



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:19 am BST

PDB ID : 3ABM  
Title : Bovine heart cytochrome c oxidase at the fully oxidized state (200-s X-ray exposure dataset)  
Authors : Aoyama, H.; Muramoto, K.; Shinzawa-Itoh, K.; Yamashita, E.; Tsukihara, T.; Ogura, T.; Yoshikawa, S.  
Deposited on : 2009-12-16  
Resolution : 1.95 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) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

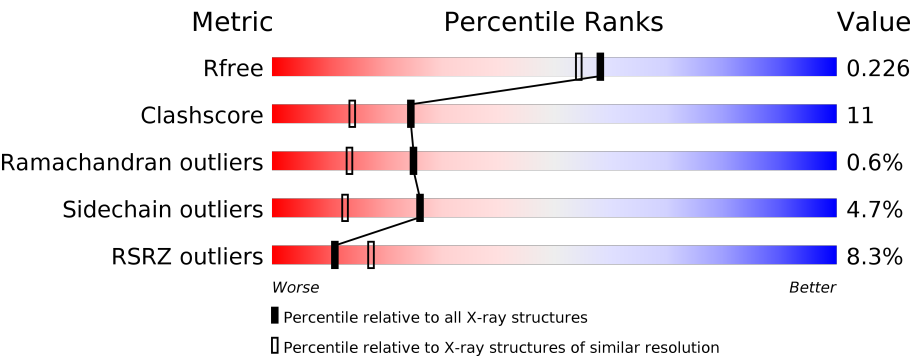
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	514	<div><div>10%</div><div><div></div><div>82%</div><div>16%</div><div>.</div></div></div>
1	N	514	<div><div>7%</div><div><div></div><div>78%</div><div>20%</div><div>.</div></div></div>
2	B	227	<div><div>%</div><div><div></div><div>74%</div><div>22%</div><div>..</div></div></div>
2	O	227	<div><div>3%</div><div><div></div><div>70%</div><div>25%</div><div>..</div></div></div>
3	C	261	<div><div>%</div><div><div></div><div>82%</div><div>16%</div><div>..</div></div></div>
3	P	261	<div><div>3%</div><div><div></div><div>83%</div><div>13%</div><div>...</div></div></div>

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Mol	Chain	Length	Quality of chain
4	D	147	
4	Q	147	
5	E	109	
5	R	109	
6	F	98	
6	S	98	
7	G	85	
7	T	85	
8	H	85	
8	U	85	
9	I	73	
9	V	73	
10	J	59	
10	W	59	
11	K	56	
11	X	56	
12	L	47	
12	Y	47	
13	M	46	
13	Z	46	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	HEA	A	515	X	-	-	-
18	HEA	A	516	X	-	-	-
18	HEA	N	515	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
18	HEA	N	516	X	-	-	-
22	CHD	B	1086	X	-	-	-
22	CHD	C	271	X	-	-	-
22	CHD	J	60	X	-	-	-
22	CHD	P	1271	X	-	-	-
22	CHD	W	1060	X	-	-	-
23	UNX	C	262	-	-	-	X
24	PEK	T	263	-	-	X	-
25	CDL	G	269	-	-	X	-
25	CDL	P	1270	-	-	X	-
26	PSC	E	230	-	-	X	-
28	DMU	G	272	X	-	-	-
28	DMU	M	526	X	-	-	-
28	DMU	P	1272	X	-	-	-
28	DMU	Z	1526	X	-	-	-



## 2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32113 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

- Molecule 5 is a protein called Cytochrome c oxidase subunit 5A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			
5	R	104	Total	C	N	O	S	0	0	0
			842	538	141	161	2			

- Molecule 6 is a protein called Cytochrome c oxidase subunit 5B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	93	Total	C	N	O	S	0	0	0
			717	447	127	138	5			
6	S	93	Total	C	N	O	S	0	0	0
			717	447	127	138	5			

- Molecule 7 is a protein called Cytochrome c oxidase subunit 6A2.

