C46-C47
20	P	1267	PGV	C23-C24-C25-C26
19	N	1521	TGL	CC2-CC1-OG3-CG3
25	P	1264	PEK	C26-C27-C28-C29
25	P	1264	PEK	C27-C28-C29-C30
26	T	1269	CDL	OA5-CA3-CA4-CA6
26	T	1269	CDL	C14-C15-C16-C17
20	C	268	PGV	C5-C6-C7-C8
25	T	263	PEK	C22-C21-O03-C01
19	Y	1522	TGL	OB1-CB1-OG2-CG2
19	A	521	TGL	C12-C13-C14-C29
20	P	1268	PGV	C4-C5-C6-C7
20	P	1268	PGV	C5-C6-C7-C8
18	N	515	HEA	C17-C18-C19-C27
25	C	264	PEK	C32-C33-C34-C35
20	C	268	PGV	C4-C5-C6-C7
19	N	1521	TGL	C12-C13-C14-C29
24	Z	1526	DMU	C28-C31-C34-C37
20	C	267	PGV	C23-C24-C25-C26
25	C	264	PEK	C17-C18-C19-C20
25	C	264	PEK	C26-C27-C28-C29
25	T	263	PEK	O04-C21-O03-C01
25	C	265	PEK	C17-C18-C19-C20
26	T	1269	CDL	C19-C20-C21-C22
25	G	1263	PEK	C22-C21-O03-C01
26	G	269	CDL	CA3-CA4-CA6-OA8
26	T	1269	CDL	CA3-CA4-CA6-OA8
26	C	270	CDL	C34-C35-C36-C37
25	C	264	PEK	C1-C2-C3-C4
25	G	1263	PEK	O04-C21-O03-C01
20	A	604	PGV	C4-C5-C6-C7
26	C	270	CDL	C38-C39-C40-C41
26	G	269	CDL	C19-C20-C21-C22
26	T	1269	CDL	C15-C16-C17-C18
26	P	1270	CDL	C38-C39-C40-C41
20	C	268	PGV	C15-C16-C17-C18
25	T	263	PEK	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	P	1264	PEK	C5-C6-C7-C8
25	P	1264	PEK	C9-C10-C11-C12
22	O	1230	PSC	C9-C10-C11-C12
25	C	265	PEK	C11-C12-C13-C14
22	B	230	PSC	C9-C10-C11-C12
25	C	264	PEK	C5-C6-C7-C8
25	C	264	PEK	C9-C10-C11-C12
25	P	1265	PEK	C11-C12-C13-C14
25	P	1265	PEK	C12-C13-C14-C15
25	G	1263	PEK	C6-C7-C8-C9
26	P	1270	CDL	C34-C35-C36-C37
26	C	270	CDL	OB5-CB3-CB4-OB6
26	P	1270	CDL	OA5-CA3-CA4-OA6
26	P	1270	CDL	OB5-CB3-CB4-OB6
25	T	263	PEK	C2-C3-C4-C5
25	T	263	PEK	C15-C16-C17-C18
18	A	515	HEA	C17-C18-C19-C27
20	P	1268	PGV	C15-C16-C17-C18
20	C	267	PGV	C31-C32-C33-C34
24	C	272	DMU	C22-C25-C28-C31
20	P	1267	PGV	C31-C32-C33-C34
22	O	1230	PSC	O03-C01-C02-O01
22	B	230	PSC	O03-C01-C02-O01
19	Y	1522	TGL	CC7-CC8-CC9-C15
25	P	1265	PEK	C17-C18-C19-C20
25	T	263	PEK	C02-C03-O11-P
25	G	1263	PEK	C02-C03-O11-P
24	P	1272	DMU	C22-C25-C28-C31
19	L	522	TGL	CC7-CC8-CC9-C15
25	P	1264	PEK	C32-C33-C34-C35
20	N	1266	PGV	C4-C5-C6-C7
23	P	1271	CHD	C13-C17-C20-C22
23	C	271	CHD	C13-C17-C20-C22
19	A	523	TGL	CA9-C20-C21-C22
26	P	1270	CDL	C43-C44-C45-C46
20	P	1268	PGV	C26-C27-C28-C29
25	G	1263	PEK	C16-C17-C18-C19
19	Q	1523	TGL	CA9-C20-C21-C22
26	C	270	CDL	C24-C25-C26-C27
26	G	269	CDL	C24-C25-C26-C27
26	C	270	CDL	C43-C44-C45-C46
23	C	271	CHD	C13-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
20	C	268	PGV	C20-C19-O03-C01
24	P	1272	DMU	O5-C6-O16-C18
24	P	1272	DMU	C34-C37-C40-C43
20	A	524	PGV	O03-C01-C02-C03
26	G	269	CDL	CB4-CB3-OB5-PB2
20	N	1524	PGV	O03-C01-C02-C03
20	C	268	PGV	O04-C19-O03-C01
20	C	268	PGV	C26-C27-C28-C29
26	C	270	CDL	OA5-CA3-CA4-OA6
23	P	1271	CHD	C13-C17-C20-C21
26	P	1270	CDL	C24-C25-C26-C27
22	O	1230	PSC	C31-C32-C33-C34
22	B	230	PSC	C31-C32-C33-C34
26	T	1269	CDL	OA6-CA4-CA6-OA8
20	C	267	PGV	C20-C21-C22-C23
20	P	1267	PGV	C20-C21-C22-C23
20	P	1267	PGV	C24-C25-C26-C27
26	T	1269	CDL	C24-C25-C26-C27
26	T	1269	CDL	C54-C55-C56-C57
20	P	1268	PGV	O04-C19-O03-C01
20	P	1268	PGV	C20-C19-O03-C01
24	M	526	DMU	C28-C31-C34-C37
20	A	524	PGV	C11-C10-C9-C8
26	G	269	CDL	CB2-OB2-PB2-OB5
26	T	1269	CDL	CB2-OB2-PB2-OB5
20	C	267	PGV	C02-C03-O11-P
26	T	1269	CDL	CB4-CB3-OB5-PB2
20	P	1267	PGV	C02-C03-O11-P
25	T	263	PEK	C03-O11-P-O13
22	O	1230	PSC	C03-O11-P-O13
22	O	1230	PSC	C04-O12-P-O13
22	O	1230	PSC	C04-C05-N-C07
22	B	230	PSC	C03-O11-P-O13
22	B	230	PSC	C04-O12-P-O13
25	G	1263	PEK	C03-O11-P-O13
20	A	524	PGV	C01-C02-C03-O11
26	C	270	CDL	OA5-CA3-CA4-CA6
20	N	1524	PGV	C01-C02-C03-O11
26	G	269	CDL	C54-C55-C56-C57
25	P	1264	PEK	O12-C04-C05-N
23	P	1271	CHD	C16-C17-C20-C22
23	C	271	CHD	C16-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
26	G	269	CDL	CB7-C71-C72-C73
20	C	267	PGV	C24-C25-C26-C27
20	A	604	PGV	C25-C26-C27-C28
25	T	263	PEK	C21-C22-C23-C24
26	T	1269	CDL	CB7-C71-C72-C73
23	P	1271	CHD	C16-C17-C20-C21
25	C	265	PEK	C30-C31-C32-C33
25	T	263	PEK	O01-C02-C03-O11
25	G	1263	PEK	O01-C02-C03-O11
25	G	1263	PEK	C21-C22-C23-C24
24	M	526	DMU	O6-C11-C9-O1
25	P	1264	PEK	C2-C1-O01-C02
25	C	264	PEK	C2-C1-O01-C02
23	C	271	CHD	C16-C17-C20-C21
22	O	1230	PSC	C04-C05-N-C06
22	B	230	PSC	C04-C05-N-C06
22	B	230	PSC	C04-C05-N-C07
19	Y	1522	TGL	CC5-CC6-CC7-CC8
25	T	263	PEK	C16-C17-C18-C19
22	O	1230	PSC	C4-C5-C6-C7
18	A	516	HEA	C2D-C3D-CAD-CBD
18	A	516	HEA	C4D-C3D-CAD-CBD
22	B	230	PSC	C4-C5-C6-C7
18	N	516	HEA	C4D-C3D-CAD-CBD
20	A	524	PGV	O03-C01-C02-O01
26	C	270	CDL	OB6-CB4-CB6-OB8
19	A	523	TGL	OG2-CG2-CG3-OG3
25	P	1264	PEK	O03-C01-C02-O01
26	P	1270	CDL	OB6-CB4-CB6-OB8
26	G	269	CDL	OA6-CA4-CA6-OA8
19	Q	1523	TGL	OG2-CG2-CG3-OG3
25	C	264	PEK	O03-C01-C02-O01
20	N	1524	PGV	O03-C01-C02-O01
22	O	1230	PSC	C11-C12-C13-C14
25	P	1265	PEK	C30-C31-C32-C33
26	T	1269	CDL	CA7-C31-C32-C33
20	N	1266	PGV	C25-C26-C27-C28
26	T	1269	CDL	C64-C65-C66-C67
19	Y	1522	TGL	OC1-CC1-OG3-CG3
26	G	269	CDL	C64-C65-C66-C67
20	N	1266	PGV	C26-C27-C28-C29
20	N	1524	PGV	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	C36-C37-C38-C39
25	P	1265	PEK	C35-C36-C37-C38
20	A	524	PGV	C20-C21-C22-C23
25	C	265	PEK	C35-C36-C37-C38
26	P	1270	CDL	OA5-CA3-CA4-CA6
24	C	272	DMU	C34-C37-C40-C43
26	G	269	CDL	CA7-C31-C32-C33
20	C	267	PGV	C1-C2-C3-C4
20	P	1267	PGV	C1-C2-C3-C4
26	G	269	CDL	C36-C37-C38-C39
26	T	1269	CDL	OA5-CA3-CA4-OA6
22	B	230	PSC	C11-C12-C13-C14
25	G	1263	PEK	C31-C32-C33-C34
26	C	270	CDL	C52-C53-C54-C55
20	A	524	PGV	C03-O11-P-O12
26	C	270	CDL	CA3-OA5-PA1-OA2
26	P	1270	CDL	CA3-OA5-PA1-OA2
20	N	1524	PGV	C03-O11-P-O12
25	T	263	PEK	C31-C32-C33-C34
26	C	270	CDL	C1-CA2-OA2-PA1
26	P	1270	CDL	C1-CA2-OA2-PA1
20	A	524	PGV	C25-C26-C27-C28
26	G	269	CDL	C12-C13-C14-C15
26	T	1269	CDL	C12-C13-C14-C15
24	C	272	DMU	O5-C6-O16-C18
20	A	604	PGV	C26-C27-C28-C29
26	P	1270	CDL	C76-C77-C78-C79
20	P	1268	PGV	O01-C02-C03-O11
19	A	521	TGL	CG2-CG3-OG3-CC1
20	N	1524	PGV	C11-C10-C9-C8
26	C	270	CDL	C76-C77-C78-C79
19	L	522	TGL	CC5-CC6-CC7-CC8
25	T	263	PEK	C32-C33-C34-C35
20	C	267	PGV	C29-C30-C31-C32
26	P	1270	CDL	C23-C24-C25-C26
20	A	604	PGV	O03-C19-C20-C21
25	G	1263	PEK	C32-C33-C34-C35
20	P	1267	PGV	C29-C30-C31-C32
26	P	1270	CDL	C52-C53-C54-C55
26	C	270	CDL	C23-C24-C25-C26
19	A	523	TGL	CG1-CG2-OG2-CB1
19	A	521	TGL	CG1-CG2-OG2-CB1

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Mol	Chain	Res	Type	Atoms
22	O	1230	PSC	C03-C02-O01-C1
19	Q	1523	TGL	CG1-CG2-OG2-CB1
22	B	230	PSC	C03-C02-O01-C1
20	P	1268	PGV	C7-C8-C9-C10
20	P	1267	PGV	C11-C12-C13-C14
20	N	1266	PGV	C9-C10-C11-C12
26	C	270	CDL	C56-C57-C58-C59
25	C	265	PEK	C12-C13-C14-C15
25	C	264	PEK	C11-C10-C9-C8
25	T	263	PEK	C33-C34-C35-C36
20	C	268	PGV	O01-C02-C03-O11
20	N	1266	PGV	O03-C19-C20-C21
22	B	230	PSC	C15-C16-C17-C18
20	P	1268	PGV	C01-C02-C03-O11
20	C	267	PGV	C11-C12-C13-C14
25	C	265	PEK	C3-C4-C5-C6
25	P	1265	PEK	C3-C4-C5-C6
20	A	604	PGV	C9-C10-C11-C12
26	P	1270	CDL	C56-C57-C58-C59
20	N	1524	PGV	C25-C26-C27-C28
25	C	265	PEK	O03-C01-C02-O01
25	P	1265	PEK	O03-C01-C02-O01
26	T	1269	CDL	C52-C53-C54-C55
25	G	1263	PEK	C33-C34-C35-C36
26	G	269	CDL	C38-C39-C40-C41
22	O	1230	PSC	C15-C16-C17-C18
19	N	1521	TGL	C13-C14-C29-C30
19	A	521	TGL	C13-C14-C29-C30
20	P	1268	PGV	C02-C03-O11-P
26	G	269	CDL	C52-C53-C54-C55
20	C	268	PGV	C7-C8-C9-C10
20	A	524	PGV	C7-C8-C9-C10
19	L	522	TGL	CB5-CB6-CB7-CB8
26	P	1270	CDL	C22-C23-C24-C25
25	T	263	PEK	C3-C4-C5-C6
20	A	604	PGV	C11-C12-C13-C14
25	G	1263	PEK	C3-C4-C5-C6
26	G	269	CDL	OA5-CA3-CA4-OA6
20	N	1266	PGV	C19-C20-C21-C22
19	L	522	TGL	OG2-CB1-CB2-CB3
19	Y	1522	TGL	OG2-CB1-CB2-CB3
20	C	268	PGV	C01-C02-C03-O11

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Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	C38-C39-C40-C41
25	P	1264	PEK	C3-C4-C5-C6
20	N	1266	PGV	C11-C12-C13-C14
20	C	267	PGV	C05-C04-O12-P
20	C	268	PGV	C02-C03-O11-P
20	C	268	PGV	C05-C04-O12-P
20	P	1268	PGV	O03-C01-C02-O01
26	C	270	CDL	C52-C51-CB5-OB6
19	N	1521	TGL	CG2-CG3-OG3-CC1
22	B	230	PSC	C7-C8-C9-C10
20	P	1267	PGV	C9-C10-C11-C12
25	P	1264	PEK	O01-C1-C2-C3
22	O	1230	PSC	O03-C19-C20-C21
22	B	230	PSC	O03-C19-C20-C21
19	Y	1522	TGL	CB5-CB6-CB7-CB8
26	G	269	CDL	CA2-OA2-PA1-OA5
26	T	1269	CDL	CA2-OA2-PA1-OA5
20	N	1524	PGV	O01-C1-C2-C3
26	C	270	CDL	C22-C23-C24-C25
20	A	524	PGV	O01-C1-C2-C3
26	P	1270	CDL	C52-C51-CB5-OB6
25	T	263	PEK	C14-C15-C16-C17
19	N	1521	TGL	CG1-CG2-OG2-CB1
20	N	1524	PGV	C7-C8-C9-C10
25	C	264	PEK	O02-C1-O01-C02
19	L	522	TGL	OG3-CC1-CC2-CC3
25	C	264	PEK	O01-C1-C2-C3
24	P	1272	DMU	C4-C3-O7-C10
26	C	270	CDL	C32-C31-CA7-OA8
19	A	523	TGL	OG2-CB1-CB2-CB3
26	P	1270	CDL	C32-C31-CA7-OA8
20	A	524	PGV	C9-C10-C11-C12
22	O	1230	PSC	C7-C8-C9-C10
20	C	267	PGV	C9-C10-C11-C12
25	C	264	PEK	C3-C4-C5-C6
20	N	1524	PGV	C9-C10-C11-C12
25	G	1263	PEK	C14-C15-C16-C17
20	P	1268	PGV	C05-C04-O12-P
19	L	522	TGL	OC1-CC1-OG3-CG3
25	C	264	PEK	C29-C30-C31-C32
19	Q	1523	TGL	OG2-CB1-CB2-CB3
22	O	1230	PSC	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
22	B	230	PSC	C12-C13-C14-C15
22	B	230	PSC	C01-C02-C03-O11
20	P	1267	PGV	C14-C15-C16-C17
20	C	268	PGV	O03-C01-C02-O01
26	C	270	CDL	C82-C83-C84-C85
18	A	516	HEA	C26-C15-C16-C17
20	A	604	PGV	C19-C20-C21-C22
19	A	523	TGL	C21-C22-C23-C24
26	P	1270	CDL	C83-C84-C85-C86
19	Q	1523	TGL	OC1-CC1-CC2-CC3
26	P	1270	CDL	C12-C11-CA5-OA6
19	Y	1522	TGL	OG3-CC1-CC2-CC3
19	Q	1523	TGL	C21-C22-C23-C24
25	P	1264	PEK	C29-C30-C31-C32
26	C	270	CDL	C32-C31-CA7-OA9
26	P	1270	CDL	C32-C31-CA7-OA9
19	Q	1523	TGL	OB1-CB1-CB2-CB3
25	C	264	PEK	O02-C1-C2-C3
26	C	270	CDL	C12-C11-CA5-OA6
26	T	1269	CDL	C39-C40-C41-C42
25	P	1265	PEK	C34-C35-C36-C37
20	A	524	PGV	O02-C1-C2-C3
19	A	523	TGL	OC1-CC1-CC2-CC3
22	O	1230	PSC	O04-C19-C20-C21
22	B	230	PSC	O04-C19-C20-C21
20	N	1524	PGV	O02-C1-C2-C3
25	C	265	PEK	C26-C27-C28-C29
22	O	1230	PSC	O01-C1-C2-C3
22	B	230	PSC	O01-C1-C2-C3
20	C	267	PGV	C14-C15-C16-C17
25	C	264	PEK	C02-C03-O11-P
26	G	269	CDL	C39-C40-C41-C42
20	A	524	PGV	C03-O11-P-O13
25	C	265	PEK	C03-O11-P-O14
25	P	1265	PEK	C03-O11-P-O14
20	N	1524	PGV	C03-O11-P-O13
22	O	1230	PSC	C01-C02-C03-O11
26	P	1270	CDL	C52-C51-CB5-OB7
22	B	230	PSC	O02-C1-C2-C3
26	P	1270	CDL	C82-C83-C84-C85
26	T	1269	CDL	C59-C60-C61-C62
25	P	1264	PEK	O02-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
22	O	1230	PSC	O02-C1-C2-C3
22	O	1230	PSC	C05-C04-O12-P
22	B	230	PSC	C05-C04-O12-P
25	P	1265	PEK	O03-C21-C22-C23
18	N	516	HEA	C26-C15-C16-C17
26	C	270	CDL	C83-C84-C85-C86
26	G	269	CDL	C11-C12-C13-C14
26	C	270	CDL	C52-C51-CB5-OB7
19	A	523	TGL	OB1-CB1-CB2-CB3
24	C	272	DMU	O5-C4-C57-O61
25	P	1265	PEK	C26-C27-C28-C29
25	C	265	PEK	O03-C21-C22-C23
20	N	1266	PGV	C31-C32-C33-C34

There are no ring outliers.

