



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 06:17 am BST

PDB ID : 1V54  
Title : Bovine heart cytochrome c oxidase at the fully oxidized state  
Authors : Tsukihara, T.; Shimokata, K.; Katayama, Y.; Shimada, H.; Muramoto, K.; Aoyama, H.; Mochizuki, M.; Shinzawa-Itoh, K.; Yamashita, E.; Yao, M.; Ishimura, Y.; Yoshikawa, S.  
Deposited on : 2003-11-21  
Resolution : 1.80 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

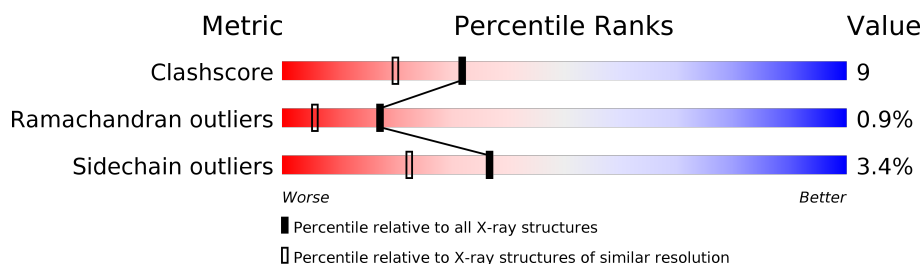
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)



















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
17	HEA	A	515	X	-	-	-
17	HEA	A	516	X	-	-	-
17	HEA	N	515	X	-	-	-
17	HEA	N	516	X	-	-	-
18	TGL	L	3522	-	-	X	-
21	CHD	C	3271	X	-	-	-
21	CHD	J	3060	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CHD	P	4271	X	-	-	-
21	CHD	W	4060	X	-	-	-
25	PSC	O	4230	-	-	X	-
27	DMU	M	3526	X	-	-	-
27	DMU	Z	4526	X	-	-	-
9	SAC	V	1	-	X	-	-

## 2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 32636 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 polypeptide I.

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 polypeptide II.

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 polypeptide III.

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 IV 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 polypeptide VIb.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

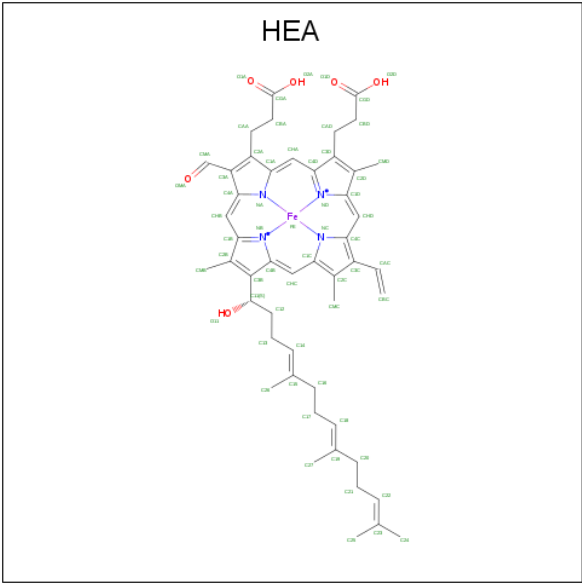
- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

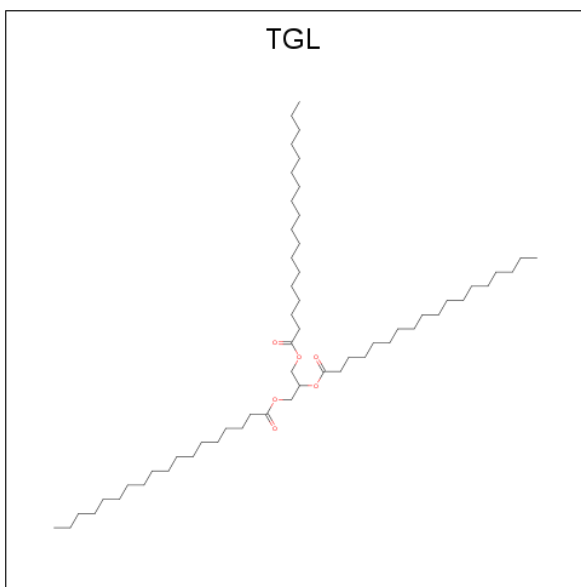
- Molecule 17 is HEME-A (three-letter code: HEA) (formula: C<sub>49</sub>H<sub>56</sub>FeN<sub>4</sub>O<sub>6</sub>).



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

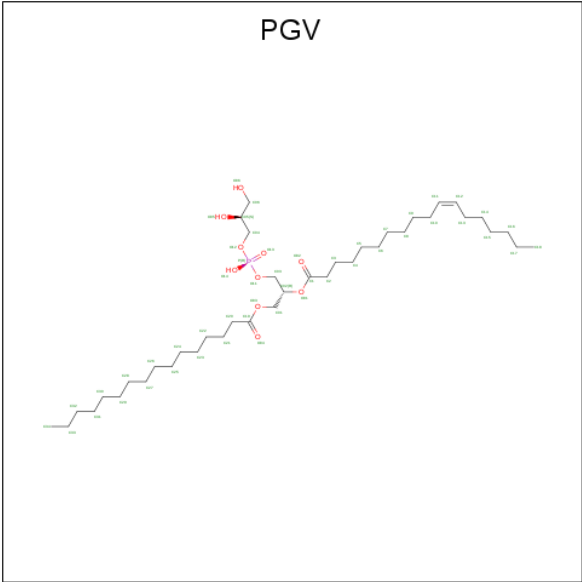
- Molecule 18 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).





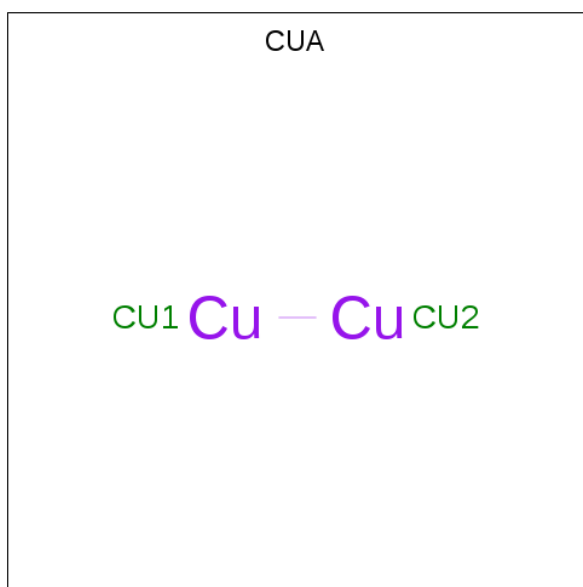
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
18	A	1	Total	C	O	0	0
			63	57	6		
18	D	1	Total	C	O	0	0
			63	57	6		
18	L	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	N	1	Total	C	O	0	0
			63	57	6		
18	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 19 is (1R)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



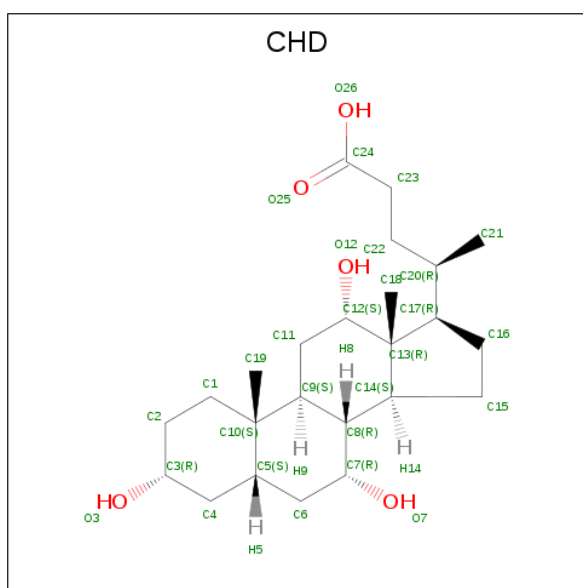
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	A	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	C	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	N	1	Total	C	O	P	0	0
			51	40	10	1		
19	P	1	Total	C	O	P	0	0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

- Molecule 20 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



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

- Molecule 21 is CHOLIC ACID (three-letter code: CHD) (formula:  $C_{24}H_{40}O_5$ ).



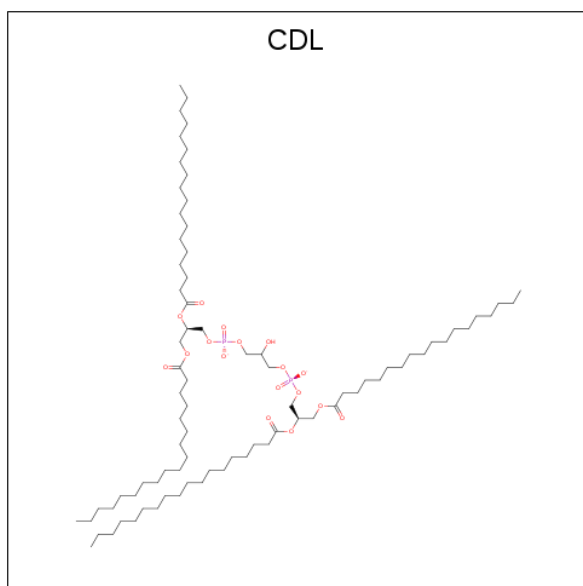
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			29	24	5		
21	C	1	Total	C	O	0	0
			29	24	5		

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

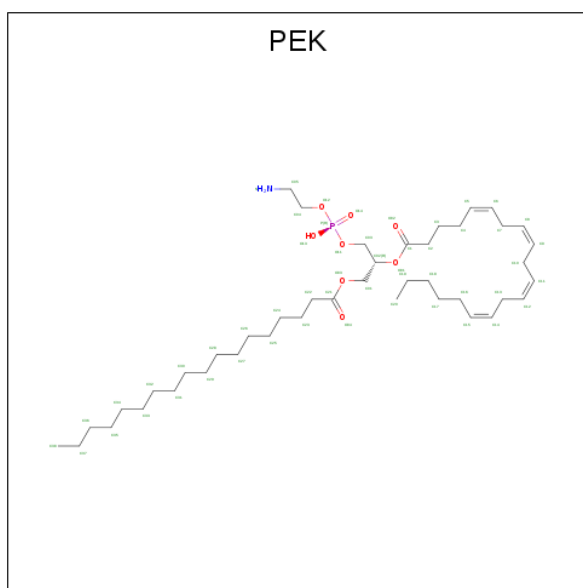
- Molecule 22 is CARDIOLIPIN (three-letter code: CDL) (formula:  $C_{81}H_{156}O_{17}P_2$ ).



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

- Molecule 23 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:  $C_{43}H_{78}NO_8P$ ).

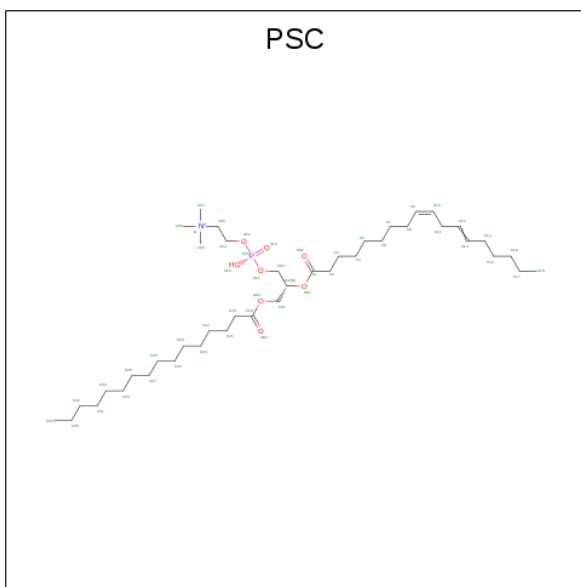


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
23	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 24 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
24	P	1	Total	X	0	0
			1	1		
24	C	1	Total	X	0	0
			1	1		

- Molecule 25 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula:  $C_{42}H_{81}NO_8P$ ).

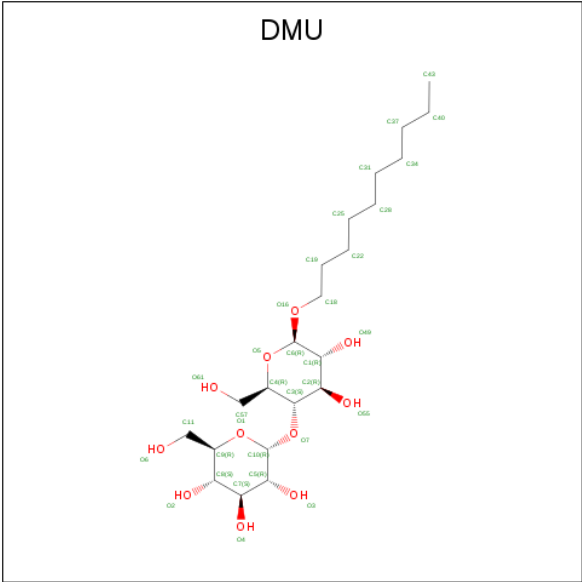


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
25	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
25	O	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 27 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



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

- Molecule 28 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	A	227	Total	O	0	0
			227	227		
28	B	180	Total	O	0	0
			180	180		
28	C	116	Total	O	0	0
			116	116		
28	D	109	Total	O	0	0
			109	109		
28	E	68	Total	O	0	0
			68	68		
28	F	80	Total	O	0	0
			80	80		
28	G	59	Total	O	0	0
			59	59		
28	H	71	Total	O	0	0
			71	71		
28	I	61	Total	O	0	0
			61	61		
28	J	21	Total	O	0	0
			21	21		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	K	37	Total 37	O 37	0	0
28	L	23	Total 23	O 23	0	0
28	M	32	Total 32	O 32	0	0
28	N	217	Total 217	O 217	0	0
28	O	146	Total 146	O 146	0	0
28	P	120	Total 120	O 120	0	0
28	Q	73	Total 73	O 73	0	0
28	R	32	Total 32	O 32	0	0
28	S	54	Total 54	O 54	0	0
28	T	58	Total 58	O 58	0	0
28	U	65	Total 65	O 65	0	0
28	V	36	Total 36	O 36	0	0
28	W	13	Total 13	O 13	0	0
28	X	29	Total 29	O 29	0	0
28	Y	25	Total 25	O 25	0	0
28	Z	18	Total 18	O 18	0	0

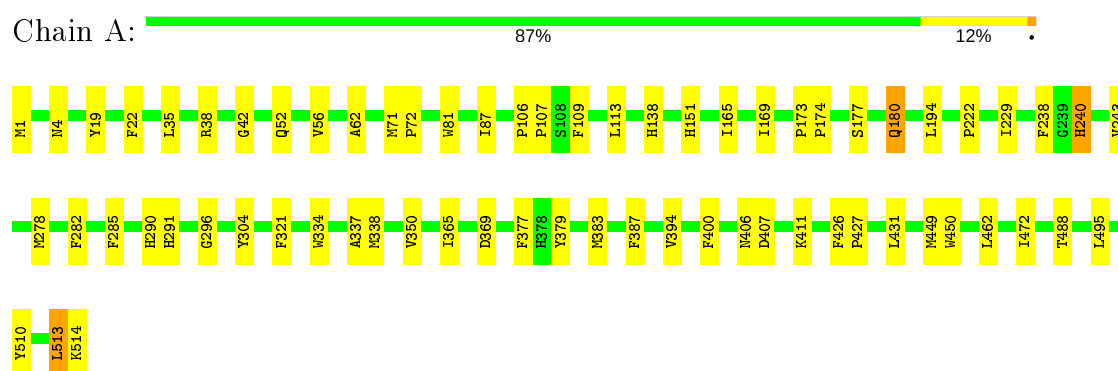


### 3 Residue-property plots

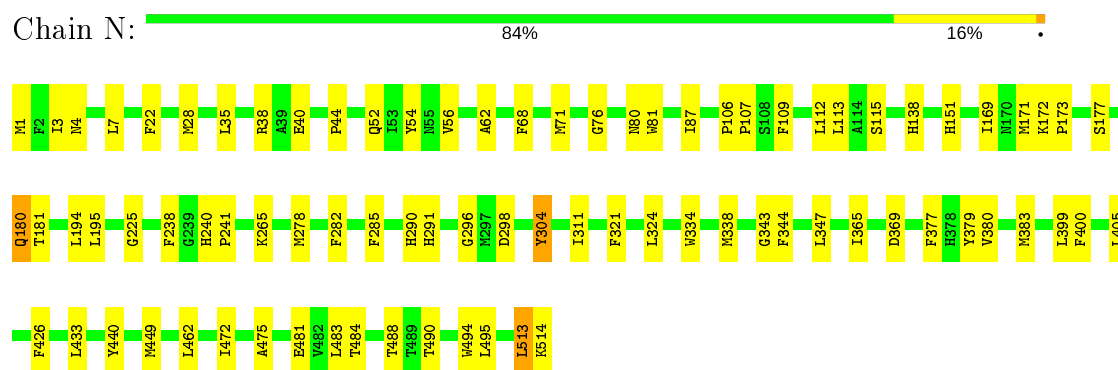
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

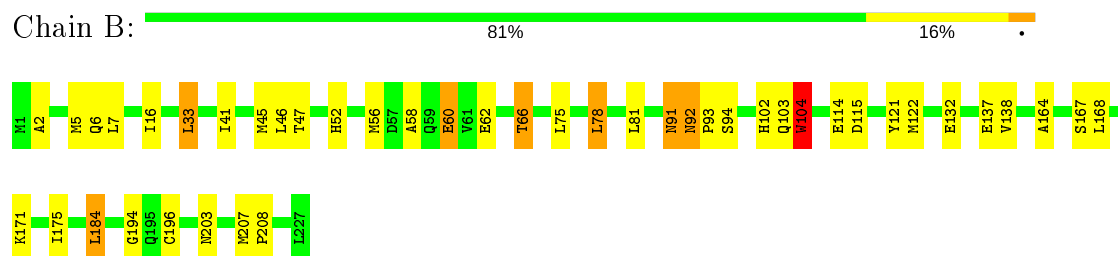
- Molecule 1: Cytochrome c oxidase polypeptide I



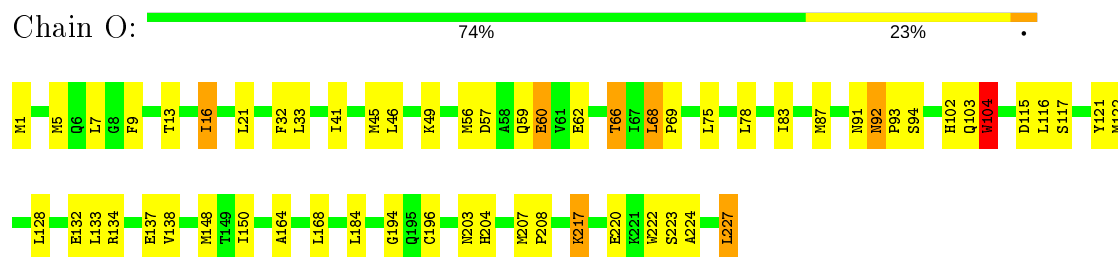
- Molecule 1: Cytochrome c oxidase polypeptide I



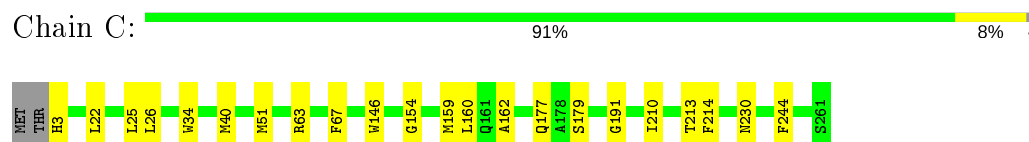
- Molecule 2: Cytochrome c oxidase polypeptide II



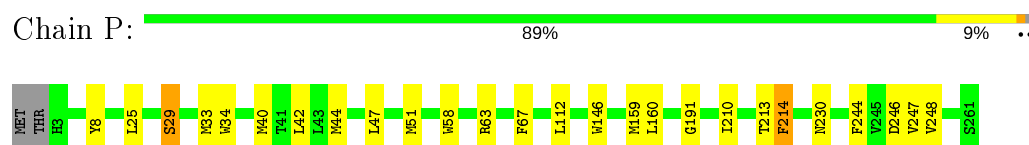
- Molecule 2: Cytochrome c oxidase polypeptide II



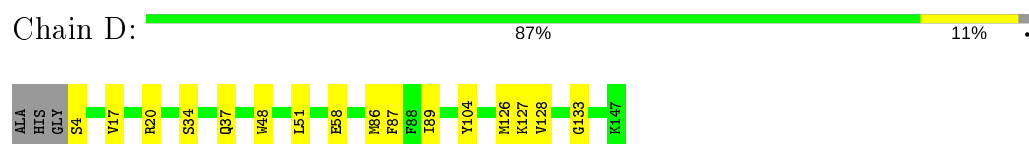
- Molecule 3: Cytochrome c oxidase polypeptide III



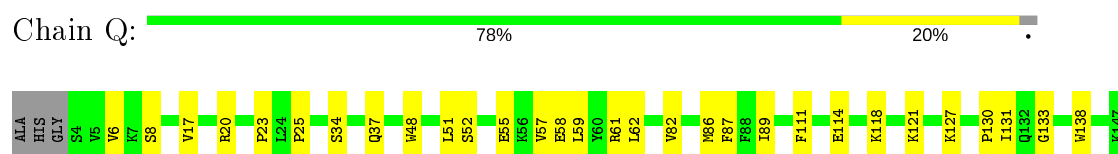
- Molecule 3: Cytochrome c oxidase polypeptide III



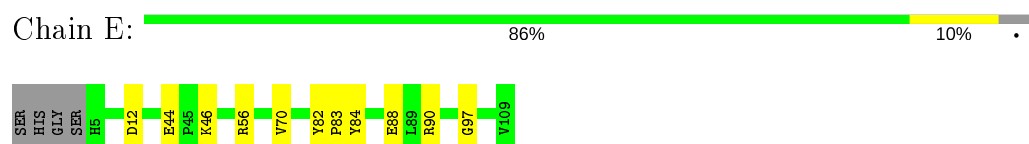
- Molecule 4: Cytochrome c oxidase subunit IV isoform 1



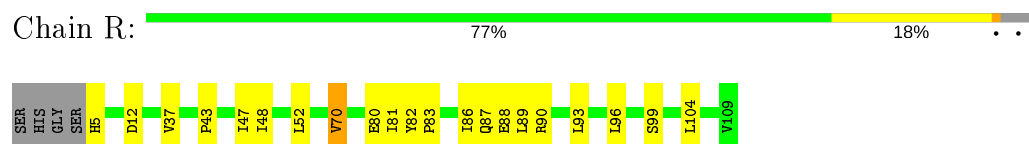
- Molecule 4: Cytochrome c oxidase subunit IV isoform 1




- Molecule 5: Cytochrome c oxidase polypeptide Va



- Molecule 5: Cytochrome c oxidase polypeptide Va




- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain F:  78% 19% ..



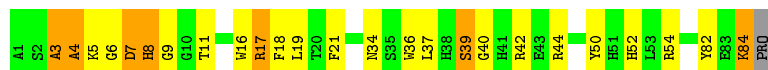
- Molecule 6: Cytochrome c oxidase polypeptide Vb

Chain S:  83% 14% ..



- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain G:  69% 21% 8% .




- Molecule 7: Cytochrome c oxidase polypeptide VIa-heart

Chain T:  72% 21% 6% .



- Molecule 8: Cytochrome c oxidase polypeptide VIb

Chain H:  82% 9% 7% .




- Molecule 8: Cytochrome c oxidase polypeptide VIb

Chain U:  74% 16% 7% .




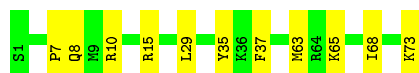
- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain I:  85% 14% .




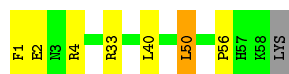
- Molecule 9: Cytochrome c oxidase polypeptide VIc

Chain V:  85% 15%



- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain J:  86% 10% ..




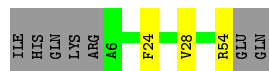
- Molecule 10: Cytochrome c oxidase polypeptide VIIa-heart

Chain W:  95% ...



- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain K:  82% 5% 13%




- Molecule 11: Cytochrome c oxidase polypeptide VIIb

Chain X:  77% 9% • 13%




- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain L:  87% 11% •

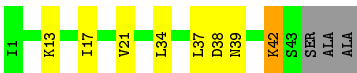
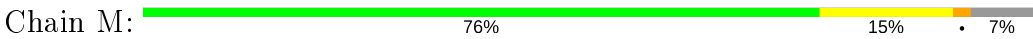


- Molecule 12: Cytochrome c oxidase polypeptide VIIc

Chain Y:  81% 15% ..



- 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, $\alpha$ , $\beta$ , $\gamma$	182.59Å 205.14Å 178.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-1.80)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.202 , 0.227	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	32636	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.51	0/4156	0.68	0/5678
1	N	0.50	0/4156	0.67	0/5678
2	B	0.48	0/1860	0.79	3/2534 (0.1%)
2	O	0.52	0/1860	0.82	3/2534 (0.1%)
3	C	0.51	0/2197	0.59	0/3005
3	P	0.48	0/2197	0.61	0/3005
4	D	0.48	0/1229	0.66	1/1658 (0.1%)
4	Q	0.51	0/1229	0.66	1/1658 (0.1%)
5	E	0.49	0/871	0.66	0/1182
5	R	0.50	0/871	0.68	0/1182
6	F	0.48	0/765	0.81	2/1038 (0.2%)
6	S	0.51	0/765	0.82	2/1038 (0.2%)
7	G	0.52	0/690	0.69	0/937
7	T	0.55	0/690	0.73	1/937 (0.1%)
8	H	0.47	0/682	0.68	0/921
8	U	0.49	0/682	0.67	0/921
9	I	0.53	0/605	0.60	0/802
9	V	0.53	0/605	0.62	0/802
10	J	0.47	0/471	0.60	0/636
10	W	0.48	0/471	0.64	0/636
11	K	0.50	0/398	0.67	0/546
11	X	0.49	0/398	0.66	0/546
12	L	0.50	0/393	0.56	0/526
12	Y	0.54	0/393	0.58	0/526
13	M	0.47	0/345	0.62	0/470
13	Z	0.43	0/345	0.61	0/470
All	All	0.50	0/29324	0.68	13/39866 (0.0%)

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

by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	N	0	2
8	U	0	1
All	All	0	5

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	94	HIS	N-CA-C	6.25	127.89	111.00
2	B	103	GLN	CA-C-N	-6.20	103.55	117.20
6	F	94	HIS	N-CA-C	5.99	127.18	111.00
7	T	33	LEU	CA-CB-CG	5.91	128.88	115.30
2	O	103	GLN	CA-C-N	-5.82	104.40	117.20
2	B	184	LEU	CA-CB-CG	5.72	128.46	115.30
6	F	93	PRO	N-CA-C	5.69	126.90	112.10
4	D	133	GLY	N-CA-C	5.63	127.17	113.10
2	B	104	TRP	N-CA-C	5.47	125.78	111.00
4	Q	133	GLY	N-CA-C	5.43	126.67	113.10
2	O	227	LEU	CA-CB-CG	5.40	127.72	115.30
6	S	93	PRO	N-CA-C	5.33	125.94	112.10
2	O	104	TRP	N-CA-C	5.27	125.23	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	19	TYR	Sidechain
1	A	240	HIS	Sidechain
1	N	240	HIS	Sidechain
1	N	304	TYR	Sidechain
8	U	11	TYR	Sidechain