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

- Molecule 8 is a protein called Cytochrome c oxidase subunit 6B1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			
8	U	75	Total	C	N	O	S	0	0	0
			628	395	114	114	5			

- Molecule 9 is a protein called Cytochrome c oxidase subunit 6C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	71	Total	C	N	O	S	0	0	0
			585	381	105	95	4			
9	V	71	Total	C	N	O	S	0	0	0
			585	381	105	95	4			

- Molecule 10 is a protein called Cytochrome c oxidase polypeptide 7A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	W	57	Total	C	N	O	S	0	0	0
			451	291	76	81	3			

- Molecule 11 is a protein called Cytochrome c oxidase subunit 7B.

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 subunit 7C.

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			

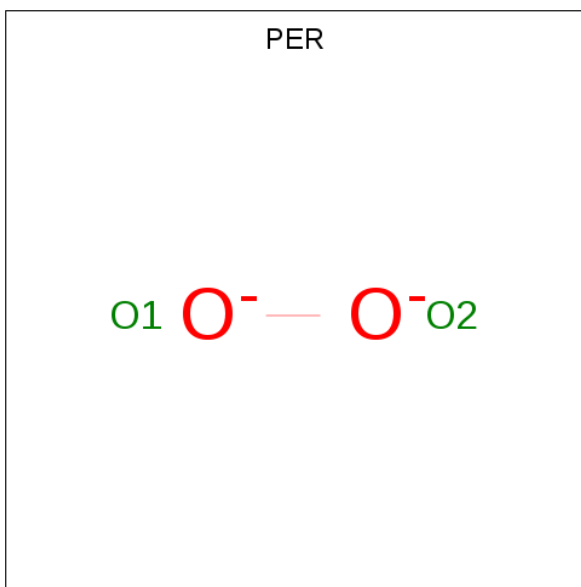
- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B.

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 PEROXIDE ION (three-letter code: PER) (formula: O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	A	1	Total O 2 2	0	0
15	N	1	Total O 2 2	0	0

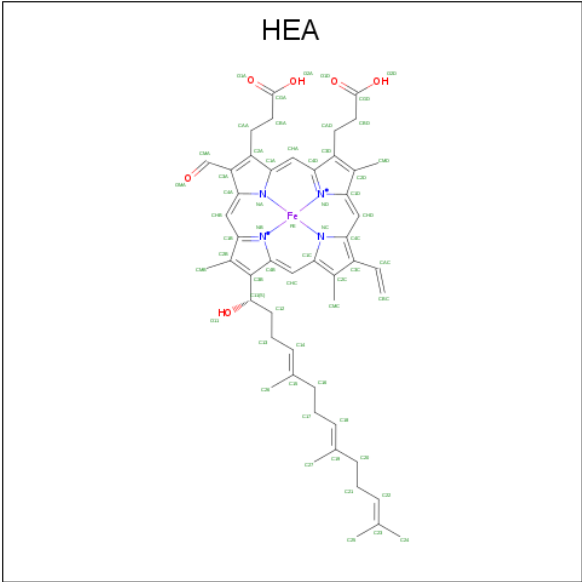
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 17 is SODIUM ION (three-letter code: NA) (formula: Na).

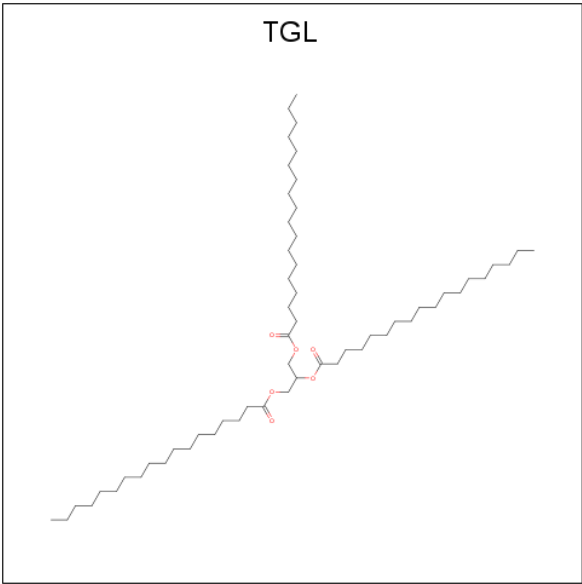
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