38 monomers are involved in 273 short contacts:

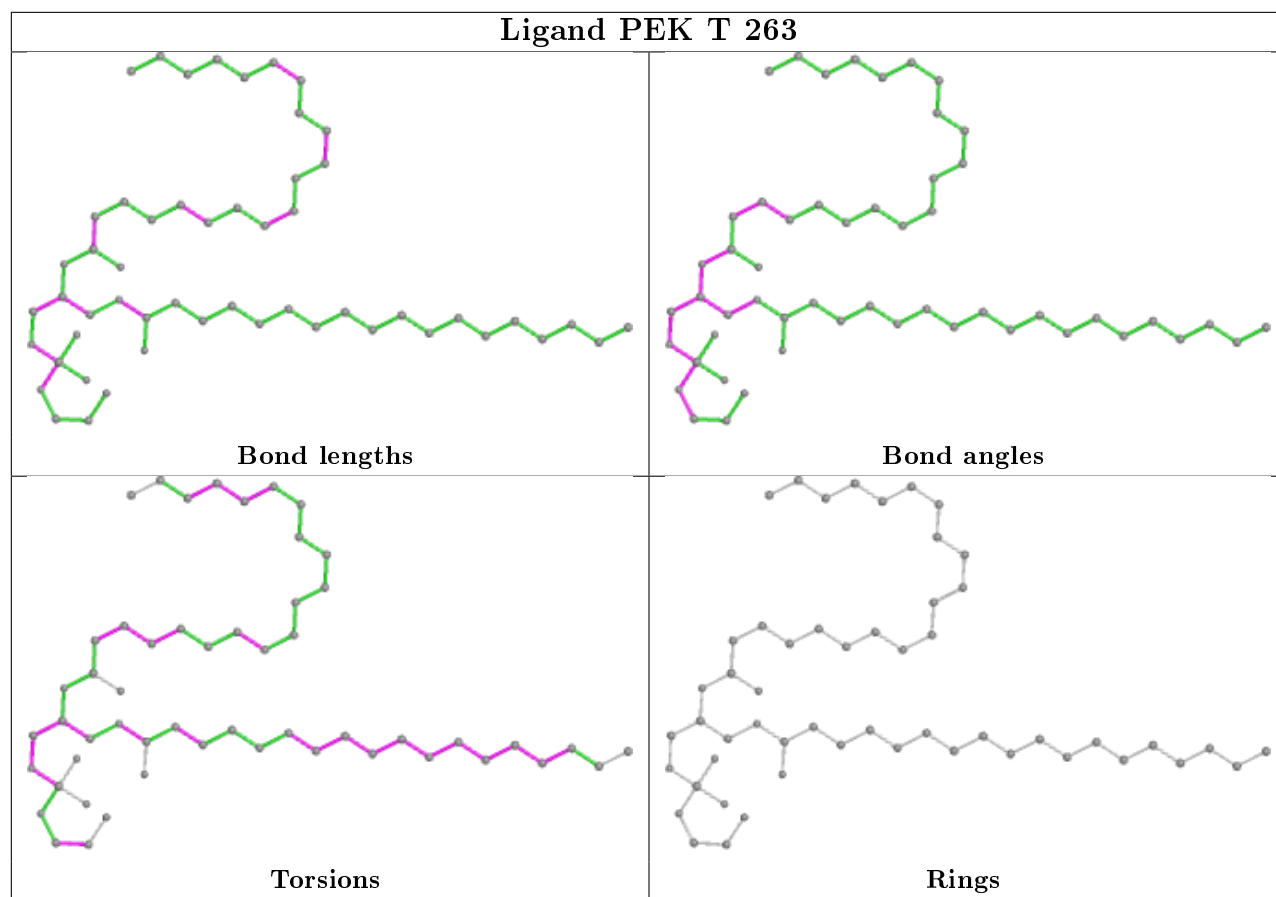
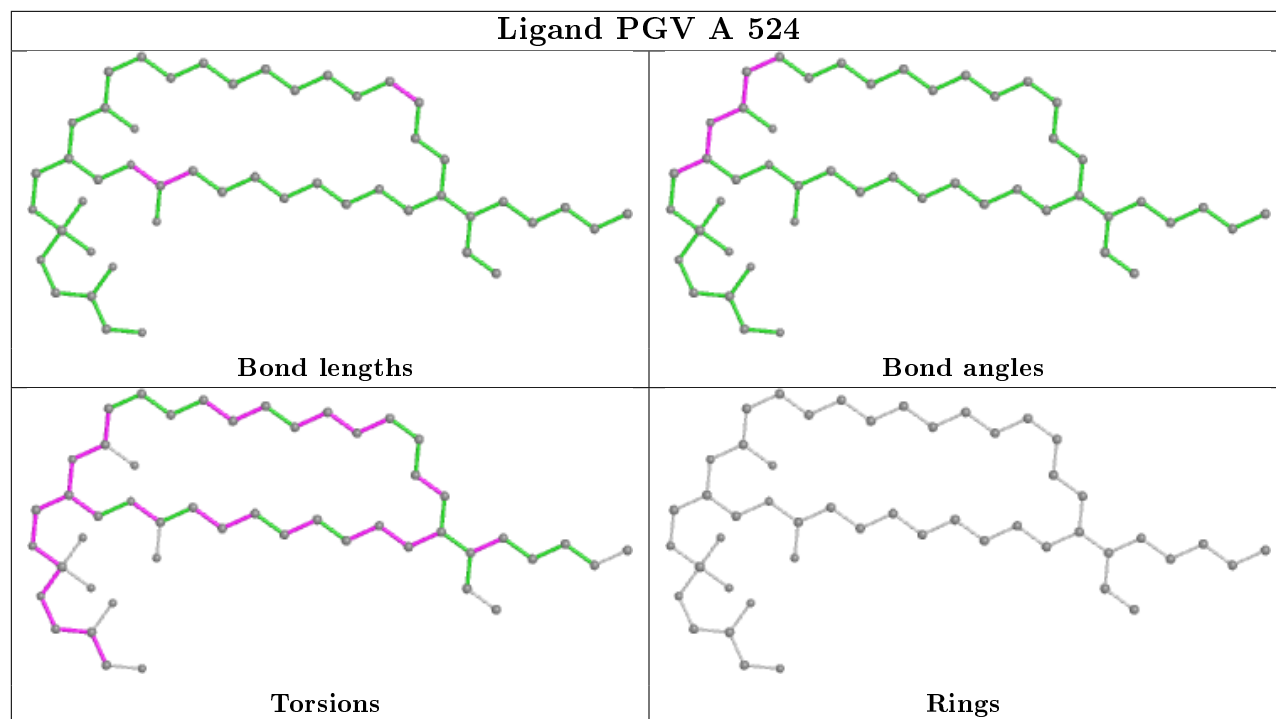
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20	A	524	PGV	8	0
25	T	263	PEK	9	0
26	C	270	CDL	16	0
19	A	523	TGL	6	0
19	N	1521	TGL	8	0
19	L	522	TGL	23	0
25	P	1264	PEK	5	0
23	B	1086	CHD	1	0
19	A	521	TGL	10	0
18	N	515	HEA	3	0
19	Y	1522	TGL	17	0
26	P	1270	CDL	18	0
26	G	269	CDL	22	0
22	O	1230	PSC	15	0
20	P	1268	PGV	2	0
18	A	516	HEA	2	0
23	J	60	CHD	3	0
18	A	515	HEA	3	0
23	O	229	CHD	1	0
25	C	265	PEK	7	0
20	N	1524	PGV	9	0
19	Q	1523	TGL	7	0
20	C	267	PGV	5	0
24	C	272	DMU	2	0