## 5.2 Too-close contacts

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



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4027	0	4001	62	0
1	N	4027	0	4001	72	0
2	B	1824	0	1833	33	0
2	O	1824	0	1833	49	0
3	C	2110	0	2027	17	0
3	P	2110	0	2027	24	0
4	D	1195	0	1183	15	0
4	Q	1195	0	1183	25	0
5	E	852	0	845	6	0
5	R	852	0	845	11	0
6	F	748	0	728	16	0
6	S	748	0	728	12	0
7	G	675	0	644	25	0
7	T	675	0	644	21	0
8	H	662	0	623	5	0
8	U	662	0	623	8	0
9	I	601	0	613	8	0
9	V	601	0	613	11	0
10	J	460	0	459	6	0
10	W	460	0	459	2	0
11	K	384	0	366	2	0
11	X	384	0	366	8	0
12	L	380	0	380	13	0
12	Y	380	0	380	10	0
13	M	335	0	352	5	0
13	Z	335	0	352	6	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	120	0	108	4	0
17	N	120	0	108	3	0
18	A	63	0	110	11	0
18	D	63	0	110	15	0
18	L	63	0	110	25	0
18	N	126	0	220	38	0
18	Q	63	0	110	15	0
19	A	102	0	152	7	0
19	C	102	0	152	7	0
19	N	102	0	152	5	0
19	P	102	0	152	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	B	2	0	0	0	0
20	O	2	0	0	0	0
21	B	29	0	39	1	0
21	C	58	0	78	3	0
21	J	29	0	39	2	0
21	O	29	0	39	1	0
21	P	58	0	78	2	0
21	W	29	0	39	2	0
22	C	100	0	156	14	0
22	G	100	0	156	14	0
22	P	100	0	156	18	0
22	T	100	0	156	15	0
23	C	106	0	154	7	0
23	G	53	0	77	10	0
23	P	106	0	154	6	0
23	T	53	0	77	9	0
24	C	1	0	0	0	0
24	P	1	0	0	0	0
25	E	52	0	80	13	0
25	O	52	0	80	21	0
26	F	1	0	0	0	0
26	S	1	0	0	0	0
27	M	33	0	36	0	0
27	Z	33	0	36	0	0
28	A	227	0	0	2	0
28	B	180	0	0	8	0
28	C	116	0	0	1	0
28	D	109	0	0	3	0
28	E	68	0	0	2	0
28	F	80	0	0	2	0
28	G	59	0	0	3	0
28	H	71	0	0	1	0
28	I	61	0	0	2	0
28	J	21	0	0	0	0
28	K	37	0	0	0	0
28	L	23	0	0	1	0
28	M	32	0	0	0	0
28	N	217	0	0	5	0
28	O	146	0	0	1	0
28	P	120	0	0	1	0
28	Q	73	0	0	5	0
28	R	32	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	S	54	0	0	3	0
28	T	58	0	0	2	0
28	U	65	0	0	1	0
28	V	36	0	0	2	0
28	W	13	0	0	0	0
28	X	29	0	0	1	0
28	Y	25	0	0	1	0
28	Z	18	0	0	0	0
All	All	32636	0	31222	551	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 (551) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:84:LYS:HD2	7:G:84:LYS:H	1.14	1.08
22:C:3270:CDL:H662	19:C:3267:PGV:H182	1.41	1.03
3:P:63:ARG:HE	22:P:4270:CDL:HA22	1.24	1.03
7:T:84:LYS:H	7:T:84:LYS:HD2	1.23	1.02
3:C:63:ARG:HE	22:C:3270:CDL:HA22	1.23	1.01
10:W:33:ARG:HG2	21:W:4060:CHD:H152	1.46	0.94
18:N:4522:TGL:HC31	12:Y:13:PHE:HA	1.51	0.93
4:D:34:SER:H	4:D:37:GLN:HE21	1.16	0.89
23:C:3264:PEK:H161	23:C:3264:PEK:H102	1.55	0.89
4:Q:114:GLU:HB3	28:Q:2622:HOH:O	1.73	0.89
6:S:94:HIS:CD2	6:S:95:GLN:H	1.93	0.87
9:I:5:ALA:HB2	28:I:2536:HOH:O	1.73	0.86
6:F:85:CYS:SG	6:F:87:THR:HG23	2.15	0.86
22:P:4270:CDL:H242	22:P:4270:CDL:H661	1.59	0.84
18:N:4521:TGL:H101	18:N:4521:TGL:H271	1.58	0.84
18:A:3521:TGL:H241	18:A:3521:TGL:HA91	1.60	0.83
7:T:5:LYS:HD2	23:T:3263:PEK:H382	1.61	0.83
22:C:3270:CDL:H242	22:C:3270:CDL:H661	1.60	0.82
22:P:4270:CDL:H662	19:P:4267:PGV:H182	1.61	0.81
25:O:4230:PSC:H21	25:O:4230:PSC:H222	1.64	0.80
12:L:20:ARG:HH12	18:L:3522:TGL:HC61	1.45	0.80
3:P:67:PHE:HE1	22:P:4270:CDL:H1	1.45	0.80
25:E:3230:PSC:H21	25:E:3230:PSC:H222	1.65	0.79
4:Q:114:GLU:HG2	28:Q:1465:HOH:O	1.81	0.79
2:O:224:ALA:O	2:O:227:LEU:HG	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:426:PHE:CE1	18:A:3521:TGL:H282	2.19	0.77
23:P:4264:PEK:H161	23:P:4264:PEK:H102	1.64	0.77
1:N:113:LEU:CD1	18:N:4522:TGL:H292	2.16	0.76
2:O:49:LYS:NZ	18:Q:4523:TGL:HC71	2.00	0.76
19:N:4524:PGV:H321	19:N:4524:PGV:H162	1.68	0.76
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.69	0.75
18:N:4521:TGL:H241	18:N:4521:TGL:HA91	1.67	0.74
2:O:56:MET:HA	25:O:4230:PSC:H202	1.70	0.74
1:N:433:LEU:HD11	18:N:4521:TGL:OB1	1.88	0.74
19:A:3524:PGV:H321	19:A:3524:PGV:H162	1.70	0.74
3:P:210:ILE:HG23	19:P:4267:PGV:H102	1.70	0.74
10:J:33:ARG:HG2	21:J:3060:CHD:H152	1.68	0.74
12:L:13:PHE:HA	18:L:3522:TGL:HC31	1.68	0.74
13:M:42:LYS:HA	13:M:42:LYS:HE3	1.68	0.74
2:O:217:LYS:HE2	2:O:217:LYS:HA	1.69	0.73
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.70	0.73
5:R:43:PRO:HB2	5:R:48:ILE:HD11	1.68	0.73
22:C:3270:CDL:C66	19:C:3267:PGV:H182	2.18	0.72
28:B:4263:HOH:O	18:D:3523:TGL:HC52	1.89	0.72
1:N:1:FME:HCN	1:N:4:ASN:H	1.55	0.72
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.72	0.72
4:D:34:SER:H	4:D:37:GLN:NE2	1.88	0.71
3:C:67:PHE:HE1	22:C:3270:CDL:H1	1.55	0.71
18:D:3523:TGL:HA81	18:D:3523:TGL:H242	1.73	0.71
6:S:85:CYS:SG	6:S:87:THR:HG23	2.31	0.70
18:Q:4523:TGL:HG12	18:Q:4523:TGL:HC21	1.73	0.70
6:S:94:HIS:CG	6:S:95:GLN:H	2.09	0.70
18:N:4521:TGL:H101	18:N:4521:TGL:C27	2.20	0.70
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.27	0.69
22:P:4270:CDL:H662	19:P:4267:PGV:C18	2.21	0.69
3:C:210:ILE:HG23	19:C:3267:PGV:H102	1.75	0.69
1:A:334:TRP:HZ3	18:D:3523:TGL:HA62	1.57	0.68
3:P:246:ASP:HB2	28:P:1524:HOH:O	1.91	0.68
7:T:38:HIS:NE2	22:T:4269:CDL:H111	2.09	0.68
7:G:5:LYS:HB3	1:N:278:MET:SD	2.33	0.68
19:P:4267:PGV:H161	19:P:4267:PGV:H12	1.76	0.68
18:D:3523:TGL:HC31	28:D:3613:HOH:O	1.93	0.67
1:N:334:TRP:CZ3	18:Q:4523:TGL:HA42	2.30	0.67
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.76	0.67
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.77	0.67
1:N:472:ILE:HD13	18:N:4522:TGL:HA92	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:84:LYS:HD2	7:G:84:LYS:N	1.99	0.67
7:T:84:LYS:H	7:T:84:LYS:CD	2.03	0.66
6:S:94:HIS:CD2	6:S:95:GLN:N	2.63	0.66
9:V:10:ARG:HD2	28:V:2590:HOH:O	1.94	0.66
12:L:20:ARG:NH2	18:L:3522:TGL:HC32	2.11	0.66
25:E:3230:PSC:C07	9:I:10:ARG:HH21	2.09	0.66
2:O:41:ILE:HD13	25:O:4230:PSC:H342	1.79	0.65
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.77	0.65
7:G:84:LYS:H	7:G:84:LYS:CD	1.97	0.65
22:C:3270:CDL:H812	19:C:3267:PGV:H181	1.79	0.65
2:B:92:ASN:HB3	28:B:4260:HOH:O	1.97	0.64
18:A:3521:TGL:H283	18:A:3521:TGL:HB92	1.79	0.64
4:D:58:GLU:HG3	28:D:3555:HOH:O	1.98	0.63
18:N:4521:TGL:HB91	2:O:32:PHE:CE2	2.33	0.63
1:N:483:LEU:HD13	4:Q:6:VAL:HB	1.80	0.63
18:Q:4523:TGL:H122	18:Q:4523:TGL:HB82	1.79	0.63
5:R:89:LEU:O	5:R:93:LEU:HG	1.99	0.63
18:D:3523:TGL:H122	18:D:3523:TGL:HB82	1.80	0.63
18:Q:4523:TGL:HA81	18:Q:4523:TGL:H242	1.80	0.62
6:S:75:HIS:H	6:S:80:GLN:HE22	1.46	0.62
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.64	0.62
6:F:92:VAL:O	6:F:92:VAL:HG23	1.99	0.62
2:O:68:LEU:HD22	25:O:4230:PSC:H171	1.82	0.62
28:N:2197:HOH:O	18:Q:4523:TGL:HG2	1.98	0.62
19:C:3267:PGV:H12	19:C:3267:PGV:H161	1.81	0.61
4:Q:58:GLU:O	4:Q:62:LEU:HG	2.00	0.61
1:N:449:MET:SD	2:O:5:MET:HG2	2.40	0.61
28:B:4247:HOH:O	18:D:3523:TGL:H352	2.00	0.61
1:N:472:ILE:HG21	18:N:4522:TGL:HA81	1.83	0.60
1:A:334:TRP:CZ3	18:D:3523:TGL:HA42	2.37	0.60
2:O:49:LYS:HZ2	18:Q:4523:TGL:HC71	1.65	0.60
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.66	0.59
2:B:41:ILE:HD13	25:E:3230:PSC:H342	1.84	0.59
1:N:472:ILE:HG21	18:N:4522:TGL:CA8	2.32	0.59
3:P:160:LEU:HD13	21:P:4271:CHD:H181	1.84	0.59
25:O:4230:PSC:C07	9:V:10:ARG:HE	2.15	0.59
9:V:65:LYS:O	11:X:54:ARG:NH1	2.35	0.59
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.67	0.59
4:Q:127:LYS:O	4:Q:130:PRO:HD3	2.02	0.59
1:A:151:HIS:CD2	23:C:3264:PEK:H382	2.38	0.59
1:N:112:LEU:HG	28:N:1389:HOH:O	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:20:ARG:NH1	18:L:3522:TGL:HC61	2.17	0.58
1:A:407:ASP:O	1:A:411:LYS:HG3	2.04	0.58
7:G:8:HIS:HD2	23:G:4263:PEK:H252	1.66	0.58
18:N:4521:TGL:H281	18:N:4521:TGL:HB81	1.83	0.58
8:U:50:VAL:HG21	28:U:2545:HOH:O	2.02	0.58
1:A:1:FME:HCN	1:A:4:ASN:H	1.68	0.58
25:E:3230:PSC:H072	9:I:10:ARG:HH21	1.67	0.58
12:L:24:MET:HG3	28:L:2411:HOH:O	2.04	0.58
1:N:81:TRP:HZ2	18:N:4522:TGL:C28	2.17	0.58
12:Y:20:ARG:NH1	28:Y:1514:HOH:O	2.36	0.58
22:P:4270:CDL:H812	19:P:4267:PGV:H181	1.86	0.57
1:A:426:PHE:CD1	18:A:3521:TGL:H282	2.38	0.57
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.39	0.57
12:L:11:ILE:HG22	18:L:3522:TGL:H271	1.86	0.57
1:A:449:MET:SD	2:B:5:MET:HG2	2.45	0.57
2:O:41:ILE:CD1	25:O:4230:PSC:H342	2.34	0.57
1:N:113:LEU:HD13	18:N:4522:TGL:H292	1.84	0.57
22:G:3269:CDL:HB32	1:N:304:TYR:HD1	1.69	0.57
1:A:282:PHE:HA	7:T:4:ALA:CB	2.35	0.57
1:A:321:PHE:CD2	25:E:3230:PSC:H341	2.40	0.57
7:G:8:HIS:CD2	23:G:4263:PEK:H252	2.39	0.57
7:G:5:LYS:HD2	23:G:4263:PEK:H382	1.87	0.56
22:T:4269:CDL:HA62	22:T:4269:CDL:H322	1.87	0.56
9:I:5:ALA:O	9:I:7:PRO:HD3	2.04	0.56
5:R:12:ASP:HA	5:R:47:ILE:HD11	1.87	0.56
19:A:3524:PGV:H141	4:D:87:PHE:CD2	2.41	0.56
1:A:296:GLY:HA2	8:H:23:GLN:OE1	2.05	0.56
2:O:59:GLN:HG3	2:O:59:GLN:O	2.06	0.56
22:G:3269:CDL:HA62	22:G:3269:CDL:H322	1.87	0.56
1:N:22:PHE:HA	18:N:4522:TGL:HB72	1.88	0.56
3:C:213:THR:HG23	22:C:3270:CDL:H762	1.88	0.55
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.88	0.55
23:C:3264:PEK:C16	23:C:3264:PEK:H102	2.34	0.55
7:T:5:LYS:CD	23:T:3263:PEK:H382	2.35	0.55
4:D:17:VAL:HG12	28:D:3556:HOH:O	2.06	0.55
5:E:84:TYR:O	5:E:88:GLU:HG2	2.07	0.55
3:C:160:LEU:HD13	21:C:3271:CHD:H181	1.88	0.55
1:A:334:TRP:CZ3	18:D:3523:TGL:HA62	2.41	0.54
1:A:472:ILE:HG21	18:L:3522:TGL:HA81	1.90	0.54
13:M:17:ILE:O	13:M:21:VAL:HG23	2.07	0.54
1:N:151:HIS:CD2	23:P:4264:PEK:H382	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:SER:H	1:A:180:GLN:HE21	1.54	0.54
1:N:54:TYR:HB2	28:N:1075:HOH:O	2.07	0.54
4:D:127:LYS:HD2	28:I:371:HOH:O	2.07	0.54
13:Z:10:THR:HA	13:Z:14:GLU:OE2	2.07	0.54
2:B:56:MET:HG2	25:E:3230:PSC:H211	1.89	0.54
19:N:4524:PGV:H41	19:N:4524:PGV:H232	1.90	0.54
17:N:515:HEA:HMC1	17:N:515:HEA:HBC1	1.90	0.54
2:B:102:HIS:O	2:B:104:TRP:N	2.41	0.53
1:A:222:PRO:HD2	28:B:4240:HOH:O	2.07	0.53
18:A:3521:TGL:HC52	2:B:7:LEU:HD12	1.90	0.53
7:G:17:ARG:HD2	28:G:289:HOH:O	2.06	0.53
10:J:40:LEU:HD12	21:J:3060:CHD:H183	1.89	0.53
28:B:4144:HOH:O	18:D:3523:TGL:HC72	2.08	0.53
7:G:8:HIS:CE1	23:G:4263:PEK:H331	2.44	0.53
3:C:3:HIS:HE1	6:F:31:TYR:OH	1.90	0.53
7:G:19:LEU:HD21	23:G:4263:PEK:H362	1.90	0.53
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.90	0.53
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.22	0.53
18:A:3521:TGL:CB9	18:A:3521:TGL:H283	2.38	0.53
4:Q:118:LYS:HG3	28:Q:1465:HOH:O	2.08	0.53
1:A:81:TRP:HZ2	18:L:3522:TGL:H282	1.74	0.53
2:O:150:ILE:HD12	2:O:184:LEU:HD22	1.91	0.53
22:T:4269:CDL:H392	22:T:4269:CDL:H161	1.90	0.53
1:N:107:PRO:HB3	3:P:25:LEU:HB2	1.91	0.53
22:P:4270:CDL:C66	19:P:4267:PGV:H182	2.36	0.52
11:X:24:PHE:O	11:X:28:VAL:HG12	2.10	0.52
7:G:3:ALA:O	7:G:4:ALA:HB2	2.09	0.52
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.92	0.52
8:H:49:ASP:O	8:H:52:VAL:HG22	2.10	0.52
12:L:20:ARG:HH12	18:L:3522:TGL:CC6	2.16	0.52
22:G:3269:CDL:H392	22:G:3269:CDL:H161	1.92	0.52
1:N:265:LYS:HE3	28:S:2510:HOH:O	2.08	0.52
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.09	0.52
1:A:1:FME:HE2	1:A:1:FME:HA	1.90	0.52
2:B:122:MET:HB2	2:B:208:PRO:HD2	1.91	0.52
1:N:52:GLN:O	1:N:56:VAL:HG23	2.10	0.52
28:B:4241:HOH:O	23:P:4265:PEK:H031	2.09	0.52
18:Q:4523:TGL:CG1	18:Q:4523:TGL:HC21	2.39	0.52
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.09	0.51
23:G:4263:PEK:H132	3:P:247:VAL:HG11	1.93	0.51
18:N:4521:TGL:HB91	2:O:32:PHE:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:56:MET:HG2	25:O:4230:PSC:H211	1.92	0.51
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.75	0.51
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.45	0.51
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.45	0.51
1:A:194:LEU:HD22	1:A:285:PHE:CE2	2.45	0.51
19:A:3524:PGV:H41	19:A:3524:PGV:H232	1.90	0.51
3:P:213:THR:HG23	22:P:4270:CDL:H762	1.92	0.51
1:N:113:LEU:HD12	18:N:4522:TGL:H292	1.93	0.51
12:L:20:ARG:HH22	18:L:3522:TGL:HC32	1.74	0.51
1:N:324:LEU:HD13	2:O:41:ILE:CG2	2.39	0.51
12:L:13:PHE:HB3	18:L:3522:TGL:HG12	1.93	0.51
6:F:25:ARG:HD2	28:F:154:HOH:O	2.10	0.51
6:F:64:GLU:O	6:F:65:ASP:HB2	2.11	0.51
3:C:191:GLY:HA3	28:G:143:HOH:O	2.11	0.50
2:O:83:ILE:O	2:O:87:MET:HG3	2.12	0.50
17:A:515:HEA:HMC1	17:A:515:HEA:HBC1	1.93	0.50
7:G:37:LEU:HD21	22:G:3269:CDL:H361	1.93	0.50
1:N:87:ILE:O	1:N:173:PRO:HD3	2.11	0.50
7:T:3:ALA:O	7:T:4:ALA:HB2	2.11	0.50
18:N:4522:TGL:CG1	12:Y:13:PHE:HB3	2.41	0.50
1:A:229:ILE:HD11	2:B:175:ILE:CD1	2.41	0.50
1:A:472:ILE:HG21	18:L:3522:TGL:CA8	2.41	0.50
1:N:488:THR:HB	1:N:495:LEU:HD13	1.92	0.50
3:P:34:TRP:CD1	3:P:40:MET:HG2	2.47	0.50
1:A:177:SER:H	1:A:180:GLN:NE2	2.10	0.50
6:S:51:SER:O	6:S:94:HIS:N	2.45	0.50
22:T:4269:CDL:H511	22:T:4269:CDL:H172	1.93	0.50
7:T:5:LYS:HB2	23:T:3263:PEK:H372	1.94	0.50
23:G:4263:PEK:H9	3:P:244:PHE:HA	1.94	0.50
2:O:49:LYS:O	4:Q:20:ARG:NH2	2.42	0.50
6:S:87:THR:HG21	28:S:1319:HOH:O	2.12	0.50
3:C:244:PHE:HA	23:T:3263:PEK:H9	1.93	0.50
11:X:54:ARG:NH2	11:X:54:ARG:HG3	2.25	0.50
22:G:3269:CDL:H511	22:G:3269:CDL:H172	1.92	0.50
18:L:3522:TGL:HC62	18:L:3522:TGL:HC22	1.93	0.50
5:R:81:ILE:HG12	9:V:7:PRO:HG2	1.93	0.50
23:C:3264:PEK:H32	23:C:3264:PEK:H71	1.93	0.50
8:U:7:LYS:O	8:U:8:ILE:HG22	2.12	0.50
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.00	0.49
2:O:102:HIS:O	2:O:104:TRP:N	2.45	0.49
2:O:122:MET:HB2	2:O:208:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:G:3269:CDL:H522	22:G:3269:CDL:H202	1.95	0.49
2:O:132:GLU:HB3	2:O:137:GLU:HG3	1.94	0.49
1:A:81:TRP:HZ2	18:L:3522:TGL:C28	2.26	0.49
7:T:8:HIS:CD2	23:T:3263:PEK:H252	2.48	0.49
1:N:379:TYR:O	1:N:383:MET:HB2	2.12	0.49
6:F:8:THR:OG1	6:F:11:GLU:HG3	2.13	0.49
7:G:34:ASN:HD22	22:G:3269:CDL:H151	1.78	0.49
1:N:514:LYS:HE2	28:S:1319:HOH:O	2.12	0.49
4:Q:89:ILE:HD12	18:Q:4523:TGL:H311	1.95	0.49
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.95	0.49
22:P:4270:CDL:H602	22:P:4270:CDL:H632	1.59	0.49
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.95	0.48
1:N:106:PRO:HB2	1:N:107:PRO:HD3	1.95	0.48
22:C:3270:CDL:HA61	28:C:3618:HOH:O	2.11	0.48
18:N:4521:TGL:OB1	18:N:4521:TGL:HB42	2.13	0.48
1:A:87:ILE:O	1:A:173:PRO:HD3	2.13	0.48
1:N:194:LEU:HD22	1:N:285:PHE:CE2	2.48	0.48
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.78	0.48
6:S:92:VAL:HG23	6:S:92:VAL:O	2.13	0.48
28:O:2266:HOH:O	8:U:61:LYS:HD3	2.12	0.48
25:O:4230:PSC:H071	9:V:10:ARG:HE	1.77	0.48
2:B:78:LEU:HD12	22:T:4269:CDL:H351	1.94	0.48
1:A:304:TYR:HD1	22:T:4269:CDL:HB32	1.79	0.48
1:A:472:ILE:HD13	18:L:3522:TGL:HA92	1.95	0.48
2:B:164:ALA:O	2:B:194:GLY:HA3	2.13	0.48
8:H:23:GLN:HG3	28:H:2167:HOH:O	2.12	0.48
25:O:4230:PSC:H212	25:O:4230:PSC:O01	2.14	0.48
2:O:49:LYS:HZ3	18:Q:4523:TGL:HC71	1.76	0.48
10:W:50:LEU:HD22	10:W:50:LEU:O	2.14	0.48
12:Y:2:HIS:ND1	12:Y:3:TYR:N	2.62	0.48
1:A:427:PRO:HG3	18:A:3521:TGL:H351	1.95	0.48
2:B:41:ILE:O	2:B:45:MET:HG2	2.14	0.48
2:O:104:TRP:HA	2:O:207:MET:SD	2.54	0.48
18:N:4521:TGL:HB91	2:O:32:PHE:HE2	1.75	0.48
19:N:4524:PGV:H141	4:Q:87:PHE:CD2	2.49	0.48
1:A:81:TRP:CZ2	18:L:3522:TGL:H282	2.49	0.47
2:B:114:GLU:HB3	28:B:4162:HOH:O	2.14	0.47
1:N:405:LEU:HD23	1:N:475:ALA:HB2	1.96	0.47
7:G:34:ASN:ND2	22:G:3269:CDL:H151	2.28	0.47
7:G:50:TYR:HB3	7:G:52:HIS:CE1	2.48	0.47
1:A:52:GLN:O	1:A:56:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:9:PHE:HB2	2:O:21:LEU:HD21	1.96	0.47
3:P:67:PHE:CE1	22:P:4270:CDL:H1	2.37	0.47
11:X:54:ARG:HH21	11:X:54:ARG:CG	2.28	0.47
2:B:81:LEU:HD13	22:T:4269:CDL:H122	1.96	0.47
2:B:33:LEU:HD13	9:I:31:PHE:CD1	2.50	0.47
7:G:4:ALA:CB	1:N:282:PHE:HA	2.44	0.47
18:N:4521:TGL:HC52	2:O:7:LEU:HD12	1.97	0.47
3:P:25:LEU:O	3:P:29:SER:HB2	2.15	0.47
22:T:4269:CDL:H152	22:T:4269:CDL:H181	1.62	0.47
1:A:278:MET:SD	7:T:5:LYS:HB3	2.54	0.47
18:D:3523:TGL:HC91	18:D:3523:TGL:HC62	1.75	0.47
25:E:3230:PSC:H62	25:E:3230:PSC:H241	1.97	0.47
1:A:365:ILE:HD11	28:A:3732:HOH:O	2.14	0.47
5:R:37:VAL:HG11	5:R:70:VAL:HG21	1.95	0.47
2:B:58:ALA:O	2:B:62:GLU:HG3	2.15	0.47
21:W:4060:CHD:H161	21:W:4060:CHD:H212	1.74	0.47
1:A:290:HIS:CD2	1:A:291:HIS:CD2	3.02	0.46
1:A:379:TYR:O	1:A:383:MET:HB2	2.14	0.46
18:N:4521:TGL:H301	18:N:4521:TGL:HA92	1.96	0.46
18:N:4521:TGL:H283	18:N:4521:TGL:HB92	1.96	0.46
23:T:3263:PEK:H371	23:T:3263:PEK:H332	1.98	0.46
7:G:39:SER:HB3	28:G:2466:HOH:O	2.15	0.46
10:J:50:LEU:HD22	10:J:50:LEU:O	2.15	0.46
1:N:377:PHE:HA	1:N:380:VAL:HG22	1.97	0.46
25:O:4230:PSC:H072	9:V:10:ARG:HE	1.81	0.46
4:Q:131:ILE:HD12	4:Q:131:ILE:H	1.81	0.46
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.98	0.46
18:A:3521:TGL:HG11	2:B:7:LEU:HB3	1.98	0.46
22:C:3270:CDL:H632	22:C:3270:CDL:H602	1.55	0.46
22:C:3270:CDL:H652	22:C:3270:CDL:H621	1.56	0.46
3:C:210:ILE:HD13	19:C:3267:PGV:H301	1.98	0.46
10:J:56:PRO:HD3	12:L:46:LYS:HE3	1.96	0.46
1:N:347:LEU:HD13	1:N:383:MET:SD	2.54	0.46
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.98	0.46
4:Q:52:SER:OG	4:Q:55:GLU:HG3	2.16	0.46
19:N:4524:PGV:H141	4:Q:87:PHE:CE2	2.51	0.46
18:N:4522:TGL:H181	18:N:4522:TGL:OA1	2.15	0.46
22:T:4269:CDL:H202	22:T:4269:CDL:H522	1.98	0.46
28:Q:1465:HOH:O	11:X:51:LYS:HD3	2.16	0.46
12:Y:20:ARG:HH21	12:Y:24:MET:CG	2.29	0.46
19:A:3524:PGV:H141	4:D:87:PHE:CE2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:44:PRO:HG2	4:Q:111:PHE:CZ	2.51	0.46
1:A:22:PHE:HA	18:L:3522:TGL:HB72	1.98	0.46
2:O:1:FME:SD	2:O:133:LEU:CD1	3.04	0.46
2:O:57:ASP:H	25:O:4230:PSC:H201	1.80	0.46
1:N:426:PHE:CE1	18:N:4521:TGL:H282	2.50	0.45
1:N:343:GLY:HA2	18:Q:4523:TGL:H202	1.98	0.45
3:P:191:GLY:HA3	28:T:1143:HOH:O	2.16	0.45
22:P:4270:CDL:H642	22:P:4270:CDL:H191	1.98	0.45
4:D:89:ILE:CD1	18:D:3523:TGL:H311	2.46	0.45
23:G:4263:PEK:H15	3:P:248:VAL:HG22	1.99	0.45
11:K:24:PHE:O	11:K:28:VAL:HG12	2.17	0.45
13:M:42:LYS:CE	13:M:42:LYS:HA	2.38	0.45
4:Q:130:PRO:HG2	4:Q:131:ILE:HD12	1.99	0.45
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.99	0.45
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.82	0.45
2:O:57:ASP:H	25:O:4230:PSC:C20	2.29	0.45
22:P:4270:CDL:CB3	22:P:4270:CDL:HB21	2.46	0.45
10:J:1:PHE:H1	10:J:1:PHE:HD1	1.64	0.45
1:N:62:ALA:HB2	17:N:515:HEA:HBD1	1.99	0.45
1:A:1:FME:HA	1:A:1:FME:CE	2.47	0.45
22:G:3269:CDL:H551	22:G:3269:CDL:H582	1.69	0.45
4:Q:48:TRP:HB2	5:R:96:LEU:O	2.16	0.45
22:C:3270:CDL:H191	22:C:3270:CDL:H642	1.99	0.45
22:C:3270:CDL:HB21	22:C:3270:CDL:CB3	2.47	0.45
1:N:171:MET:HG2	3:P:8:TYR:CE1	2.51	0.45
1:N:28:MET:HE2	17:N:515:HEA:H271	1.97	0.45
18:L:3522:TGL:OA1	18:L:3522:TGL:H181	2.17	0.45
6:S:55:LYS:HA	6:S:74:LEU:O	2.17	0.45
1:N:321:PHE:CD2	25:O:4230:PSC:H341	2.52	0.45
1:N:365:ILE:HD11	28:N:2145:HOH:O	2.16	0.45
22:T:4269:CDL:H582	22:T:4269:CDL:H551	1.68	0.45
2:B:47:THR:HB	18:D:3523:TGL:H332	1.99	0.44
3:C:22:LEU:O	3:C:26:LEU:HG	2.17	0.44
6:F:92:VAL:O	6:F:92:VAL:CG2	2.63	0.44
18:L:3522:TGL:H122	18:L:3522:TGL:H291	1.66	0.44
25:O:4230:PSC:H221	25:O:4230:PSC:H251	1.75	0.44
13:Z:32:TRP:CZ3	13:Z:40:TYR:OH	2.70	0.44
2:B:91:ASN:HD22	2:B:92:ASN:N	2.15	0.44
18:N:4521:TGL:H222	18:N:4521:TGL:HA91	1.57	0.44
21:P:4271:CHD:H112	21:P:4271:CHD:H12A	1.65	0.44
4:Q:17:VAL:HG12	28:Q:2237:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.65	0.44
3:P:146:TRP:CZ2	7:T:17:ARG:HG3	2.52	0.44
9:V:15:ARG:HD2	28:V:2350:HOH:O	2.17	0.44
19:A:3524:PGV:H81	19:A:3524:PGV:H262	2.00	0.44
2:B:94:SER:HB2	28:B:4194:HOH:O	2.17	0.44
4:D:126:MET:HA	9:I:68:ILE:HD13	2.00	0.44
18:N:4522:TGL:HG12	12:Y:13:PHE:HB3	1.98	0.44
18:L:3522:TGL:HG12	18:L:3522:TGL:CC1	2.48	0.44
1:A:106:PRO:HB2	1:A:107:PRO:HD3	1.99	0.44
23:G:4263:PEK:H332	23:G:4263:PEK:H371	2.00	0.44
1:N:344:PHE:C	1:N:344:PHE:CD1	2.91	0.44
4:Q:86:MET:HG2	18:Q:4523:TGL:H312	1.98	0.44
23:C:3265:PEK:H131	23:C:3265:PEK:H102	1.79	0.44
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.83	0.44
18:N:4521:TGL:HB81	18:N:4521:TGL:C28	2.48	0.44
1:N:400:PHE:HB3	18:N:4522:TGL:H282	1.99	0.44
18:N:4522:TGL:HB52	18:N:4522:TGL:HB81	1.65	0.44
4:Q:82:VAL:O	4:Q:86:MET:HG3	2.17	0.44
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.53	0.44
2:O:68:LEU:CB	2:O:69:PRO:HD3	2.48	0.44
5:R:87:GLN:HG2	5:R:88:GLU:N	2.32	0.44
1:A:350:VAL:HG21	18:A:3521:TGL:H271	2.00	0.44
4:D:34:SER:N	4:D:37:GLN:HE21	1.99	0.44
25:E:3230:PSC:H232	25:E:3230:PSC:H201	1.85	0.44
18:N:4521:TGL:CA9	18:N:4521:TGL:H241	2.41	0.44
2:O:56:MET:HA	25:O:4230:PSC:C20	2.44	0.44
2:O:62:GLU:O	2:O:66:THR:HB	2.18	0.44
13:Z:13:LYS:O	13:Z:17:ILE:HG13	2.17	0.44
1:A:35:LEU:HD11	1:A:462:LEU:HD13	1.99	0.44
2:B:104:TRP:HA	2:B:207:MET:SD	2.58	0.44
25:O:4230:PSC:H241	25:O:4230:PSC:H62	1.98	0.44
3:P:47:LEU:O	3:P:51:MET:HG2	2.18	0.44
22:T:4269:CDL:H631	22:T:4269:CDL:H662	1.85	0.44
9:V:63:MET:HB3	9:V:68:ILE:CD1	2.45	0.44
1:A:383:MET:O	1:A:387:PHE:HB2	2.18	0.43
1:A:488:THR:HB	1:A:495:LEU:HD13	2.00	0.43
6:F:52:ILE:HA	6:F:94:HIS:HA	1.99	0.43
22:G:3269:CDL:H212	1:N:311:ILE:HD12	2.00	0.43
12:L:11:ILE:CG2	18:L:3522:TGL:H271	2.48	0.43
19:N:4524:PGV:H032	19:N:4524:PGV:O05	2.18	0.43
7:T:19:LEU:HD21	23:T:3263:PEK:H362	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:PHE:CD1	17:A:516:HEA:HAD1	2.53	0.43
2:B:62:GLU:O	2:B:66:THR:HB	2.19	0.43
18:N:4521:TGL:H283	18:N:4521:TGL:CB9	2.49	0.43
25:E:3230:PSC:O01	25:E:3230:PSC:H212	2.17	0.43
7:G:7:ASP:O	7:G:9:GLY:N	2.51	0.43
1:N:35:LEU:HD11	1:N:462:LEU:HD13	2.00	0.43
4:D:86:MET:HG2	18:D:3523:TGL:H312	2.00	0.43
18:L:3522:TGL:HB81	18:L:3522:TGL:HB52	1.63	0.43
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.82	0.43
3:C:177:GLN:HA	3:C:177:GLN:OE1	2.19	0.43
1:N:225:GLY:HA3	3:P:112:LEU:HD21	2.01	0.43
5:R:99:SER:HB2	5:R:104:LEU:HD21	2.01	0.43
5:R:82:TYR:N	5:R:83:PRO:CD	2.81	0.43
6:S:52:ILE:O	6:S:94:HIS:ND1	2.52	0.43
1:N:481:GLU:HB2	13:Z:4:LYS:HE2	1.99	0.43
1:A:431:LEU:HD21	1:A:450:TRP:HB2	2.01	0.43
3:C:34:TRP:CD1	3:C:40:MET:HG2	2.53	0.43
7:G:44:ARG:HD2	7:G:82:TYR:CE1	2.54	0.43
22:T:4269:CDL:H601	22:T:4269:CDL:H571	1.70	0.43
23:C:3265:PEK:H383	22:G:3269:CDL:H272	2.01	0.43
2:O:1:FME:SD	2:O:133:LEU:HD13	2.58	0.43
4:Q:131:ILE:N	4:Q:131:ILE:HD12	2.34	0.43
5:E:97:GLY:HA2	28:E:3252:HOH:O	2.19	0.43
1:N:81:TRP:CZ2	18:N:4522:TGL:C28	3.00	0.43
2:O:164:ALA:O	2:O:194:GLY:HA3	2.18	0.43
2:O:41:ILE:O	2:O:45:MET:HG2	2.18	0.43
4:Q:23:PRO:O	4:Q:25:PRO:HD3	2.18	0.43
22:T:4269:CDL:H732	22:T:4269:CDL:H762	1.94	0.43
18:N:4522:TGL:HA41	12:Y:25:MET:HG2	1.99	0.43
1:A:400:PHE:HB2	18:L:3522:TGL:H252	2.00	0.43
2:B:56:MET:HA	25:E:3230:PSC:H202	2.01	0.43
4:Q:57:VAL:O	4:Q:61:ARG:HG2	2.19	0.43
8:U:37:HIS:CD2	8:U:76:ARG:CZ	3.02	0.43
2:B:52:HIS:HE1	25:E:3230:PSC:H02	1.83	0.42
6:F:55:LYS:HA	6:F:74:LEU:O	2.18	0.42
13:M:42:LYS:HE3	13:M:42:LYS:CA	2.46	0.42
2:O:220:GLU:O	2:O:223:SER:HB2	2.18	0.42
1:N:334:TRP:HZ3	18:Q:4523:TGL:HA62	1.83	0.42
1:N:324:LEU:HD13	2:O:41:ILE:HG22	2.01	0.42
1:N:513:LEU:HD22	1:N:513:LEU:HA	1.89	0.42
3:P:58:TRP:CZ3	19:P:4267:PGV:H81	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:63:ARG:HE	22:P:4270:CDL:CA2	2.11	0.42
4:Q:89:ILE:CD1	18:Q:4523:TGL:H311	2.49	0.42
1:A:240:HIS:O	1:A:243:VAL:HG22	2.19	0.42
10:J:2:GLU:HB2	10:J:4:ARG:NH1	2.35	0.42
1:N:399:LEU:HB2	1:N:494:TRP:CZ3	2.55	0.42
6:S:94:HIS:CG	6:S:95:GLN:N	2.84	0.42
1:A:165:ILE:O	1:A:169:ILE:HG12	2.18	0.42
18:A:3521:TGL:OB1	18:A:3521:TGL:HB42	2.18	0.42
18:D:3523:TGL:HB21	18:D:3523:TGL:OG1	2.19	0.42
1:N:112:LEU:HD23	1:N:112:LEU:C	2.40	0.42
2:O:121:TYR:O	2:O:138:VAL:HA	2.18	0.42
12:Y:20:ARG:HH21	12:Y:24:MET:HG3	1.85	0.42
3:C:146:TRP:CD2	3:C:162:ALA:HB2	2.55	0.42
25:E:3230:PSC:C14	25:E:3230:PSC:H343	2.49	0.42
7:G:7:ASP:O	1:N:169:ILE:HD12	2.20	0.42
2:O:116:LEU:HD12	2:O:117:SER:N	2.35	0.42
23:C:3265:PEK:H232	7:G:21:PHE:CD2	2.54	0.42
6:F:25:ARG:HB3	28:F:145:HOH:O	2.19	0.42
7:G:5:LYS:HB2	23:G:4263:PEK:H372	2.02	0.42
13:Z:28:LEU:HB2	13:Z:29:PRO:HD3	2.01	0.42
1:A:426:PHE:HE1	18:A:3521:TGL:H282	1.74	0.42
12:L:13:PHE:HB3	18:L:3522:TGL:CG1	2.49	0.42
5:R:48:ILE:O	5:R:52:LEU:HG	2.20	0.42
25:O:4230:PSC:H201	25:O:4230:PSC:H232	1.84	0.42
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.82	0.42
4:Q:138:TRP:CH2	11:X:50:PRO:HG2	2.54	0.42
25:E:3230:PSC:H221	25:E:3230:PSC:H251	1.73	0.42
22:G:3269:CDL:H152	22:G:3269:CDL:H181	1.63	0.42
18:N:4522:TGL:H232	18:N:4522:TGL:H272	2.02	0.42
7:T:7:ASP:O	7:T:9:GLY:N	2.52	0.42
5:E:46:LYS:HG2	28:E:3281:HOH:O	2.19	0.41
1:A:62:ALA:HB2	17:A:515:HEA:HBD1	2.01	0.41
2:B:92:ASN:HA	2:B:93:PRO:HD2	1.92	0.41
22:C:3270:CDL:H312	22:C:3270:CDL:H151	2.02	0.41
8:H:60:TYR:C	8:H:60:TYR:CD1	2.92	0.41
1:N:3:ILE:HG23	1:N:7:LEU:HD22	2.02	0.41
22:P:4270:CDL:H312	22:P:4270:CDL:H151	2.03	0.41
1:A:174:PRO:HB2	6:F:35:ALA:HB2	2.02	0.41
21:C:3271:CHD:H222	21:C:3271:CHD:H162	1.79	0.41
28:A:3739:HOH:O	4:D:20:ARG:HG3	2.21	0.41
9:I:65:LYS:O	11:K:54:ARG:NH1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:265:LYS:HB2	1:N:490:THR:HG21	2.02	0.41
21:O:3085:CHD:H212	21:O:3085:CHD:H12	2.01	0.41
22:P:4270:CDL:H372	22:P:4270:CDL:H192	2.02	0.41
7:T:2:SER:O	7:T:3:ALA:HB3	2.21	0.41
11:X:8:ASP:HB2	28:X:2472:HOH:O	2.19	0.41
21:C:3271:CHD:H112	21:C:3271:CHD:H12A	1.63	0.41
18:D:3523:TGL:HA52	18:D:3523:TGL:HB71	2.03	0.41
1:N:426:PHE:CD1	18:N:4521:TGL:H282	2.56	0.41
1:N:440:TYR:HE2	2:O:204:HIS:CE1	2.37	0.41
9:V:35:TYR:C	9:V:37:PHE:H	2.24	0.41
1:A:42:GLY:HA3	4:D:104:TYR:OH	2.21	0.41
1:A:514:LYS:HA	6:F:38:ALA:HB3	2.03	0.41
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.20	0.41
12:L:20:ARG:HH22	18:L:3522:TGL:CC6	2.33	0.41
2:O:116:LEU:HD21	2:O:222:TRP:CH2	2.55	0.41
23:P:4264:PEK:H71	23:P:4264:PEK:H32	2.01	0.41
5:R:86:ILE:HA	5:R:86:ILE:HD13	1.88	0.41
19:A:3524:PGV:H032	19:A:3524:PGV:O05	2.19	0.41
1:A:406:ASN:HD21	19:A:3524:PGV:C3	2.34	0.41
3:C:51:MET:SD	22:C:3270:CDL:H622	2.61	0.41
4:D:126:MET:HG3	4:D:128:VAL:HG23	2.02	0.41
1:A:510:TYR:CD2	6:F:49:VAL:HG13	2.56	0.41
22:G:3269:CDL:HB32	1:N:304:TYR:CD1	2.51	0.41
18:Q:4523:TGL:HB31	18:Q:4523:TGL:HA32	2.03	0.41
7:T:8:HIS:CE1	23:T:3263:PEK:H331	2.56	0.41
18:N:4522:TGL:H342	12:Y:28:PHE:HA	2.03	0.41
2:B:168:LEU:HD13	2:B:184:LEU:HG	2.03	0.41
19:C:3268:PGV:H202	19:C:3268:PGV:H231	1.83	0.41
25:O:4230:PSC:H343	25:O:4230:PSC:C14	2.51	0.41
8:U:9:LYS:HB3	8:U:10:ASN:H	1.57	0.41
2:B:121:TYR:O	2:B:138:VAL:HA	2.21	0.41
2:B:2:ALA:HA	2:B:6:GLN:OE1	2.21	0.41
1:N:177:SER:H	1:N:180:GLN:NE2	2.19	0.41
18:N:4521:TGL:H101	18:N:4521:TGL:C28	2.50	0.41
2:O:13:THR:HB	2:O:168:LEU:HD23	2.03	0.41
22:P:4270:CDL:H561	22:P:4270:CDL:H532	1.83	0.41
3:C:154:GLY:HA2	6:F:6:VAL:HB	2.03	0.41
22:G:3269:CDL:H601	22:G:3269:CDL:H571	1.71	0.41
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.50	0.41
18:N:4522:TGL:CC6	18:N:4522:TGL:HC22	2.51	0.41
1:N:76:GLY:O	1:N:80:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:214:PHE:CD1	19:P:4267:PGV:H71	2.55	0.41
23:P:4265:PEK:H383	22:T:4269:CDL:H272	2.03	0.41
3:P:51:MET:SD	22:P:4270:CDL:H622	2.61	0.41
9:V:73:LYS:HE3	9:V:73:LYS:HB3	1.86	0.41
1:A:35:LEU:HA	1:A:35:LEU:HD23	1.95	0.41
1:A:426:PHE:HB3	1:A:427:PRO:HD3	2.03	0.41
21:B:4085:CHD:H12	21:B:4085:CHD:H212	2.03	0.41
25:O:4230:PSC:H042	25:O:4230:PSC:H062	1.86	0.41
7:T:17:ARG:HD3	28:T:1289:HOH:O	2.21	0.41
8:U:64:CYS:HA	8:U:65:PRO:HD3	1.98	0.41
9:I:35:TYR:C	9:I:37:PHE:H	2.25	0.41
25:O:4230:PSC:H212	25:O:4230:PSC:C02	2.51	0.41
3:P:40:MET:O	3:P:44:MET:HG2	2.21	0.41
4:Q:51:LEU:HD21	4:Q:59:LEU:CD1	2.51	0.41
13:Z:42:LYS:HE3	13:Z:43:SER:N	2.36	0.41
6:F:51:SER:O	6:F:94:HIS:N	2.54	0.40
23:P:4264:PEK:C16	23:P:4264:PEK:H102	2.43	0.40
4:D:48:TRP:CH2	5:E:56:ARG:HA	2.56	0.40
25:O:4230:PSC:H343	25:O:4230:PSC:C13	2.51	0.40
8:U:50:VAL:O	8:U:50:VAL:HG12	2.21	0.40
8:H:36:PHE:CD1	8:H:57:ARG:HB2	2.56	0.40
1:A:113:LEU:CD1	18:L:3522:TGL:H292	2.51	0.40
13:M:37:LEU:HA	13:M:37:LEU:HD23	1.85	0.40
22:P:4270:CDL:H641	22:P:4270:CDL:H231	2.02	0.40
7:T:25:LEU:HD23	7:T:25:LEU:HA	1.89	0.40
7:T:31:CYS:SG	22:T:4269:CDL:H532	2.61	0.40
7:T:8:HIS:CD2	23:T:3263:PEK:H231	2.55	0.40
1:A:513:LEU:HA	1:A:513:LEU:HD22	1.81	0.40
17:A:515:HEA:HMB1	17:A:515:HEA:H11	1.98	0.40
1:N:40:GLU:HG2	1:N:54:TYR:CD2	2.57	0.40
1:N:71:MET:HE1	1:N:195:LEU:HD21	2.04	0.40
2:O:68:LEU:HB3	2:O:69:PRO:HD3	2.04	0.40
2:B:16:ILE:HA	2:B:16:ILE:HD13	1.84	0.40
1:N:298:ASP:HB3	28:N:1369:HOH:O	2.21	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	496 (97%)	16 (3%)	0	100	100
1	N	512/514 (100%)	500 (98%)	12 (2%)	0	100	100
2	B	225/227 (99%)	208 (92%)	14 (6%)	3 (1%)	12	3
2	O	225/227 (99%)	206 (92%)	16 (7%)	3 (1%)	12	3
3	C	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
5	E	103/109 (94%)	103 (100%)	0	0	100	100
5	R	103/109 (94%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	4	0
6	S	96/98 (98%)	89 (93%)	4 (4%)	3 (3%)	4	0
7	G	81/85 (95%)	68 (84%)	6 (7%)	7 (9%)	1	0
7	T	81/85 (95%)	65 (80%)	9 (11%)	7 (9%)	1	0
8	H	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	5	1
8	U	77/85 (91%)	70 (91%)	5 (6%)	2 (3%)	5	1
9	I	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
9	V	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
10	J	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
10	W	56/59 (95%)	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/46 (89%)	41 (100%)	0	0	100	100
All	All	3504/3614 (97%)	3350 (96%)	124 (4%)	30 (1%)	17	6