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



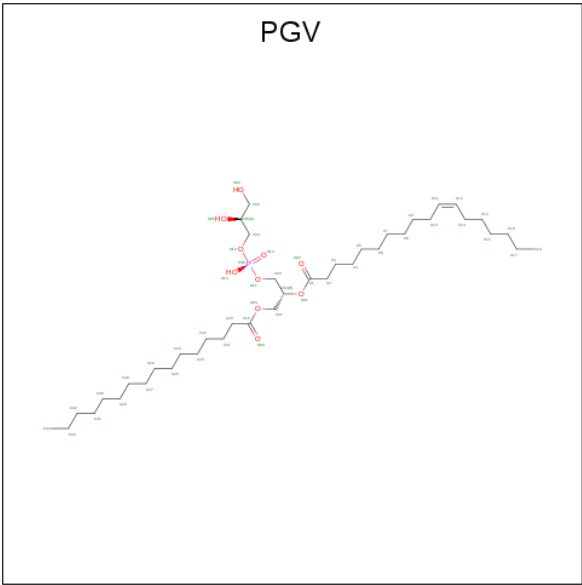
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 19 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
19	A	1	Total	C	O	0	0
			63	57	6		
19	D	1	Total	C	O	0	0
			63	57	6		
19	L	1	Total	C	O	0	0
			63	57	6		
19	O	1	Total	C	O	0	0
			63	57	6		
19	O	1	Total	C	O	0	0
			63	57	6		
19	Y	1	Total	C	O	0	0
			63	57	6		

- Molecule 20 is (1R)-2-{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL (11E)-OCTADEC-11-ENOATE (three-letter code: PGV) (formula: C<sub>40</sub>H<sub>77</sub>O<sub>10</sub>P).



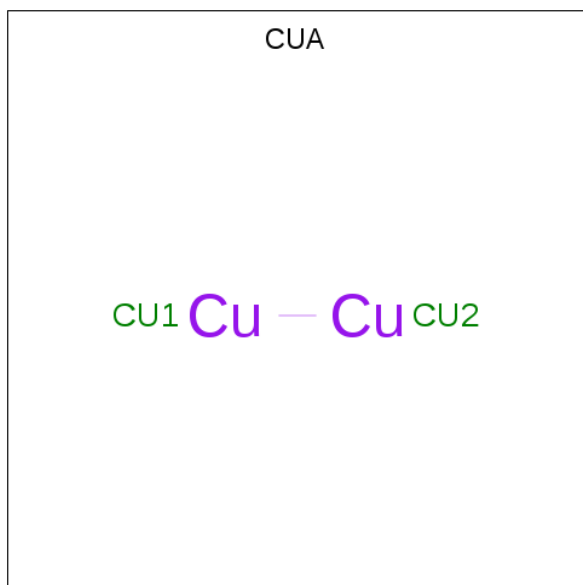
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	H	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		

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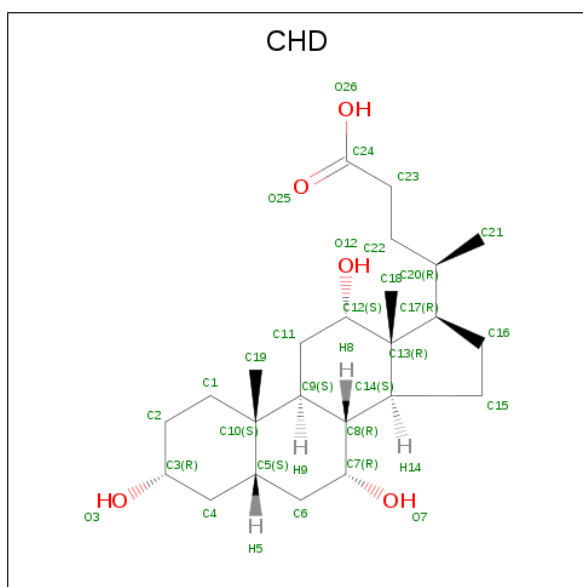
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		

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



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

- Molecule 22 is CHOLIC ACID (three-letter code: CHD) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>5</sub>).