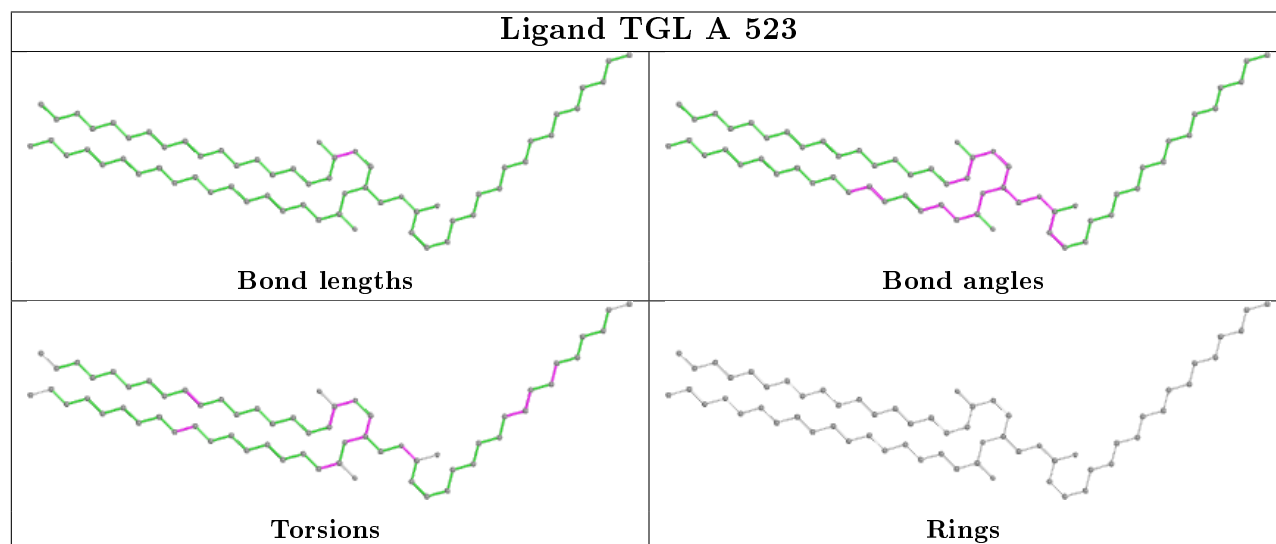
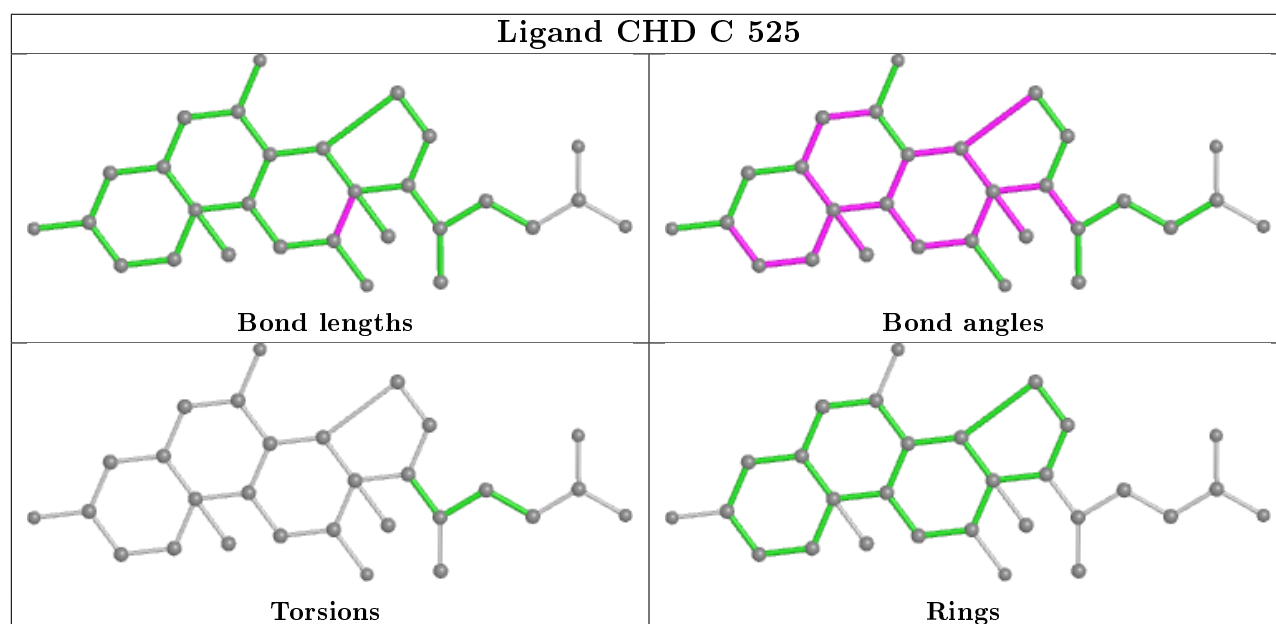
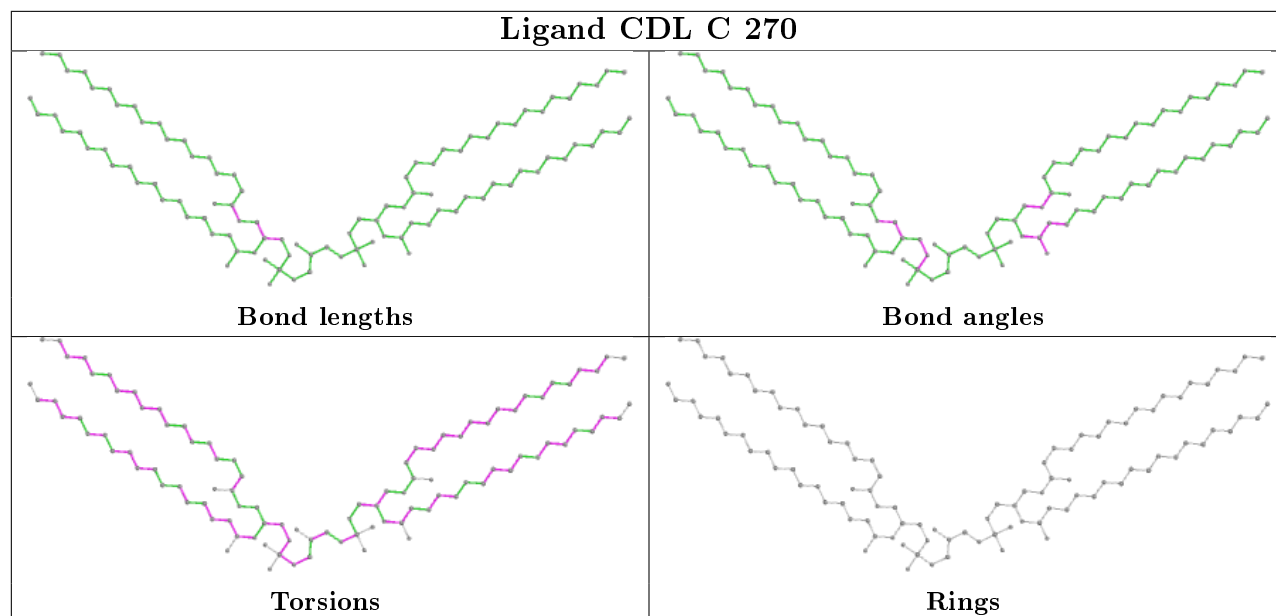
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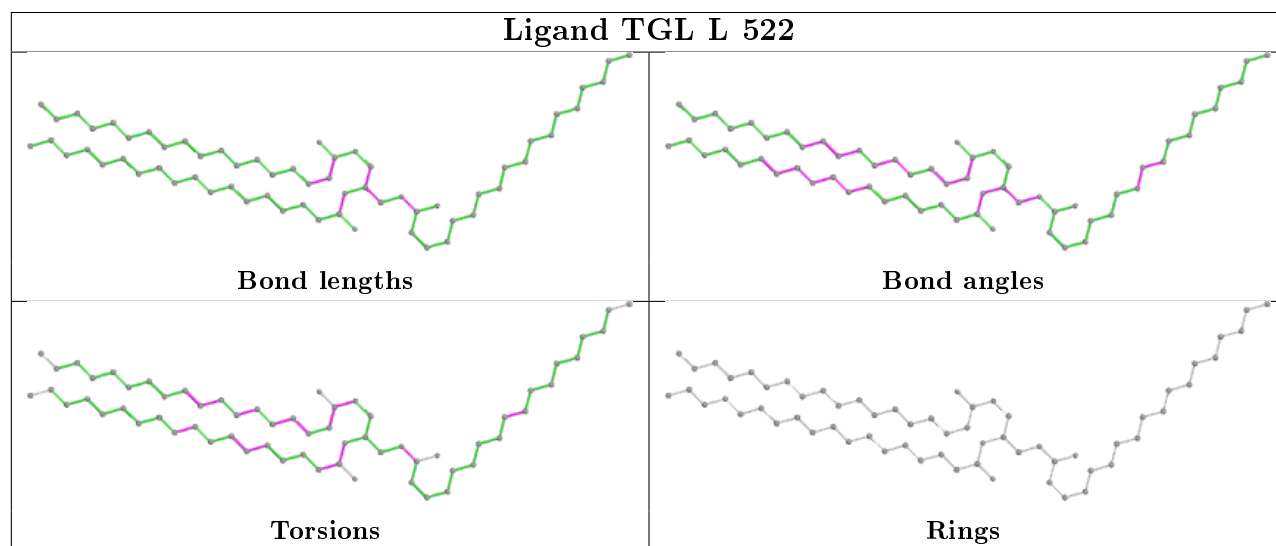
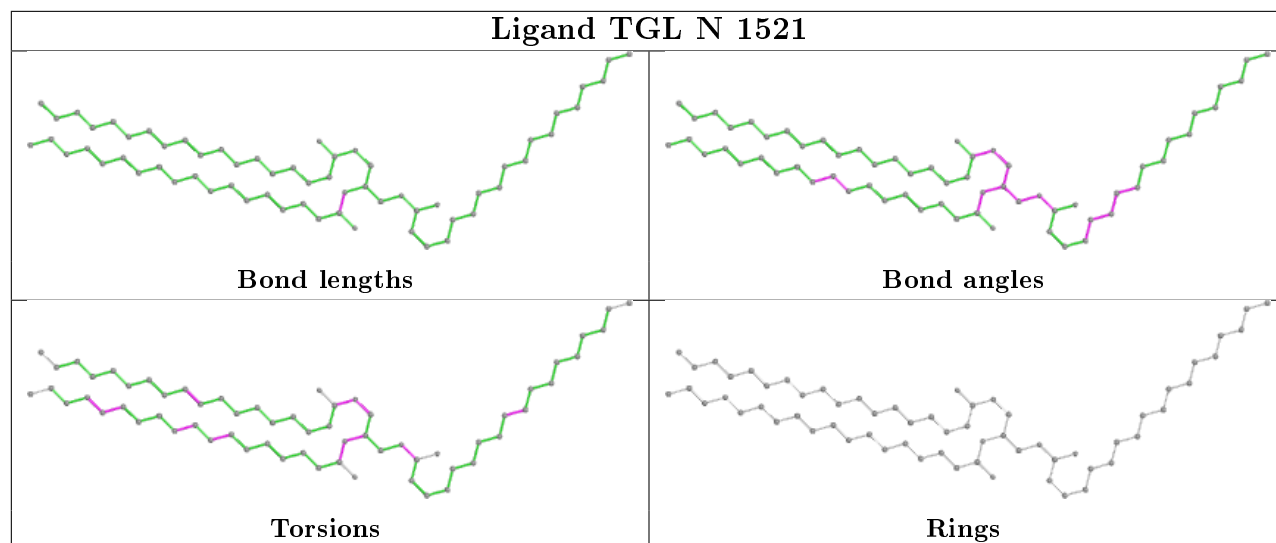
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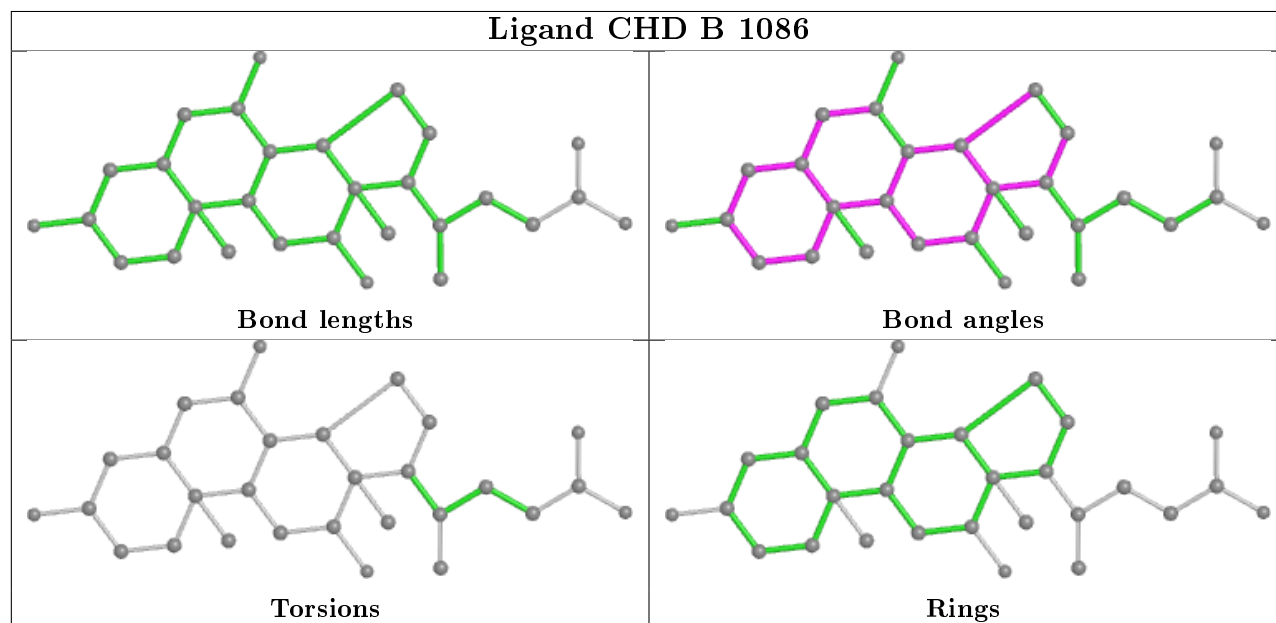
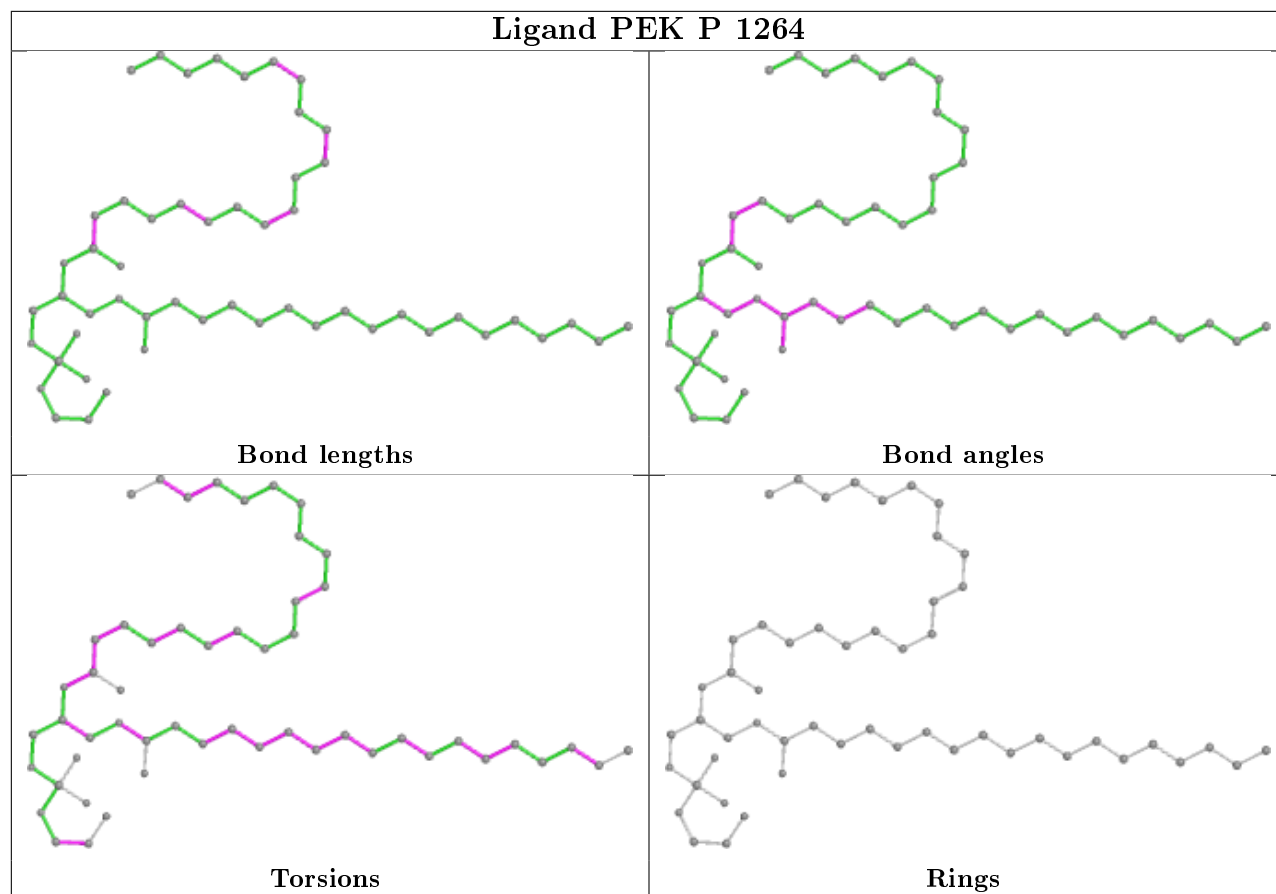
Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	230	PSC	14	0
23	P	1271	CHD	1	0
18	N	516	HEA	1	0
20	P	1267	PGV	4	0
20	C	268	PGV	2	0
26	T	1269	CDL	19	0
20	N	1266	PGV	1	0
23	W	1060	CHD	5	0
20	A	604	PGV	1	0
23	C	271	CHD	7	0
25	C	264	PEK	4	0
25	G	1263	PEK	9	0
25	P	1265	PEK	7	0
24	P	1272	DMU	8	0

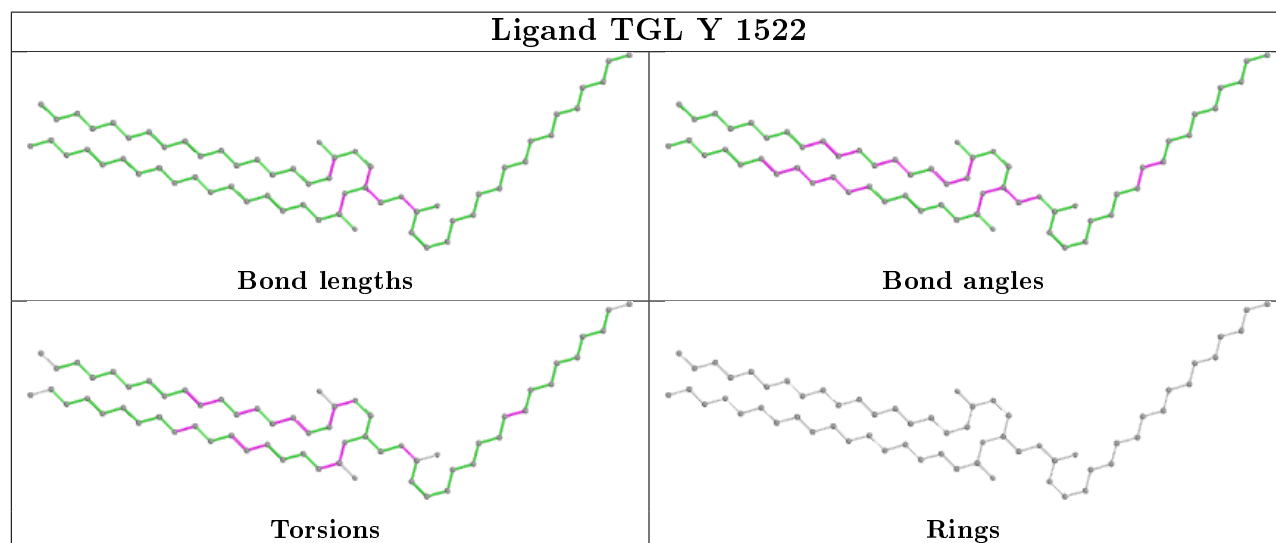
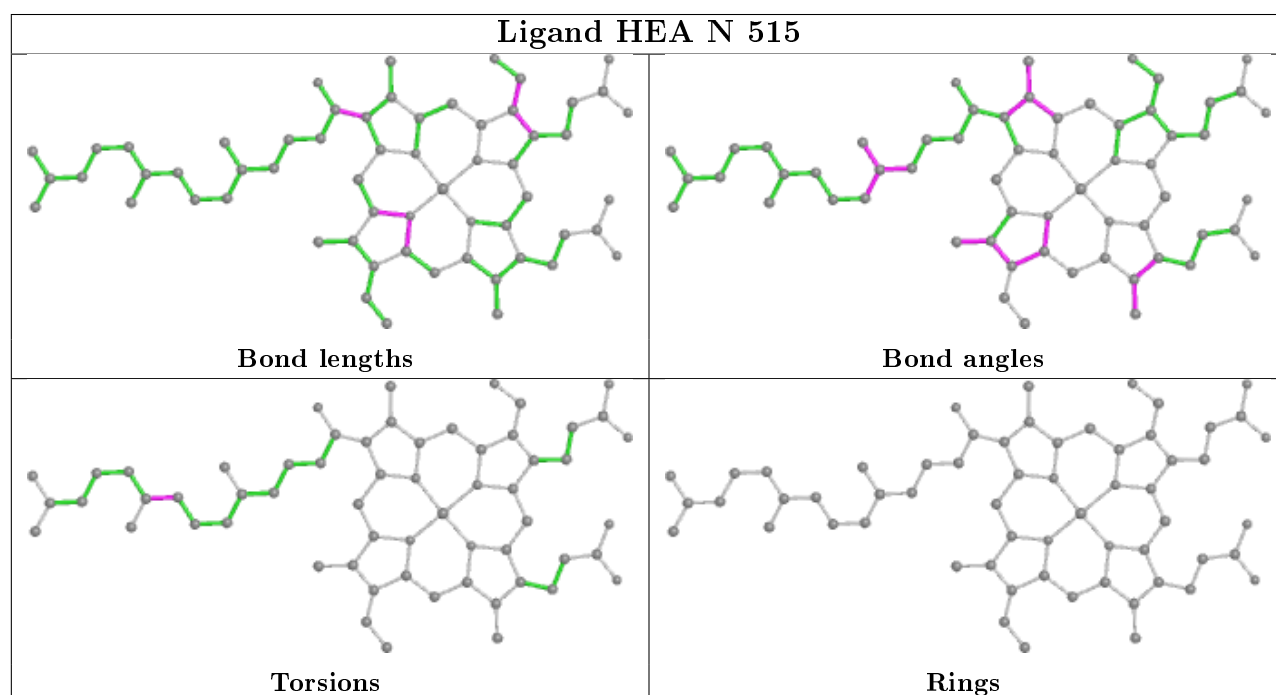
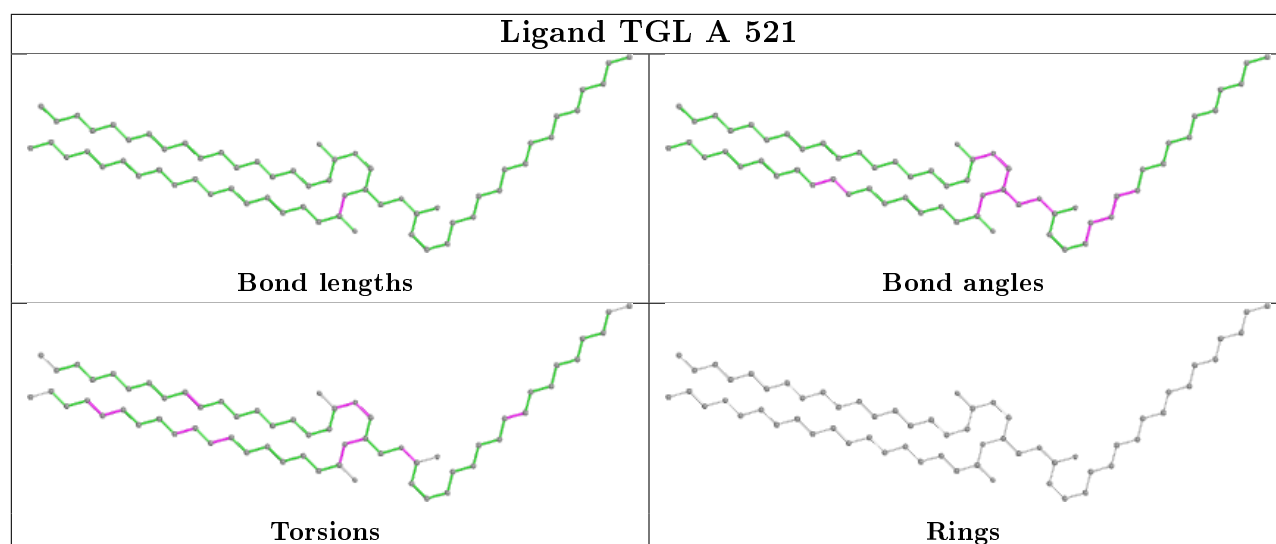
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