All (30) 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
6	F	94	HIS
7	G	3	ALA
7	G	40	GLY
8	H	8	ILE
2	O	104	TRP
7	T	3	ALA
8	U	8	ILE
2	B	104	TRP
2	O	60	GLU
7	T	40	GLY
6	F	96	LEU
8	H	46	LYS
6	S	96	LEU
7	G	6	GLY
7	T	6	GLY
8	U	46	LYS
2	O	92	ASN
2	B	92	ASN

### 5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	418 (98%)	8 (2%)	57	46
1	N	426/426 (100%)	415 (97%)	11 (3%)	46	32
2	B	210/210 (100%)	200 (95%)	10 (5%)	25	11
2	O	210/210 (100%)	197 (94%)	13 (6%)	18	6
3	C	224/226 (99%)	220 (98%)	4 (2%)	59	48
3	P	224/226 (99%)	219 (98%)	5 (2%)	52	39
4	D	128/129 (99%)	126 (98%)	2 (2%)	62	54
4	Q	128/129 (99%)	126 (98%)	2 (2%)	62	54
5	E	92/95 (97%)	90 (98%)	2 (2%)	52	39
5	R	92/95 (97%)	88 (96%)	4 (4%)	29	14
6	F	81/81 (100%)	79 (98%)	2 (2%)	47	34
6	S	81/81 (100%)	77 (95%)	4 (5%)	25	11
7	G	67/68 (98%)	61 (91%)	6 (9%)	9	2
7	T	67/68 (98%)	62 (92%)	5 (8%)	13	4
8	H	71/75 (95%)	69 (97%)	2 (3%)	43	30
8	U	71/75 (95%)	67 (94%)	4 (6%)	21	8
9	I	57/57 (100%)	53 (93%)	4 (7%)	15	5
9	V	57/57 (100%)	55 (96%)	2 (4%)	36	21
10	J	49/50 (98%)	48 (98%)	1 (2%)	55	44
10	W	49/50 (98%)	48 (98%)	1 (2%)	55	44
11	K	39/46 (85%)	39 (100%)	0	100	100
11	X	39/46 (85%)	38 (97%)	1 (3%)	46	32
12	L	39/40 (98%)	39 (100%)	0	100	100
12	Y	39/40 (98%)	37 (95%)	2 (5%)	24	10
13	M	37/38 (97%)	32 (86%)	5 (14%)	4	1
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	1
All	All	3040/3082 (99%)	2936 (97%)	104 (3%)	37	22

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN
1	A	238	PHE
1	A	338	MET
1	A	369	ASP
1	A	513	LEU
2	B	33	LEU
2	B	60	GLU
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	104	TRP
2	B	115	ASP
2	B	167	SER
2	B	171	LYS
3	C	159	MET
3	C	179	SER
3	C	214	PHE
3	C	230	ASN
4	D	4	SER
4	D	51	LEU
5	E	70	VAL
5	E	90	ARG
6	F	48	LEU
6	F	87	THR
7	G	17	ARG
7	G	18	PHE
7	G	36	TRP
7	G	42	ARG
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
9	I	61	GLU
10	J	50	LEU
13	M	13	LYS
13	M	34	LEU

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Mol	Chain	Res	Type
13	M	38	ASP
13	M	39	ASN
13	M	42	LYS
1	N	38	ARG
1	N	109	PHE
1	N	115	SER
1	N	138	HIS
1	N	180	GLN
1	N	238	PHE
1	N	241	PRO
1	N	338	MET
1	N	369	ASP
1	N	484	THR
1	N	513	LEU
2	O	16	ILE
2	O	33	LEU
2	O	60	GLU
2	O	66	THR
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	104	TRP
2	O	115	ASP
2	O	148	MET
2	O	217	LYS
3	P	29	SER
3	P	33	MET
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	8	SER
4	Q	121	LYS
5	R	5	HIS
5	R	70	VAL
5	R	80	GLU
5	R	90	ARG
6	S	48	LEU
6	S	53	THR
6	S	54	ASN
6	S	80	GLN

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Mol	Chain	Res	Type
7	T	18	PHE
7	T	38	HIS
7	T	42	ARG
7	T	43	GLU
7	T	54	ARG
8	U	9	LYS
8	U	21	PRO
8	U	29	CYS
8	U	60	TYR
9	V	8	GLN
9	V	29	LEU
10	W	50	LEU
11	X	54	ARG
12	Y	20	ARG
12	Y	26	THR
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS

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

Mol	Chain	Res	Type
1	A	80	ASN
1	A	98	ASN
1	A	151	HIS
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	10	GLN
2	B	181	GLN
3	C	3	HIS
3	C	50	ASN
3	C	68	GLN
4	D	37	GLN
4	D	109	HIS
5	E	94	ASN
7	G	8	HIS
7	G	34	ASN
9	I	8	GLN
11	K	35	GLN
1	N	80	ASN

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Mol	Chain	Res	Type
1	N	98	ASN
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	91	ASN
2	O	181	GLN
2	O	195	GLN
3	P	3	HIS
3	P	68	GLN
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN
6	S	54	ASN
6	S	80	GLN
6	S	94	HIS
9	V	8	GLN
10	W	57	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	FME	N	1	1	8,9,10	0.79	0	7,9,11	1.87	2 (28%)
1	FME	A	1	1	8,9,10	0.64	0	7,9,11	1.17	1 (14%)
7	TPO	T	11	7	8,10,11	1.32	1 (12%)	10,14,16	1.07	0
2	FME	O	1	2	8,9,10	0.66	0	7,9,11	1.88	2 (28%)
7	TPO	G	11	7	8,10,11	1.38	1 (12%)	10,14,16	1.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	SAC	V	1	9	7,8,9	2.71	2 (28%)	8,9,11	3.24	5 (62%)
2	FME	B	1	2	8,9,10	0.86	0	7,9,11	2.49	2 (28%)
9	SAC	I	1	9	7,8,9	2.61	2 (28%)	8,9,11	2.92	4 (50%)

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

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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	V	1	SAC	OAC-C1A	5.22	1.35	1.23
9	I	1	SAC	OAC-C1A	5.14	1.34	1.23
9	V	1	SAC	CA-N	4.43	1.52	1.46
9	I	1	SAC	CA-N	4.33	1.52	1.46
7	T	11	TPO	CB-CA	2.64	1.59	1.53
7	G	11	TPO	CB-CA	2.37	1.59	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	1	SAC	CA-N-C1A	-6.99	110.25	123.15
9	I	1	SAC	CA-N-C1A	-5.71	112.62	123.15
2	B	1	FME	CA-N-CN	-4.79	115.46	122.82
2	B	1	FME	C-CA-N	4.26	117.43	109.73
1	N	1	FME	CA-N-CN	-4.24	116.30	122.82
9	I	1	SAC	CB-CA-N	3.72	118.90	110.55
2	O	1	FME	C-CA-N	3.68	116.38	109.73
9	I	1	SAC	C-CA-N	-3.53	103.36	109.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	V	1	SAC	C-CA-N	-3.48	103.46	109.73
2	O	1	FME	CA-N-CN	-2.96	118.27	122.82
9	V	1	SAC	C2A-C1A-N	2.88	120.97	116.10
9	V	1	SAC	CB-CA-N	2.59	116.36	110.55
9	V	1	SAC	OAC-C1A-C2A	-2.18	118.00	122.06
1	A	1	FME	CA-N-CN	-2.17	119.48	122.82
1	N	1	FME	O-C-CA	-2.07	119.35	124.78
9	I	1	SAC	C2A-C1A-N	2.01	119.50	116.10

There are no chirality outliers.

All (23) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	N	1	FME	1	0
1	A	1	FME	3	0
7	T	11	TPO	1	0
2	O	1	FME	2	0
7	G	11	TPO	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 42 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	$\# Z  > 2$
21	CHD	C	3271	-	29,32,32	0.80	1 (3%)	48,51,51	3.71	22 (45%)
22	CDL	G	3269	-	99,99,99	0.96	5 (5%)	105,111,111	0.93	7 (6%)
21	CHD	O	3085	-	29,32,32	0.76	0	48,51,51	1.93	18 (37%)
19	PGV	P	4267	-	50,50,50	0.98	2 (4%)	53,56,56	1.05	3 (5%)
23	PEK	C	3265	-	52,52,52	1.64	11 (21%)	55,57,57	0.99	4 (7%)
19	PGV	P	4268	-	50,50,50	1.11	4 (8%)	53,56,56	0.66	0
27	DMU	Z	4526	-	34,34,34	3.22	8 (23%)	45,45,45	4.29	19 (42%)
23	PEK	P	4265	-	52,52,52	1.68	12 (23%)	55,57,57	0.96	5 (9%)
19	PGV	C	3268	-	50,50,50	1.10	4 (8%)	53,56,56	0.64	0
21	CHD	C	3525	-	29,32,32	0.80	0	48,51,51	1.63	12 (25%)
21	CHD	B	4085	-	29,32,32	0.72	0	48,51,51	1.91	14 (29%)
25	PSC	E	3230	-	51,51,51	1.22	3 (5%)	57,59,59	1.02	4 (7%)
23	PEK	C	3264	-	52,52,52	1.47	4 (7%)	55,57,57	1.28	7 (12%)
23	PEK	P	4264	-	52,52,52	1.46	5 (9%)	55,57,57	1.35	10 (18%)
21	CHD	P	4525	-	29,32,32	0.83	1 (3%)	48,51,51	1.69	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	PGV	N	4524	-	50,50,50	1.11	4 (8%)	53,56,56	1.17	7 (13%)
18	TGL	D	3523	-	62,62,62	1.15	3 (4%)	65,65,65	1.11	6 (9%)
18	TGL	N	4522	-	62,62,62	1.41	6 (9%)	65,65,65	1.13	5 (7%)
17	HEA	A	515	1	44,67,67	1.27	5 (11%)	37,103,103	1.52	8 (21%)
25	PSC	O	4230	-	51,51,51	1.19	3 (5%)	57,59,59	1.03	4 (7%)
20	CUA	B	228	2	0,1,1	0.00	-	-		
19	PGV	N	4266	-	50,50,50	1.02	3 (6%)	53,56,56	0.99	3 (5%)
18	TGL	L	3522	-	62,62,62	1.38	7 (11%)	65,65,65	1.22	6 (9%)
18	TGL	Q	4523	-	62,62,62	1.14	3 (4%)	65,65,65	1.05	4 (6%)
22	CDL	P	4270	-	99,99,99	0.81	3 (3%)	105,111,111	0.87	5 (4%)
19	PGV	C	3267	-	50,50,50	0.80	1 (2%)	53,56,56	0.93	4 (7%)
27	DMU	M	3526	-	34,34,34	3.24	8 (23%)	45,45,45	4.33	19 (42%)
19	PGV	A	3524	-	50,50,50	1.11	6 (12%)	53,56,56	1.23	7 (13%)
17	HEA	A	516	1	44,67,67	1.30	5 (11%)	37,103,103	1.39	6 (16%)
19	PGV	A	3266	-	50,50,50	0.90	1 (2%)	53,56,56	0.77	2 (3%)
22	CDL	C	3270	-	99,99,99	0.78	3 (3%)	105,111,111	0.90	5 (4%)
17	HEA	N	516	1	44,67,67	1.40	6 (13%)	37,103,103	1.37	6 (16%)
18	TGL	N	4521	-	62,62,62	1.00	4 (6%)	65,65,65	1.10	4 (6%)
21	CHD	J	3060	-	29,32,32	0.86	1 (3%)	48,51,51	3.34	24 (50%)
21	CHD	W	4060	-	29,32,32	0.95	2 (6%)	48,51,51	3.30	25 (52%)
21	CHD	P	4271	-	29,32,32	0.76	0	48,51,51	3.64	22 (45%)
23	PEK	G	4263	-	52,52,52	1.68	9 (17%)	55,57,57	1.00	3 (5%)
22	CDL	T	4269	-	99,99,99	0.92	4 (4%)	105,111,111	0.94	9 (8%)
17	HEA	N	515	1	44,67,67	1.36	6 (13%)	37,103,103	1.58	12 (32%)
23	PEK	T	3263	-	52,52,52	1.68	11 (21%)	55,57,57	0.99	3 (5%)
20	CUA	O	228	2	0,1,1	0.00	-	-		
18	TGL	A	3521	-	62,62,62	0.98	4 (6%)	65,65,65	1.13	6 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CHD	C	3271	-	5/5/12/12	6/7/74/74	0/4/4/4
22	CDL	G	3269	-	-	69/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CHD	O	3085	-	-	0/7/74/74	0/4/4/4
19	PGV	P	4267	-	-	15/55/55/55	-
23	PEK	C	3265	-	-	24/56/56/56	-
19	PGV	P	4268	-	-	33/55/55/55	-
27	DMU	Z	4526	-	5/5/10/10	6/19/59/59	0/2/2/2
23	PEK	P	4265	-	-	24/56/56/56	-
19	PGV	C	3268	-	-	33/55/55/55	-
19	PGV	N	4266	-	-	15/55/55/55	-
21	CHD	C	3525	-	-	0/7/74/74	0/4/4/4
21	CHD	B	4085	-	-	0/7/74/74	0/4/4/4
25	PSC	E	3230	-	-	39/55/55/55	-
23	PEK	C	3264	-	-	17/56/56/56	-
19	PGV	N	4524	-	-	29/55/55/55	-
21	CHD	P	4525	-	-	0/7/74/74	0/4/4/4
23	PEK	P	4264	-	-	17/56/56/56	-
18	TGL	D	3523	-	-	29/65/65/65	-
21	CHD	W	4060	-	5/5/12/12	6/7/74/74	0/4/4/4
27	DMU	M	3526	-	5/5/10/10	6/19/59/59	0/2/2/2
25	PSC	O	4230	-	-	40/55/55/55	-
18	TGL	N	4522	-	-	34/65/65/65	-
18	TGL	L	3522	-	-	33/65/65/65	-
18	TGL	Q	4523	-	-	27/65/65/65	-
22	CDL	P	4270	-	-	72/110/110/110	-
19	PGV	C	3267	-	-	18/55/55/55	-
17	HEA	A	515	1	3/3/7/16	3/24/76/76	-
19	PGV	A	3524	-	-	29/55/55/55	-
17	HEA	A	516	1	3/3/7/16	1/24/76/76	-
19	PGV	A	3266	-	-	12/55/55/55	-
22	CDL	C	3270	-	-	71/110/110/110	-
17	HEA	N	516	1	3/3/7/16	1/24/76/76	-
18	TGL	N	4521	-	-	32/65/65/65	-
21	CHD	J	3060	-	5/5/12/12	6/7/74/74	0/4/4/4
21	CHD	P	4271	-	5/5/12/12	6/7/74/74	0/4/4/4
23	PEK	G	4263	-	-	23/56/56/56	-
22	CDL	T	4269	-	-	68/110/110/110	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	HEA	N	515	1	3/3/7/16	3/24/76/76	-
23	PEK	T	3263	-	-	23/56/56/56	-
18	TGL	A	3521	-	-	32/65/65/65	-

All (168) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	M	3526	DMU	O7-C3	-8.28	1.22	1.43
27	Z	4526	DMU	O7-C3	-8.08	1.22	1.43
27	Z	4526	DMU	O16-C6	-7.57	1.27	1.40
27	M	3526	DMU	O16-C6	-7.13	1.28	1.40
27	M	3526	DMU	O1-C9	-7.08	1.27	1.44
27	Z	4526	DMU	O1-C9	-7.01	1.27	1.44
27	M	3526	DMU	O5-C4	-6.77	1.27	1.44
27	Z	4526	DMU	O5-C4	-6.38	1.28	1.44
27	M	3526	DMU	O16-C18	-6.28	1.25	1.43
27	Z	4526	DMU	O7-C10	-6.18	1.24	1.41
27	M	3526	DMU	O7-C10	-6.13	1.24	1.41
27	Z	4526	DMU	O1-C10	-5.91	1.26	1.41
27	Z	4526	DMU	O16-C18	-5.87	1.26	1.43
18	L	3522	TGL	OG2-CB1	5.82	1.50	1.34
27	M	3526	DMU	O1-C10	-5.66	1.27	1.41
18	N	4522	TGL	OG2-CB1	5.44	1.49	1.34
18	N	4522	TGL	OG1-CA1	5.10	1.48	1.33
18	D	3523	TGL	OG1-CA1	5.03	1.48	1.33
23	P	4264	PEK	C12-C11	4.77	1.59	1.31
18	L	3522	TGL	OG1-CA1	4.66	1.47	1.33
23	C	3264	PEK	C15-C14	4.66	1.58	1.31
23	G	4263	PEK	C12-C11	4.65	1.58	1.31
27	M	3526	DMU	O5-C6	-4.61	1.30	1.41
23	P	4264	PEK	C15-C14	4.57	1.58	1.31
23	C	3264	PEK	C12-C11	4.53	1.58	1.31
18	Q	4523	TGL	OG1-CA1	4.52	1.46	1.33
18	N	4522	TGL	OG3-CC1	4.45	1.46	1.33
23	T	3263	PEK	C12-C11	4.44	1.57	1.31
27	Z	4526	DMU	O5-C6	-4.44	1.30	1.41
17	N	516	HEA	C3B-C11	-4.42	1.49	1.52
25	O	4230	PSC	C10-C9	4.37	1.57	1.31
18	D	3523	TGL	OG3-CC1	4.36	1.46	1.33
23	T	3263	PEK	C6-C5	4.33	1.56	1.31
19	P	4268	PGV	C12-C11	4.33	1.56	1.31
23	C	3265	PEK	C6-C5	4.32	1.56	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	4265	PEK	C12-C11	4.31	1.56	1.31
18	Q	4523	TGL	OG2-CB1	4.30	1.46	1.34
25	O	4230	PSC	C13-C12	4.29	1.56	1.31
23	G	4263	PEK	C6-C5	4.27	1.56	1.31
23	C	3265	PEK	C12-C11	4.26	1.56	1.31
25	E	3230	PSC	C10-C9	4.26	1.56	1.31
23	P	4265	PEK	C6-C5	4.25	1.56	1.31
19	C	3268	PGV	C12-C11	4.22	1.56	1.31
23	G	4263	PEK	C15-C14	4.20	1.56	1.31
23	P	4265	PEK	C9-C8	4.20	1.56	1.31
23	C	3265	PEK	C9-C8	4.17	1.55	1.31
23	T	3263	PEK	C9-C8	4.15	1.55	1.31
23	T	3263	PEK	C15-C14	4.15	1.55	1.31
18	N	4521	TGL	OG2-CB1	4.11	1.45	1.34
23	C	3264	PEK	C6-C5	4.11	1.55	1.31
25	E	3230	PSC	C13-C12	4.11	1.55	1.31
23	C	3264	PEK	C9-C8	4.09	1.55	1.31
19	N	4524	PGV	C12-C11	4.09	1.55	1.31
18	L	3522	TGL	OG3-CC1	4.08	1.45	1.33
19	A	3266	PGV	C12-C11	4.07	1.55	1.31
23	P	4264	PEK	C9-C8	4.06	1.55	1.31
23	G	4263	PEK	C9-C8	4.05	1.55	1.31
19	A	3524	PGV	C12-C11	4.05	1.55	1.31
23	C	3265	PEK	C15-C14	4.03	1.55	1.31
17	N	515	HEA	C3B-C11	-4.02	1.49	1.52
23	P	4264	PEK	C6-C5	4.00	1.54	1.31
23	P	4265	PEK	C15-C14	3.96	1.54	1.31
19	N	4266	PGV	C12-C11	3.92	1.54	1.31
18	Q	4523	TGL	OG3-CC1	3.86	1.44	1.33
18	A	3521	TGL	OG2-CB1	3.69	1.44	1.34
19	P	4267	PGV	C12-C11	3.63	1.52	1.31
18	D	3523	TGL	OG2-CB1	3.62	1.44	1.34
23	T	3263	PEK	O03-C21	3.58	1.43	1.33
17	N	516	HEA	C3A-CMA	-3.44	1.38	1.46
23	G	4263	PEK	C03-C02	3.41	1.61	1.50
17	A	515	HEA	C3B-C11	-3.41	1.50	1.52
18	A	3521	TGL	OG1-CA1	3.39	1.43	1.33
17	A	516	HEA	C3C-C2C	-3.38	1.35	1.40
17	A	516	HEA	C3A-C2A	-3.37	1.35	1.40
23	P	4265	PEK	O03-C21	3.35	1.43	1.33
22	T	4269	CDL	CB6-CB4	3.32	1.60	1.50
23	T	3263	PEK	C03-C02	3.28	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	G	4263	PEK	O03-C21	3.21	1.42	1.33
17	N	515	HEA	C3A-C2A	-3.20	1.35	1.40
23	G	4263	PEK	C01-C02	3.20	1.60	1.50
21	W	4060	CHD	C13-C17	3.19	1.61	1.55
17	N	515	HEA	C3A-CMA	-3.19	1.39	1.46
18	N	4521	TGL	OG1-CA1	3.15	1.42	1.33
22	G	3269	CDL	CB6-CB4	3.13	1.60	1.50
17	A	515	HEA	C4D-ND	3.10	1.42	1.36
22	G	3269	CDL	OA6-CA5	3.06	1.42	1.34
17	A	516	HEA	C3A-CMA	-3.04	1.39	1.46
23	C	3265	PEK	C03-C02	2.95	1.59	1.50
18	A	3521	TGL	OG3-CC1	2.93	1.41	1.33
17	A	515	HEA	C3A-CMA	-2.92	1.39	1.46
23	C	3265	PEK	O03-C21	2.89	1.41	1.33
19	P	4268	PGV	C2-C1	2.89	1.59	1.50
19	C	3267	PGV	C12-C11	2.88	1.48	1.31
18	N	4521	TGL	OG3-CC1	2.88	1.41	1.33
23	T	3263	PEK	C01-C02	2.87	1.59	1.50
21	J	3060	CHD	C13-C17	2.83	1.60	1.55
17	N	516	HEA	C3A-C2A	-2.83	1.36	1.40
23	P	4265	PEK	C03-C02	2.83	1.59	1.50
23	G	4263	PEK	C22-C21	2.79	1.58	1.50
19	C	3268	PGV	C2-C1	2.79	1.58	1.50
19	N	4524	PGV	P-O11	2.71	1.70	1.59
19	A	3524	PGV	P-O11	2.71	1.70	1.59
19	P	4268	PGV	O01-C1	2.69	1.41	1.34
23	T	3263	PEK	C22-C21	2.64	1.58	1.50
19	C	3268	PGV	O01-C1	2.62	1.41	1.34
23	P	4265	PEK	P-O11	2.61	1.69	1.59
22	P	4270	CDL	CA6-CA4	2.59	1.58	1.50
18	N	4521	TGL	OG1-CG1	-2.59	1.39	1.45
17	N	516	HEA	C4D-ND	2.59	1.41	1.36
23	P	4265	PEK	C2-C1	2.50	1.58	1.50
23	T	3263	PEK	P-O11	2.50	1.69	1.59
18	N	4522	TGL	OG3-CG3	2.50	1.50	1.45
23	P	4265	PEK	C01-C02	2.49	1.58	1.50
18	L	3522	TGL	OG2-CG2	2.46	1.52	1.46
22	T	4269	CDL	OA6-CA5	2.46	1.41	1.34
23	P	4265	PEK	P-O12	2.45	1.69	1.59
23	C	3265	PEK	C01-C02	2.45	1.58	1.50
23	P	4265	PEK	O01-C1	2.45	1.41	1.34
22	G	3269	CDL	CB3-CB4	2.43	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	3521	TGL	OG1-CG1	-2.43	1.39	1.45
23	C	3265	PEK	P-O11	2.43	1.69	1.59
25	E	3230	PSC	C2-C1	2.41	1.57	1.50
18	N	4522	TGL	CB2-CB1	2.39	1.57	1.50
22	G	3269	CDL	C11-CA5	2.39	1.57	1.50
18	N	4522	TGL	CC2-CC1	2.37	1.57	1.50
22	T	4269	CDL	CB3-CB4	2.35	1.57	1.50
22	T	4269	CDL	C11-CA5	2.35	1.57	1.50
22	C	3270	CDL	CA6-CA4	2.33	1.57	1.50
17	A	516	HEA	C3B-C11	-2.33	1.51	1.52
19	N	4524	PGV	C20-C19	2.33	1.57	1.50
17	A	515	HEA	C3C-CAC	2.31	1.52	1.47
23	C	3265	PEK	C2-C1	2.31	1.57	1.50
18	L	3522	TGL	OG3-CG3	2.30	1.50	1.45
17	N	515	HEA	C1C-NC	2.24	1.40	1.36
23	G	4263	PEK	P-O11	2.24	1.68	1.59
19	A	3524	PGV	C20-C19	2.23	1.57	1.50
25	O	4230	PSC	C2-C1	2.23	1.57	1.50
17	A	516	HEA	C4D-ND	2.22	1.40	1.36
19	N	4266	PGV	O03-C19	2.22	1.39	1.33
23	C	3265	PEK	O01-C1	2.20	1.40	1.34
23	P	4264	PEK	O03-C01	-2.20	1.40	1.45
23	T	3263	PEK	C2-C1	2.20	1.57	1.50
18	L	3522	TGL	CC2-CC1	2.19	1.57	1.50
19	N	4266	PGV	C01-C02	2.18	1.57	1.50
21	C	3271	CHD	C10-C9	-2.18	1.52	1.56
22	P	4270	CDL	CA3-CA4	2.17	1.57	1.50
23	P	4265	PEK	C22-C21	2.17	1.57	1.50
23	C	3265	PEK	P-O12	2.16	1.68	1.59
19	P	4267	PGV	O03-C19	2.15	1.39	1.33
17	N	516	HEA	C1D-C2D	2.14	1.47	1.42
22	G	3269	CDL	CA6-CA4	2.14	1.57	1.50
22	C	3270	CDL	CA3-CA4	2.13	1.57	1.50
22	C	3270	CDL	OA8-CA7	2.13	1.39	1.33
22	P	4270	CDL	OA8-CA7	2.13	1.39	1.33
21	P	4525	CHD	C8-C9	2.11	1.58	1.53
19	A	3524	PGV	C01-C02	2.08	1.57	1.50
19	A	3524	PGV	P-O12	2.07	1.67	1.59
18	L	3522	TGL	CG3-CG2	2.07	1.57	1.50
19	P	4268	PGV	C03-C02	2.07	1.57	1.50
21	W	4060	CHD	C20-C17	2.06	1.58	1.54
23	T	3263	PEK	O01-C1	2.05	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	N	515	HEA	C1D-C2D	2.04	1.47	1.42
17	N	516	HEA	C1B-NB	2.03	1.40	1.36
19	A	3524	PGV	O03-C19	2.02	1.39	1.33
17	N	515	HEA	C4D-ND	2.01	1.40	1.36
19	N	4524	PGV	C01-C02	2.01	1.56	1.50
19	C	3268	PGV	C03-C02	2.01	1.56	1.50
17	A	515	HEA	C3B-C2B	-2.01	1.34	1.41