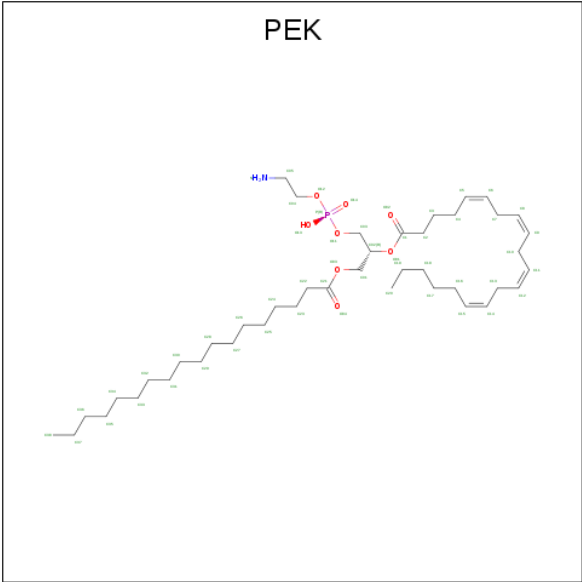
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
22	B	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	C	1	Total C O 29 24 5	0	0
22	J	1	Total C O 29 24 5	0	0
22	O	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	P	1	Total C O 29 24 5	0	0
22	W	1	Total C O 29 24 5	0	0

- Molecule 23 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

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

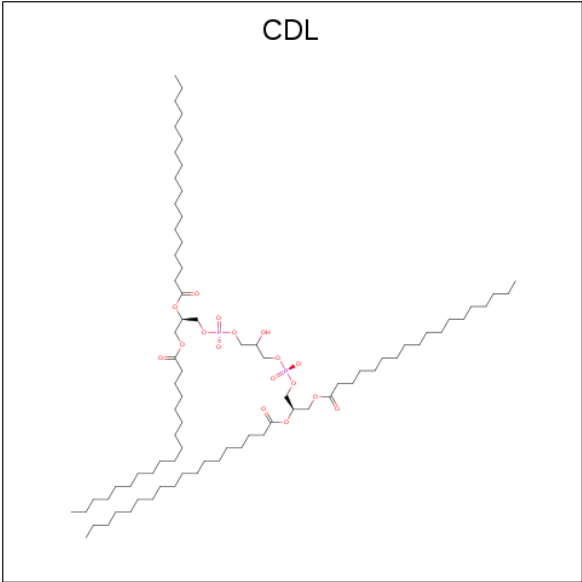
- Molecule 24 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(STEAROYLOXY)METHYL]ETHYL (5E,8E,11E,14E)-ICOSA-5,8,11,14-TETRAENOATE (three-letter code: PEK) (formula: C<sub>43</sub>H<sub>78</sub>NO<sub>8</sub>P).





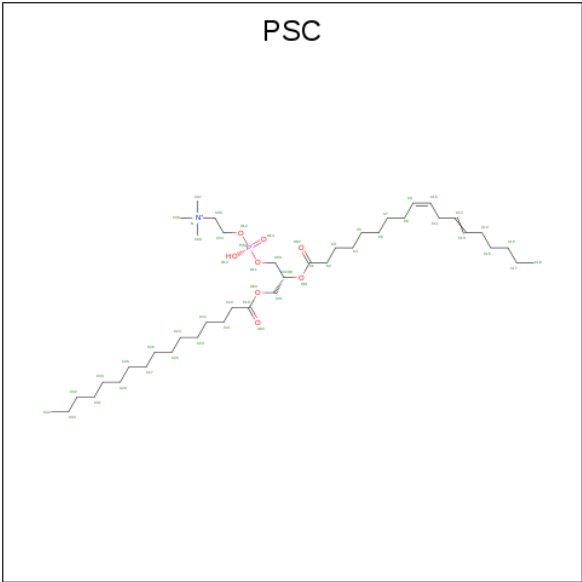
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
24	C	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
24	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 25 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



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

- Molecule 26 is (7R,17E,20E)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY)METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSA-17,20-DIEN-1-AMINIUM 4-OXIDE (three-letter code: PSC) (formula: C<sub>42</sub>H<sub>81</sub>NO<sub>8</sub>P).