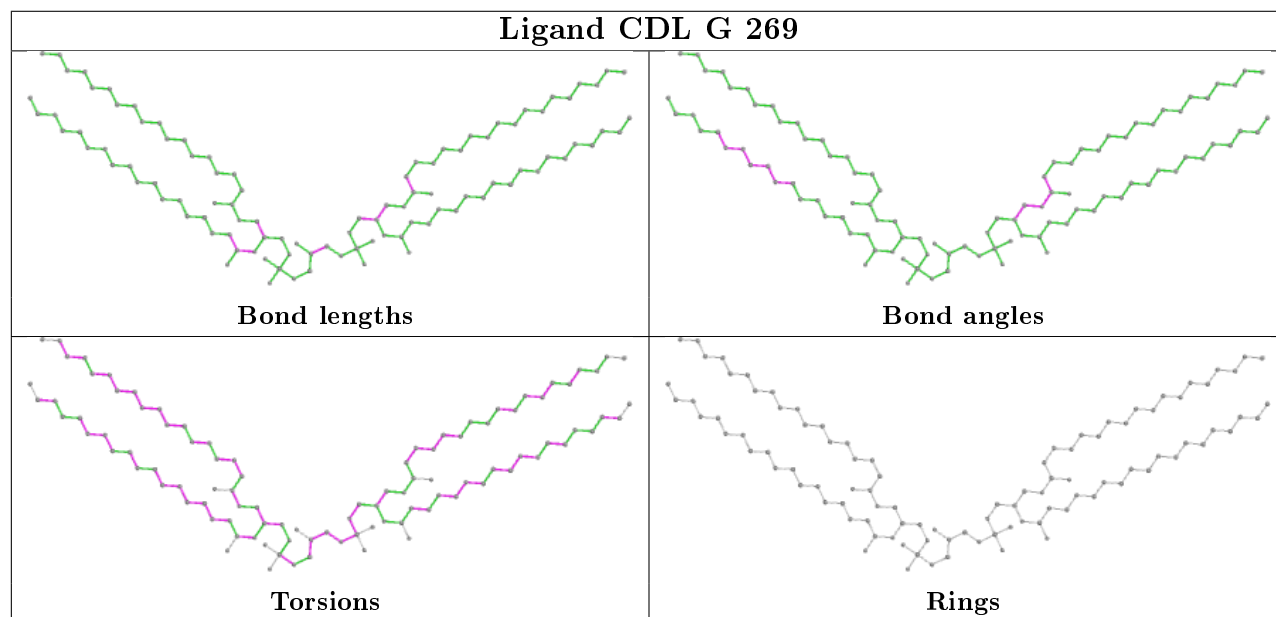
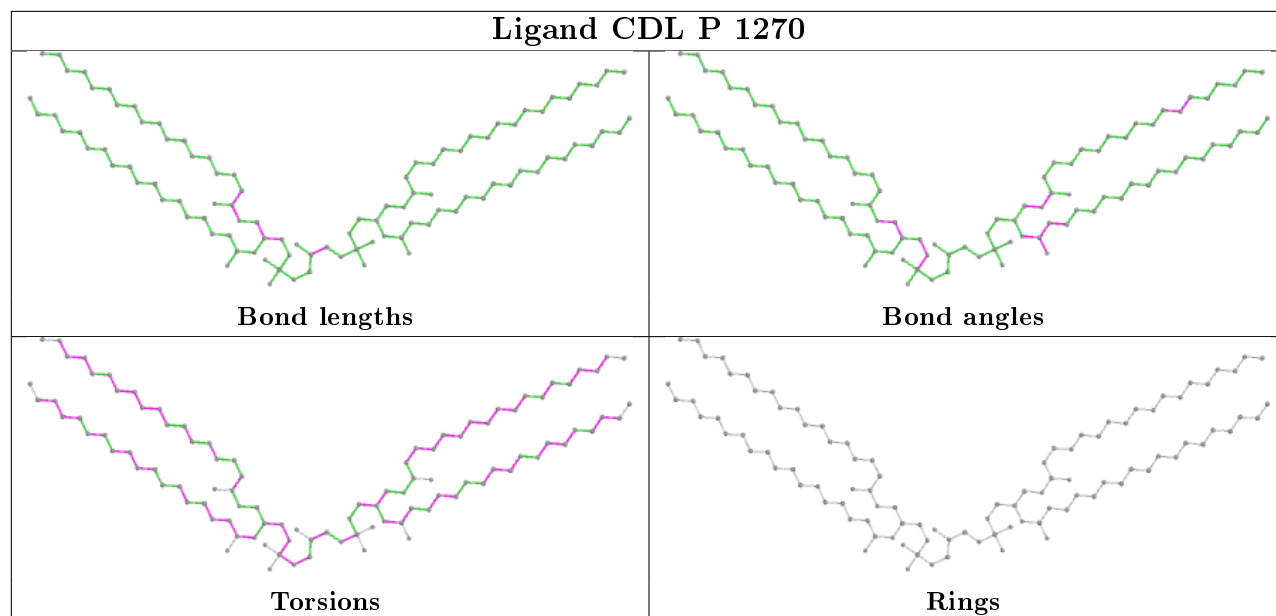




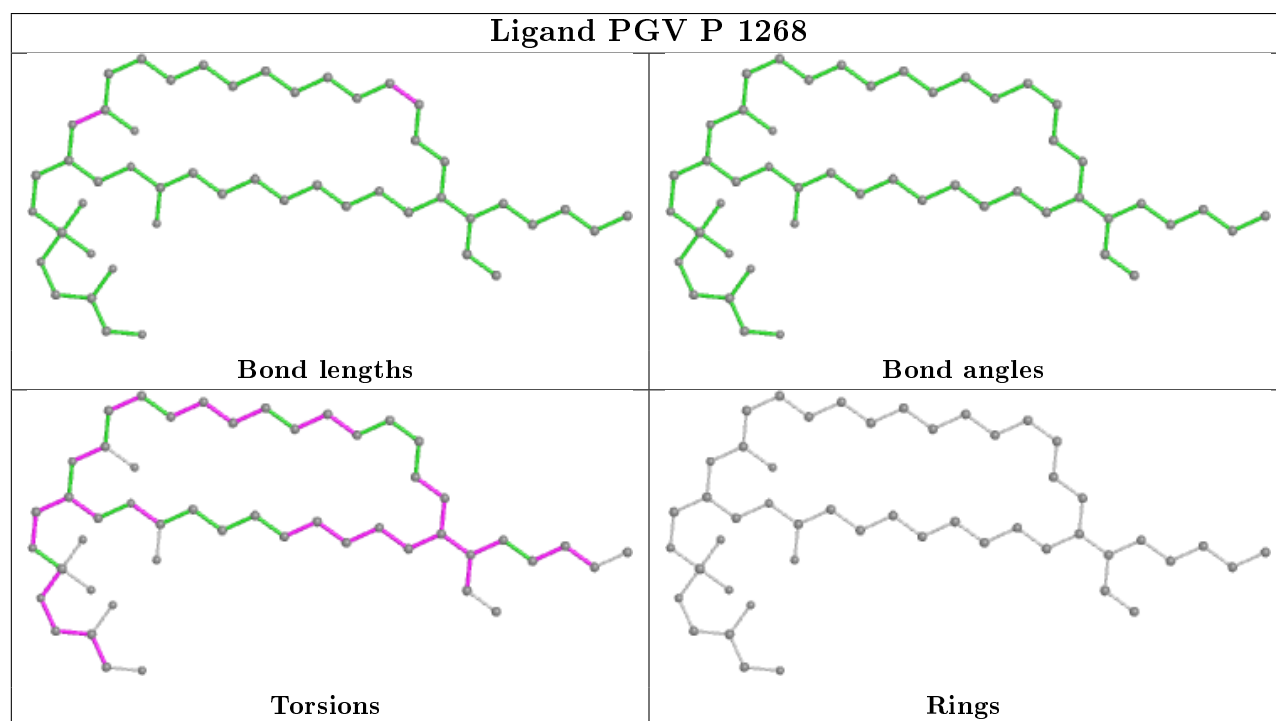
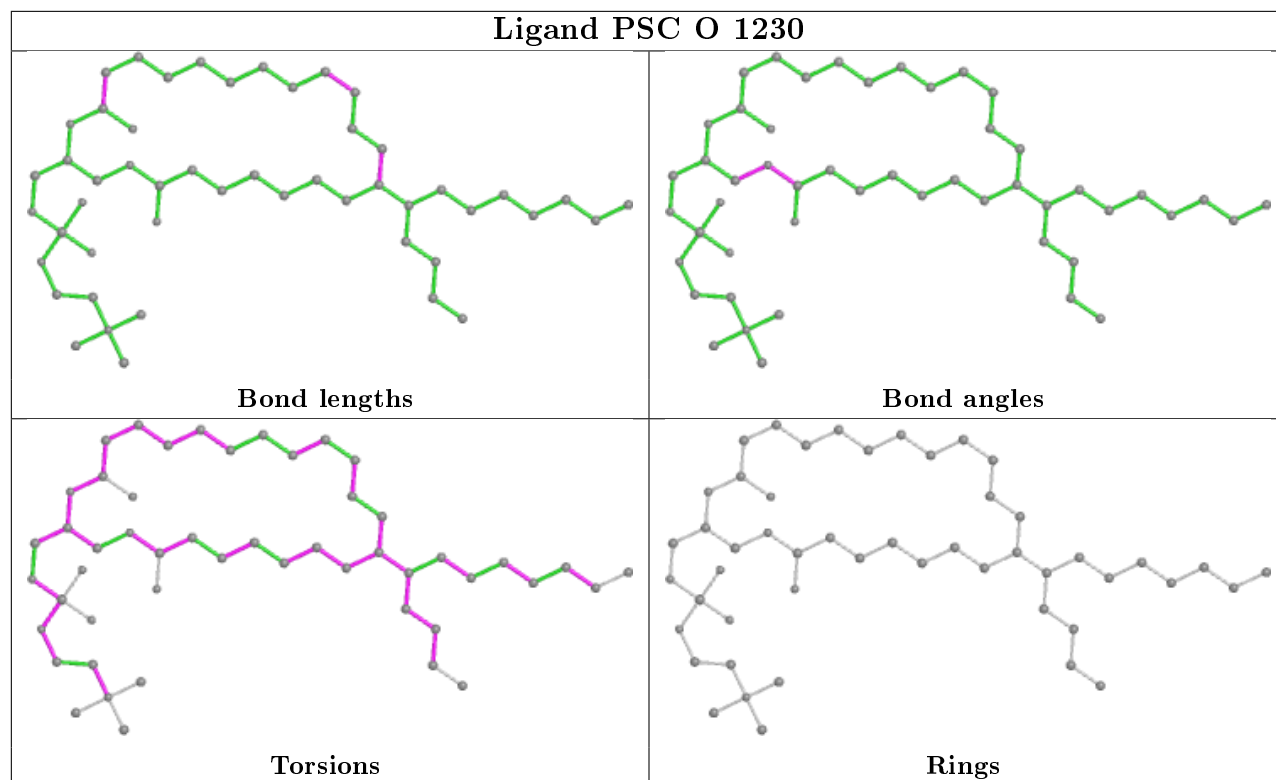


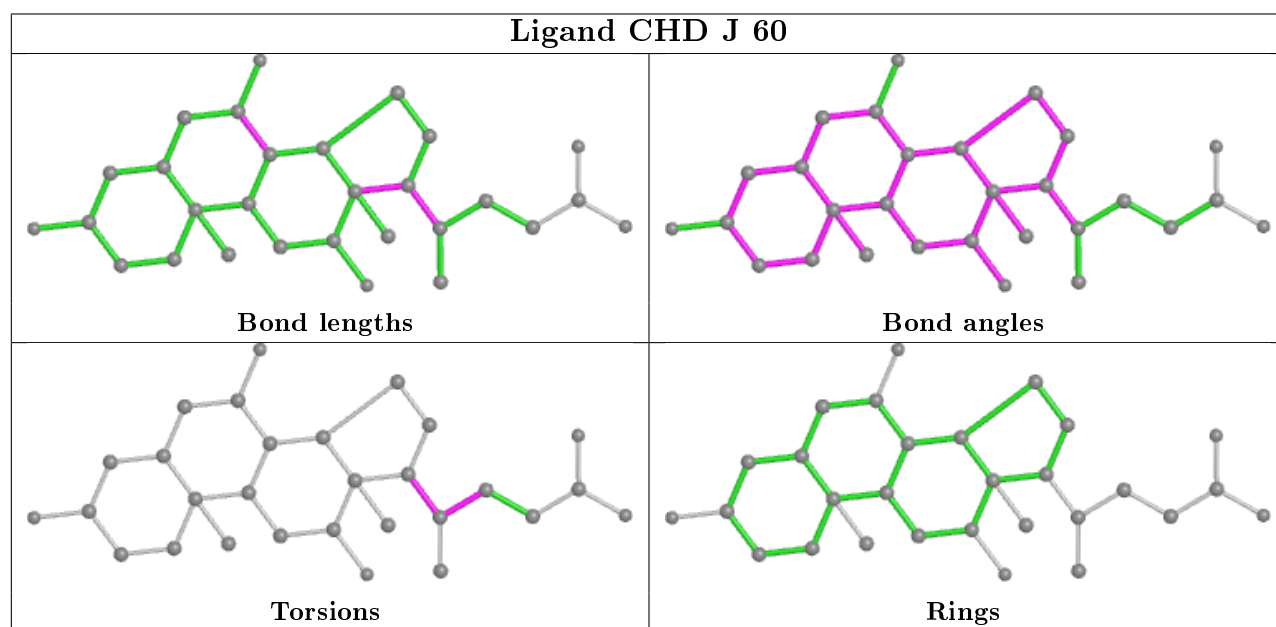
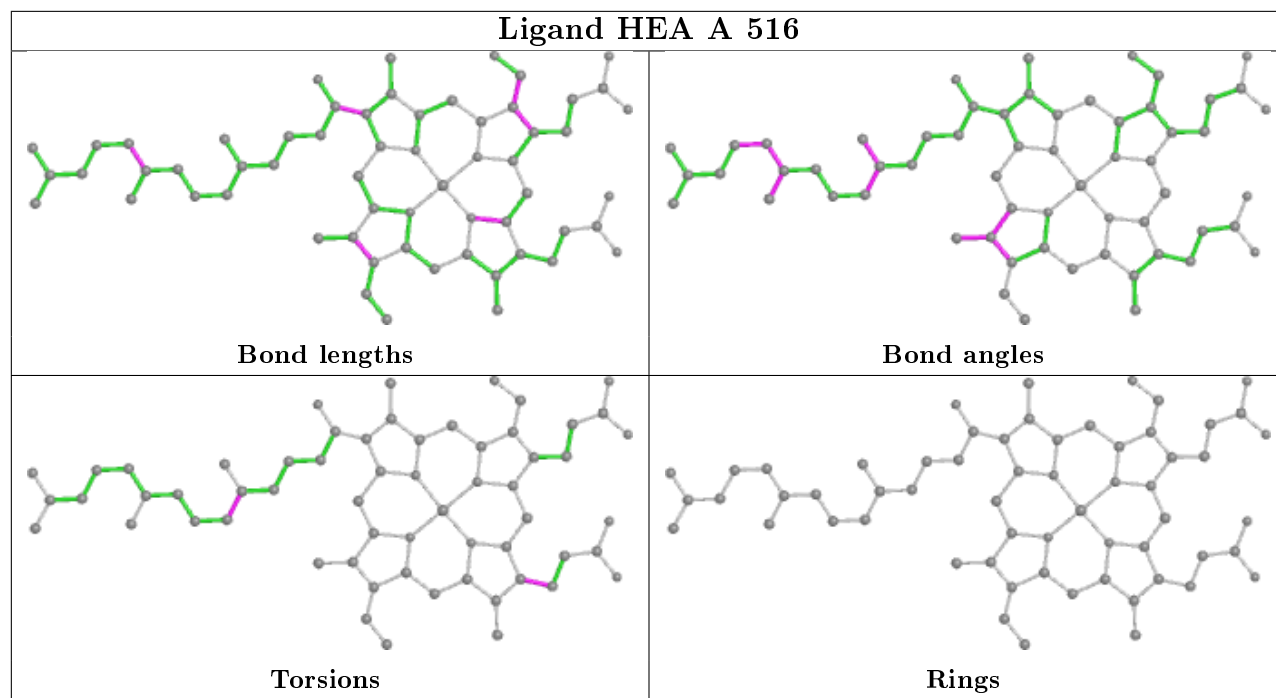