All (339) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	M	3526	DMU	C10-C5-C7	10.54	131.95	110.00
21	C	3271	CHD	C17-C13-C14	10.46	110.64	100.09
27	Z	4526	DMU	C10-C5-C7	10.44	131.73	110.00
21	P	4271	CHD	C10-C9-C8	10.21	122.78	111.82
21	P	4271	CHD	C17-C13-C14	10.05	110.22	100.09
27	Z	4526	DMU	C1-C2-C3	9.99	132.50	109.68
21	C	3271	CHD	C17-C13-C12	-9.97	108.56	117.67
27	M	3526	DMU	C1-C2-C3	9.96	132.43	109.68
21	P	4271	CHD	C17-C13-C12	-9.86	108.66	117.67
21	C	3271	CHD	C10-C9-C8	9.83	122.37	111.82
21	J	3060	CHD	C17-C13-C14	9.63	109.81	100.09
21	W	4060	CHD	C17-C13-C14	9.29	109.46	100.09
21	C	3271	CHD	C19-C10-C9	-8.48	99.50	111.18
27	M	3526	DMU	C6-O5-C4	8.41	130.20	113.69
27	Z	4526	DMU	C6-O5-C4	8.09	129.56	113.69
27	M	3526	DMU	C8-C7-C5	-7.93	96.98	110.82
27	Z	4526	DMU	C8-C7-C5	-7.90	97.03	110.82
21	P	4271	CHD	C19-C10-C9	-7.73	100.53	111.18
27	M	3526	DMU	O1-C9-C8	7.57	123.43	109.69
27	Z	4526	DMU	O5-C4-C3	7.39	125.34	109.75
27	Z	4526	DMU	O1-C9-C11	7.34	124.68	106.44
27	Z	4526	DMU	O1-C9-C8	7.27	122.90	109.69
27	M	3526	DMU	C7-C8-C9	7.19	123.06	110.24
27	M	3526	DMU	O5-C4-C3	7.14	124.81	109.75
27	M	3526	DMU	O1-C9-C11	7.06	124.00	106.44
27	Z	4526	DMU	C7-C8-C9	7.04	122.79	110.24
21	W	4060	CHD	C13-C17-C20	6.99	127.84	119.50
21	J	3060	CHD	C13-C17-C20	6.97	127.82	119.50
27	M	3526	DMU	O5-C4-C57	6.96	123.75	106.44
27	Z	4526	DMU	O5-C4-C57	6.84	123.45	106.44
21	W	4060	CHD	C10-C9-C8	6.61	118.91	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	P	4271	CHD	C1-C10-C5	6.57	117.48	107.77
21	J	3060	CHD	C10-C9-C8	6.52	118.82	111.82
27	M	3526	DMU	C18-O16-C6	6.46	124.56	113.84
21	C	3271	CHD	C1-C10-C5	6.41	117.25	107.77
27	M	3526	DMU	O7-C3-C2	6.09	123.47	107.28
27	Z	4526	DMU	O7-C3-C2	6.01	123.27	107.28
27	Z	4526	DMU	C18-O16-C6	5.80	123.46	113.84
21	C	3271	CHD	C9-C8-C7	5.73	118.73	111.88
21	P	4271	CHD	C9-C8-C7	5.66	118.65	111.88
27	Z	4526	DMU	O5-C6-O16	5.59	123.21	109.97
21	W	4060	CHD	C15-C14-C8	-5.57	110.54	118.33
21	J	3060	CHD	C15-C14-C8	-5.57	110.54	118.33
21	W	4060	CHD	C6-C5-C10	5.44	118.44	112.66
21	J	3060	CHD	C4-C3-C2	5.42	117.03	110.55
27	Z	4526	DMU	O5-C6-C1	5.39	121.77	110.35
21	J	3060	CHD	C6-C5-C10	5.36	118.35	112.66
21	W	4060	CHD	C11-C12-C13	5.30	116.69	111.24
21	C	3271	CHD	C4-C5-C10	5.29	118.28	112.66
27	M	3526	DMU	O5-C6-C1	5.20	121.35	110.35
21	P	4271	CHD	C15-C14-C8	-5.17	111.11	118.33
21	C	3271	CHD	C15-C14-C8	-5.16	111.12	118.33
27	M	3526	DMU	O5-C6-O16	5.16	122.18	109.97
21	J	3060	CHD	C9-C8-C7	5.13	118.01	111.88
21	W	4060	CHD	C9-C8-C7	5.03	117.89	111.88
21	J	3060	CHD	C18-C13-C14	-5.01	103.38	111.21
27	M	3526	DMU	O16-C6-C1	4.96	116.04	108.30
21	J	3060	CHD	C11-C12-C13	4.90	116.27	111.24
21	P	4271	CHD	C4-C5-C10	4.88	117.83	112.66
21	C	3271	CHD	C19-C10-C1	-4.87	100.41	108.26
21	P	4271	CHD	C19-C10-C1	-4.85	100.44	108.26
21	W	4060	CHD	C4-C3-C2	4.85	116.34	110.55
21	J	3060	CHD	C1-C10-C5	4.84	114.93	107.77
21	W	4060	CHD	C18-C13-C14	-4.74	103.79	111.21
18	D	3523	TGL	OG2-CB1-CB2	4.67	121.57	111.50
18	N	4521	TGL	OG2-CB1-CB2	4.66	121.55	111.50
27	Z	4526	DMU	O7-C3-C4	4.58	121.99	109.45
21	W	4060	CHD	C1-C10-C5	4.56	114.52	107.77
21	W	4060	CHD	C5-C6-C7	4.53	119.47	114.46
18	A	3521	TGL	OG2-CB1-CB2	4.49	121.19	111.50
21	C	3271	CHD	C4-C3-C2	4.39	115.80	110.55
18	L	3522	TGL	OG3-CG3-CG2	4.32	121.02	108.43
21	P	4525	CHD	C13-C17-C20	4.29	124.61	119.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	J	3060	CHD	C5-C6-C7	4.26	119.16	114.46
27	M	3526	DMU	O7-C3-C4	4.23	121.05	109.45
19	N	4266	PGV	C01-O03-C19	-4.20	101.55	117.12
18	Q	4523	TGL	OG2-CB1-CB2	4.10	120.35	111.50
27	Z	4526	DMU	O16-C6-C1	4.09	114.68	108.30
21	P	4271	CHD	C4-C3-C2	4.08	115.42	110.55
18	L	3522	TGL	OG2-CB1-CB2	4.08	120.28	111.50
27	M	3526	DMU	O7-C10-C5	4.02	118.52	108.10
21	C	3525	CHD	C13-C17-C20	4.01	124.28	119.50
27	Z	4526	DMU	O7-C10-C5	3.96	118.37	108.10
21	B	4085	CHD	C16-C17-C13	-3.95	99.68	103.55
21	J	3060	CHD	C17-C13-C12	-3.94	114.07	117.67
18	N	4522	TGL	OG3-CG3-CG2	3.92	119.85	108.43
21	C	3271	CHD	C14-C13-C12	3.85	110.98	107.40
21	W	4060	CHD	C2-C1-C10	3.84	119.37	112.78
21	O	3085	CHD	C10-C9-C8	3.75	115.85	111.82
21	B	4085	CHD	C15-C14-C8	-3.71	113.14	118.33
21	B	4085	CHD	C15-C14-C13	-3.69	99.93	103.55
23	T	3263	PEK	P-O11-C03	3.67	143.22	121.68
21	J	3060	CHD	C2-C1-C10	3.66	119.06	112.78
21	O	3085	CHD	C16-C17-C13	-3.66	99.97	103.55
21	P	4525	CHD	C15-C14-C8	-3.64	113.24	118.33
21	W	4060	CHD	C17-C13-C12	-3.64	114.34	117.67
21	O	3085	CHD	C15-C14-C8	-3.63	113.26	118.33
23	C	3264	PEK	C30-C29-C28	-3.62	96.05	114.42
21	P	4271	CHD	C14-C13-C12	3.62	110.77	107.40
21	B	4085	CHD	O3-C3-C4	-3.57	102.74	109.85
18	N	4522	TGL	OG2-CB1-CB2	3.56	119.16	111.50
21	O	3085	CHD	C5-C4-C3	3.55	117.97	112.76
21	J	3060	CHD	C19-C10-C9	-3.55	106.29	111.18
23	C	3264	PEK	O03-C21-C22	-3.54	100.78	111.91
21	O	3085	CHD	C5-C6-C7	3.54	118.37	114.46
23	G	4263	PEK	P-O11-C03	3.52	142.34	121.68
21	W	4060	CHD	C5-C4-C3	3.52	117.93	112.76
19	A	3524	PGV	C02-O01-C1	3.49	126.38	117.79
21	J	3060	CHD	C11-C9-C10	3.45	117.28	113.73
21	B	4085	CHD	C1-C2-C3	3.42	114.86	110.47
17	N	516	HEA	C27-C19-C20	3.41	121.00	115.27
19	A	3524	PGV	P-O11-C03	3.40	141.60	121.68
21	W	4060	CHD	C11-C9-C10	3.36	117.19	113.73
23	P	4264	PEK	C30-C29-C28	-3.35	97.41	114.42
21	J	3060	CHD	C5-C4-C3	3.32	117.64	112.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	3265	PEK	P-O11-C03	3.32	141.13	121.68
19	N	4524	PGV	P-O11-C03	3.31	141.06	121.68
21	C	3525	CHD	C14-C13-C12	-3.28	104.34	107.40
19	P	4267	PGV	C9-C10-C11	-3.27	93.69	112.43
23	P	4265	PEK	P-O11-C03	3.25	140.76	121.68
21	C	3525	CHD	C15-C14-C8	-3.24	113.80	118.33
21	B	4085	CHD	C14-C13-C12	-3.23	104.39	107.40
27	M	3526	DMU	C10-O7-C3	3.23	125.95	117.96
21	J	3060	CHD	C1-C2-C3	3.18	114.55	110.47
21	W	4060	CHD	C1-C2-C3	3.16	114.52	110.47
17	A	516	HEA	C27-C19-C20	3.15	120.57	115.27
23	P	4264	PEK	O03-C21-C22	-3.15	102.03	111.91
21	P	4525	CHD	C1-C10-C5	3.15	112.42	107.77
21	C	3271	CHD	C1-C10-C9	3.14	116.29	111.35
21	W	4060	CHD	C19-C10-C9	-3.13	106.86	111.18
19	A	3524	PGV	P-O12-C04	3.13	140.05	121.68
21	P	4271	CHD	C5-C6-C7	3.13	117.92	114.46
21	P	4525	CHD	C14-C8-C9	-3.08	105.48	109.71
21	P	4271	CHD	C5-C4-C3	3.08	117.28	112.76
21	W	4060	CHD	C16-C15-C14	3.06	111.20	105.13
21	P	4525	CHD	C5-C6-C7	3.06	117.84	114.46
21	O	3085	CHD	C14-C13-C12	-3.05	104.56	107.40
19	N	4524	PGV	P-O12-C04	3.03	139.42	121.68
27	Z	4526	DMU	O7-C10-O1	3.02	119.11	110.67
21	B	4085	CHD	C10-C9-C8	3.01	115.05	111.82
17	N	515	HEA	C27-C19-C18	-2.99	116.02	123.68
21	O	3085	CHD	C15-C14-C13	-2.98	100.63	103.55
21	P	4271	CHD	C1-C10-C9	2.96	116.01	111.35
25	E	3230	PSC	C16-C15-C14	2.96	126.67	113.79
27	Z	4526	DMU	C2-C3-C4	-2.94	104.18	110.93
21	J	3060	CHD	C16-C15-C14	2.93	110.94	105.13
23	P	4264	PEK	C3-C2-C1	-2.92	103.00	113.62
21	B	4085	CHD	C1-C10-C5	2.91	112.08	107.77
17	A	516	HEA	CMC-C2C-C3C	2.91	130.13	124.68
17	A	515	HEA	C27-C19-C18	-2.90	116.25	123.68
21	C	3271	CHD	C5-C4-C3	2.90	117.01	112.76
19	N	4524	PGV	C02-O01-C1	2.88	124.89	117.79
19	A	3524	PGV	C03-C02-C01	2.86	118.55	111.79
19	N	4524	PGV	C03-C02-C01	2.86	118.54	111.79
22	C	3270	CDL	OB6-CB5-C51	-2.85	105.36	111.50
21	C	3525	CHD	C14-C8-C9	-2.84	105.81	109.71
27	M	3526	DMU	C2-C3-C4	-2.83	104.45	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	3264	PEK	C27-C26-C25	-2.82	100.11	114.42
21	C	3271	CHD	C6-C5-C10	2.81	115.64	112.66
23	G	4263	PEK	O03-C01-C02	2.81	116.61	108.43
21	B	4085	CHD	C19-C10-C1	-2.81	103.74	108.26
21	J	3060	CHD	C15-C16-C17	2.81	110.70	105.13
21	P	4271	CHD	C15-C16-C17	2.80	110.68	105.13
21	C	3525	CHD	C1-C10-C5	2.79	111.89	107.77
21	P	4271	CHD	C6-C5-C10	2.79	115.62	112.66
21	B	4085	CHD	C5-C4-C3	2.79	116.85	112.76
25	O	4230	PSC	C16-C15-C14	2.79	125.93	113.79
21	O	3085	CHD	C1-C10-C5	2.76	111.85	107.77
21	O	3085	CHD	C1-C2-C3	2.76	114.01	110.47
21	O	3085	CHD	O3-C3-C4	-2.76	104.35	109.85
21	B	4085	CHD	C14-C8-C9	-2.72	105.98	109.71
21	C	3271	CHD	C18-C13-C14	-2.72	106.95	111.21
19	A	3524	PGV	C3-C2-C1	-2.72	103.74	113.62
22	T	4269	CDL	C19-C18-C17	2.72	128.21	114.42
21	O	3085	CHD	C14-C8-C9	-2.71	105.99	109.71
21	P	4525	CHD	C6-C5-C10	2.71	115.54	112.66
21	C	3271	CHD	C16-C15-C14	2.71	110.50	105.13
21	P	4525	CHD	C1-C2-C3	2.71	113.94	110.47
17	N	515	HEA	C17-C18-C19	-2.71	121.14	127.66
21	C	3271	CHD	C1-C2-C3	2.71	113.94	110.47
25	O	4230	PSC	C01-O03-C19	-2.70	107.11	117.12
21	J	3060	CHD	C14-C13-C12	2.70	109.92	107.40
27	M	3526	DMU	O7-C10-O1	2.70	118.22	110.67
21	W	4060	CHD	C15-C16-C17	2.70	110.48	105.13
22	G	3269	CDL	C19-C18-C17	2.70	128.12	114.42
21	C	3271	CHD	C15-C16-C17	2.69	110.47	105.13
22	P	4270	CDL	CB6-OB8-CB7	-2.69	107.18	117.12
19	C	3267	PGV	C9-C10-C11	-2.68	97.05	112.43
17	N	515	HEA	CMB-C2B-C1B	-2.68	124.35	128.46
23	P	4264	PEK	C32-C31-C30	-2.67	100.89	114.42
19	P	4267	PGV	O01-C1-C2	-2.66	105.76	111.50
21	C	3271	CHD	O12-C12-C13	2.66	115.53	111.03
25	E	3230	PSC	C01-O03-C19	-2.65	107.30	117.12
21	P	4525	CHD	C9-C11-C12	2.65	117.80	114.30
21	C	3271	CHD	C5-C6-C7	2.65	117.38	114.46
17	N	515	HEA	CMC-C2C-C3C	2.64	129.62	124.68
23	C	3264	PEK	C32-C31-C30	-2.63	101.05	114.42
23	T	3263	PEK	C03-C02-C01	2.63	118.02	111.79
23	T	3263	PEK	O03-C01-C02	2.63	116.09	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	J	3060	CHD	C6-C5-C4	2.62	114.21	111.19
17	N	516	HEA	CMB-C2B-C1B	-2.62	124.43	128.46
17	N	516	HEA	C3C-C4C-NC	2.62	112.59	109.21
21	O	3085	CHD	C19-C10-C1	-2.62	104.05	108.26
21	C	3271	CHD	C14-C8-C7	2.60	115.25	111.81
21	W	4060	CHD	C14-C13-C12	2.59	109.82	107.40
21	P	4271	CHD	C1-C2-C3	2.59	113.79	110.47
21	P	4271	CHD	C16-C15-C14	2.58	110.24	105.13
23	P	4264	PEK	C34-C33-C32	-2.57	101.36	114.42
21	W	4060	CHD	C19-C10-C5	-2.57	106.00	110.36
17	A	515	HEA	C17-C18-C19	-2.56	121.49	127.66
25	O	4230	PSC	C15-C14-C13	2.56	127.10	112.43
21	C	3525	CHD	C5-C6-C7	2.56	117.28	114.46
22	C	3270	CDL	CB6-OB8-CB7	-2.53	107.74	117.12
23	C	3265	PEK	O03-C01-C02	2.53	115.80	108.43
21	P	4271	CHD	O12-C12-C13	2.53	115.30	111.03
17	A	516	HEA	C4B-C3B-C2B	-2.53	105.10	106.87
17	A	515	HEA	CMD-C2D-C3D	2.52	129.69	124.94
17	N	515	HEA	C20-C19-C18	2.52	126.21	121.12
18	L	3522	TGL	OG3-CC1-OC1	-2.51	117.25	123.59
17	N	515	HEA	C4B-C3B-C2B	-2.50	105.12	106.87
23	C	3264	PEK	C3-C2-C1	-2.50	104.54	113.62
19	N	4524	PGV	C3-C2-C1	-2.50	104.54	113.62
23	G	4263	PEK	C03-C02-C01	2.49	117.67	111.79
22	G	3269	CDL	C22-C21-C20	2.47	126.99	114.42
19	A	3266	PGV	C01-O03-C19	-2.47	107.98	117.12
17	A	515	HEA	CMB-C2B-C1B	-2.47	124.67	128.46
19	P	4267	PGV	C14-C13-C12	-2.47	98.30	112.43
19	N	4524	PGV	O01-C02-C03	2.47	117.33	108.40
27	Z	4526	DMU	C10-O7-C3	2.46	124.06	117.96
21	P	4271	CHD	C14-C8-C7	2.46	115.07	111.81
21	C	3525	CHD	C19-C10-C9	-2.45	107.80	111.18
22	T	4269	CDL	C22-C21-C20	2.44	126.82	114.42
23	P	4264	PEK	C25-C24-C23	-2.44	102.04	114.42
17	N	515	HEA	CMD-C2D-C3D	2.44	129.54	124.94
23	P	4265	PEK	O03-C01-C02	2.43	115.51	108.43
19	A	3524	PGV	O01-C02-C03	2.43	117.18	108.40
17	A	515	HEA	CMC-C2C-C3C	2.42	129.21	124.68
18	D	3523	TGL	CB6-CB5-CB4	2.42	126.73	114.42
25	E	3230	PSC	C15-C14-C13	2.42	126.31	112.43
21	P	4271	CHD	C18-C13-C14	-2.42	107.42	111.21
18	N	4522	TGL	OG1-CA1-CA2	2.41	119.48	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	W	4060	CHD	C14-C8-C7	2.41	115.00	111.81
23	C	3264	PEK	O03-C21-O04	2.40	129.66	123.59
18	N	4522	TGL	OG3-CC1-OC1	-2.40	117.53	123.59
23	C	3264	PEK	C25-C24-C23	-2.40	102.25	114.42
18	A	3521	TGL	OG3-CC1-CC2	2.40	119.43	111.91
22	C	3270	CDL	C52-C51-CB5	-2.39	104.91	113.62
23	P	4264	PEK	C27-C26-C25	-2.39	102.28	114.42
21	C	3525	CHD	C10-C9-C8	2.38	114.37	111.82
22	C	3270	CDL	OB6-CB5-OB7	2.36	129.40	123.70
18	N	4521	TGL	OG3-CC1-OC1	-2.35	117.65	123.59
21	W	4060	CHD	C6-C5-C4	2.35	113.90	111.19
22	G	3269	CDL	C20-C19-C18	2.35	126.35	114.42
21	J	3060	CHD	C14-C8-C7	2.35	114.92	111.81
18	L	3522	TGL	OG1-CA1-CA2	2.35	119.27	111.91
21	J	3060	CHD	C19-C10-C5	-2.34	106.39	110.36
22	T	4269	CDL	C23-C22-C21	2.34	126.30	114.42
18	A	3521	TGL	OG3-CC1-OC1	-2.34	117.69	123.59
19	N	4266	PGV	C3-C2-C1	-2.31	105.22	113.62
18	A	3521	TGL	CB6-CB5-CB4	2.31	126.15	114.42
17	A	516	HEA	CMC-C2C-C1C	-2.30	124.93	128.46
17	A	515	HEA	C20-C19-C18	2.29	125.76	121.12
23	P	4265	PEK	P-O12-C04	2.29	132.86	121.59
21	W	4060	CHD	C4-C5-C10	2.29	115.09	112.66
23	P	4264	PEK	C28-C27-C26	-2.29	102.81	114.42
22	P	4270	CDL	C52-C51-CB5	-2.28	105.31	113.62
19	C	3267	PGV	C3-C2-C1	-2.28	105.34	113.62
17	A	516	HEA	C1B-C2B-C3B	2.27	108.58	107.00
23	C	3265	PEK	P-O12-C04	2.27	132.77	121.59
21	J	3060	CHD	C4-C5-C10	2.26	115.06	112.66
22	T	4269	CDL	C20-C19-C18	2.25	125.86	114.42
23	P	4264	PEK	O03-C21-O04	2.25	129.27	123.59
17	N	516	HEA	C4B-C3B-C2B	-2.25	105.30	106.87
22	P	4270	CDL	OB6-CB5-C51	-2.24	106.68	111.50
18	D	3523	TGL	CB5-CB4-CB3	2.23	125.77	114.42
19	A	3524	PGV	O01-C1-C2	-2.23	106.69	111.50
19	A	3266	PGV	O01-C1-C2	-2.23	106.69	111.50
22	G	3269	CDL	C23-C22-C21	2.23	125.75	114.42
17	N	515	HEA	C26-C15-C14	-2.23	117.96	123.68
17	A	515	HEA	C21-C20-C19	-2.21	105.70	112.98
21	B	4085	CHD	C9-C11-C12	2.21	117.22	114.30
19	N	4524	PGV	O01-C1-C2	-2.21	106.74	111.50
22	T	4269	CDL	OB8-CB6-CB4	2.21	114.85	108.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	3270	CDL	OA8-CA6-CA4	2.21	114.85	108.43
23	C	3265	PEK	C11-C10-C9	2.20	122.86	112.02
19	C	3267	PGV	O01-C1-C2	-2.20	106.76	111.50
21	O	3085	CHD	C1-C10-C9	2.20	114.81	111.35
18	A	3521	TGL	CC6-CC5-CC4	2.19	125.54	114.42
22	G	3269	CDL	C80-C79-C78	2.18	125.47	114.42
22	T	4269	CDL	C80-C79-C78	2.17	125.45	114.42
17	N	515	HEA	C13-C14-C15	-2.17	122.44	127.66
23	P	4265	PEK	C11-C10-C9	2.16	122.68	112.02
18	Q	4523	TGL	CB6-CB5-CB4	2.16	125.40	114.42
18	Q	4523	TGL	OG3-CC1-OC1	-2.16	118.14	123.59
21	P	4525	CHD	C17-C13-C12	2.16	119.64	117.67
21	B	4085	CHD	C17-C13-C14	2.15	102.27	100.09
18	A	3521	TGL	CB5-CB4-CB3	2.15	125.34	114.42
17	A	515	HEA	C13-C14-C15	-2.15	122.49	127.66
21	O	3085	CHD	C9-C11-C12	2.14	117.12	114.30
21	C	3271	CHD	C9-C10-C5	2.13	111.58	108.58
21	C	3525	CHD	C16-C17-C13	-2.13	101.47	103.55
18	Q	4523	TGL	OG1-CA1-CA2	2.12	118.57	111.91
22	G	3269	CDL	OB8-CB6-CB4	2.12	114.59	108.43
21	C	3525	CHD	C2-C1-C10	2.11	116.40	112.78
17	N	515	HEA	CMC-C2C-C1C	-2.11	125.22	128.46
19	N	4266	PGV	C22-C21-C20	2.11	120.76	113.19
17	N	515	HEA	C21-C20-C19	-2.10	106.05	112.98
18	N	4521	TGL	CB5-CB4-CB3	2.09	125.05	114.42
17	N	516	HEA	C20-C19-C18	-2.09	116.89	121.12
18	D	3523	TGL	OG2-CB1-OB1	-2.09	118.66	123.70
22	P	4270	CDL	OB6-CB5-OB7	2.09	128.74	123.70
21	O	3085	CHD	C18-C13-C14	2.08	114.47	111.21
22	G	3269	CDL	C79-C78-C77	2.08	124.98	114.42
18	N	4522	TGL	OG1-CG1-CG2	2.08	114.48	108.43
21	W	4060	CHD	C13-C14-C8	2.08	117.39	114.74
22	T	4269	CDL	OB8-CB7-C71	-2.08	105.39	111.91
21	B	4085	CHD	C5-C6-C7	2.07	116.75	114.46
23	P	4265	PEK	C8-C7-C6	2.06	122.19	112.02
25	E	3230	PSC	P-O12-C04	2.06	131.75	121.59
17	N	515	HEA	C16-C15-C14	2.06	125.29	121.12
21	O	3085	CHD	C4-C5-C10	-2.06	110.47	112.66
18	D	3523	TGL	OG1-CA1-CA2	2.05	118.36	111.91
19	C	3267	PGV	C8-C7-C6	-2.05	104.00	114.42
21	C	3525	CHD	O12-C12-C13	-2.05	107.56	111.03
22	T	4269	CDL	C83-C82-C81	2.05	124.81	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	D	3523	TGL	OG3-CC1-CC2	2.04	118.32	111.91
21	O	3085	CHD	C13-C17-C20	-2.04	117.06	119.50
17	A	516	HEA	CMB-C2B-C1B	-2.04	125.33	128.46
21	O	3085	CHD	C18-C13-C12	-2.04	106.99	109.07
21	C	3525	CHD	C6-C5-C10	2.03	114.82	112.66
18	L	3522	TGL	CC6-CC5-CC4	2.03	124.74	114.42
18	N	4521	TGL	CB6-CB5-CB4	2.03	124.73	114.42
22	T	4269	CDL	C79-C78-C77	2.03	124.71	114.42
22	P	4270	CDL	OA8-CA6-CA4	2.02	114.33	108.43
23	P	4264	PEK	O03-C01-C02	-2.02	102.56	108.43
21	P	4271	CHD	C9-C10-C5	2.02	111.41	108.58
18	L	3522	TGL	CA7-CA6-CA5	-2.01	104.22	114.42
17	N	516	HEA	C1B-C2B-C3B	2.01	108.39	107.00
25	O	4230	PSC	P-O12-C04	2.00	131.44	121.59

All (42) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
27	Z	4526	DMU	C4
27	Z	4526	DMU	C6
27	Z	4526	DMU	C5
27	Z	4526	DMU	C2
27	Z	4526	DMU	C9
21	C	3271	CHD	C12
21	C	3271	CHD	C8
21	C	3271	CHD	C3
21	C	3271	CHD	C9
21	C	3271	CHD	C14
17	A	515	HEA	ND
17	A	515	HEA	NA
17	A	515	HEA	NB
27	M	3526	DMU	C4
27	M	3526	DMU	C6
27	M	3526	DMU	C5
27	M	3526	DMU	C2
27	M	3526	DMU	C9
17	N	516	HEA	ND
17	N	516	HEA	NA
17	N	516	HEA	NB
17	A	516	HEA	ND
17	A	516	HEA	NA
17	A	516	HEA	NB

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Mol	Chain	Res	Type	Atom
21	W	4060	CHD	C12
21	W	4060	CHD	C8
21	W	4060	CHD	C9
21	W	4060	CHD	C14
21	W	4060	CHD	C17
21	P	4271	CHD	C12
21	P	4271	CHD	C8
21	P	4271	CHD	C3
21	P	4271	CHD	C9
21	P	4271	CHD	C14
17	N	515	HEA	ND
17	N	515	HEA	NA
17	N	515	HEA	NB
21	J	3060	CHD	C12
21	J	3060	CHD	C8
21	J	3060	CHD	C9
21	J	3060	CHD	C14
21	J	3060	CHD	C17

All (902) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	G	3269	CDL	CB2-C1-CA2-OA2
22	G	3269	CDL	CA2-OA2-PA1-OA3
22	G	3269	CDL	C1-CB2-OB2-PB2
22	G	3269	CDL	CB3-OB5-PB2-OB3
22	G	3269	CDL	CB3-OB5-PB2-OB4
22	G	3269	CDL	OB6-CB4-CB6-OB8
23	C	3265	PEK	C03-O11-P-O13
23	C	3265	PEK	C04-O12-P-O11
23	C	3265	PEK	C04-O12-P-O13
23	C	3265	PEK	C04-O12-P-O14
19	P	4268	PGV	C04-O12-P-O11
19	P	4268	PGV	C04-O12-P-O13
19	P	4268	PGV	C04-O12-P-O14
27	Z	4526	DMU	O5-C6-O16-C18
23	P	4265	PEK	C03-O11-P-O13
23	P	4265	PEK	C04-O12-P-O11
23	P	4265	PEK	C04-O12-P-O13
23	P	4265	PEK	C04-O12-P-O14
19	C	3268	PGV	C04-O12-P-O11
19	C	3268	PGV	C04-O12-P-O13

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Mol	Chain	Res	Type	Atoms
19	C	3268	PGV	C04-O12-P-O14
25	E	3230	PSC	C03-O11-P-O14
25	E	3230	PSC	C04-O12-P-O14
25	E	3230	PSC	C13-C14-C15-C16
19	N	4524	PGV	C02-C03-O11-P
19	N	4524	PGV	C05-C04-O12-P
19	N	4524	PGV	C04-C05-C06-O06
19	N	4524	PGV	O05-C05-C06-O06
19	N	4524	PGV	C2-C1-O01-C02
18	D	3523	TGL	CB2-CB1-OG2-CG2
18	D	3523	TGL	OB1-CB1-OG2-CG2
25	O	4230	PSC	C03-O11-P-O14
25	O	4230	PSC	C04-O12-P-O14
25	O	4230	PSC	C13-C14-C15-C16
18	L	3522	TGL	CG2-CG3-OG3-CC1
18	Q	4523	TGL	OB1-CB1-OG2-CG2
22	P	4270	CDL	CA2-OA2-PA1-OA3
22	P	4270	CDL	CA3-OA5-PA1-OA2
22	P	4270	CDL	CA3-OA5-PA1-OA3
22	P	4270	CDL	CB2-OB2-PB2-OB3
22	P	4270	CDL	CB2-OB2-PB2-OB4
22	P	4270	CDL	CB2-OB2-PB2-OB5
27	M	3526	DMU	O5-C6-O16-C18
19	A	3524	PGV	C02-C03-O11-P
19	A	3524	PGV	C05-C04-O12-P
19	A	3524	PGV	C04-C05-C06-O06
19	A	3524	PGV	O05-C05-C06-O06
19	A	3524	PGV	C2-C1-O01-C02
22	C	3270	CDL	CA2-OA2-PA1-OA3
22	C	3270	CDL	CA3-OA5-PA1-OA2
22	C	3270	CDL	CA3-OA5-PA1-OA3
22	C	3270	CDL	CB2-OB2-PB2-OB3
22	C	3270	CDL	CB2-OB2-PB2-OB4
22	C	3270	CDL	CB2-OB2-PB2-OB5
18	N	4521	TGL	OB1-CB1-OG2-CG2
21	W	4060	CHD	C16-C17-C20-C21
21	W	4060	CHD	C16-C17-C20-C22
23	G	4263	PEK	C04-O12-P-O13
23	G	4263	PEK	C04-O12-P-O14
23	G	4263	PEK	O12-C04-C05-N
22	T	4269	CDL	CB2-C1-CA2-OA2
22	T	4269	CDL	CA2-OA2-PA1-OA3

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Mol	Chain	Res	Type	Atoms
22	T	4269	CDL	C1-CB2-OB2-PB2
22	T	4269	CDL	CB3-OB5-PB2-OB3
22	T	4269	CDL	CB3-OB5-PB2-OB4
22	T	4269	CDL	OB6-CB4-CB6-OB8
23	T	3263	PEK	C04-O12-P-O13
23	T	3263	PEK	C04-O12-P-O14
23	T	3263	PEK	O12-C04-C05-N
21	J	3060	CHD	C16-C17-C20-C21
21	J	3060	CHD	C16-C17-C20-C22
18	A	3521	TGL	CB2-CB1-OG2-CG2
18	A	3521	TGL	OB1-CB1-OG2-CG2
18	A	3521	TGL	OG1-CG1-CG2-OG2
18	A	3521	TGL	OC1-CC1-OG3-CG3
18	N	4522	TGL	CG2-CG3-OG3-CC1
19	N	4524	PGV	O04-C19-O03-C01
18	D	3523	TGL	OC1-CC1-OG3-CG3
18	Q	4523	TGL	OC1-CC1-OG3-CG3
19	A	3524	PGV	O04-C19-O03-C01
18	N	4521	TGL	OC1-CC1-OG3-CG3
25	E	3230	PSC	O02-C1-O01-C02
19	N	4524	PGV	O02-C1-O01-C02
25	O	4230	PSC	O02-C1-O01-C02
22	P	4270	CDL	OA7-CA5-OA6-CA4
19	A	3524	PGV	O02-C1-O01-C02
22	C	3270	CDL	OA7-CA5-OA6-CA4
18	Q	4523	TGL	CB2-CB1-OG2-CG2
18	N	4521	TGL	CB2-CB1-OG2-CG2
22	T	4269	CDL	OA9-CA7-OA8-CA6
22	G	3269	CDL	C17-C18-C19-C20
22	G	3269	CDL	C20-C21-C22-C23
22	G	3269	CDL	C37-C38-C39-C40
22	G	3269	CDL	C40-C41-C42-C43
22	G	3269	CDL	C57-C58-C59-C60
22	G	3269	CDL	C60-C61-C62-C63
22	G	3269	CDL	C80-C81-C82-C83
18	D	3523	TGL	CB3-CB4-CB5-CB6
18	N	4522	TGL	CB3-CB4-CB5-CB6
18	L	3522	TGL	CB3-CB4-CB5-CB6
18	Q	4523	TGL	CB3-CB4-CB5-CB6
22	P	4270	CDL	C17-C18-C19-C20
22	P	4270	CDL	C20-C21-C22-C23
22	P	4270	CDL	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
22	P	4270	CDL	C57-C58-C59-C60
22	P	4270	CDL	C60-C61-C62-C63
22	P	4270	CDL	C77-C78-C79-C80
22	P	4270	CDL	C80-C81-C82-C83
22	C	3270	CDL	C17-C18-C19-C20
22	C	3270	CDL	C20-C21-C22-C23
22	C	3270	CDL	C40-C41-C42-C43
22	C	3270	CDL	C57-C58-C59-C60
22	C	3270	CDL	C60-C61-C62-C63
22	C	3270	CDL	C77-C78-C79-C80
22	C	3270	CDL	C80-C81-C82-C83
18	N	4521	TGL	CB3-CB4-CB5-CB6
22	T	4269	CDL	C17-C18-C19-C20
22	T	4269	CDL	C20-C21-C22-C23
22	T	4269	CDL	C37-C38-C39-C40
22	T	4269	CDL	C40-C41-C42-C43
22	T	4269	CDL	C57-C58-C59-C60
22	T	4269	CDL	C60-C61-C62-C63
22	T	4269	CDL	C77-C78-C79-C80
18	A	3521	TGL	CB3-CB4-CB5-CB6
22	G	3269	CDL	C31-CA7-OA8-CA6
19	N	4524	PGV	C20-C19-O03-C01
18	L	3522	TGL	CA2-CA1-OG1-CG1
18	Q	4523	TGL	CC2-CC1-OG3-CG3
19	A	3524	PGV	C20-C19-O03-C01
18	N	4521	TGL	CA2-CA1-OG1-CG1
22	T	4269	CDL	C31-CA7-OA8-CA6
22	G	3269	CDL	C77-C78-C79-C80
22	T	4269	CDL	C80-C81-C82-C83
22	P	4270	CDL	C37-C38-C39-C40
22	C	3270	CDL	C37-C38-C39-C40
22	G	3269	CDL	OA9-CA7-OA8-CA6
18	N	4521	TGL	OA1-CA1-OG1-CG1
18	D	3523	TGL	CC2-CC3-CC4-CC5
22	G	3269	CDL	O1-C1-CA2-OA2
22	T	4269	CDL	O1-C1-CA2-OA2
18	N	4522	TGL	CA2-CA1-OG1-CG1
18	N	4521	TGL	CC2-CC1-OG3-CG3
27	M	3526	DMU	O6-C11-C9-C8
22	P	4270	CDL	C11-CA5-OA6-CA4
22	C	3270	CDL	C11-CA5-OA6-CA4
27	Z	4526	DMU	O6-C11-C9-C8

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Mol	Chain	Res	Type	Atoms
25	E	3230	PSC	C20-C21-C22-C23
22	T	4269	CDL	C73-C74-C75-C76
18	L	3522	TGL	OA1-CA1-OG1-CG1
22	G	3269	CDL	C52-C53-C54-C55
18	N	4522	TGL	CC2-CC3-CC4-CC5
25	O	4230	PSC	C20-C21-C22-C23
22	T	4269	CDL	C52-C53-C54-C55
22	G	3269	CDL	C73-C74-C75-C76
18	N	4521	TGL	CA9-C20-C21-C22
18	D	3523	TGL	CC2-CC1-OG3-CG3
18	A	3521	TGL	CC2-CC1-OG3-CG3
27	Z	4526	DMU	O5-C4-C57-O61
27	M	3526	DMU	O5-C4-C57-O61
18	N	4522	TGL	OA1-CA1-OG1-CG1
18	N	4522	TGL	OC1-CC1-OG3-CG3
22	P	4270	CDL	C23-C24-C25-C26
22	C	3270	CDL	C23-C24-C25-C26
22	C	3270	CDL	C62-C63-C64-C65
18	A	3521	TGL	CA9-C20-C21-C22
22	P	4270	CDL	C62-C63-C64-C65
22	G	3269	CDL	CA2-C1-CB2-OB2
19	P	4268	PGV	O12-C04-C05-C06
19	C	3268	PGV	O12-C04-C05-C06
22	P	4270	CDL	CA2-C1-CB2-OB2
22	C	3270	CDL	CA2-C1-CB2-OB2
22	T	4269	CDL	CA2-C1-CB2-OB2
18	L	3522	TGL	OC1-CC1-OG3-CG3
25	E	3230	PSC	C22-C23-C24-C25
25	E	3230	PSC	C20-C19-O03-C01
25	O	4230	PSC	C20-C19-O03-C01
21	W	4060	CHD	C13-C17-C20-C22
21	J	3060	CHD	C13-C17-C20-C22
22	G	3269	CDL	C15-C16-C17-C18
25	O	4230	PSC	C22-C23-C24-C25
22	T	4269	CDL	C15-C16-C17-C18
22	G	3269	CDL	O1-C1-CB2-OB2
19	P	4268	PGV	O12-C04-C05-O05
19	C	3268	PGV	O12-C04-C05-O05
22	T	4269	CDL	O1-C1-CB2-OB2
19	N	4524	PGV	C20-C21-C22-C23
19	A	3524	PGV	C20-C21-C22-C23
25	E	3230	PSC	C2-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
25	O	4230	PSC	C2-C1-O01-C02
18	L	3522	TGL	CC2-CC3-CC4-CC5
18	Q	4523	TGL	CC2-CC3-CC4-CC5
25	E	3230	PSC	O04-C19-O03-C01
25	O	4230	PSC	O04-C19-O03-C01
21	W	4060	CHD	C17-C20-C22-C23
21	J	3060	CHD	C17-C20-C22-C23
23	C	3265	PEK	C22-C21-O03-C01
23	P	4265	PEK	C22-C21-O03-C01
21	W	4060	CHD	C21-C20-C22-C23
21	J	3060	CHD	C21-C20-C22-C23
18	N	4522	TGL	CB5-CB6-CB7-CB8
23	P	4265	PEK	C1-C2-C3-C4
25	O	4230	PSC	C1-C2-C3-C4
18	Q	4523	TGL	CA1-CA2-CA3-CA4
25	E	3230	PSC	C1-C2-C3-C4
19	N	4524	PGV	C1-C2-C3-C4
18	D	3523	TGL	CA1-CA2-CA3-CA4
18	L	3522	TGL	CB1-CB2-CB3-CB4
19	A	3524	PGV	C1-C2-C3-C4
23	G	4263	PEK	C1-C2-C3-C4
23	T	3263	PEK	C1-C2-C3-C4
18	L	3522	TGL	CB5-CB6-CB7-CB8
18	A	3521	TGL	CA2-CA1-OG1-CG1
27	Z	4526	DMU	O16-C18-C19-C22
23	C	3265	PEK	C1-C2-C3-C4
22	P	4270	CDL	CB7-C71-C72-C73
22	C	3270	CDL	CB7-C71-C72-C73
27	M	3526	DMU	O16-C18-C19-C22
23	C	3265	PEK	O04-C21-O03-C01
19	N	4266	PGV	C19-C20-C21-C22
23	P	4265	PEK	O04-C21-O03-C01
23	C	3264	PEK	C1-C2-C3-C4
18	N	4522	TGL	CB1-CB2-CB3-CB4
22	P	4270	CDL	O1-C1-CB2-OB2
22	C	3270	CDL	O1-C1-CB2-OB2
21	W	4060	CHD	C13-C17-C20-C21
21	J	3060	CHD	C13-C17-C20-C21
21	P	4271	CHD	C17-C20-C22-C23
25	E	3230	PSC	C11-C12-C13-C14
25	O	4230	PSC	C11-C12-C13-C14
22	P	4270	CDL	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
22	C	3270	CDL	C14-C15-C16-C17
22	G	3269	CDL	CA2-OA2-PA1-OA5
22	G	3269	CDL	CB3-OB5-PB2-OB2
22	P	4270	CDL	CA2-OA2-PA1-OA5
22	C	3270	CDL	CA2-OA2-PA1-OA5
23	G	4263	PEK	C04-O12-P-O11
22	T	4269	CDL	CA2-OA2-PA1-OA5
22	T	4269	CDL	CB3-OB5-PB2-OB2
23	T	3263	PEK	C04-O12-P-O11
23	P	4264	PEK	C1-C2-C3-C4
19	N	4266	PGV	C5-C6-C7-C8
19	N	4266	PGV	C15-C16-C17-C18
18	Q	4523	TGL	C12-C13-C14-C29
18	N	4521	TGL	CB4-CB5-CB6-CB7
22	T	4269	CDL	C13-C14-C15-C16
22	G	3269	CDL	C11-CA5-OA6-CA4
22	T	4269	CDL	C11-CA5-OA6-CA4
21	C	3271	CHD	C17-C20-C22-C23
19	P	4268	PGV	C14-C15-C16-C17
19	C	3268	PGV	C14-C15-C16-C17
25	E	3230	PSC	C2-C3-C4-C5
25	E	3230	PSC	C29-C30-C31-C32
25	O	4230	PSC	C29-C30-C31-C32
18	Q	4523	TGL	CB6-CB7-CB8-CB9
18	N	4521	TGL	C22-C23-C24-C25
18	A	3521	TGL	C21-C20-CA9-CA8
18	A	3521	TGL	CC4-CC5-CC6-CC7
18	A	3521	TGL	C23-C24-C25-C26
18	A	3521	TGL	OA1-CA1-OG1-CG1
22	G	3269	CDL	C13-C14-C15-C16
18	D	3523	TGL	C12-C13-C14-C29
25	O	4230	PSC	C2-C3-C4-C5
19	N	4266	PGV	C6-C7-C8-C9
18	L	3522	TGL	C24-C25-C26-C27
22	P	4270	CDL	C11-C12-C13-C14
19	A	3266	PGV	C29-C30-C31-C32
22	C	3270	CDL	C11-C12-C13-C14
22	G	3269	CDL	OA7-CA5-OA6-CA4
22	T	4269	CDL	OA7-CA5-OA6-CA4
23	P	4265	PEK	C25-C26-C27-C28
19	N	4266	PGV	C29-C30-C31-C32
18	A	3521	TGL	C12-C13-C14-C29