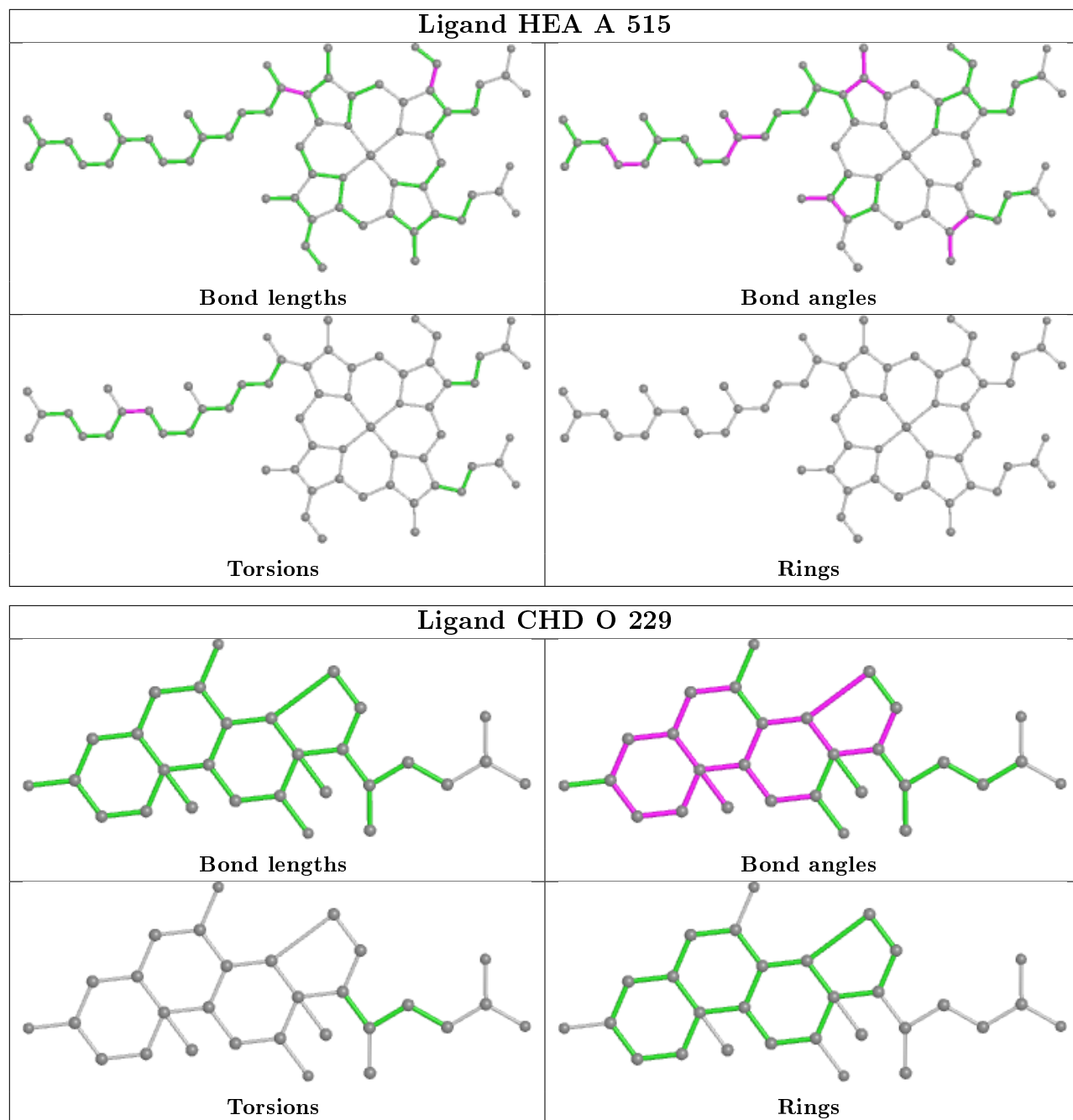




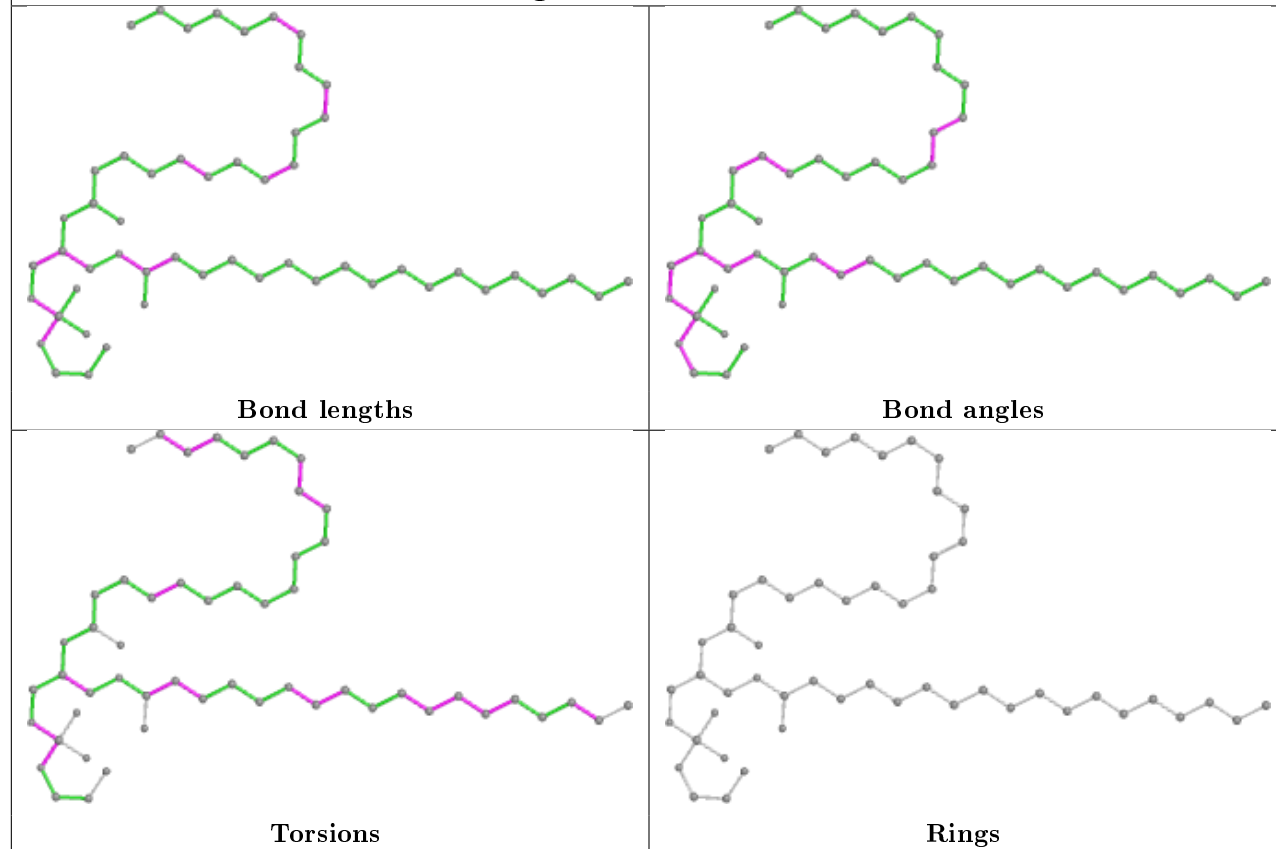




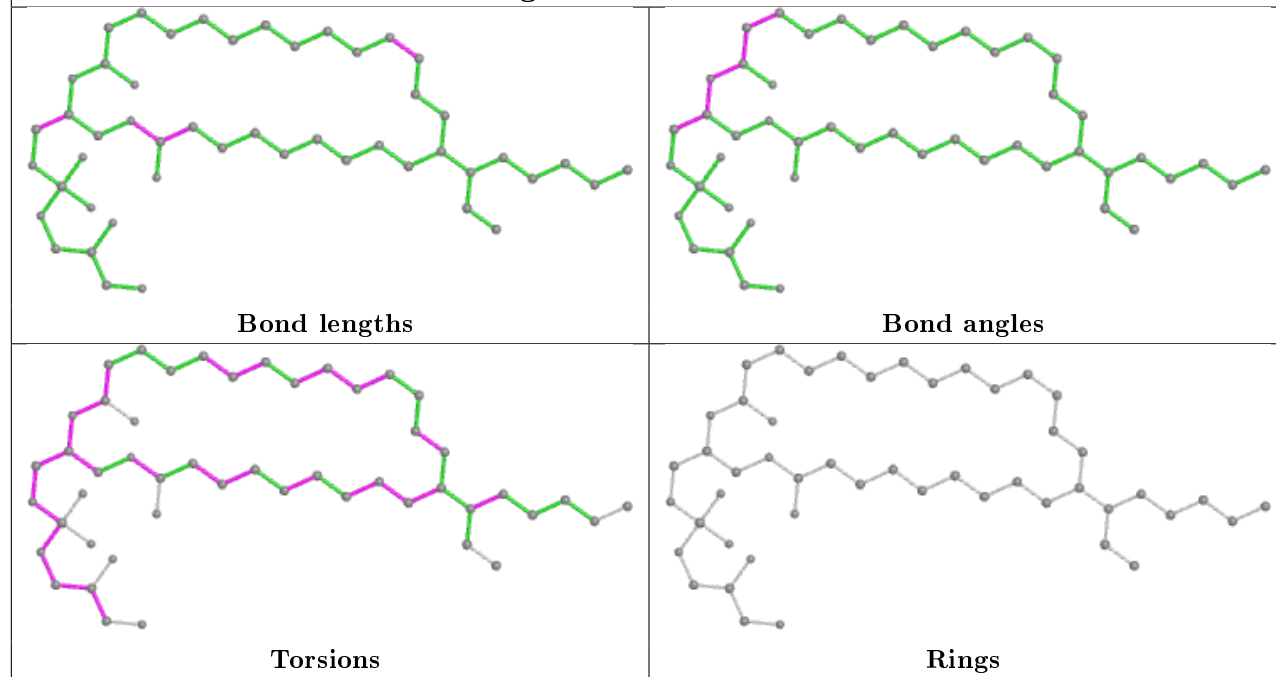


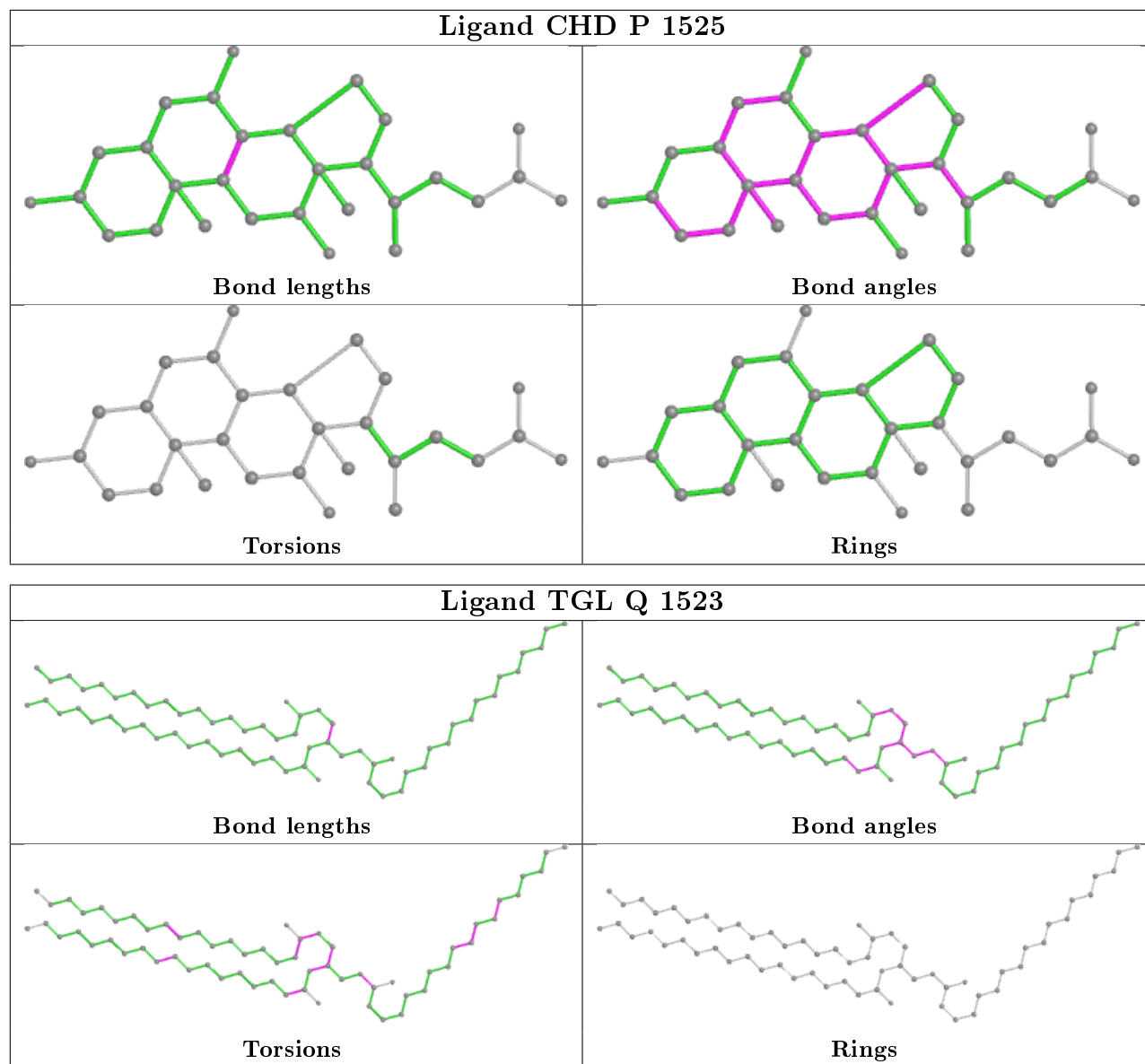


## Ligand PEK C 265

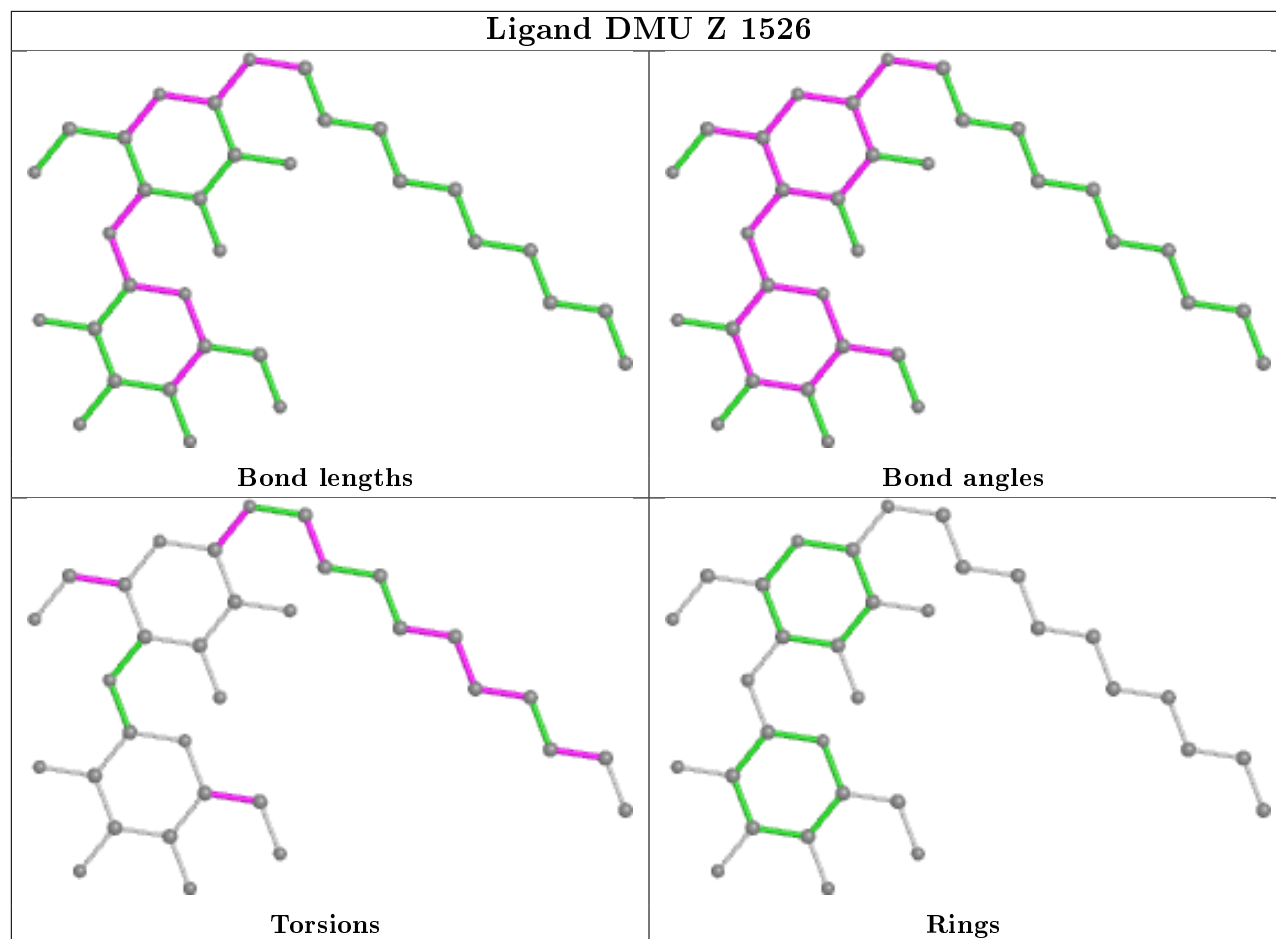


## Ligand PGV N 1524

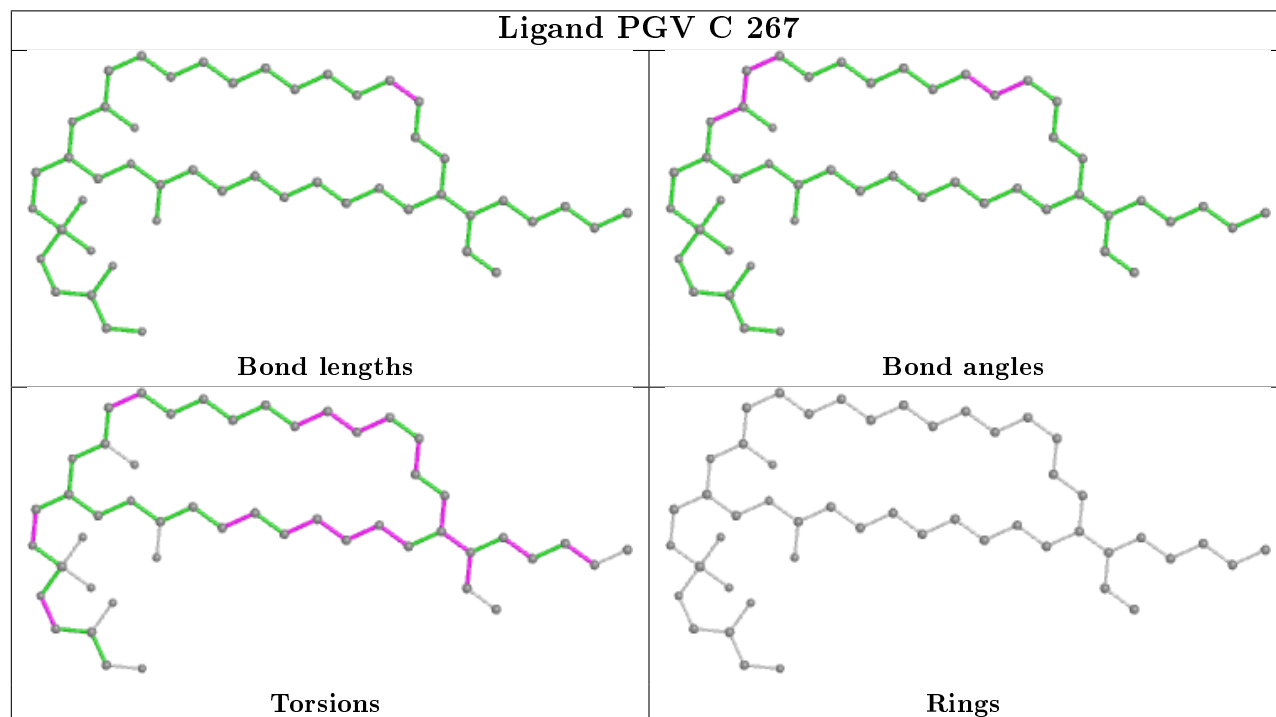




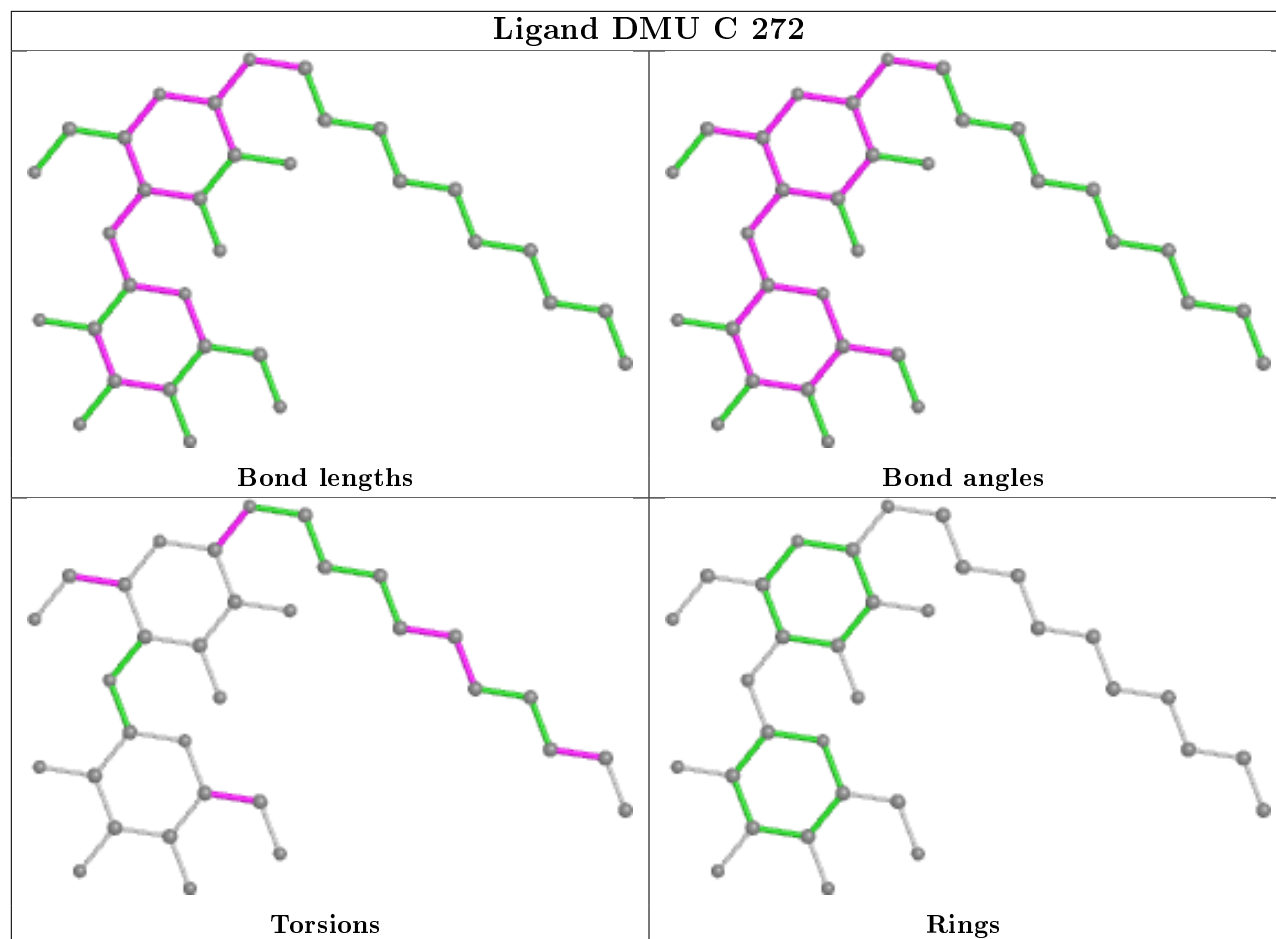
## Ligand DMU Z 1526



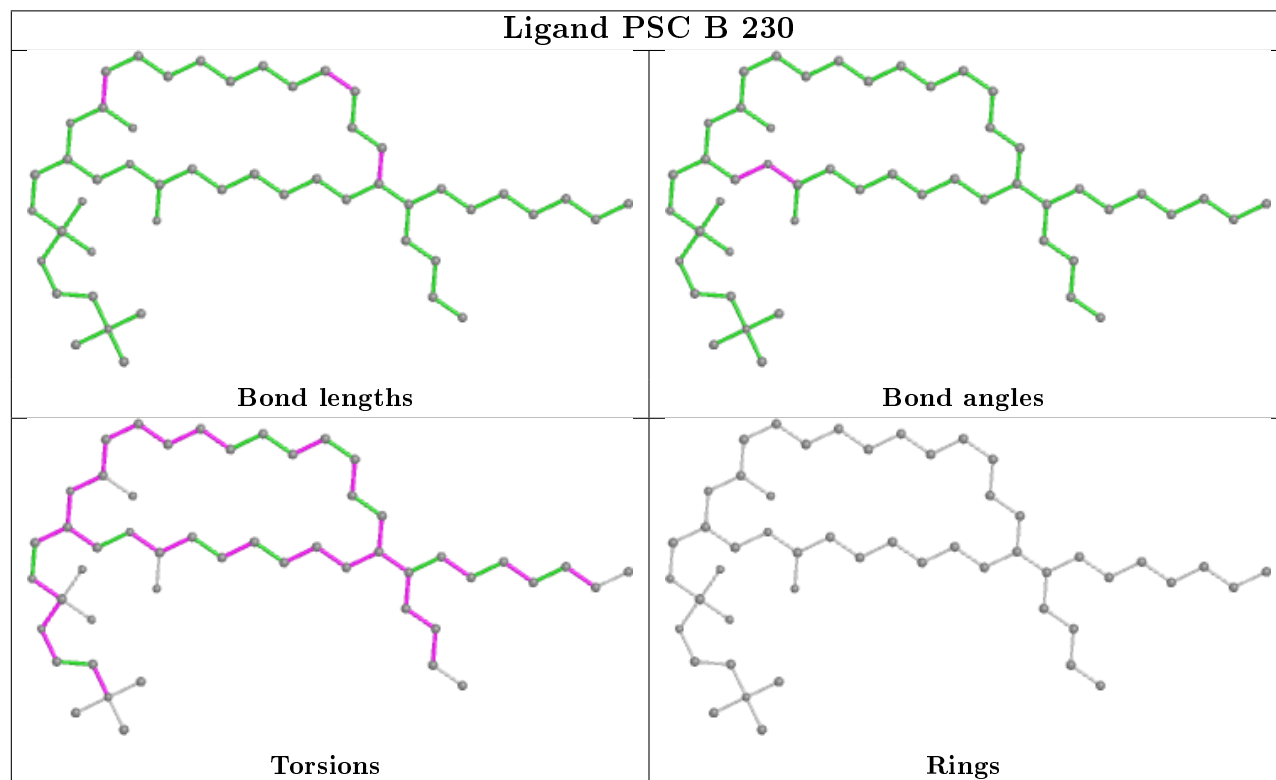
## Ligand PGV C 267



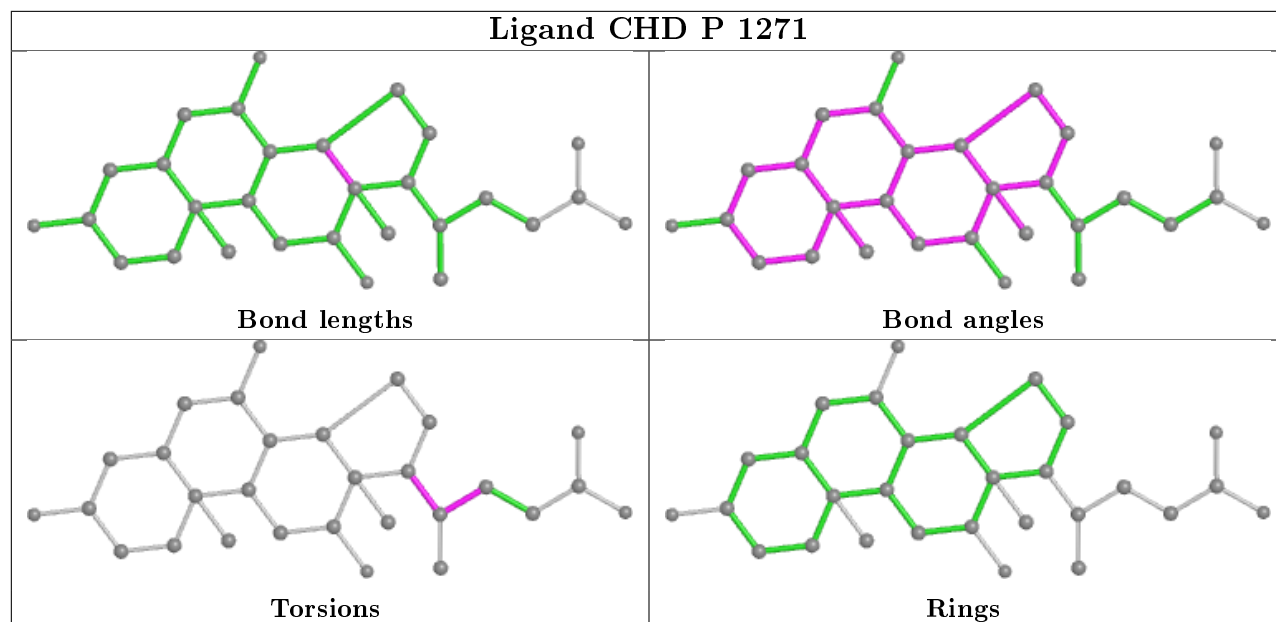
## Ligand DMU C 272



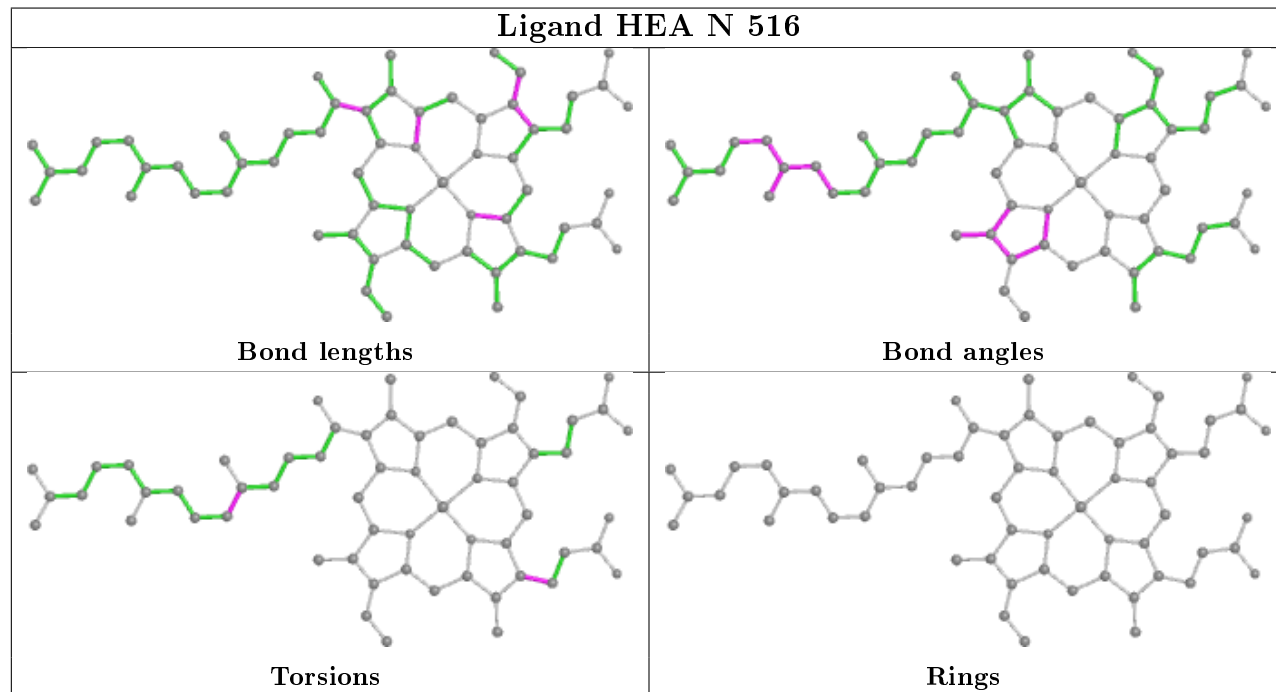
## Ligand PSC B 230



## Ligand CHD P 1271

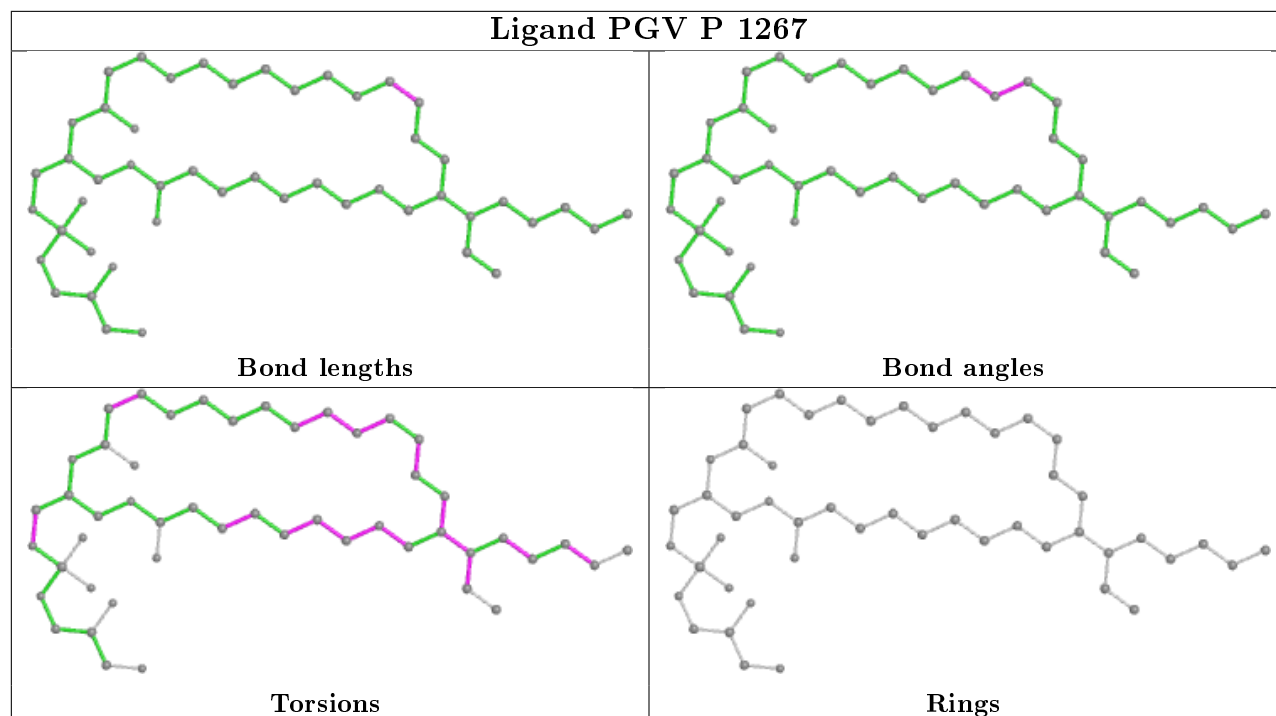