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Mol	Chain	Res	Type	Atoms
18	A	3521	TGL	C20-C21-C22-C23
18	L	3522	TGL	C22-C23-C24-C25
27	Z	4526	DMU	C25-C28-C31-C34
18	N	4522	TGL	CC6-CC7-CC8-CC9
18	Q	4523	TGL	C16-C15-CC9-CC8
27	M	3526	DMU	C25-C28-C31-C34
23	G	4263	PEK	C31-C32-C33-C34
22	G	3269	CDL	C79-C80-C81-C82
23	C	3265	PEK	C25-C26-C27-C28
19	A	3266	PGV	C6-C7-C8-C9
19	A	3266	PGV	C23-C24-C25-C26
18	N	4521	TGL	C14-C29-C30-C31
22	G	3269	CDL	C82-C83-C84-C85
19	A	3266	PGV	C5-C6-C7-C8
22	T	4269	CDL	C79-C80-C81-C82
23	T	3263	PEK	C31-C32-C33-C34
22	G	3269	CDL	CA5-C11-C12-C13
22	T	4269	CDL	CA5-C11-C12-C13
19	P	4267	PGV	C22-C23-C24-C25
19	P	4268	PGV	C30-C31-C32-C33
19	C	3268	PGV	C30-C31-C32-C33
18	D	3523	TGL	C16-C15-CC9-CC8
18	N	4522	TGL	C16-C15-CC9-CC8
18	L	3522	TGL	C21-C22-C23-C24
22	C	3270	CDL	C75-C76-C77-C78
23	G	4263	PEK	C25-C26-C27-C28
23	G	4263	PEK	C27-C28-C29-C30
23	T	3263	PEK	C25-C26-C27-C28
23	T	3263	PEK	C27-C28-C29-C30
18	A	3521	TGL	CB4-CB5-CB6-CB7
22	P	4270	CDL	C75-C76-C77-C78
19	P	4268	PGV	C04-C05-C06-O06
19	C	3268	PGV	C04-C05-C06-O06
22	C	3270	CDL	C59-C60-C61-C62
22	T	4269	CDL	C82-C83-C84-C85
21	P	4271	CHD	C21-C20-C22-C23
19	C	3267	PGV	C11-C10-C9-C8
23	T	3263	PEK	C21-C22-C23-C24
23	C	3265	PEK	C31-C32-C33-C34
19	P	4268	PGV	C2-C3-C4-C5
19	P	4268	PGV	C13-C14-C15-C16
19	P	4268	PGV	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
23	P	4265	PEK	C31-C32-C33-C34
19	C	3268	PGV	C2-C3-C4-C5
19	C	3268	PGV	C23-C24-C25-C26
19	C	3268	PGV	C25-C26-C27-C28
23	C	3264	PEK	C22-C23-C24-C25
19	N	4524	PGV	C22-C23-C24-C25
18	D	3523	TGL	CB6-CB7-CB8-CB9
18	N	4522	TGL	C22-C23-C24-C25
18	L	3522	TGL	C17-C18-C19-C33
18	L	3522	TGL	C19-C33-C34-C35
22	P	4270	CDL	C59-C60-C61-C62
19	C	3267	PGV	C22-C23-C24-C25
19	A	3524	PGV	C2-C3-C4-C5
19	A	3524	PGV	C22-C23-C24-C25
19	P	4268	PGV	C25-C26-C27-C28
19	C	3268	PGV	C13-C14-C15-C16
19	N	4524	PGV	C2-C3-C4-C5
18	L	3522	TGL	C18-C19-C33-C34
18	Q	4523	TGL	CB5-CB6-CB7-CB8
19	A	3266	PGV	C7-C8-C9-C10
18	N	4521	TGL	C17-C18-C19-C33
18	N	4521	TGL	C23-C24-C25-C26
23	P	4264	PEK	C16-C17-C18-C19
22	P	4270	CDL	C63-C64-C65-C66
22	P	4270	CDL	C72-C73-C74-C75
22	C	3270	CDL	C51-C52-C53-C54
23	G	4263	PEK	C21-C22-C23-C24
23	C	3264	PEK	C16-C17-C18-C19
19	N	4524	PGV	C13-C14-C15-C16
18	N	4522	TGL	C24-C25-C26-C27
19	N	4266	PGV	C7-C8-C9-C10
22	P	4270	CDL	C61-C62-C63-C64
22	C	3270	CDL	C61-C62-C63-C64
22	C	3270	CDL	C63-C64-C65-C66
22	C	3270	CDL	C74-C75-C76-C77
18	N	4522	TGL	C17-C18-C19-C33
22	P	4270	CDL	C73-C74-C75-C76
19	A	3524	PGV	C13-C14-C15-C16
22	C	3270	CDL	C73-C74-C75-C76
22	T	4269	CDL	C56-C57-C58-C59
21	C	3271	CHD	C21-C20-C22-C23
17	A	515	HEA	C21-C22-C23-C25

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Mol	Chain	Res	Type	Atoms
22	G	3269	CDL	C14-C15-C16-C17
22	G	3269	CDL	C33-C34-C35-C36
22	G	3269	CDL	C56-C57-C58-C59
19	P	4267	PGV	C13-C14-C15-C16
18	L	3522	TGL	CC6-CC7-CC8-CC9
22	C	3270	CDL	C72-C73-C74-C75
18	A	3521	TGL	C14-C29-C30-C31
22	P	4270	CDL	C51-C52-C53-C54
22	P	4270	CDL	C74-C75-C76-C77
22	T	4269	CDL	C14-C15-C16-C17
18	N	4521	TGL	CB1-CB2-CB3-CB4
22	T	4269	CDL	C33-C34-C35-C36
19	P	4268	PGV	C24-C25-C26-C27
18	L	3522	TGL	CC3-CC4-CC5-CC6
19	A	3524	PGV	C14-C15-C16-C17
27	Z	4526	DMU	C22-C25-C28-C31
23	P	4264	PEK	C22-C23-C24-C25
19	N	4524	PGV	C14-C15-C16-C17
18	L	3522	TGL	CA7-CA8-CA9-C20
18	L	3522	TGL	C21-C20-CA9-CA8
19	C	3268	PGV	C24-C25-C26-C27
23	P	4265	PEK	C32-C33-C34-C35
22	P	4270	CDL	C71-C72-C73-C74
22	C	3270	CDL	C71-C72-C73-C74
22	C	3270	CDL	OB7-CB5-OB6-CB4
17	N	515	HEA	C21-C22-C23-C25
27	M	3526	DMU	C22-C25-C28-C31
18	N	4521	TGL	CC4-CC5-CC6-CC7
23	C	3265	PEK	C29-C30-C31-C32
25	E	3230	PSC	C3-C4-C5-C6
18	D	3523	TGL	CB5-CB6-CB7-CB8
18	D	3523	TGL	C18-C19-C33-C34
19	A	3266	PGV	C15-C16-C17-C18
22	T	4269	CDL	C43-C44-C45-C46
19	N	4524	PGV	C19-C20-C21-C22
19	A	3524	PGV	C19-C20-C21-C22
23	C	3265	PEK	C32-C33-C34-C35
19	P	4268	PGV	C7-C8-C9-C10
18	N	4522	TGL	CC2-CC1-OG3-CG3
22	G	3269	CDL	C43-C44-C45-C46
19	P	4267	PGV	C25-C26-C27-C28
25	O	4230	PSC	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
18	N	4521	TGL	C20-C21-C22-C23
23	P	4265	PEK	C29-C30-C31-C32
19	C	3267	PGV	C25-C26-C27-C28
18	A	3521	TGL	C17-C18-C19-C33
19	P	4268	PGV	C4-C5-C6-C7
18	D	3523	TGL	CB4-CB5-CB6-CB7
18	N	4522	TGL	CA7-CA8-CA9-C20
19	P	4267	PGV	C11-C10-C9-C8
19	C	3268	PGV	O02-C1-O01-C02
22	P	4270	CDL	OB7-CB5-OB6-CB4
23	G	4263	PEK	O02-C1-O01-C02
19	C	3268	PGV	C20-C21-C22-C23
22	C	3270	CDL	C55-C56-C57-C58
19	C	3268	PGV	C7-C8-C9-C10
19	N	4266	PGV	C23-C24-C25-C26
19	A	3524	PGV	C24-C25-C26-C27
19	N	4524	PGV	C24-C25-C26-C27
18	N	4521	TGL	C12-C13-C14-C29
22	T	4269	CDL	CA7-C31-C32-C33
19	C	3268	PGV	C4-C5-C6-C7
22	P	4270	CDL	C55-C56-C57-C58
19	P	4268	PGV	C2-C1-O01-C02
22	P	4270	CDL	C51-CB5-OB6-CB4
22	C	3270	CDL	C51-CB5-OB6-CB4
23	G	4263	PEK	C2-C1-O01-C02
23	T	3263	PEK	C2-C1-O01-C02
19	C	3268	PGV	C28-C29-C30-C31
22	P	4270	CDL	C12-C13-C14-C15
19	P	4268	PGV	O02-C1-O01-C02
23	T	3263	PEK	O02-C1-O01-C02
22	G	3269	CDL	CA7-C31-C32-C33
18	A	3521	TGL	CA1-CA2-CA3-CA4
19	P	4268	PGV	C20-C21-C22-C23
22	C	3270	CDL	C12-C13-C14-C15
22	C	3270	CDL	C19-C20-C21-C22
18	D	3523	TGL	OG1-CG1-CG2-OG2
19	P	4268	PGV	C28-C29-C30-C31
22	P	4270	CDL	C19-C20-C21-C22
23	G	4263	PEK	C22-C23-C24-C25
18	N	4522	TGL	C21-C22-C23-C24
23	C	3265	PEK	C2-C3-C4-C5
23	P	4265	PEK	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
19	P	4268	PGV	C19-C20-C21-C22
18	L	3522	TGL	C16-C15-CC9-CC8
22	G	3269	CDL	C41-C42-C43-C44
22	C	3270	CDL	C16-C17-C18-C19
18	N	4521	TGL	C19-C33-C34-C35
23	T	3263	PEK	C16-C17-C18-C19
23	T	3263	PEK	C22-C23-C24-C25
25	E	3230	PSC	C27-C28-C29-C30
23	P	4264	PEK	C23-C24-C25-C26
25	O	4230	PSC	C27-C28-C29-C30
22	C	3270	CDL	C32-C33-C34-C35
19	C	3268	PGV	C2-C1-O01-C02
22	G	3269	CDL	C21-C22-C23-C24
19	C	3268	PGV	C29-C30-C31-C32
22	P	4270	CDL	C16-C17-C18-C19
22	P	4270	CDL	C32-C33-C34-C35
22	C	3270	CDL	C18-C19-C20-C21
22	T	4269	CDL	C41-C42-C43-C44
18	N	4522	TGL	CB9-C10-C11-C12
22	P	4270	CDL	OA5-CA3-CA4-CA6
22	P	4270	CDL	OB5-CB3-CB4-CB6
22	C	3270	CDL	OA5-CA3-CA4-CA6
22	C	3270	CDL	OB5-CB3-CB4-CB6
22	T	4269	CDL	C21-C22-C23-C24
22	P	4270	CDL	C18-C19-C20-C21
18	N	4521	TGL	CC5-CC6-CC7-CC8
19	P	4268	PGV	C29-C30-C31-C32
23	C	3264	PEK	C23-C24-C25-C26
18	N	4522	TGL	C18-C19-C33-C34
19	C	3267	PGV	C23-C24-C25-C26
22	T	4269	CDL	C72-C73-C74-C75
18	A	3521	TGL	C22-C23-C24-C25
19	N	4524	PGV	C28-C29-C30-C31
23	C	3265	PEK	C16-C17-C18-C19
22	G	3269	CDL	C72-C73-C74-C75
23	G	4263	PEK	C16-C17-C18-C19
19	P	4268	PGV	C22-C23-C24-C25
23	P	4265	PEK	C16-C17-C18-C19
18	D	3523	TGL	C15-C16-C17-C18
22	G	3269	CDL	CA3-CA4-CA6-OA8
22	G	3269	CDL	CB3-CB4-CB6-OB8
19	C	3268	PGV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
23	P	4264	PEK	O03-C01-C02-C03
18	D	3523	TGL	OG1-CG1-CG2-CG3
22	P	4270	CDL	CB3-CB4-CB6-OB8
22	C	3270	CDL	CB3-CB4-CB6-OB8
22	T	4269	CDL	CA3-CA4-CA6-OA8
22	T	4269	CDL	CB3-CB4-CB6-OB8
19	P	4267	PGV	C24-C25-C26-C27
18	Q	4523	TGL	CA9-C20-C21-C22
23	C	3264	PEK	O04-C21-O03-C01
18	L	3522	TGL	C29-C30-C31-C32
22	C	3270	CDL	C84-C85-C86-C87
22	G	3269	CDL	CB7-C71-C72-C73
18	N	4522	TGL	C21-C20-CA9-CA8
17	A	515	HEA	C15-C16-C17-C18
19	N	4266	PGV	C30-C31-C32-C33
22	P	4270	CDL	C84-C85-C86-C87
19	P	4268	PGV	O05-C05-C06-O06
19	C	3268	PGV	O05-C05-C06-O06
18	N	4522	TGL	C19-C33-C34-C35
19	C	3267	PGV	C13-C14-C15-C16
19	C	3268	PGV	C19-C20-C21-C22
18	N	4521	TGL	CC1-CC2-CC3-CC4
19	P	4267	PGV	C31-C32-C33-C34
19	A	3524	PGV	C28-C29-C30-C31
22	C	3270	CDL	C44-C45-C46-C47
22	P	4270	CDL	C44-C45-C46-C47
22	G	3269	CDL	C44-C45-C46-C47
18	D	3523	TGL	C33-C34-C35-C36
22	T	4269	CDL	C44-C45-C46-C47
18	A	3521	TGL	C16-C15-CC9-CC8
19	C	3267	PGV	C31-C32-C33-C34
18	N	4521	TGL	CC2-CC3-CC4-CC5
23	C	3264	PEK	C22-C21-O03-C01
19	P	4267	PGV	C23-C24-C25-C26
25	O	4230	PSC	C24-C25-C26-C27
25	E	3230	PSC	C24-C25-C26-C27
22	T	4269	CDL	CB7-C71-C72-C73
18	L	3522	TGL	CC7-CC8-CC9-C15
18	L	3522	TGL	C33-C34-C35-C36
18	N	4522	TGL	C33-C34-C35-C36
18	N	4521	TGL	C25-C26-C27-C28
22	C	3270	CDL	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
22	G	3269	CDL	C58-C59-C60-C61
22	C	3270	CDL	C34-C35-C36-C37
22	T	4269	CDL	C58-C59-C60-C61
18	L	3522	TGL	CC2-CC1-OG3-CG3
18	N	4522	TGL	CB4-CB5-CB6-CB7
19	C	3267	PGV	C7-C8-C9-C10
19	A	3266	PGV	C31-C32-C33-C34
18	N	4522	TGL	C29-C30-C31-C32
22	P	4270	CDL	C38-C39-C40-C41
22	P	4270	CDL	C34-C35-C36-C37
19	N	4524	PGV	C21-C22-C23-C24
23	P	4265	PEK	C22-C23-C24-C25
22	C	3270	CDL	C36-C37-C38-C39
22	G	3269	CDL	OA5-CA3-CA4-CA6
22	T	4269	CDL	OA5-CA3-CA4-CA6
22	T	4269	CDL	C39-C40-C41-C42
23	G	4263	PEK	C30-C31-C32-C33
23	T	3263	PEK	C30-C31-C32-C33
18	N	4521	TGL	CB6-CB7-CB8-CB9
22	P	4270	CDL	CA4-CA3-OA5-PA1
22	C	3270	CDL	CA4-CA3-OA5-PA1
22	G	3269	CDL	C39-C40-C41-C42
18	N	4522	TGL	CC5-CC6-CC7-CC8
19	A	3524	PGV	C21-C22-C23-C24
22	P	4270	CDL	C36-C37-C38-C39
23	T	3263	PEK	C32-C33-C34-C35
19	P	4268	PGV	C3-C4-C5-C6
18	N	4521	TGL	C13-C14-C29-C30
19	N	4266	PGV	C31-C32-C33-C34
18	L	3522	TGL	C25-C26-C27-C28
19	C	3267	PGV	C24-C25-C26-C27
18	N	4521	TGL	C21-C20-CA9-CA8
18	A	3521	TGL	CC2-CC3-CC4-CC5
23	C	3265	PEK	O03-C01-C02-C03
23	P	4265	PEK	O03-C01-C02-C03
23	C	3264	PEK	O03-C01-C02-C03
22	P	4270	CDL	CA3-CA4-CA6-OA8
22	C	3270	CDL	CA3-CA4-CA6-OA8
22	G	3269	CDL	C35-C36-C37-C38
18	D	3523	TGL	CA9-C20-C21-C22
18	N	4522	TGL	C20-C21-C22-C23
23	G	4263	PEK	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
19	C	3268	PGV	C3-C4-C5-C6
22	T	4269	CDL	C19-C20-C21-C22
23	G	4263	PEK	C28-C29-C30-C31
22	G	3269	CDL	C38-C39-C40-C41
22	P	4270	CDL	C42-C43-C44-C45
18	N	4521	TGL	C16-C17-C18-C19
25	E	3230	PSC	C9-C10-C11-C12
23	C	3264	PEK	C5-C6-C7-C8
23	C	3264	PEK	C9-C10-C11-C12
23	P	4264	PEK	C5-C6-C7-C8
23	P	4264	PEK	C9-C10-C11-C12
25	O	4230	PSC	C9-C10-C11-C12
23	G	4263	PEK	C6-C7-C8-C9
23	T	3263	PEK	C6-C7-C8-C9
23	C	3265	PEK	C22-C23-C24-C25
18	Q	4523	TGL	C23-C24-C25-C26
22	T	4269	CDL	C35-C36-C37-C38
23	T	3263	PEK	C28-C29-C30-C31
19	C	3268	PGV	O01-C02-C03-O11
22	P	4270	CDL	OB5-CB3-CB4-OB6
22	C	3270	CDL	OB5-CB3-CB4-OB6
22	G	3269	CDL	C19-C20-C21-C22
19	N	4524	PGV	C26-C27-C28-C29
22	C	3270	CDL	C42-C43-C44-C45
23	C	3264	PEK	C17-C18-C19-C20
18	L	3522	TGL	CC5-CC6-CC7-CC8
22	C	3270	CDL	C13-C14-C15-C16
18	A	3521	TGL	C16-C17-C18-C19
22	P	4270	CDL	OB6-CB4-CB6-OB8
22	C	3270	CDL	OB6-CB4-CB6-OB8
19	P	4267	PGV	C5-C6-C7-C8
18	A	3521	TGL	C25-C26-C27-C28
17	N	515	HEA	C15-C16-C17-C18
22	P	4270	CDL	C13-C14-C15-C16
22	T	4269	CDL	C38-C39-C40-C41
18	Q	4523	TGL	C33-C34-C35-C36
19	N	4266	PGV	C25-C26-C27-C28
19	P	4267	PGV	C02-C03-O11-P
19	P	4268	PGV	C02-C03-O11-P
19	C	3268	PGV	C02-C03-O11-P
18	N	4522	TGL	CC4-CC5-CC6-CC7
25	O	4230	PSC	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
23	T	3263	PEK	C35-C36-C37-C38
25	E	3230	PSC	C15-C16-C17-C18
18	L	3522	TGL	C12-C13-C14-C29
19	C	3267	PGV	C20-C21-C22-C23
18	N	4521	TGL	CC7-CC8-CC9-C15
19	P	4267	PGV	C30-C31-C32-C33
18	Q	4523	TGL	CB4-CB5-CB6-CB7
22	P	4270	CDL	C78-C79-C80-C81
19	A	3266	PGV	C30-C31-C32-C33
18	N	4522	TGL	C25-C26-C27-C28
18	N	4521	TGL	C16-C15-CC9-CC8
23	G	4263	PEK	C35-C36-C37-C38
25	E	3230	PSC	C14-C15-C16-C17
19	A	3266	PGV	C25-C26-C27-C28
23	P	4264	PEK	C17-C18-C19-C20
19	A	3524	PGV	C26-C27-C28-C29
22	C	3270	CDL	C78-C79-C80-C81
23	C	3264	PEK	C35-C36-C37-C38
25	O	4230	PSC	C14-C15-C16-C17
19	N	4524	PGV	C03-C02-O01-C1
19	A	3524	PGV	C03-C02-O01-C1
19	P	4268	PGV	C5-C6-C7-C8
19	A	3524	PGV	C25-C26-C27-C28
22	T	4269	CDL	C63-C64-C65-C66
22	G	3269	CDL	C63-C64-C65-C66
18	A	3521	TGL	C13-C14-C29-C30
25	E	3230	PSC	O03-C01-C02-C03
25	O	4230	PSC	O03-C01-C02-C03
18	A	3521	TGL	OG1-CG1-CG2-CG3
22	G	3269	CDL	OA5-CA3-CA4-OA6
19	P	4268	PGV	O01-C02-C03-O11
22	C	3270	CDL	OA5-CA3-CA4-OA6
21	C	3271	CHD	C13-C17-C20-C21
21	P	4271	CHD	C13-C17-C20-C21
19	C	3268	PGV	C5-C6-C7-C8
18	A	3521	TGL	CC5-CC6-CC7-CC8
23	P	4265	PEK	C30-C31-C32-C33
25	O	4230	PSC	C23-C24-C25-C26
22	G	3269	CDL	C54-C55-C56-C57
22	T	4269	CDL	C54-C55-C56-C57
25	E	3230	PSC	O03-C01-C02-O01
23	P	4264	PEK	O03-C01-C02-O01

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Mol	Chain	Res	Type	Atoms
25	O	4230	PSC	O03-C01-C02-O01
22	P	4270	CDL	OA6-CA4-CA6-OA8
22	C	3270	CDL	OA6-CA4-CA6-OA8
25	O	4230	PSC	C04-C05-N-C08
23	C	3265	PEK	C30-C31-C32-C33
25	E	3230	PSC	C23-C24-C25-C26
21	C	3271	CHD	C13-C17-C20-C22
19	N	4266	PGV	C20-C21-C22-C23
23	P	4264	PEK	O04-C21-O03-C01
23	T	3263	PEK	C17-C18-C19-C20
19	N	4524	PGV	C25-C26-C27-C28
18	N	4522	TGL	C13-C14-C29-C30
18	Q	4523	TGL	C15-C16-C17-C18
21	P	4271	CHD	C13-C17-C20-C22
19	C	3267	PGV	C15-C16-C17-C18
23	G	4263	PEK	C17-C18-C19-C20
22	G	3269	CDL	C12-C13-C14-C15
23	G	4263	PEK	C2-C3-C4-C5
23	T	3263	PEK	C2-C3-C4-C5
22	G	3269	CDL	CB2-OB2-PB2-OB5
23	C	3265	PEK	C03-O11-P-O12
25	E	3230	PSC	C04-O12-P-O11
25	O	4230	PSC	C04-O12-P-O11
22	T	4269	CDL	CB2-OB2-PB2-OB5
18	L	3522	TGL	CB6-CB7-CB8-CB9
22	G	3269	CDL	CB4-CB3-OB5-PB2
19	C	3267	PGV	C02-C03-O11-P
22	T	4269	CDL	CB4-CB3-OB5-PB2
22	G	3269	CDL	CA2-OA2-PA1-OA4
23	C	3265	PEK	C03-O11-P-O14
23	P	4265	PEK	C03-O11-P-O14
25	E	3230	PSC	C04-O12-P-O13
25	O	4230	PSC	C04-O12-P-O13
22	P	4270	CDL	CA2-OA2-PA1-OA4
22	C	3270	CDL	CA2-OA2-PA1-OA4
22	T	4269	CDL	CA2-OA2-PA1-OA4
22	T	4269	CDL	CB5-C51-C52-C53
19	P	4268	PGV	C01-C02-C03-O11
19	C	3268	PGV	C01-C02-C03-O11
22	C	3270	CDL	C39-C40-C41-C42
22	T	4269	CDL	C12-C13-C14-C15
17	A	515	HEA	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
22	T	4269	CDL	C23-C24-C25-C26
21	P	4271	CHD	C16-C17-C20-C22
19	A	3524	PGV	C12-C13-C14-C15
22	G	3269	CDL	CB5-C51-C52-C53
22	G	3269	CDL	C23-C24-C25-C26
19	N	4524	PGV	O01-C02-C03-O11
22	P	4270	CDL	OA5-CA3-CA4-OA6
22	T	4269	CDL	OA5-CA3-CA4-OA6
18	A	3521	TGL	CC7-CC8-CC9-C15
19	N	4524	PGV	C5-C6-C7-C8
22	T	4269	CDL	C71-C72-C73-C74
19	C	3268	PGV	C27-C28-C29-C30
18	L	3522	TGL	CB9-C10-C11-C12
22	P	4270	CDL	C82-C83-C84-C85
22	G	3269	CDL	C71-C72-C73-C74
18	N	4522	TGL	CC7-CC8-CC9-C15
25	O	4230	PSC	C4-C5-C6-C7
22	P	4270	CDL	C39-C40-C41-C42
21	C	3271	CHD	C16-C17-C20-C22
22	G	3269	CDL	OA6-CA4-CA6-OA8
23	C	3265	PEK	O03-C01-C02-O01
23	P	4265	PEK	O03-C01-C02-O01
23	C	3264	PEK	O03-C01-C02-O01
19	N	4524	PGV	O03-C01-C02-O01
19	A	3524	PGV	O03-C01-C02-O01
22	T	4269	CDL	OA6-CA4-CA6-OA8
22	C	3270	CDL	C82-C83-C84-C85
19	P	4268	PGV	C27-C28-C29-C30
23	P	4264	PEK	C26-C27-C28-C29
19	N	4266	PGV	C26-C27-C28-C29
22	T	4269	CDL	C22-C23-C24-C25
25	E	3230	PSC	C4-C5-C6-C7
25	E	3230	PSC	C04-C05-N-C08
25	O	4230	PSC	C04-C05-N-C06
25	O	4230	PSC	C04-C05-N-C07
21	P	4271	CHD	C16-C17-C20-C21
22	T	4269	CDL	C55-C56-C57-C58
17	N	515	HEA	C21-C22-C23-C24
19	C	3267	PGV	C30-C31-C32-C33
22	C	3270	CDL	C52-C53-C54-C55
19	P	4267	PGV	C20-C21-C22-C23
25	E	3230	PSC	C03-C02-O01-C1

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Mol	Chain	Res	Type	Atoms
25	O	4230	PSC	C03-C02-O01-C1
18	N	4521	TGL	C21-C22-C23-C24
18	D	3523	TGL	C23-C24-C25-C26
19	A	3524	PGV	C5-C6-C7-C8
19	A	3524	PGV	O01-C02-C03-O11
19	P	4267	PGV	C29-C30-C31-C32
25	E	3230	PSC	C04-C05-N-C07
19	A	3266	PGV	C11-C12-C13-C14
21	C	3271	CHD	C16-C17-C20-C21
23	P	4265	PEK	C03-O11-P-O12
19	P	4267	PGV	C11-C12-C13-C14
23	G	4263	PEK	C14-C15-C16-C17
22	G	3269	CDL	C22-C23-C24-C25
23	C	3264	PEK	C26-C27-C28-C29
22	P	4270	CDL	C1-CA2-OA2-PA1
18	D	3523	TGL	CC6-CC7-CC8-CC9
23	C	3264	PEK	C3-C4-C5-C6
19	N	4266	PGV	C9-C10-C11-C12
23	T	3263	PEK	C14-C15-C16-C17
22	G	3269	CDL	C55-C56-C57-C58
18	N	4522	TGL	CC1-CC2-CC3-CC4
22	P	4270	CDL	C52-C53-C54-C55
23	P	4264	PEK	C3-C4-C5-C6
19	C	3268	PGV	C21-C22-C23-C24
23	C	3265	PEK	C26-C27-C28-C29
23	P	4264	PEK	C35-C36-C37-C38
22	G	3269	CDL	C53-C54-C55-C56
23	C	3265	PEK	C17-C18-C19-C20
19	P	4268	PGV	C21-C22-C23-C24
18	A	3521	TGL	C24-C25-C26-C27
22	G	3269	CDL	C11-C12-C13-C14
23	P	4265	PEK	C17-C18-C19-C20
23	P	4265	PEK	C26-C27-C28-C29
23	P	4265	PEK	C34-C35-C36-C37
22	T	4269	CDL	C53-C54-C55-C56
19	C	3267	PGV	C05-C04-O12-P
22	C	3270	CDL	C1-CA2-OA2-PA1
18	Q	4523	TGL	CC9-C15-C16-C17
22	T	4269	CDL	C31-C32-C33-C34
22	T	4269	CDL	C11-C12-C13-C14
19	N	4524	PGV	C12-C13-C14-C15
18	D	3523	TGL	CC5-CC6-CC7-CC8

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Mol	Chain	Res	Type	Atoms
22	G	3269	CDL	C31-C32-C33-C34
22	P	4270	CDL	C15-C16-C17-C18
19	A	3524	PGV	C31-C32-C33-C34
18	N	4522	TGL	OB1-CB1-OG2-CG2
22	G	3269	CDL	C36-C37-C38-C39
25	O	4230	PSC	C03-O11-P-O12
22	T	4269	CDL	C84-C85-C86-C87
23	P	4264	PEK	C31-C32-C33-C34
22	P	4270	CDL	C54-C55-C56-C57
22	C	3270	CDL	C54-C55-C56-C57
18	Q	4523	TGL	OG1-CG1-CG2-OG2
18	N	4521	TGL	OG1-CG1-CG2-OG2
18	Q	4523	TGL	CB9-C10-C11-C12
22	C	3270	CDL	C15-C16-C17-C18
22	T	4269	CDL	C36-C37-C38-C39
19	N	4524	PGV	O12-C04-C05-C06
22	G	3269	CDL	C62-C63-C64-C65
18	D	3523	TGL	C21-C22-C23-C24
19	C	3267	PGV	C1-C2-C3-C4
22	G	3269	CDL	C84-C85-C86-C87
18	L	3522	TGL	CB4-CB5-CB6-CB7
19	N	4524	PGV	C31-C32-C33-C34
18	N	4521	TGL	CC3-CC4-CC5-CC6
18	L	3522	TGL	OG2-CB1-CB2-CB3
18	N	4522	TGL	OG1-CA1-CA2-CA3
18	L	3522	TGL	OG1-CA1-CA2-CA3
18	Q	4523	TGL	OG1-CA1-CA2-CA3
18	Q	4523	TGL	CC7-CC8-CC9-C15
22	T	4269	CDL	C62-C63-C64-C65
19	A	3266	PGV	O03-C19-C20-C21
23	C	3265	PEK	C34-C35-C36-C37
19	A	3266	PGV	C9-C10-C11-C12
25	E	3230	PSC	C04-C05-N-C06
18	A	3521	TGL	CC3-CC4-CC5-CC6
19	A	3524	PGV	C01-C02-C03-O11
25	E	3230	PSC	C31-C32-C33-C34
23	C	3264	PEK	O01-C1-C2-C3
22	C	3270	CDL	C12-C11-CA5-OA6
19	C	3267	PGV	C29-C30-C31-C32
22	P	4270	CDL	C12-C11-CA5-OA6
25	O	4230	PSC	C19-C20-C21-C22
23	P	4264	PEK	O01-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
23	C	3265	PEK	C3-C4-C5-C6
23	P	4265	PEK	C3-C4-C5-C6
25	E	3230	PSC	C7-C8-C9-C10
22	P	4270	CDL	C32-C31-CA7-OA8
19	C	3267	PGV	C14-C15-C16-C17
19	N	4524	PGV	O01-C1-C2-C3
22	P	4270	CDL	C52-C51-CB5-OB6
22	C	3270	CDL	C52-C51-CB5-OB6
19	P	4268	PGV	C9-C10-C11-C12
19	N	4266	PGV	C11-C12-C13-C14
19	C	3267	PGV	C11-C12-C13-C14
19	C	3268	PGV	C31-C32-C33-C34
18	Q	4523	TGL	CC6-CC7-CC8-CC9
19	P	4268	PGV	C31-C32-C33-C34
18	D	3523	TGL	C19-C33-C34-C35
25	O	4230	PSC	C31-C32-C33-C34
19	P	4267	PGV	C9-C10-C11-C12
19	C	3268	PGV	C9-C10-C11-C12
25	O	4230	PSC	C7-C8-C9-C10
19	C	3267	PGV	C9-C10-C11-C12
19	A	3524	PGV	O12-C04-C05-C06
18	Q	4523	TGL	OG3-CC1-CC2-CC3
22	C	3270	CDL	C32-C31-CA7-OA8
19	N	4266	PGV	C4-C5-C6-C7
19	N	4524	PGV	C01-C02-C03-O11
18	A	3521	TGL	OG3-CC1-CC2-CC3
23	G	4263	PEK	C3-C4-C5-C6
19	P	4267	PGV	C21-C22-C23-C24
18	Q	4523	TGL	OG2-CB1-CB2-CB3
22	G	3269	CDL	C76-C77-C78-C79
18	N	4522	TGL	CC9-C15-C16-C17
23	P	4264	PEK	C22-C21-O03-C01
18	N	4521	TGL	OG3-CC1-CC2-CC3
23	C	3264	PEK	O02-C1-C2-C3
19	A	3524	PGV	O01-C1-C2-C3
22	P	4270	CDL	C32-C31-CA7-OA9
22	C	3270	CDL	C32-C31-CA7-OA9
18	Q	4523	TGL	CC5-CC6-CC7-CC8
25	O	4230	PSC	O02-C1-C2-C3
22	C	3270	CDL	C52-C51-CB5-OB7
18	N	4522	TGL	CB2-CB1-OG2-CG2
23	T	3263	PEK	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
22	P	4270	CDL	C52-C51-CB5-OB7
25	O	4230	PSC	O01-C1-C2-C3
25	E	3230	PSC	C03-O11-P-O12
25	E	3230	PSC	O02-C1-C2-C3
25	E	3230	PSC	O01-C1-C2-C3
23	P	4264	PEK	O02-C1-C2-C3
18	Q	4523	TGL	OB1-CB1-CB2-CB3
23	C	3265	PEK	C35-C36-C37-C38
19	P	4268	PGV	C03-O11-P-O13
19	C	3268	PGV	C03-O11-P-O13
25	E	3230	PSC	C03-O11-P-O13
25	O	4230	PSC	C03-O11-P-O13
25	E	3230	PSC	C01-C02-C03-O11
25	O	4230	PSC	C01-C02-C03-O11
23	P	4265	PEK	C35-C36-C37-C38
23	C	3264	PEK	O12-C04-C05-N
18	A	3521	TGL	OC1-CC1-CC2-CC3
18	L	3522	TGL	C13-C14-C29-C30
18	L	3522	TGL	OB1-CB1-OG2-CG2
23	T	3263	PEK	C33-C34-C35-C36
25	O	4230	PSC	C12-C13-C14-C15
17	N	516	HEA	C26-C15-C16-C17
25	E	3230	PSC	C05-C04-O12-P
25	O	4230	PSC	C05-C04-O12-P
18	D	3523	TGL	OC1-CC1-CC2-CC3
22	P	4270	CDL	C43-C44-C45-C46
25	E	3230	PSC	C12-C13-C14-C15
18	D	3523	TGL	OG2-CB1-CB2-CB3
18	D	3523	TGL	OG3-CC1-CC2-CC3
18	A	3521	TGL	OG2-CB1-CB2-CB3
18	D	3523	TGL	C29-C30-C31-C32
22	T	4269	CDL	OB9-CB7-OB8-CB6
17	A	516	HEA	C26-C15-C16-C17
22	C	3270	CDL	C76-C77-C78-C79
18	D	3523	TGL	CC9-C15-C16-C17
18	Q	4523	TGL	C11-C10-CB9-CB8
25	O	4230	PSC	O03-C19-C20-C21
25	E	3230	PSC	O03-C19-C20-C21
18	D	3523	TGL	OG1-CA1-CA2-CA3
22	G	3269	CDL	OB9-CB7-OB8-CB6
22	P	4270	CDL	C76-C77-C78-C79
23	G	4263	PEK	O01-C1-C2-C3

There are no ring outliers.