## Ligand HEA N 516

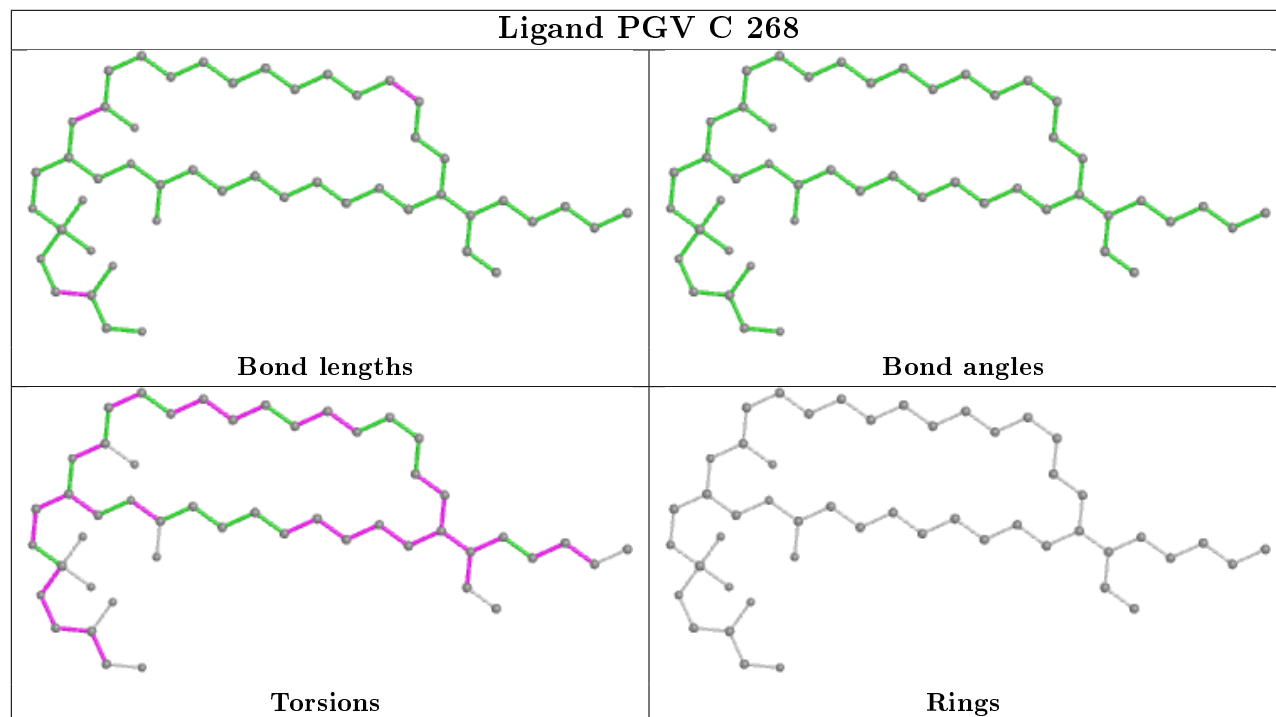


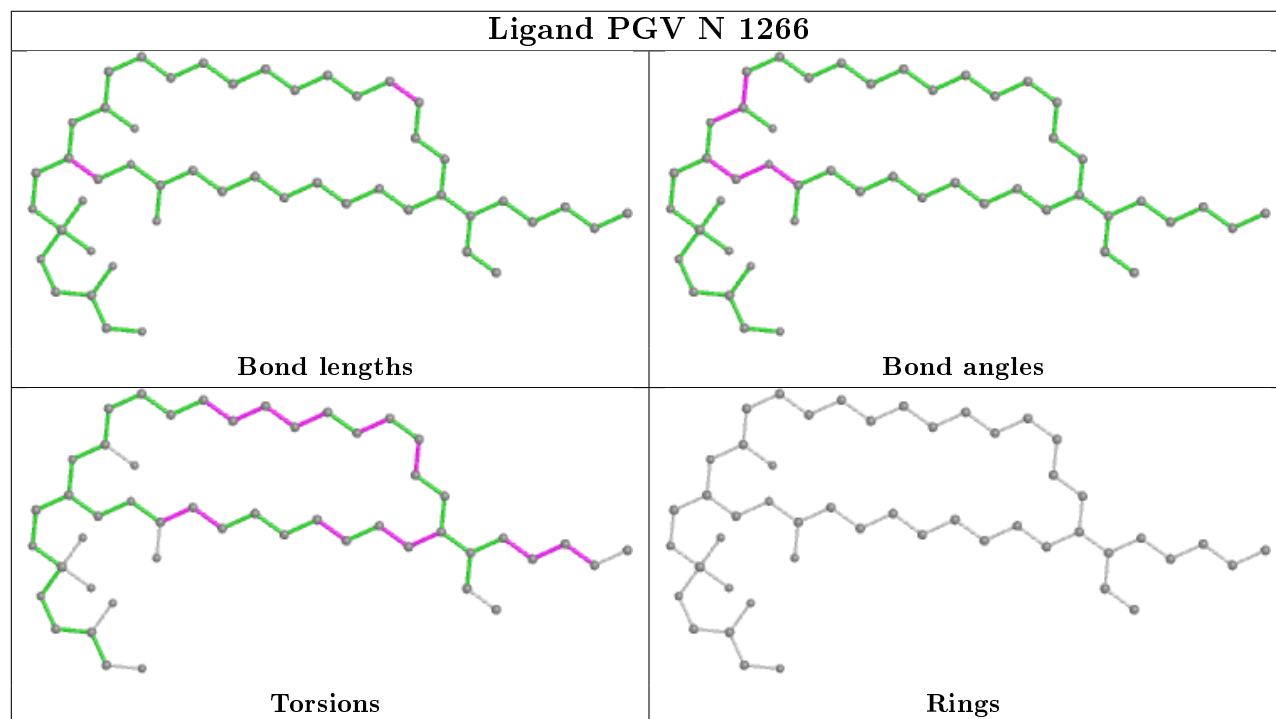
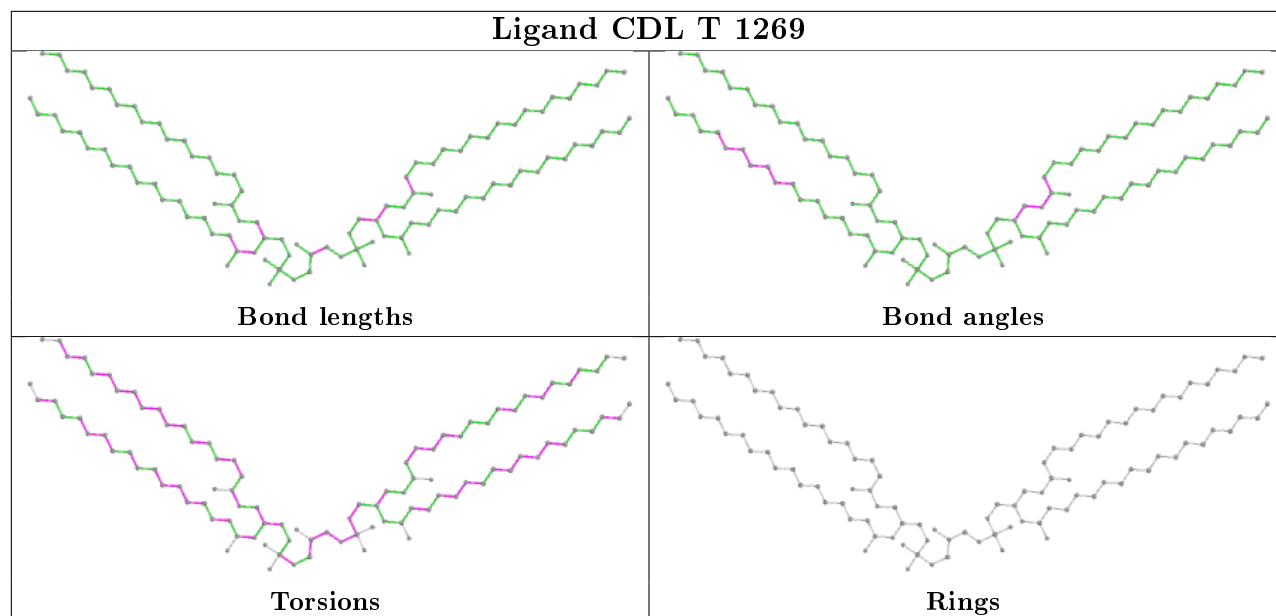


## Ligand PGV P 1267

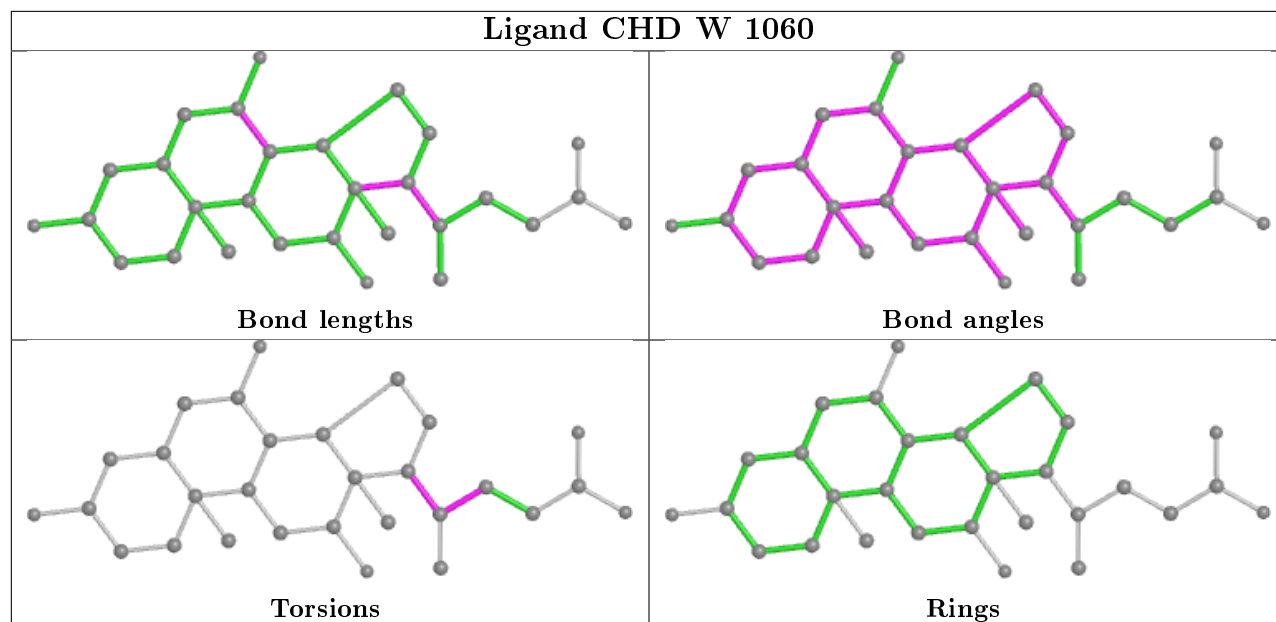


## Ligand PGV C 268

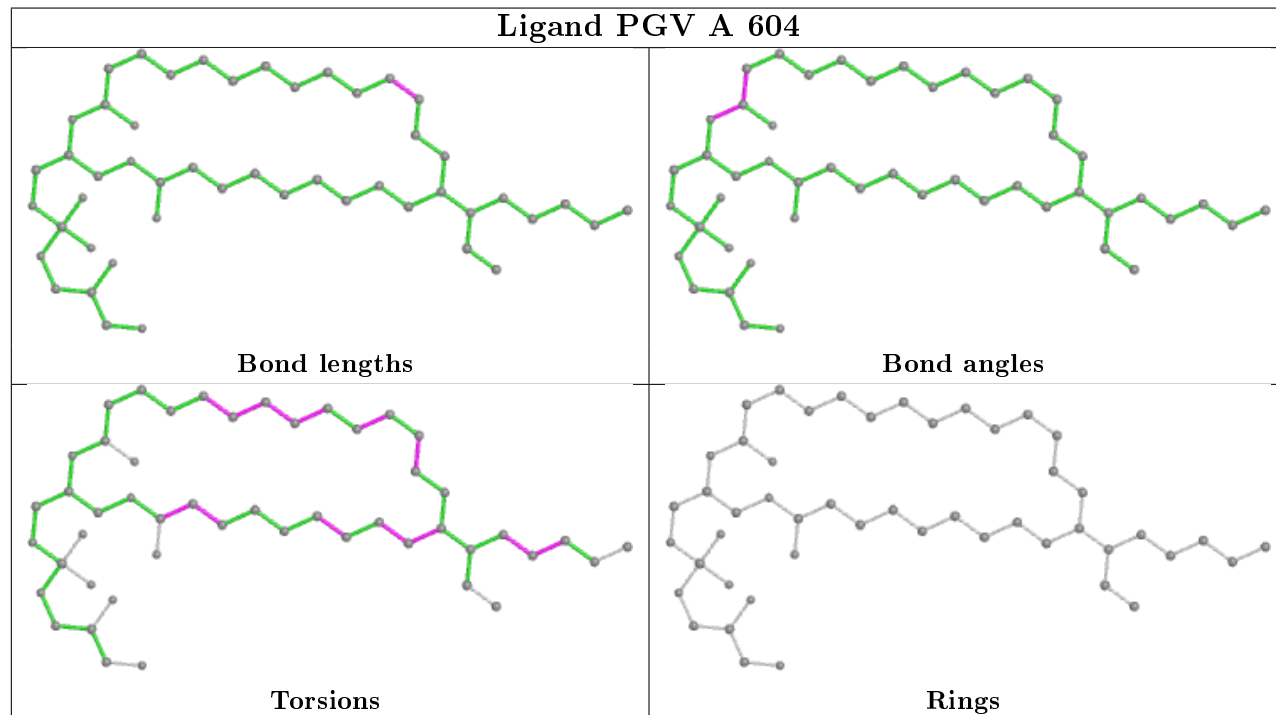


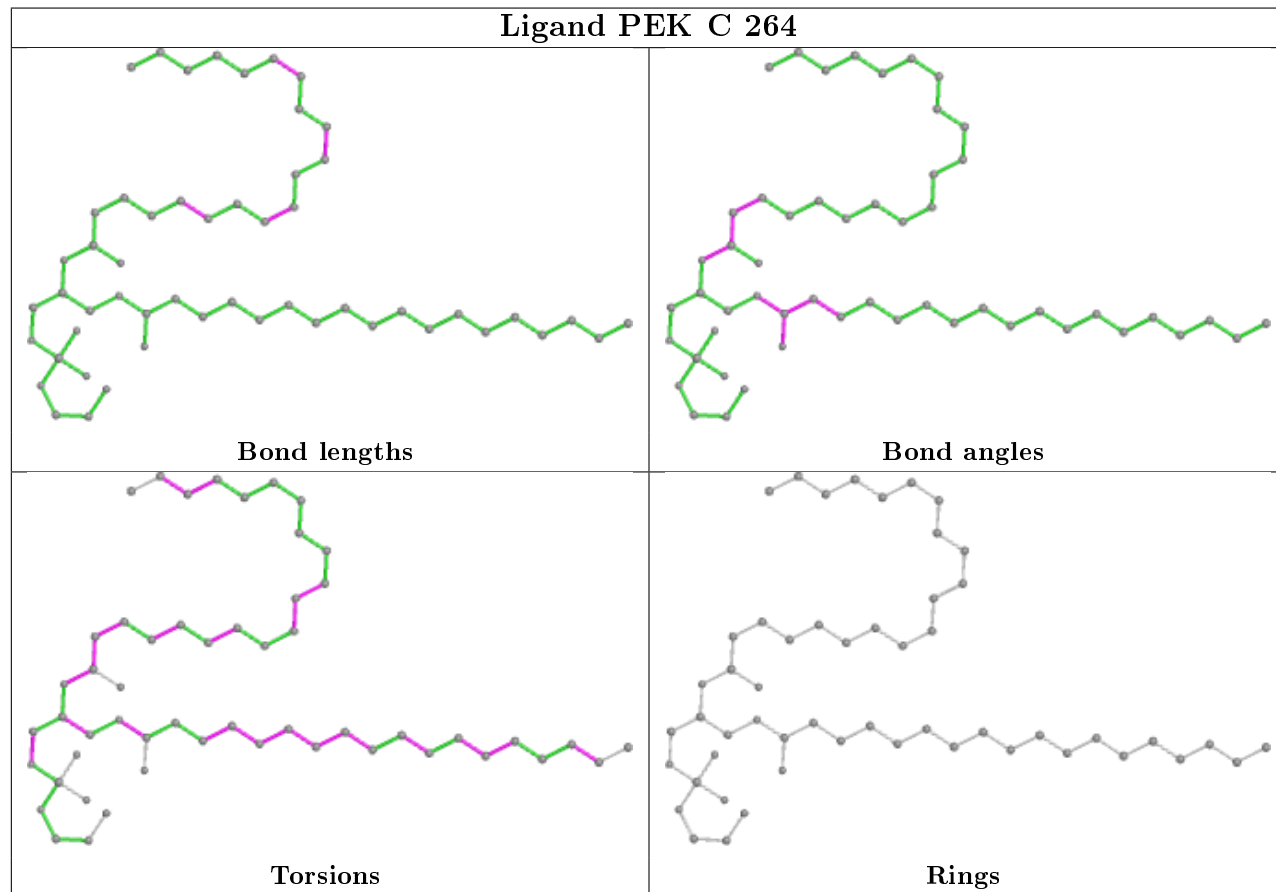
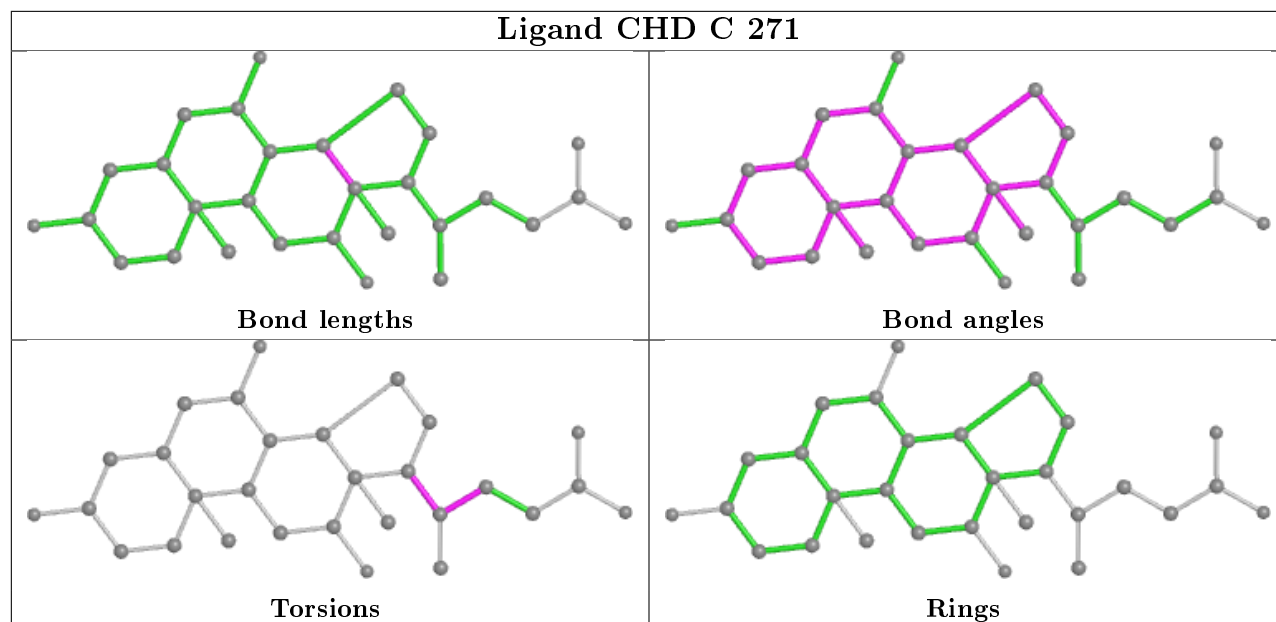