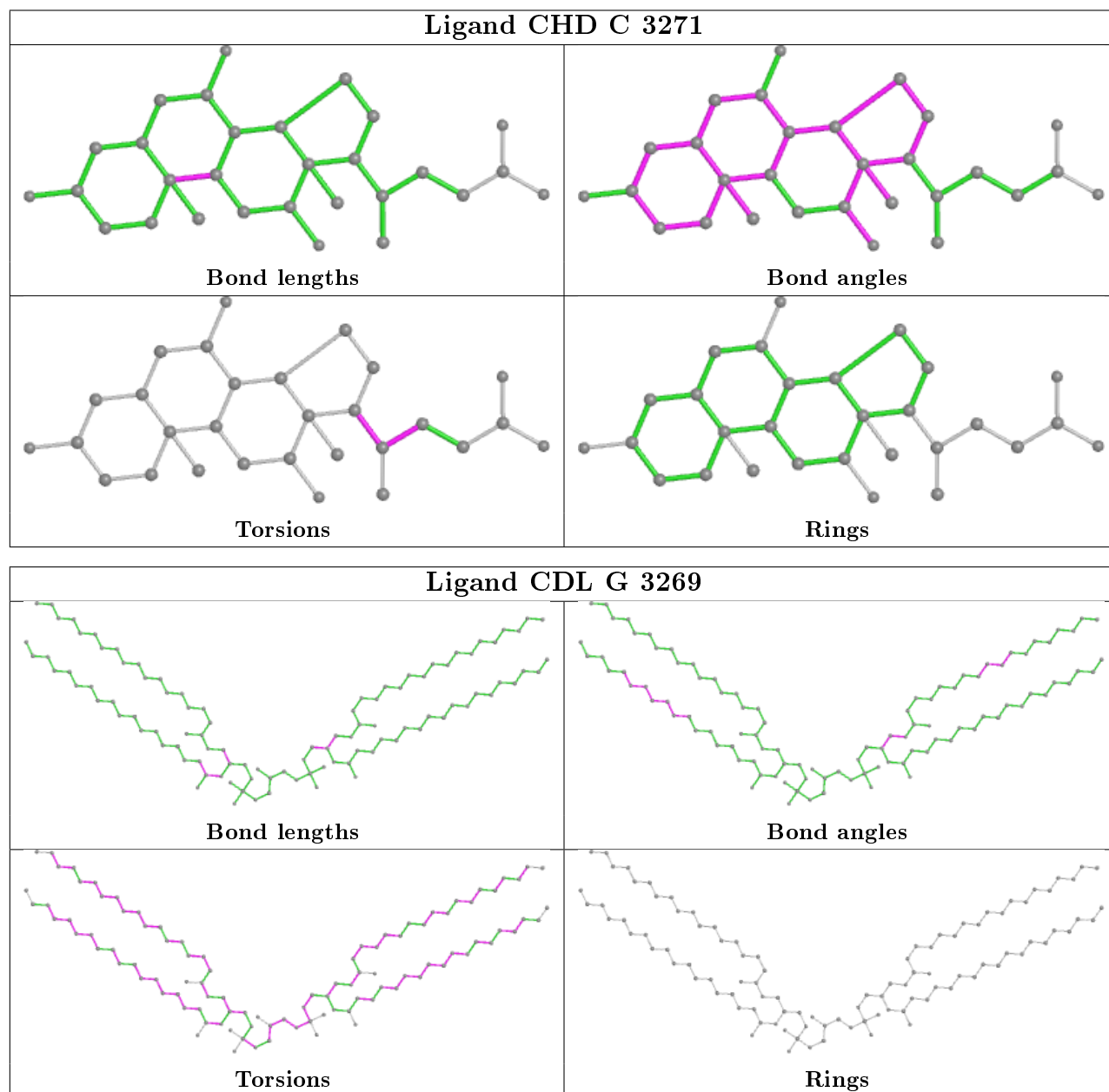
32 monomers are involved in 267 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	C	3271	CHD	3	0
22	G	3269	CDL	14	0
21	O	3085	CHD	1	0
19	P	4267	PGV	8	0
23	C	3265	PEK	3	0
23	P	4265	PEK	2	0
19	C	3268	PGV	1	0
21	B	4085	CHD	1	0
25	E	3230	PSC	13	0
23	C	3264	PEK	4	0
23	P	4264	PEK	4	0
19	N	4524	PGV	5	0
18	D	3523	TGL	15	0
18	N	4522	TGL	19	0
17	A	515	HEA	3	0
25	O	4230	PSC	21	0
18	L	3522	TGL	25	0
18	Q	4523	TGL	15	0
22	P	4270	CDL	18	0
19	C	3267	PGV	6	0
19	A	3524	PGV	7	0
17	A	516	HEA	1	0
22	C	3270	CDL	14	0
18	N	4521	TGL	19	0
21	J	3060	CHD	2	0
21	W	4060	CHD	2	0
21	P	4271	CHD	2	0
23	G	4263	PEK	10	0
22	T	4269	CDL	15	0
17	N	515	HEA	3	0
23	T	3263	PEK	9	0
18	A	3521	TGL	11	0

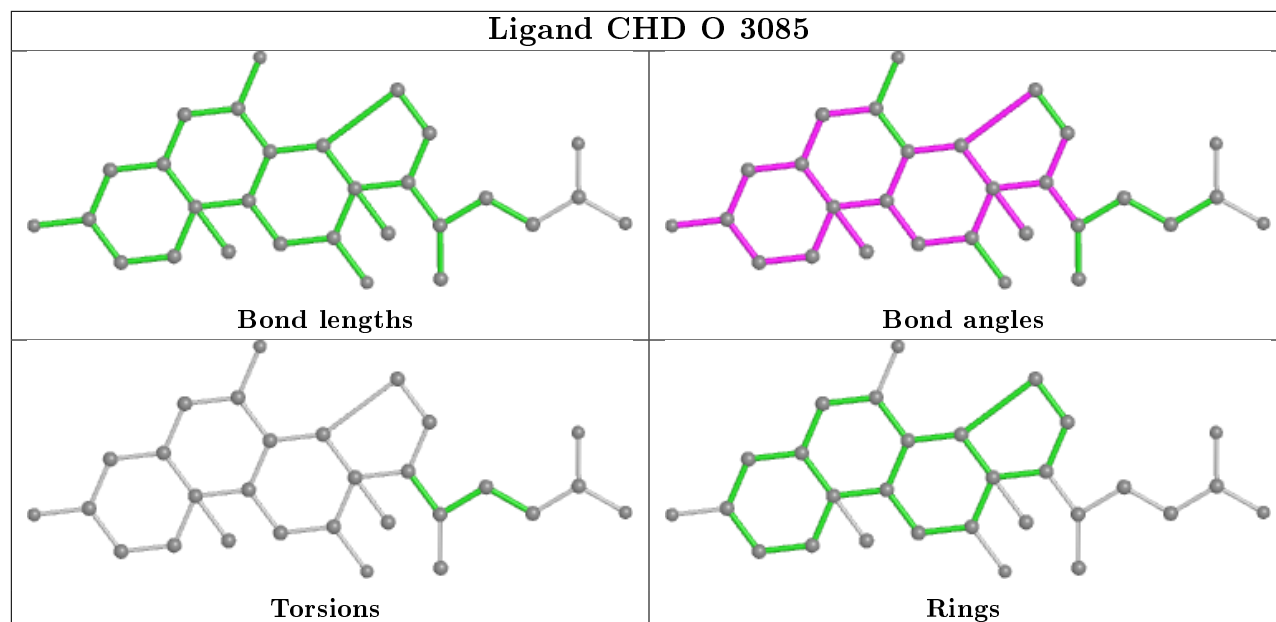
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the



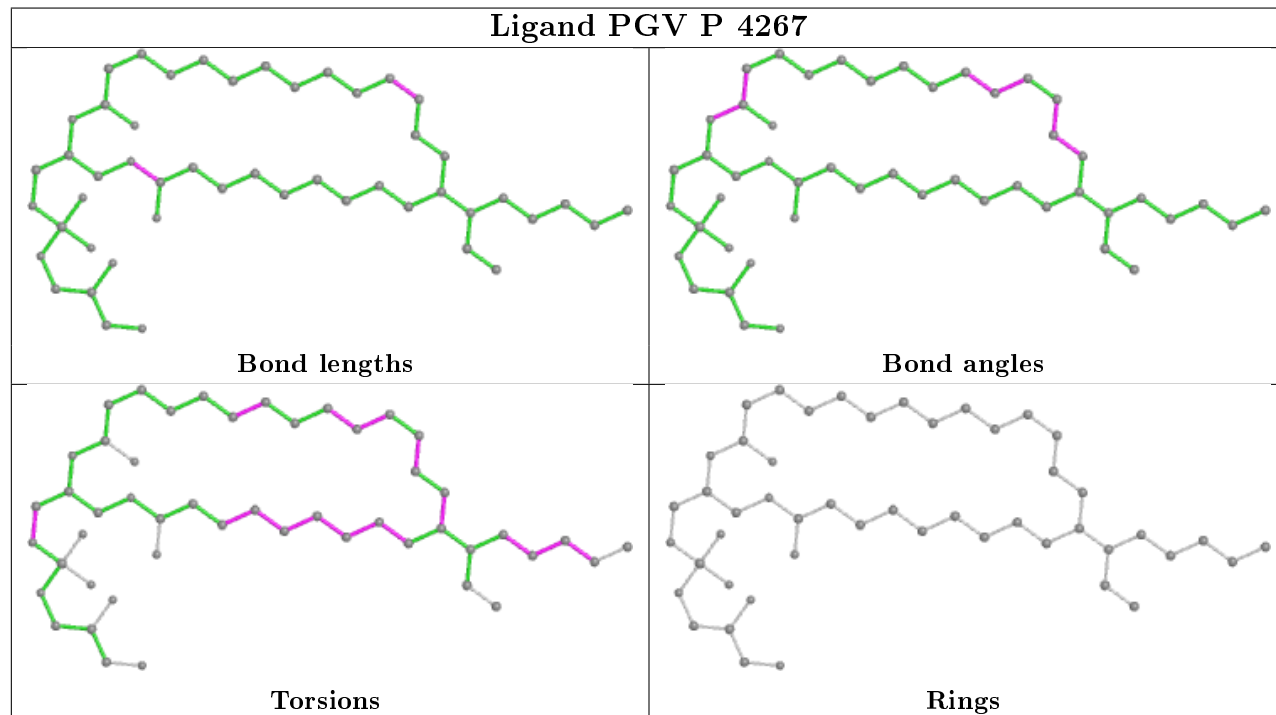
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



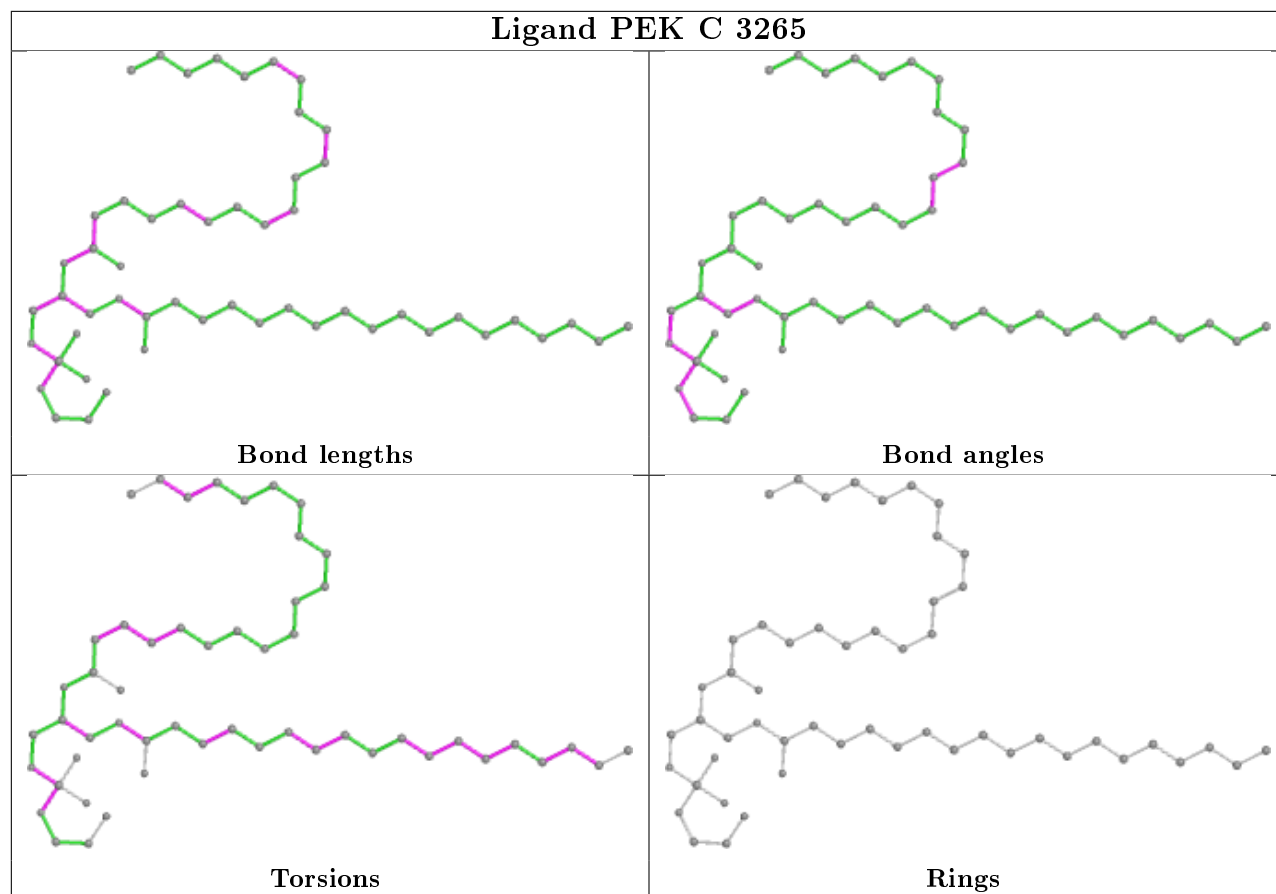
## Ligand CHD O 3085



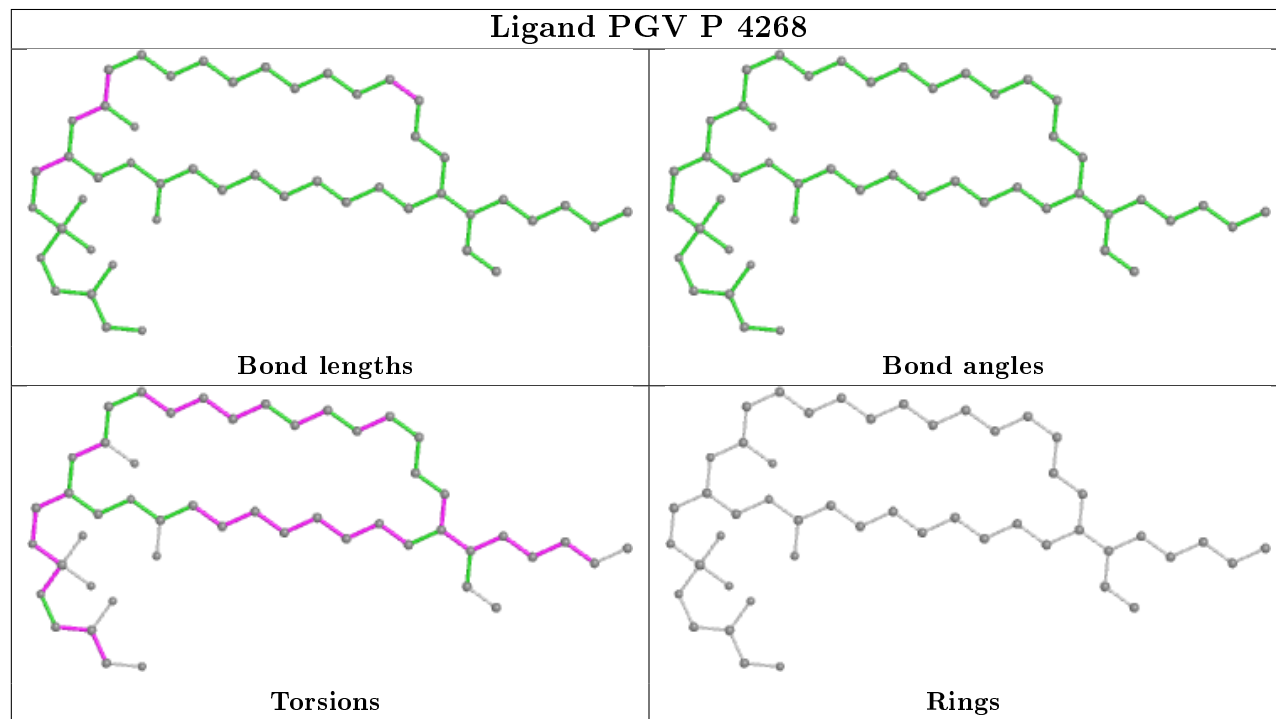
## Ligand PGV P 4267

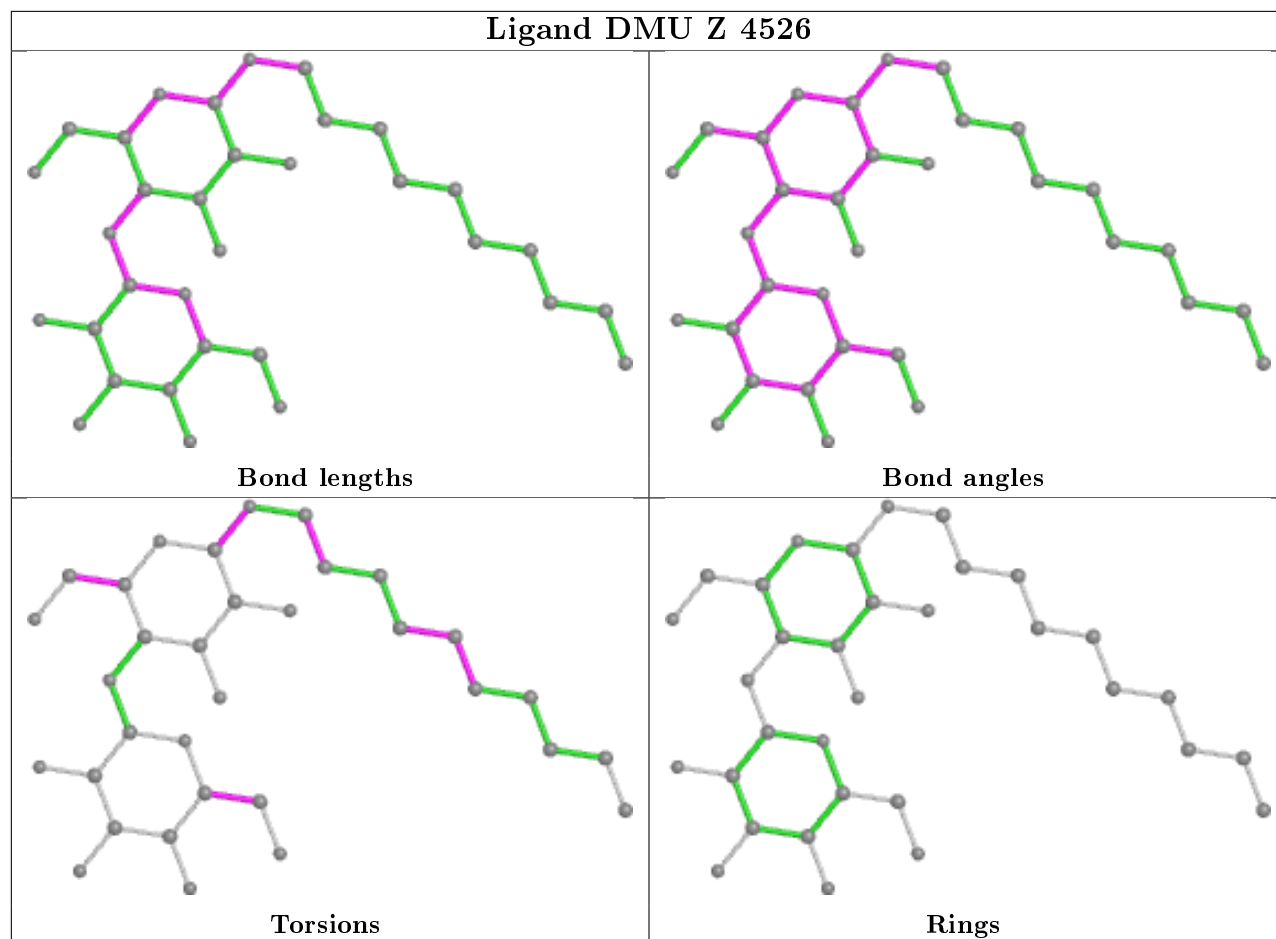


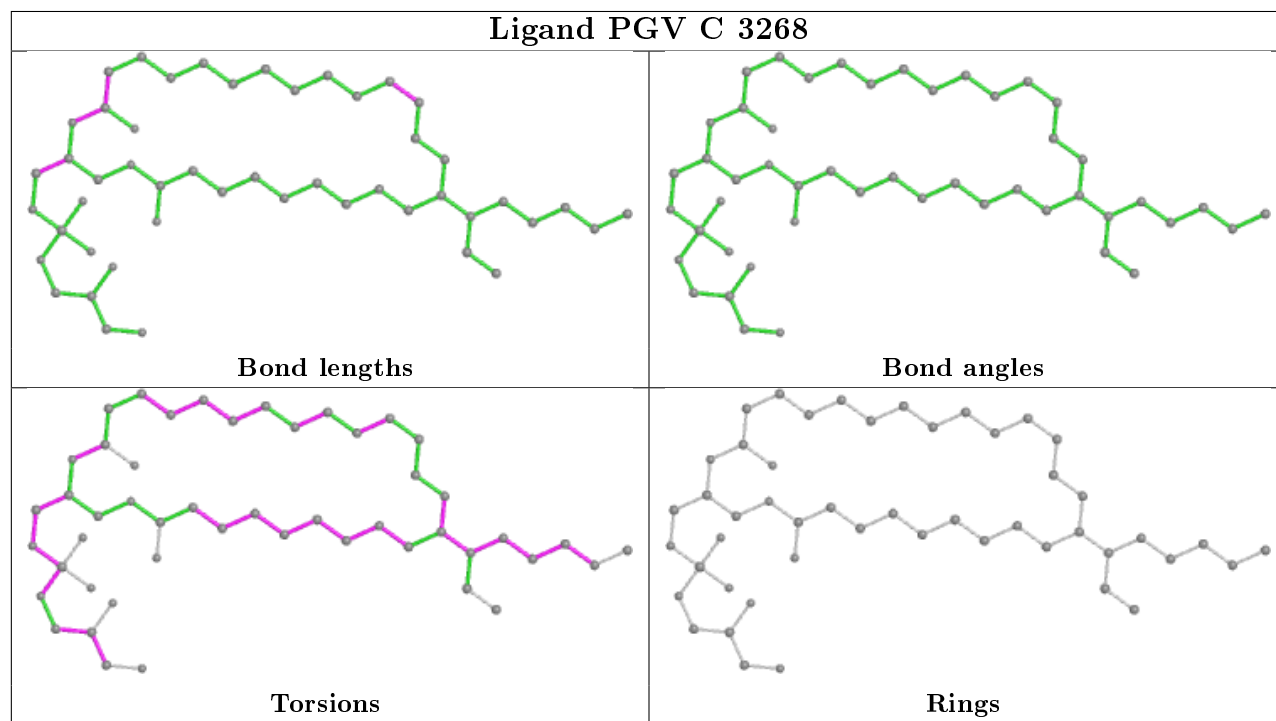
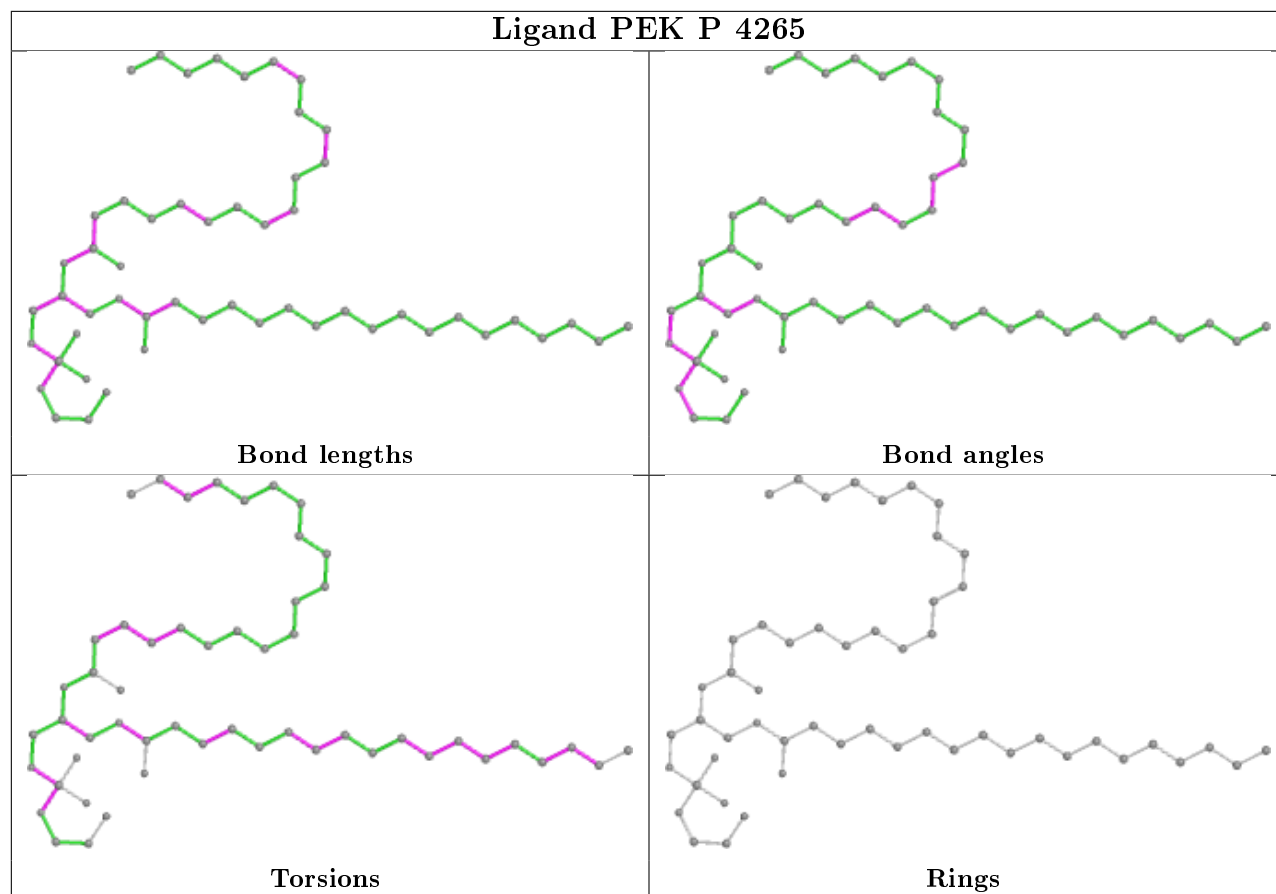
## Ligand PEK C 3265



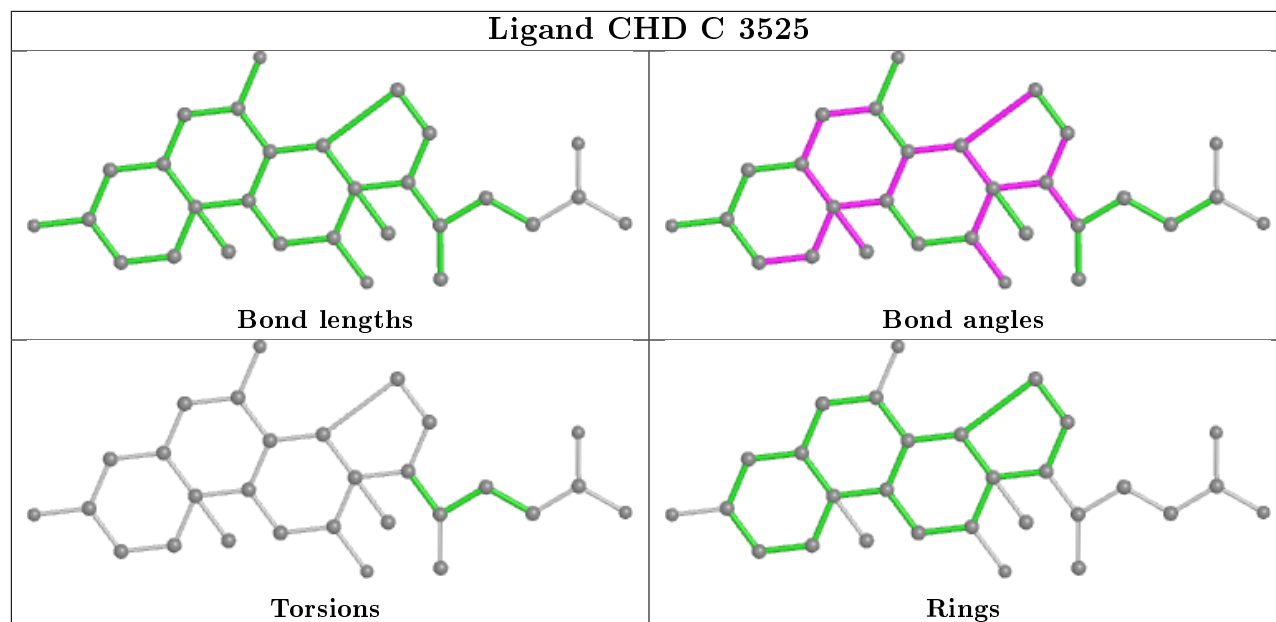
## Ligand PGV P 4268



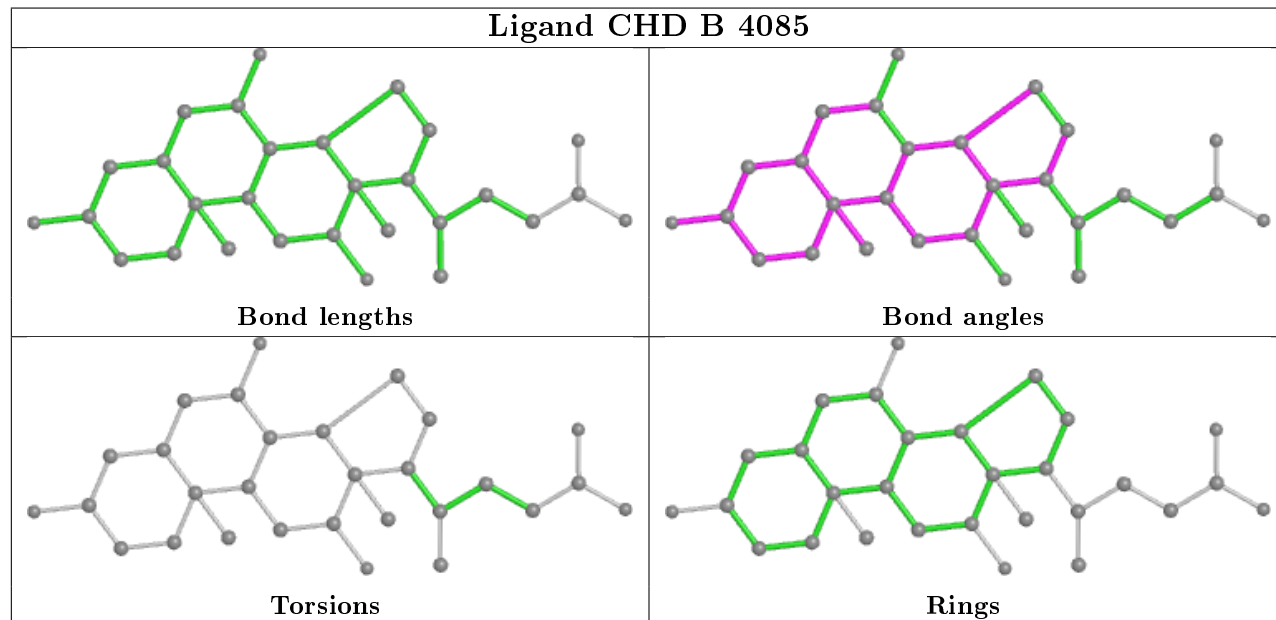


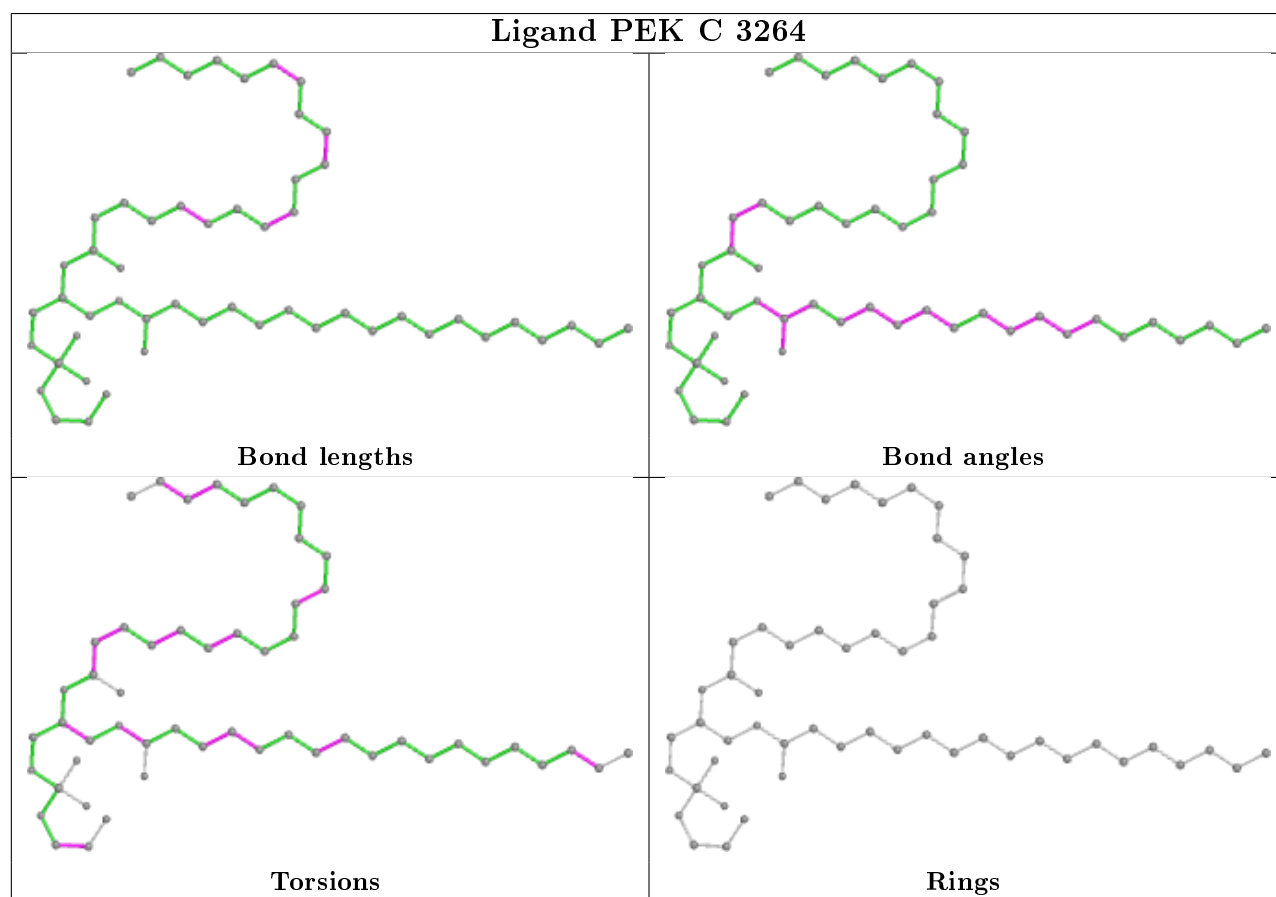
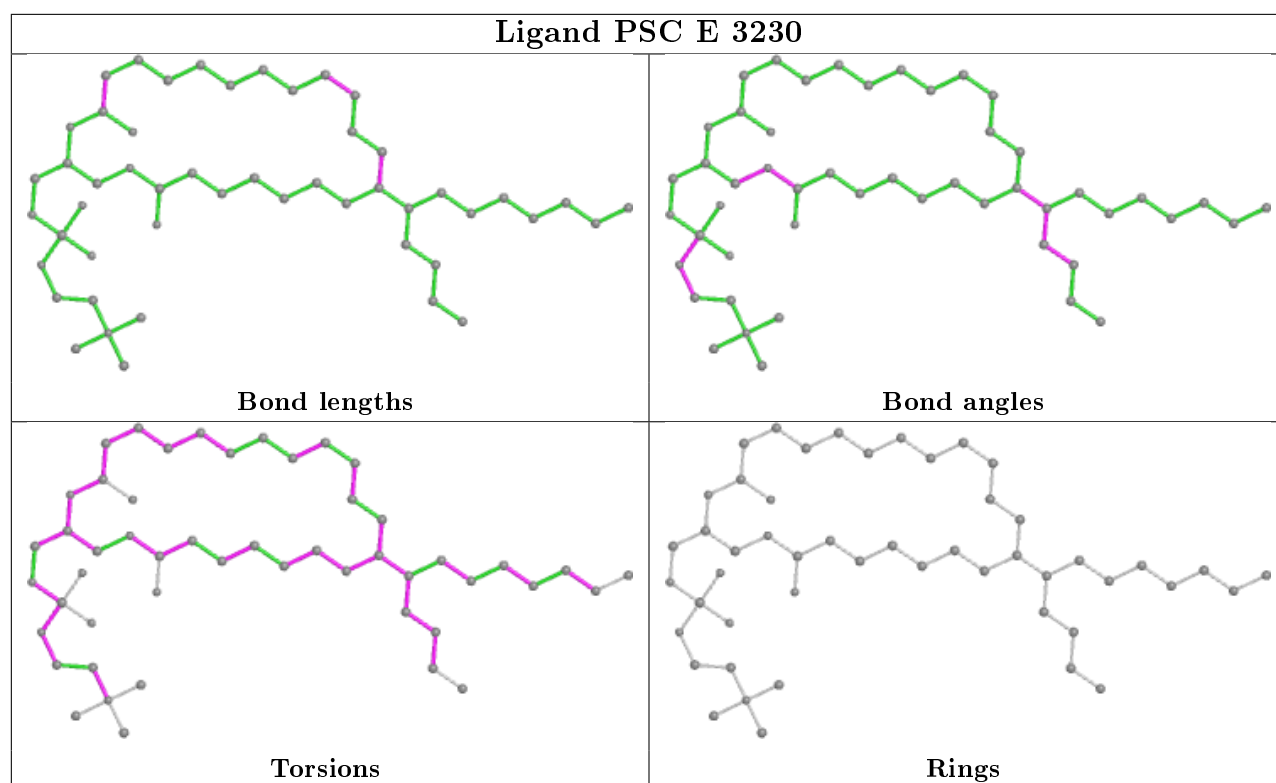


## Ligand CHD C 3525

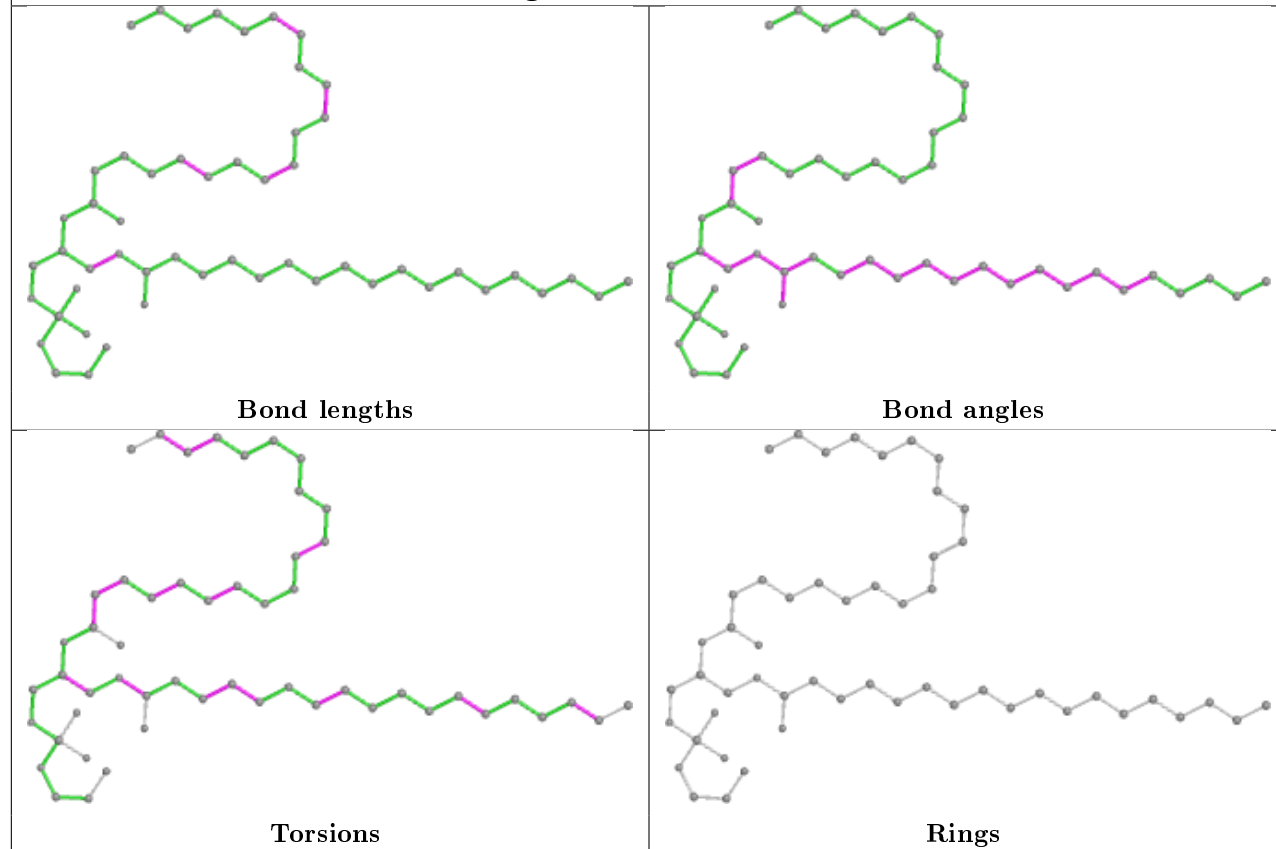


## Ligand CHD B 4085

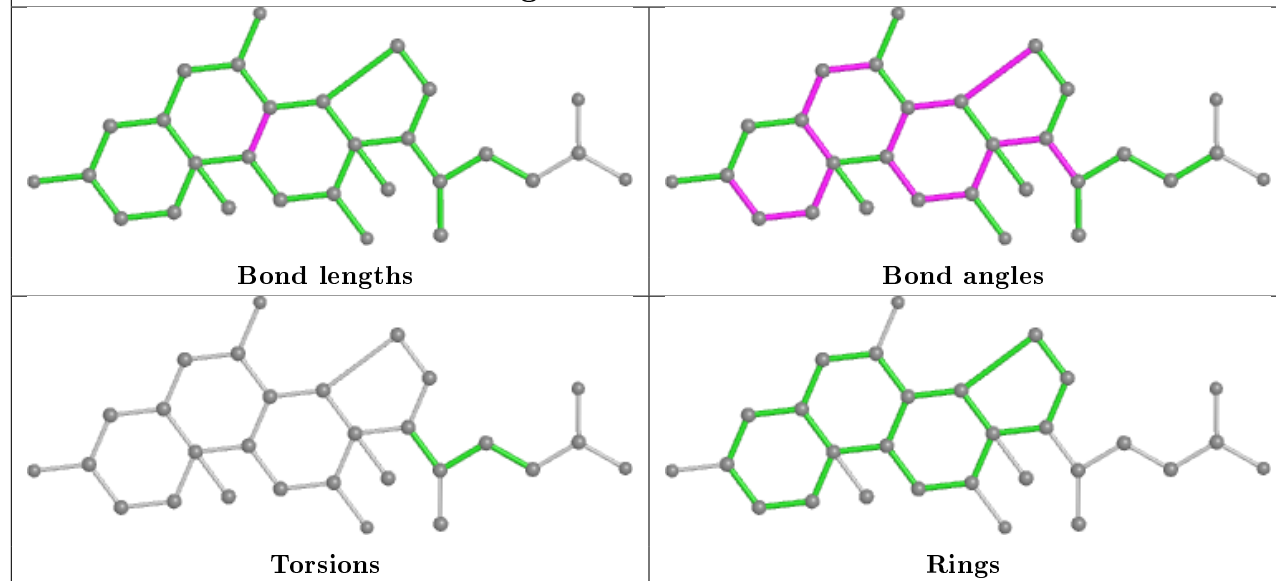




## Ligand PEK P 4264

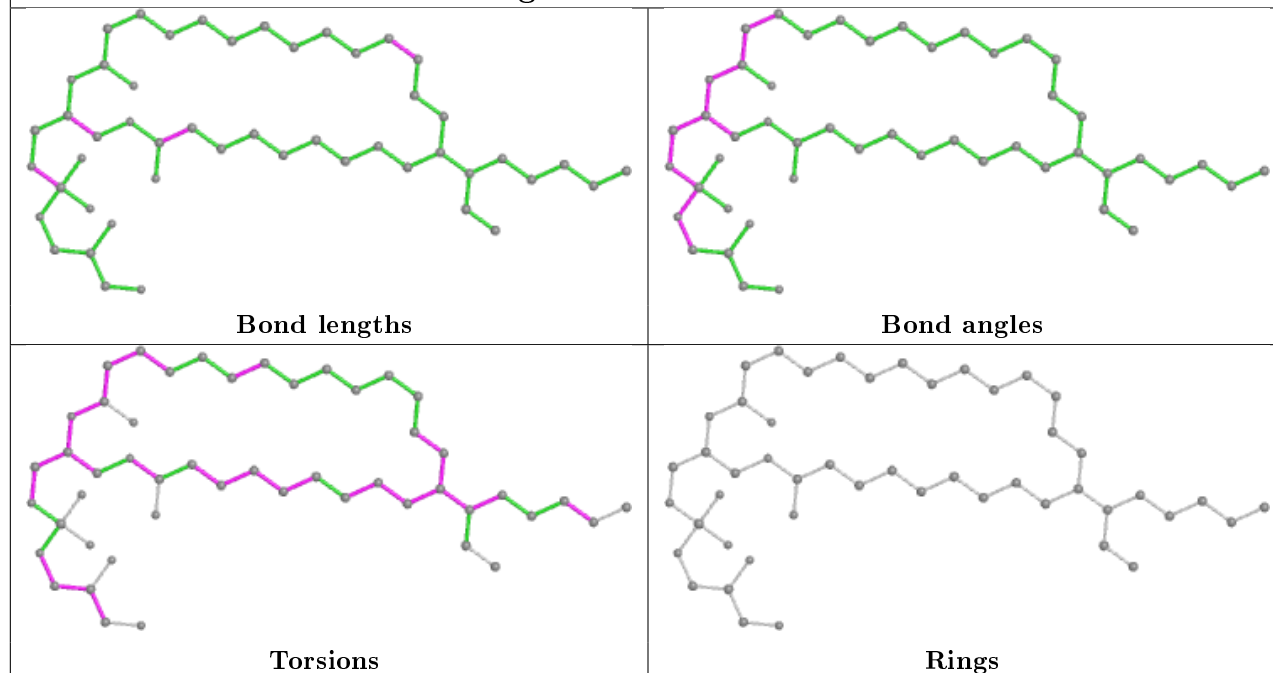


## Ligand CHD P 4525

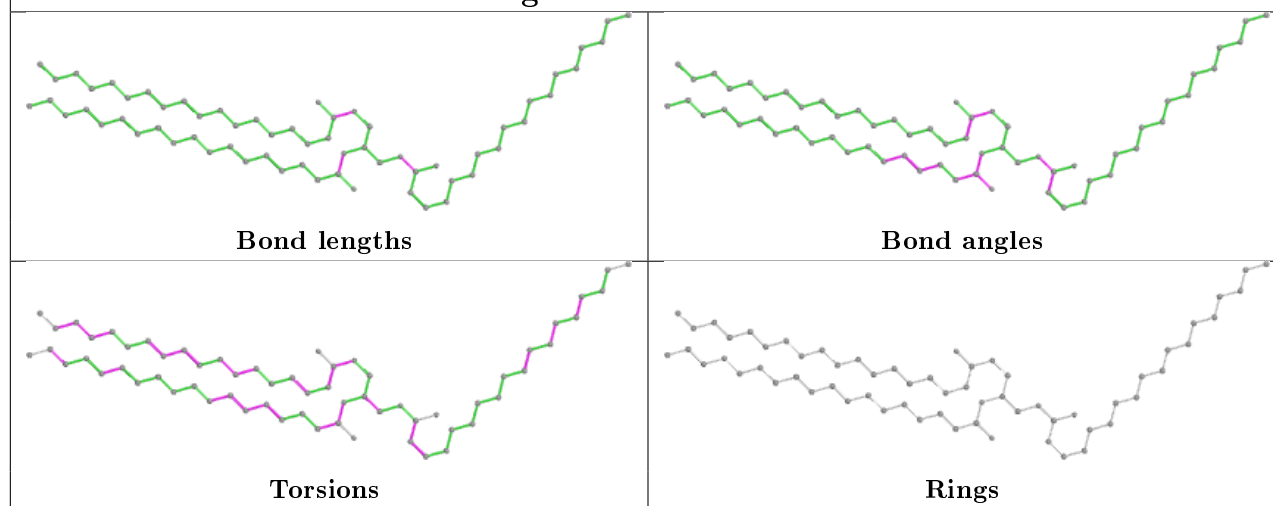


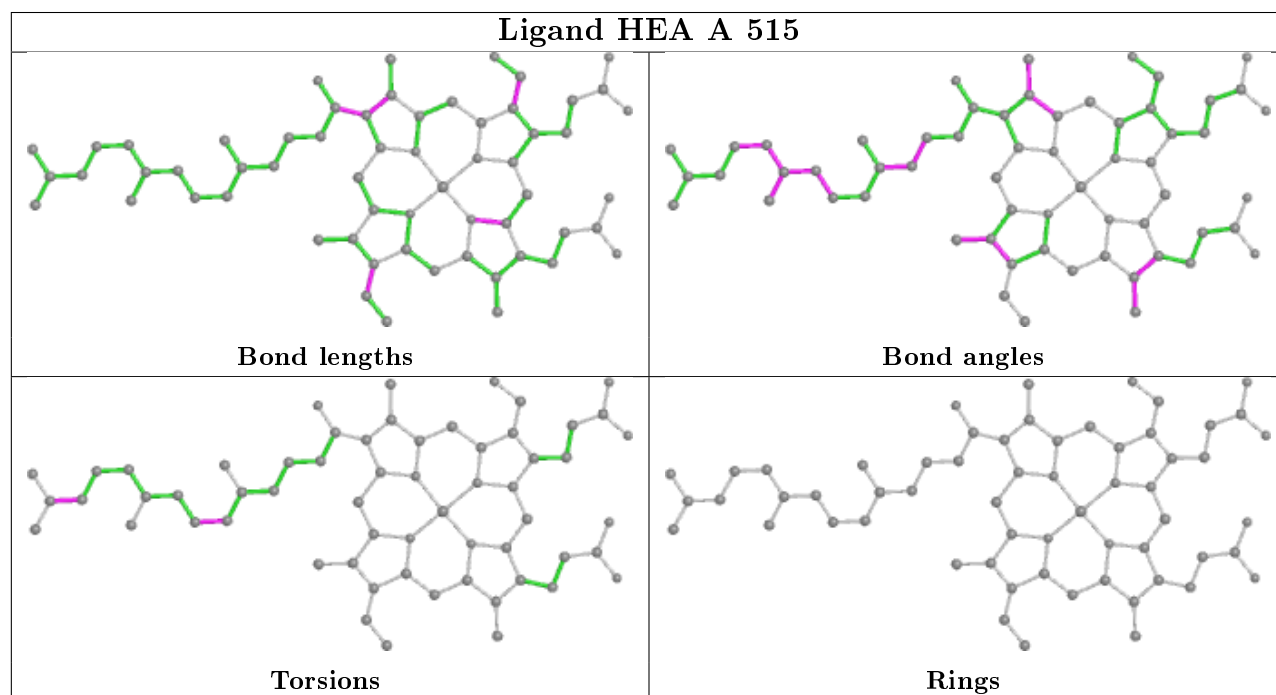
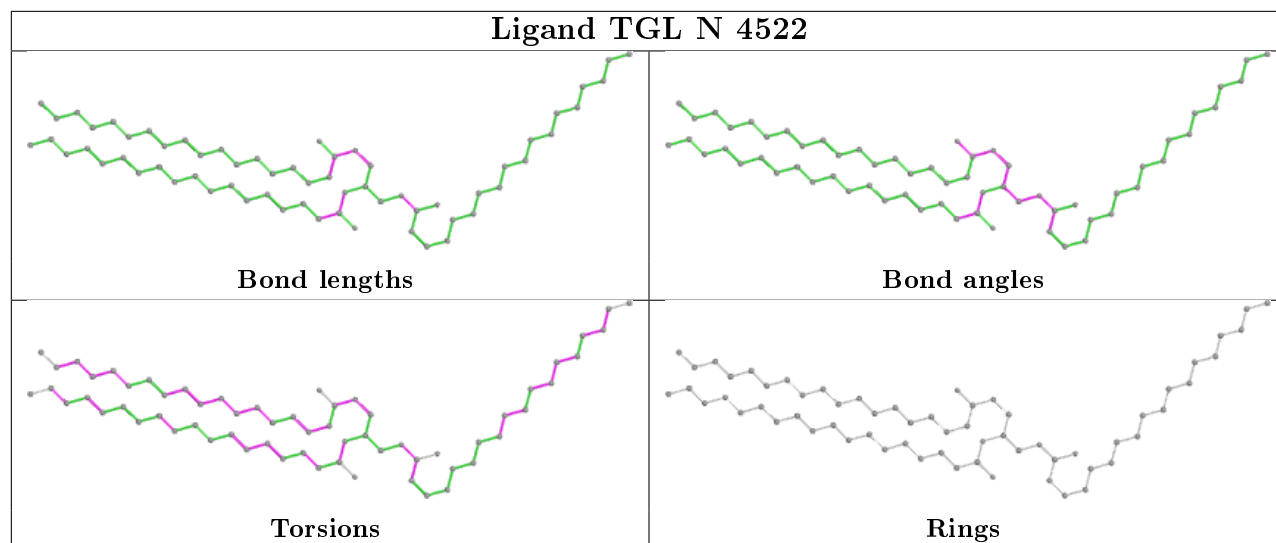


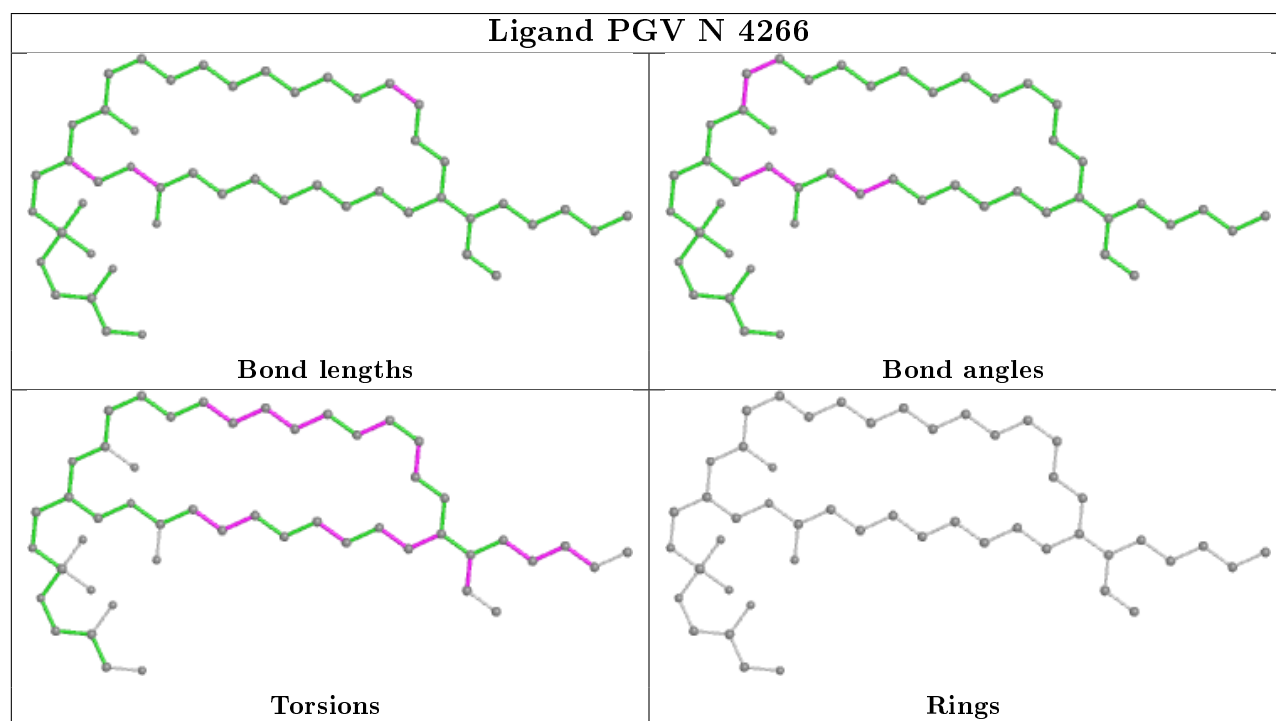
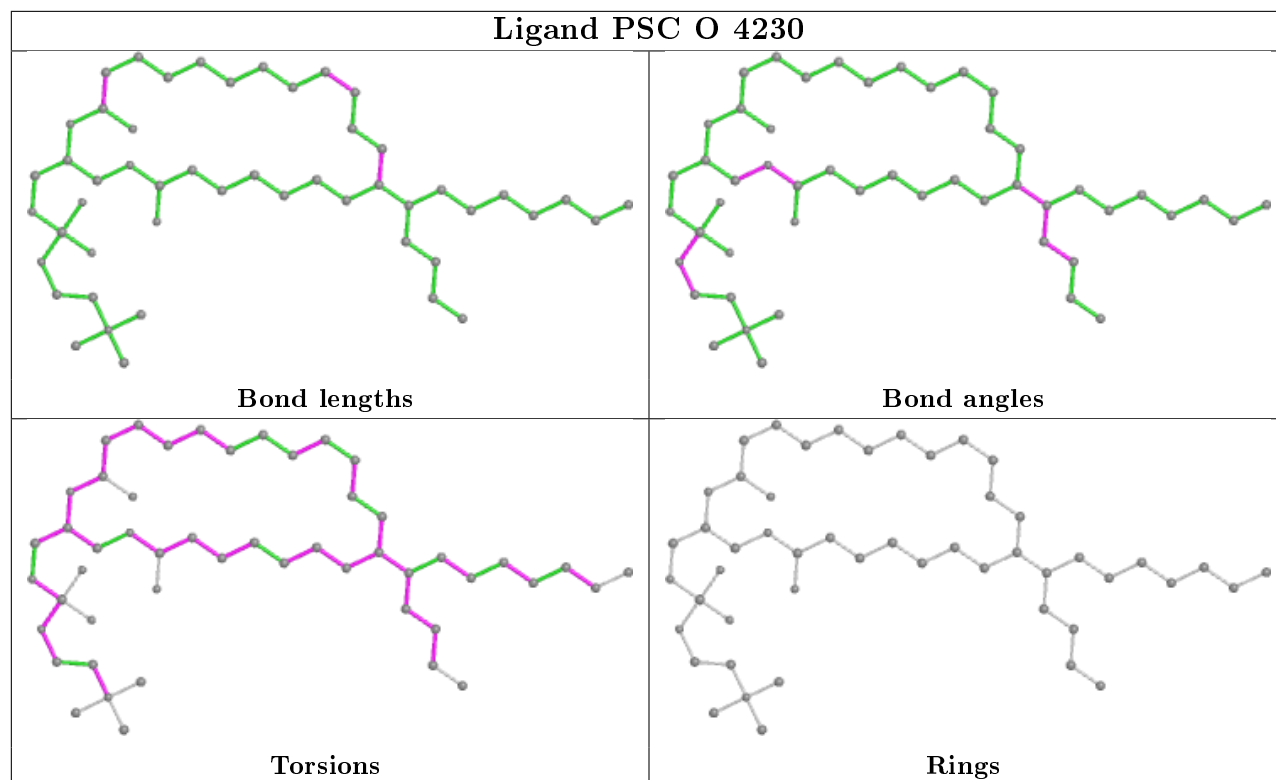
## Ligand PGV N 4524

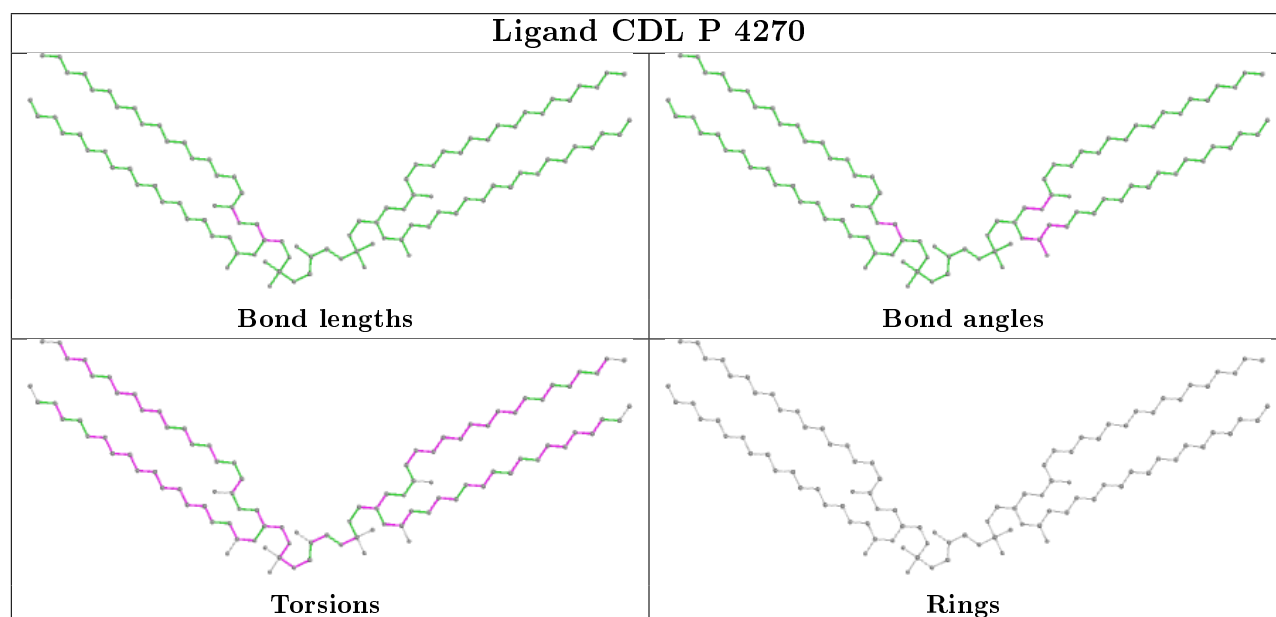
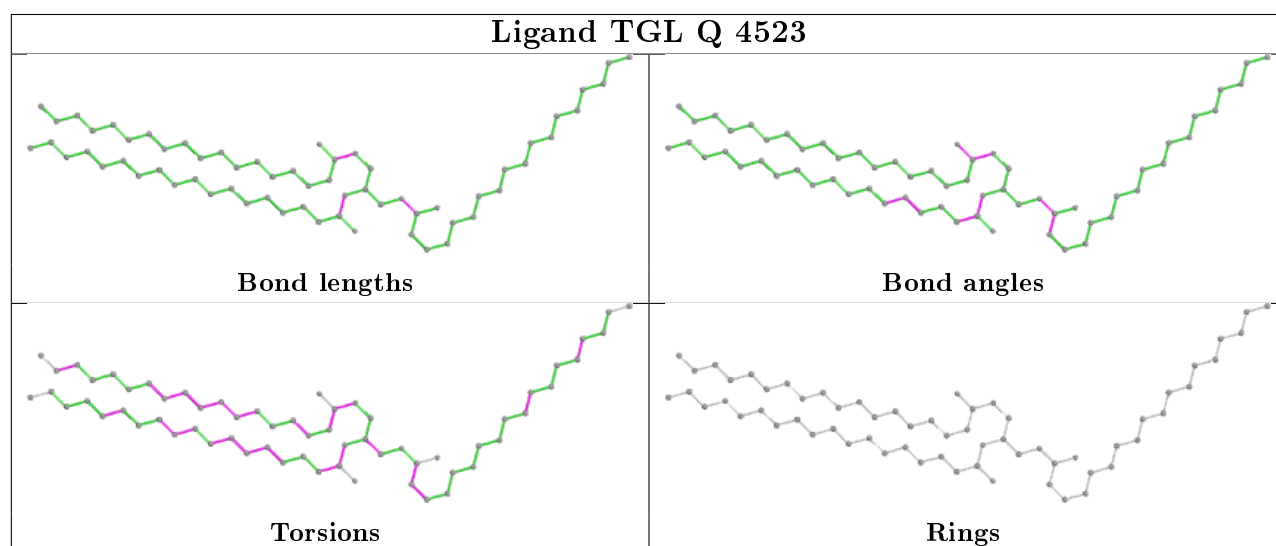
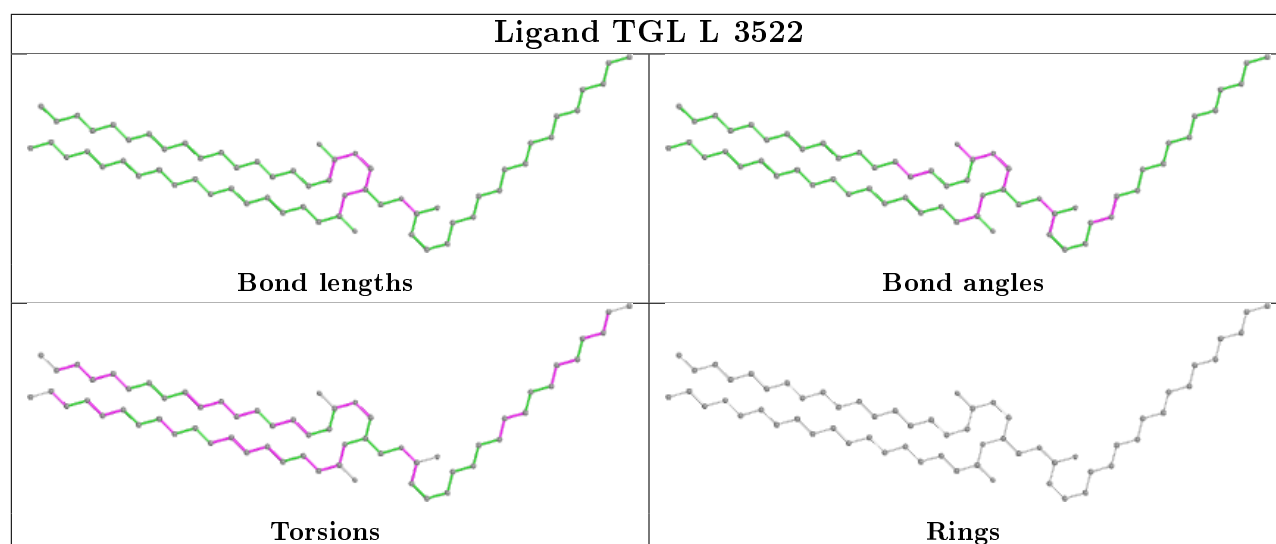