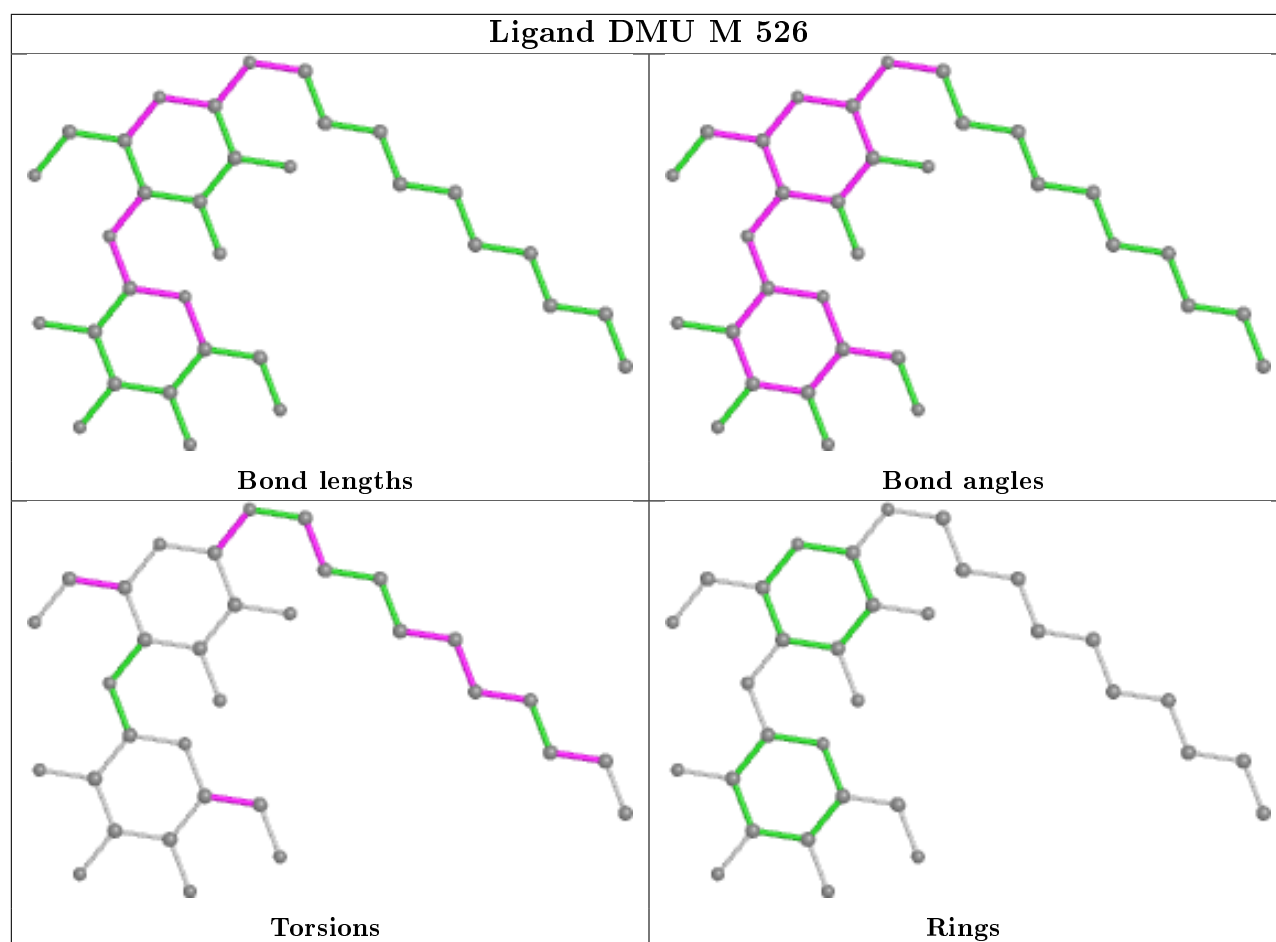
## Ligand CHD W 1060

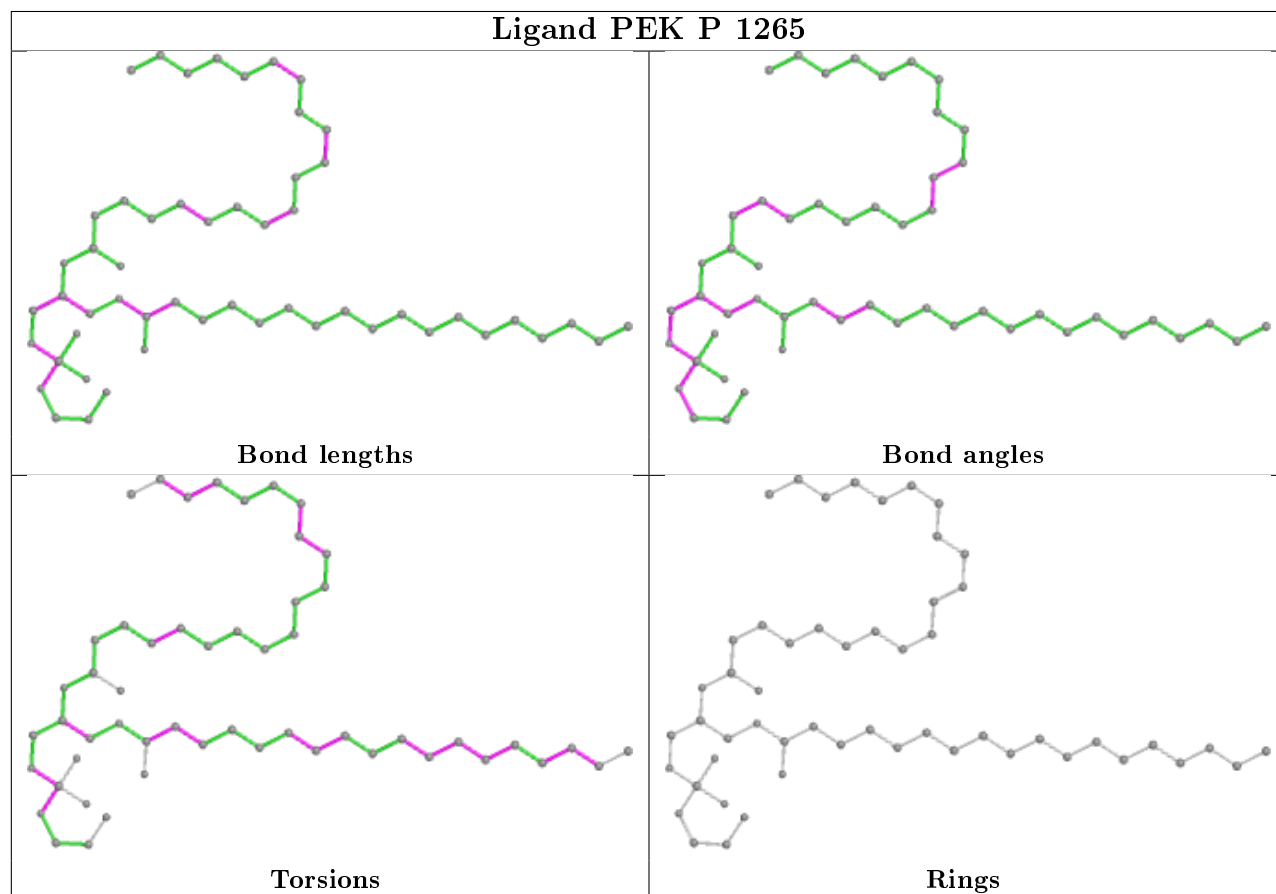
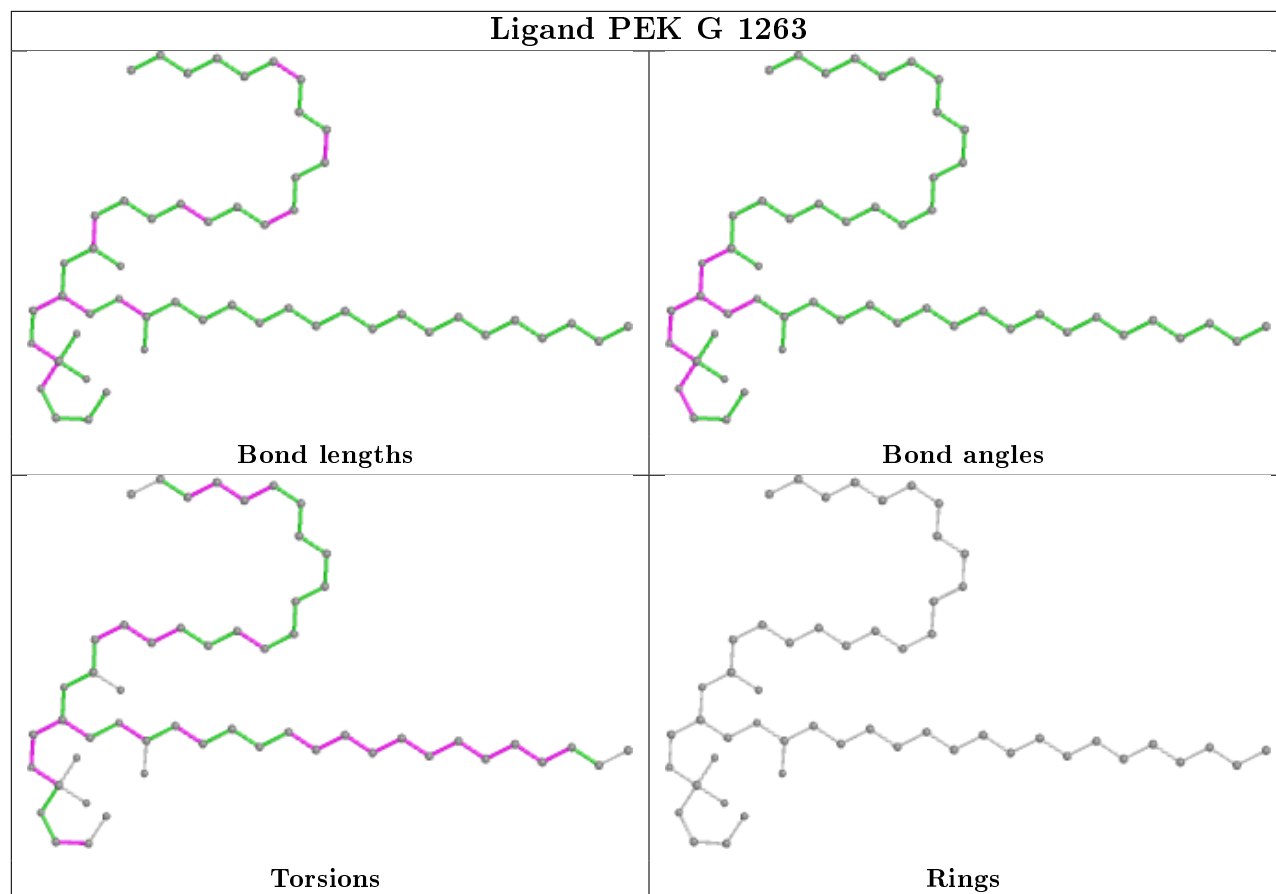


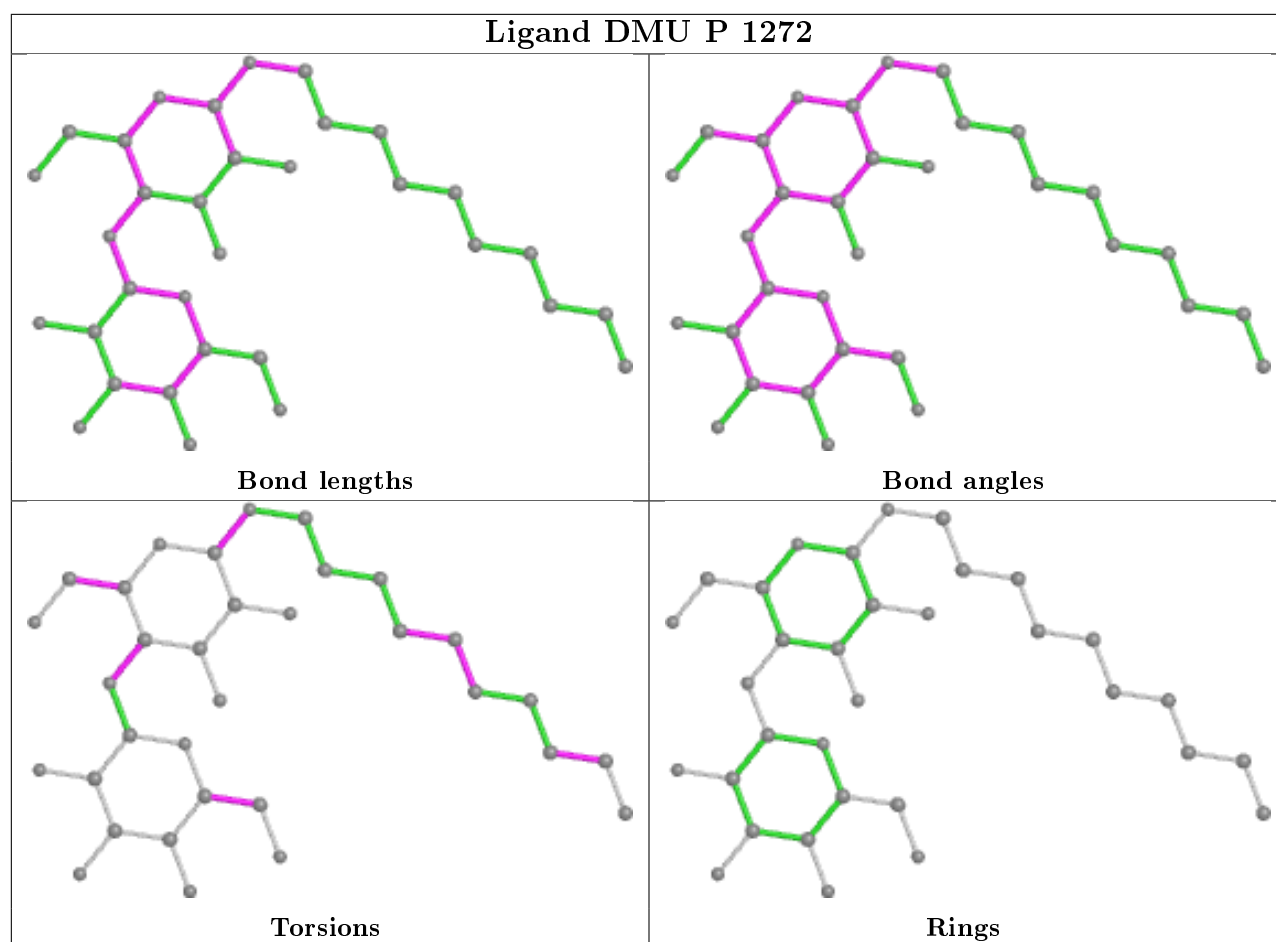
## Ligand PGV A 604











## 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.