## Ligand TGL D 3523

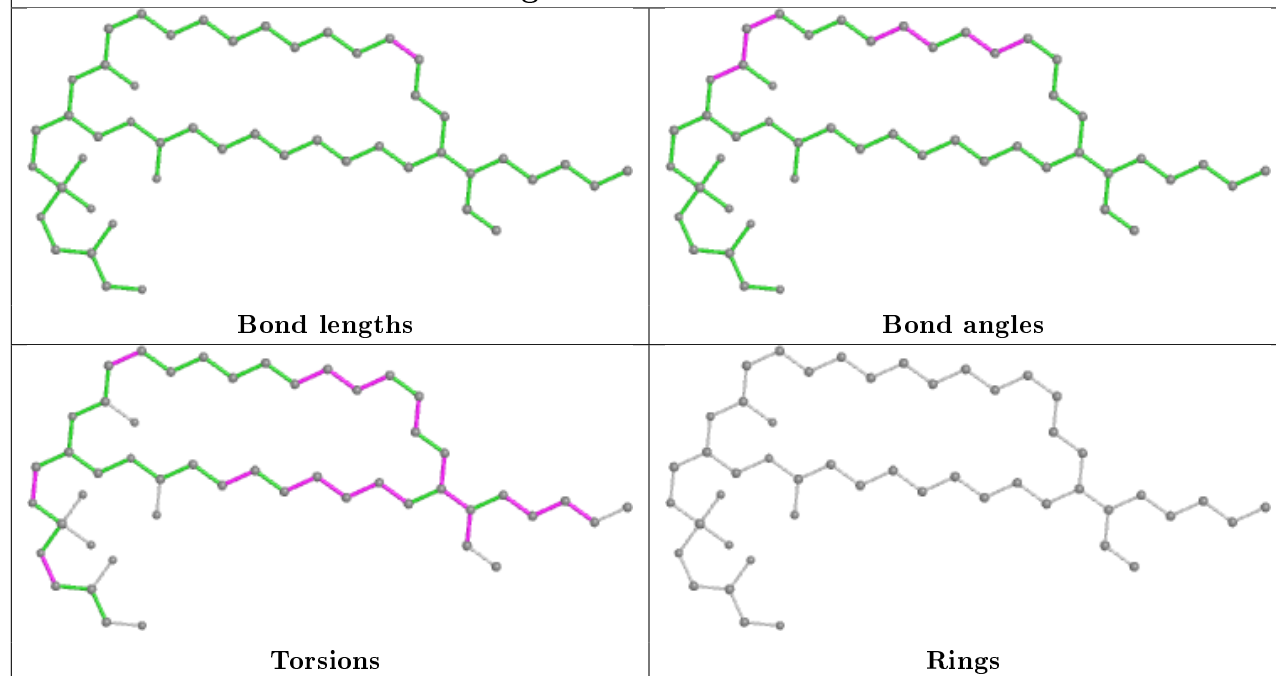




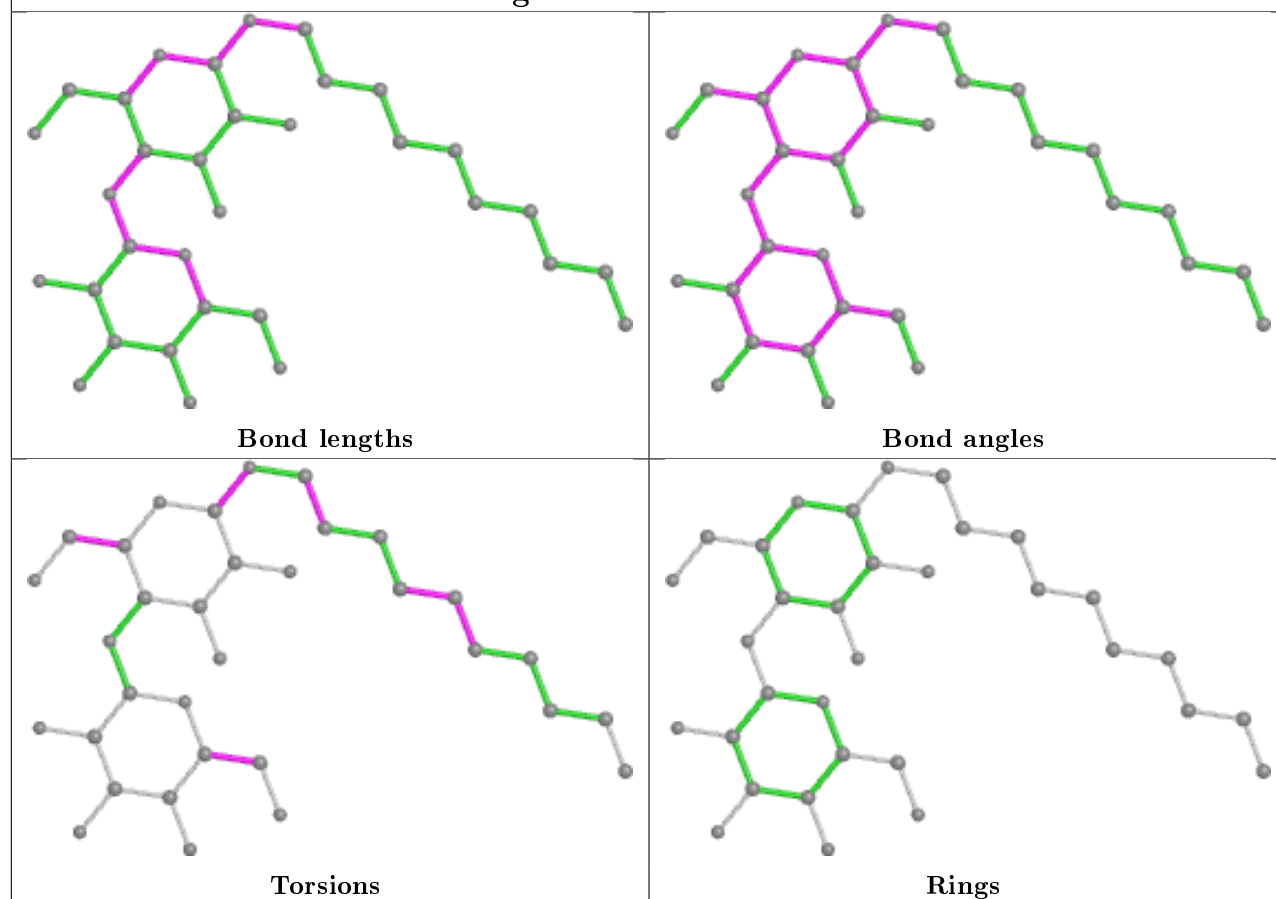




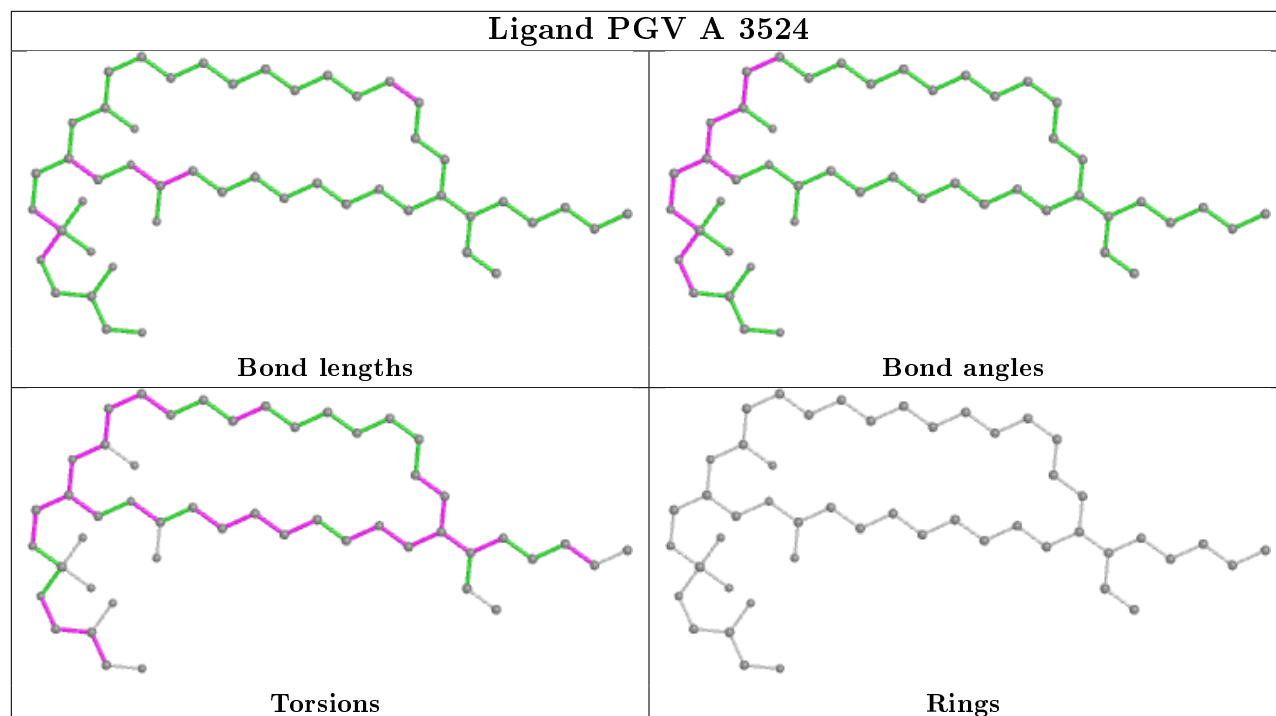
## Ligand PGV C 3267



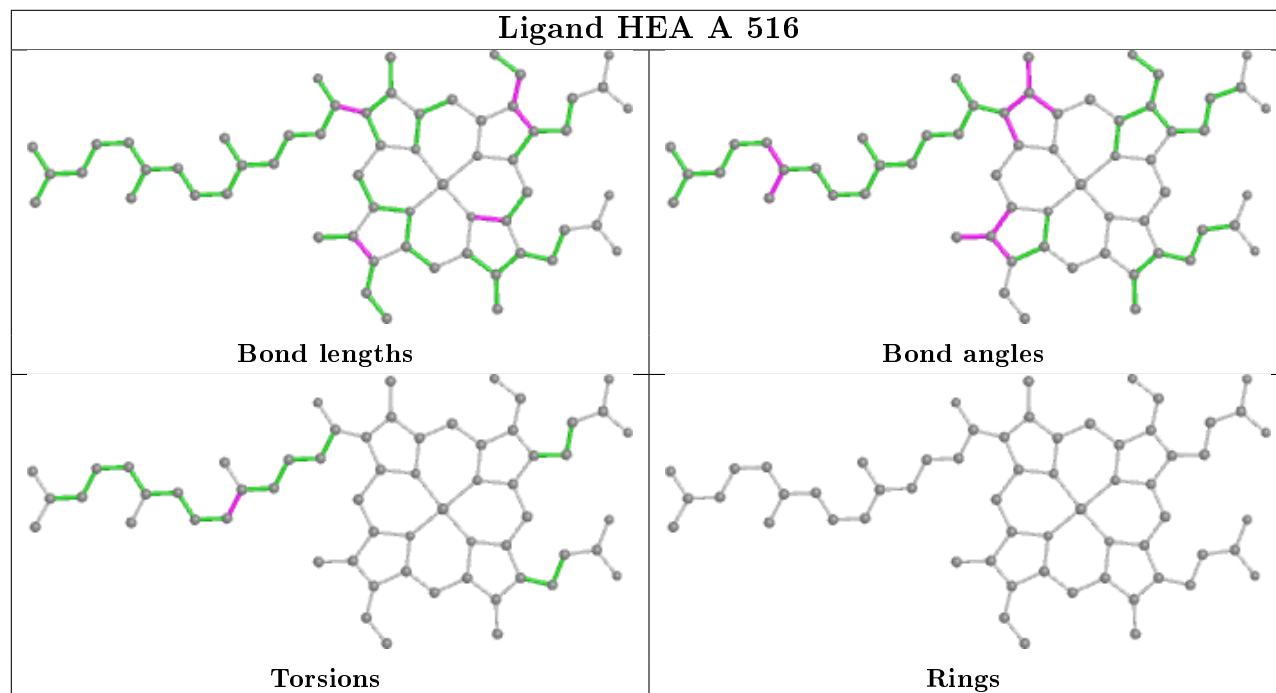
## Ligand DMU M 3526

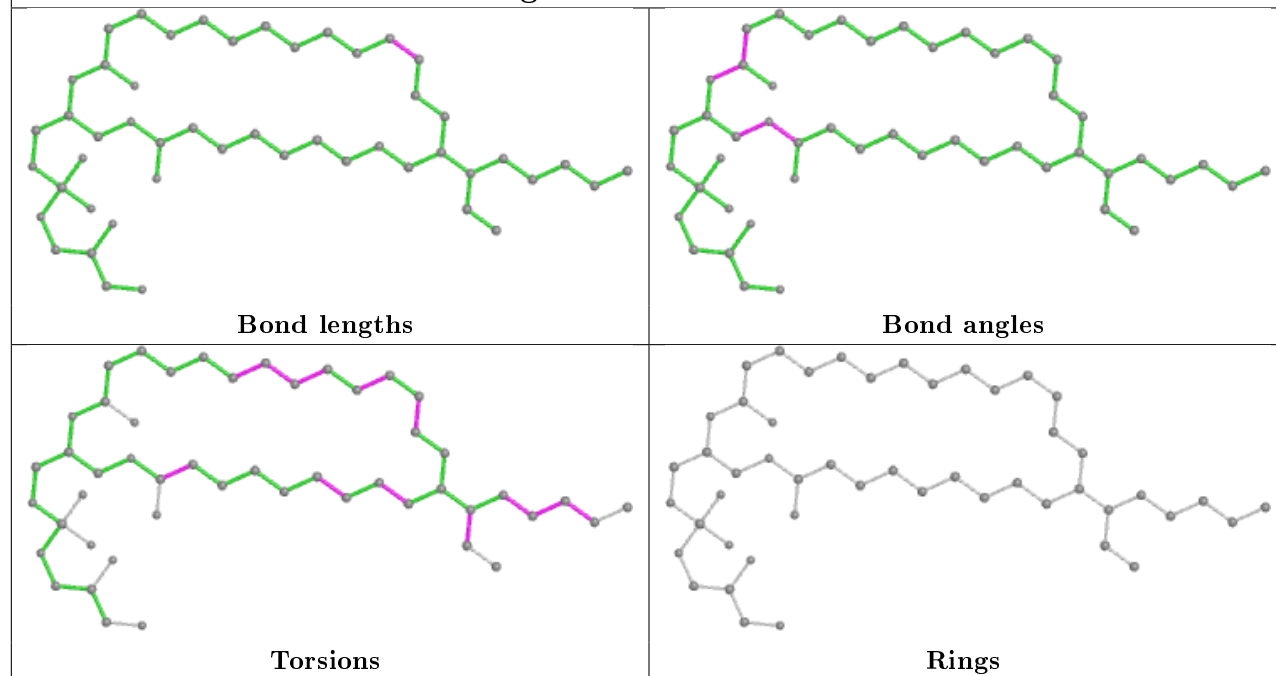
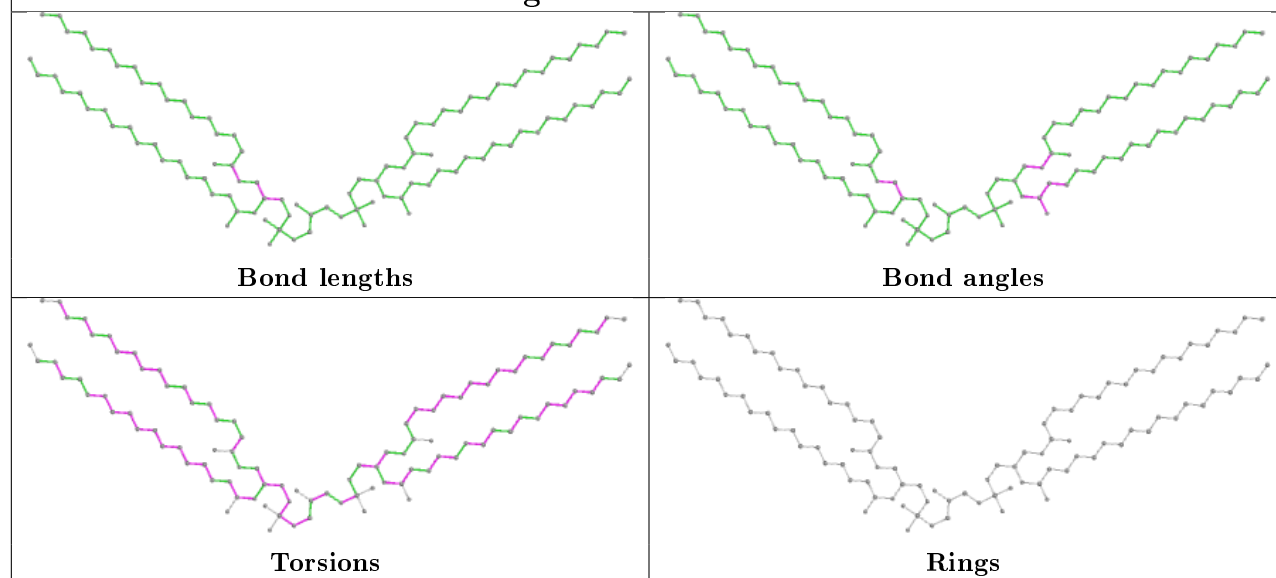


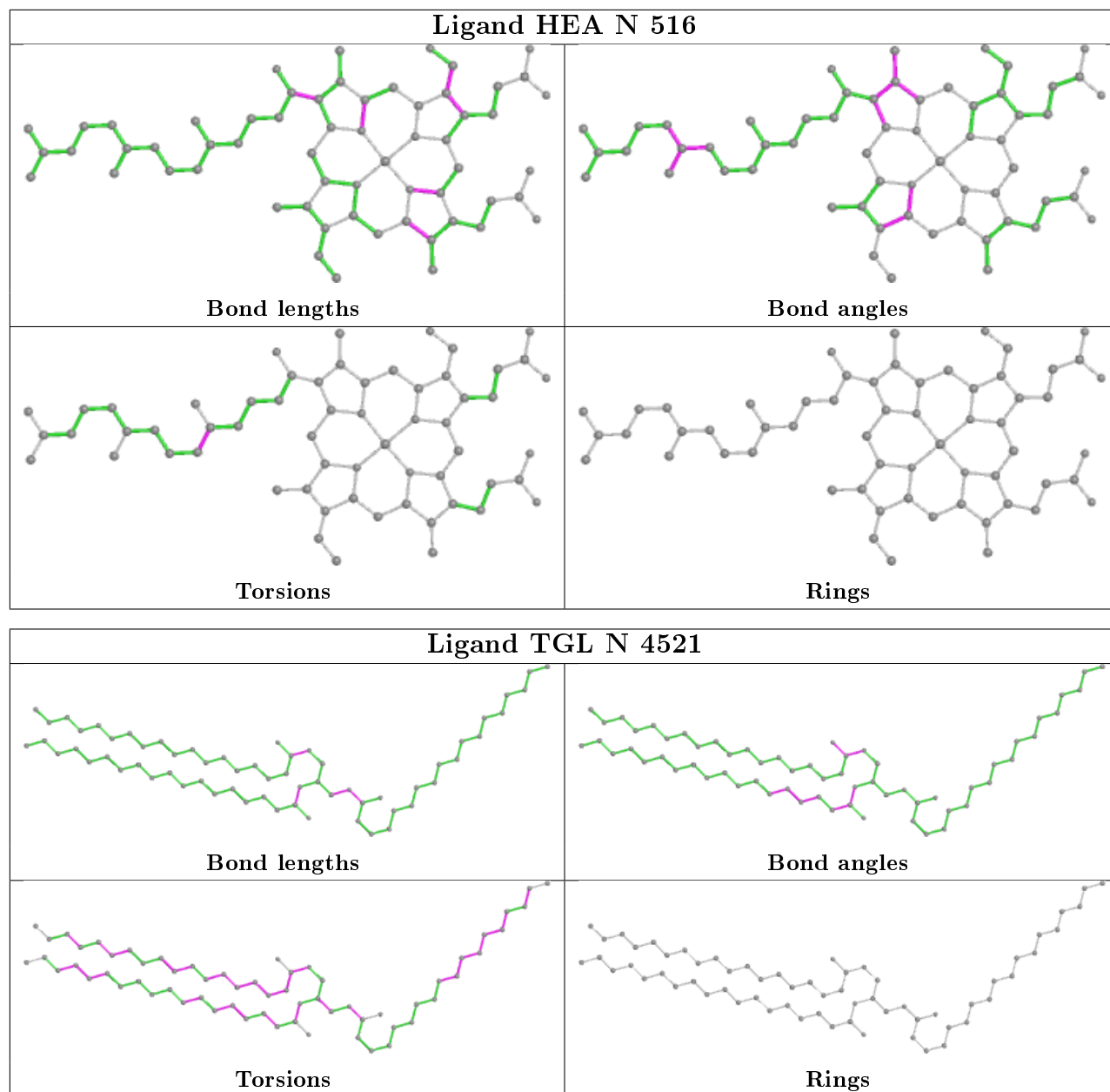
## Ligand PGV A 3524



## Ligand HEA A 516

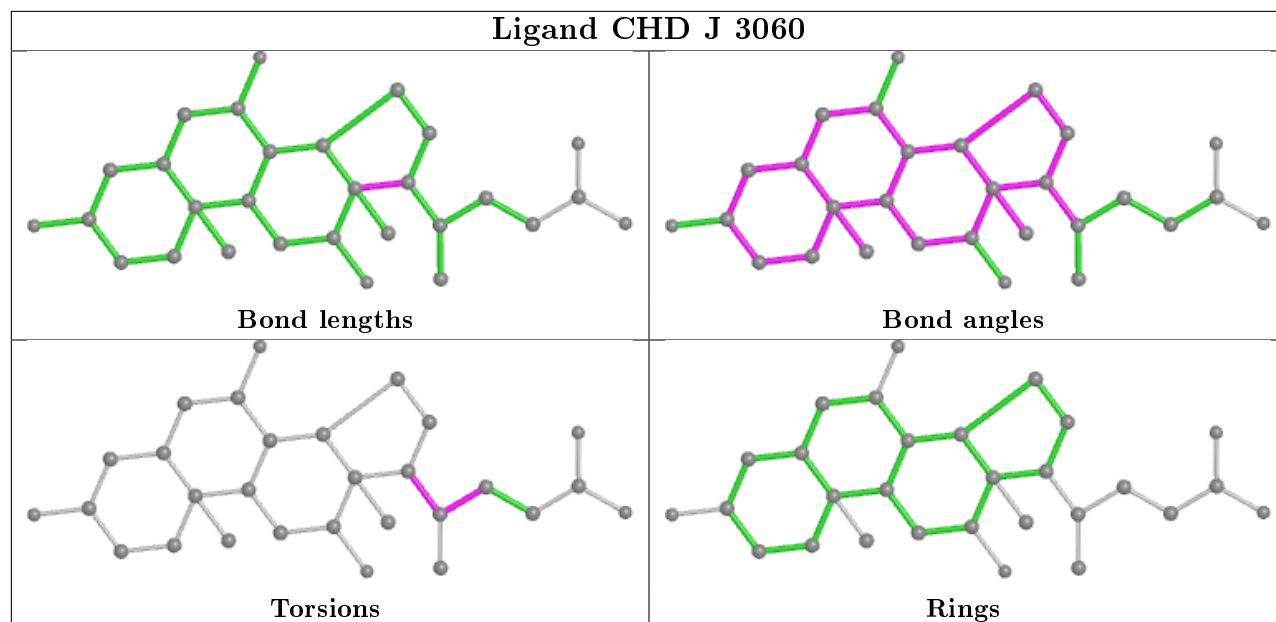


**Ligand PGV A 3266****Ligand CDL C 3270**

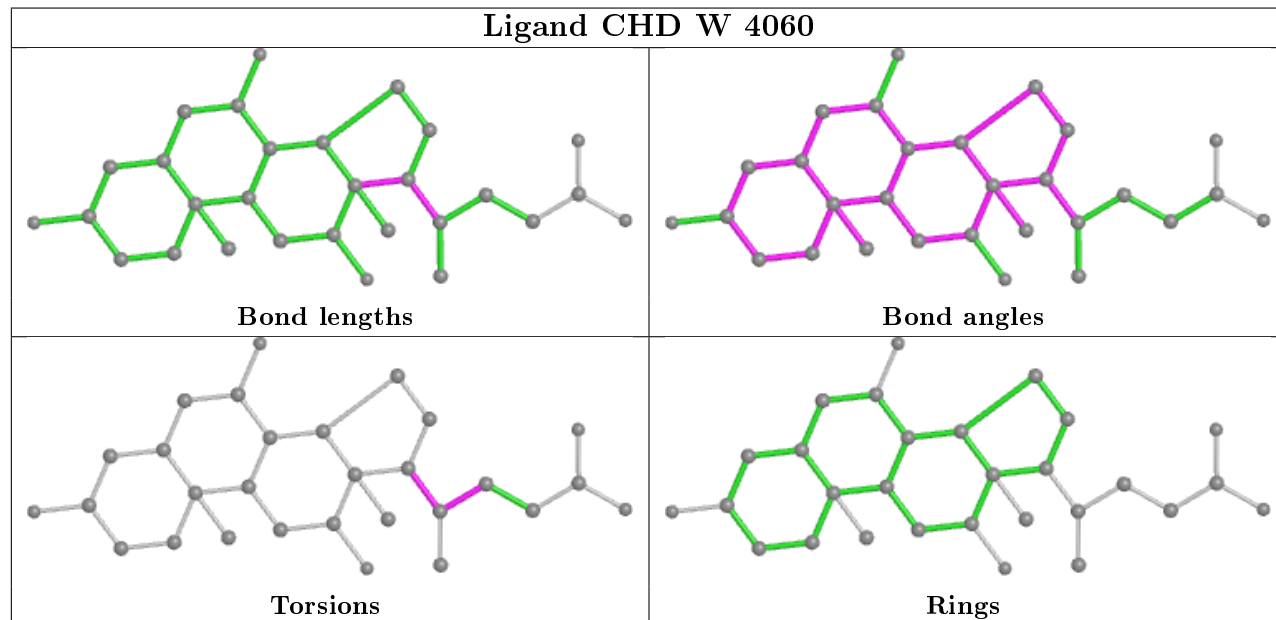


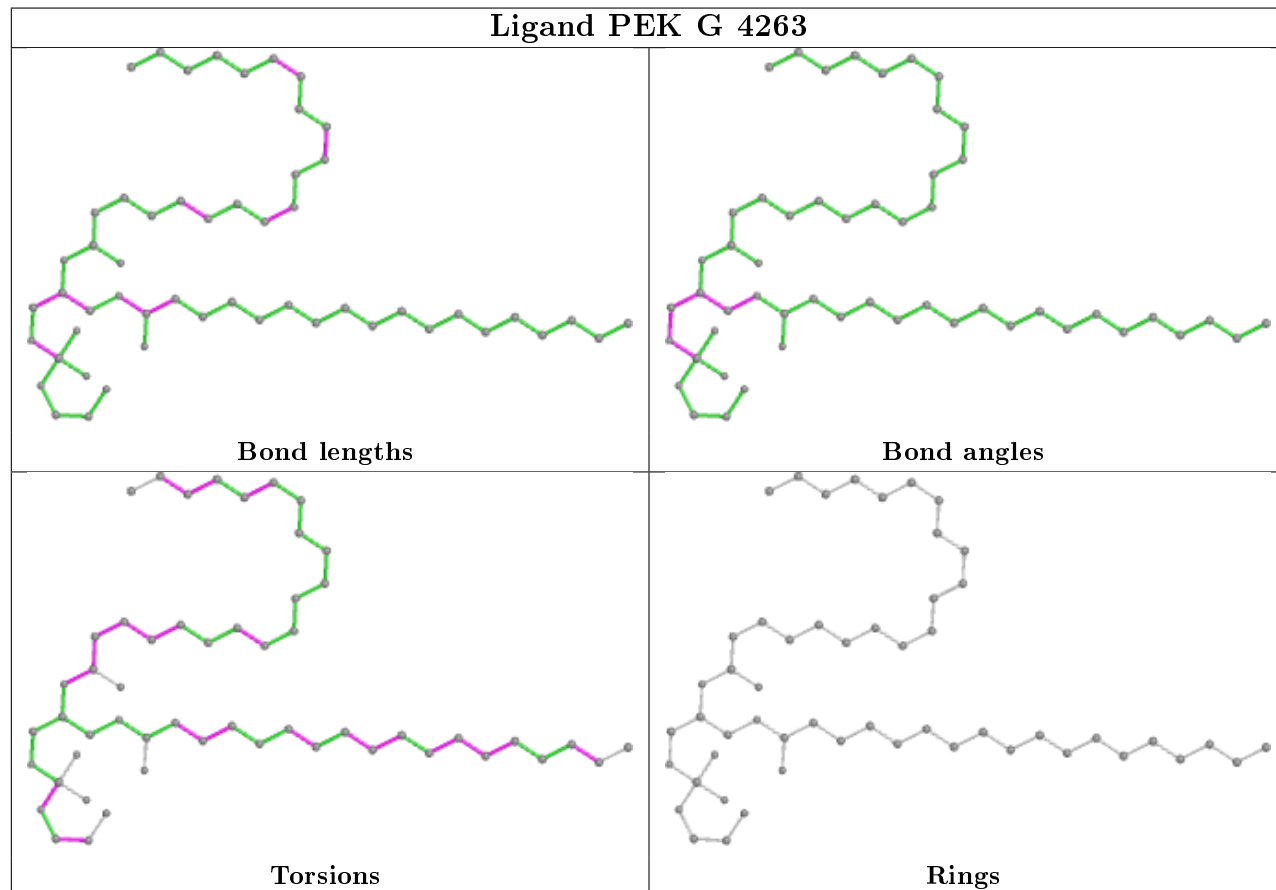
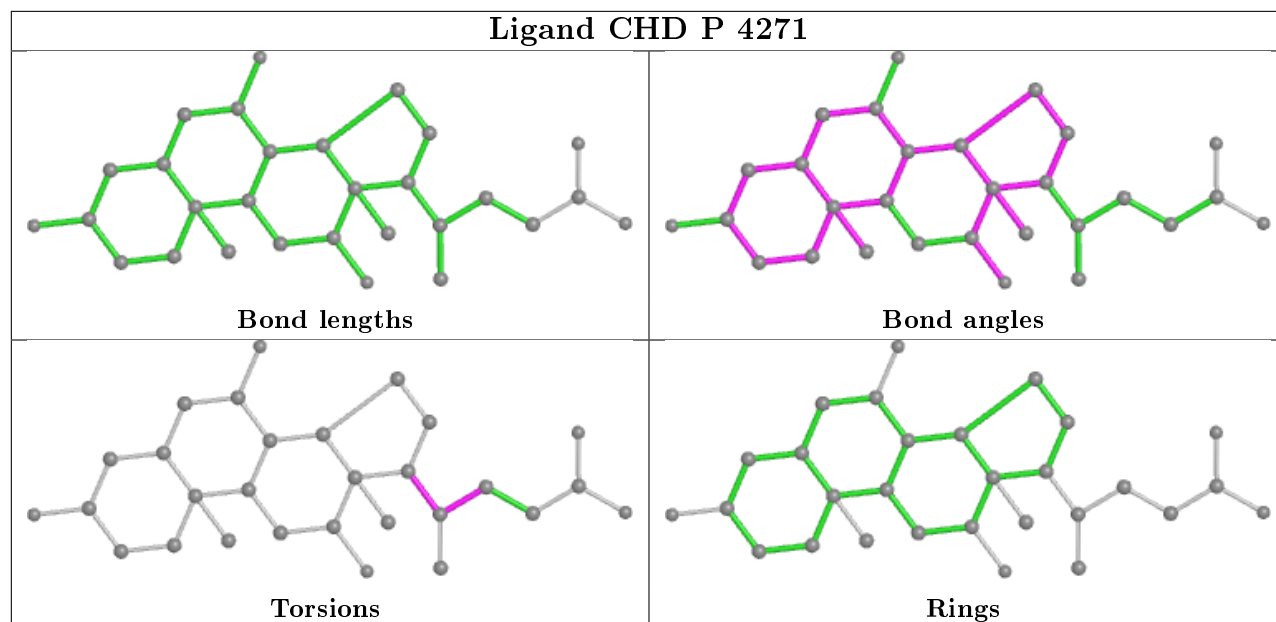


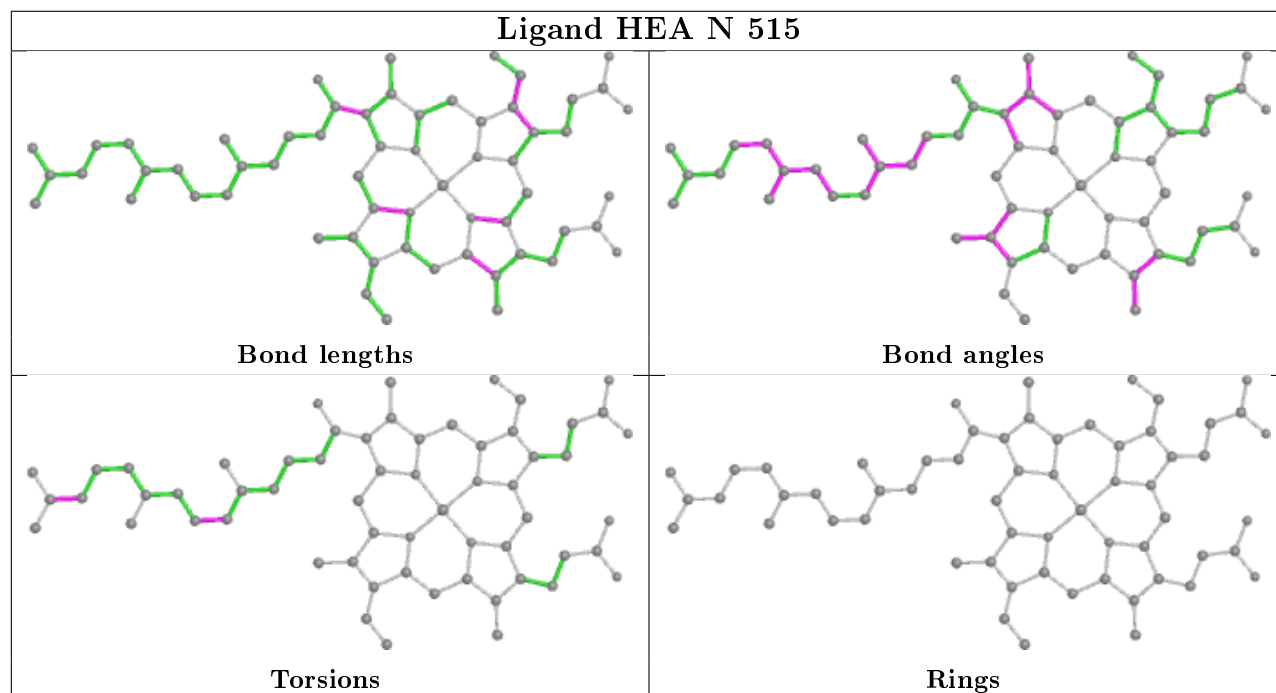
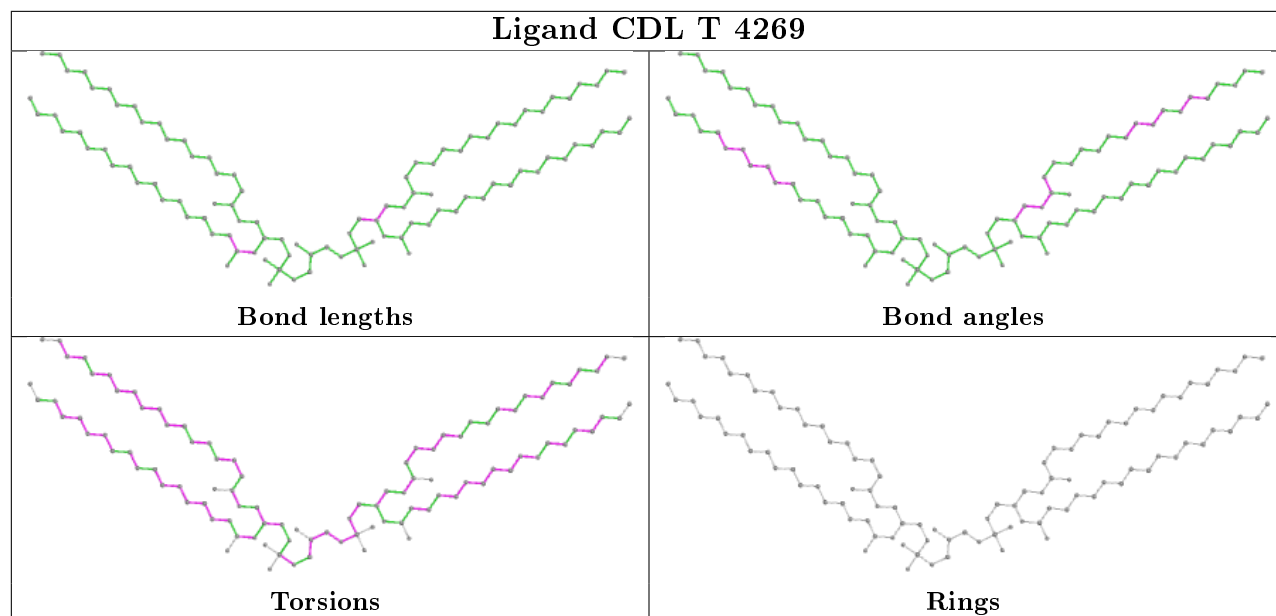
## Ligand CHD J 3060

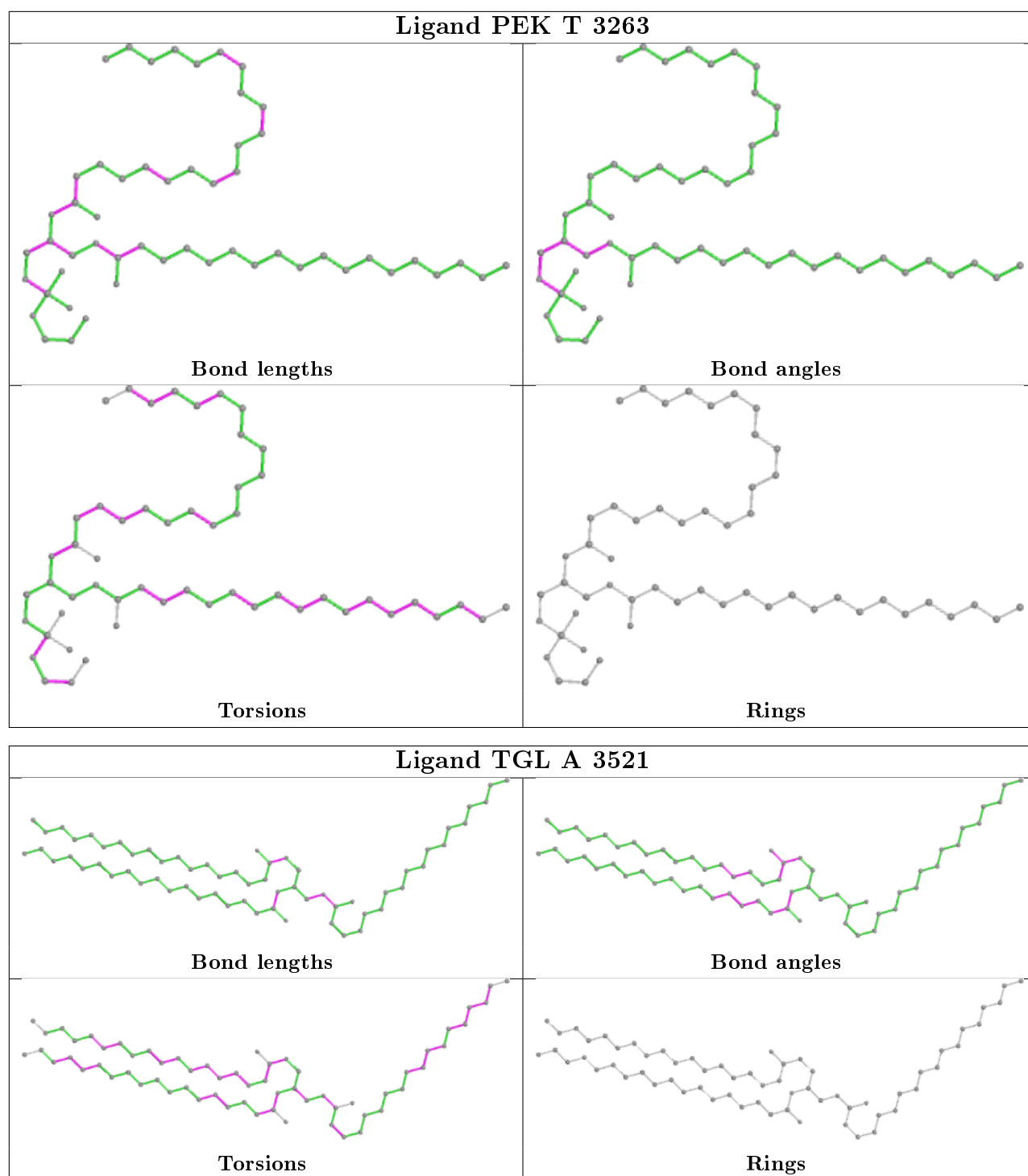


## Ligand CHD W 4060









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.