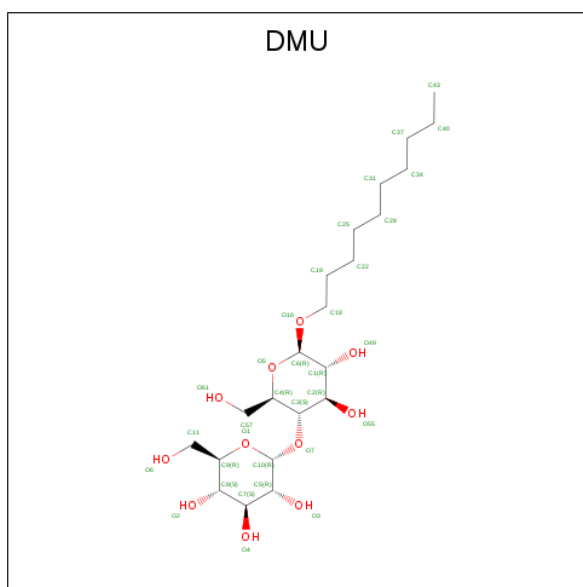


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
26	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
26	R	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

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

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

- Molecule 28 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
28	G	1	Total	C	O	0	0
			33	22	11		
28	M	1	Total	C	O	0	0
			33	22	11		
28	P	1	Total	C	O	0	0
			33	22	11		
28	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 29 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
29	A	203	Total O 203 203	0	0
29	B	131	Total O 131 131	0	0
29	C	90	Total O 90 90	0	0
29	D	96	Total O 96 96	0	0
29	E	62	Total O 62 62	0	0
29	F	70	Total O 70 70	0	0
29	G	41	Total O 41 41	0	0
29	H	46	Total O 46 46	0	0
29	I	44	Total O 44 44	0	0
29	J	17	Total O 17 17	0	0
29	K	22	Total O 22 22	0	0
29	L	23	Total O 23 23	0	0
29	M	19	Total O 19 19	0	0
29	N	196	Total O 196 196	0	0
29	O	106	Total O 106 106	0	0
29	P	89	Total O 89 89	0	0
29	Q	54	Total O 54 54	0	0
29	R	52	Total O 52 52	0	0
29	S	62	Total O 62 62	0	0
29	T	39	Total O 39 39	0	0
29	U	39	Total O 39 39	0	0
29	V	16	Total O 16 16	0	0

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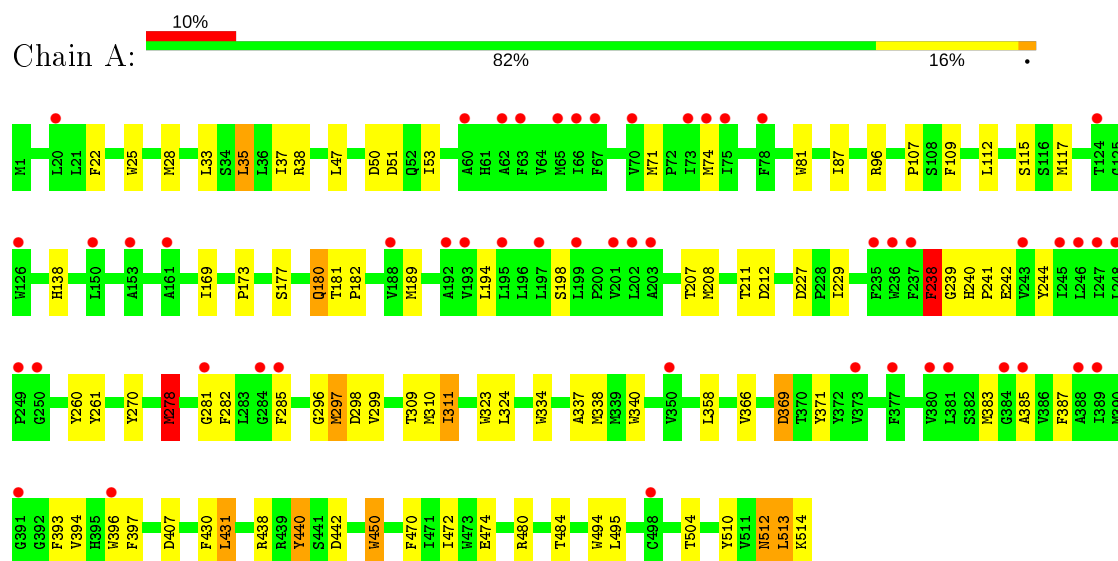
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	W	15	Total 15	O 15	0	0
29	X	16	Total 16	O 16	0	0
29	Y	19	Total 19	O 19	0	0
29	Z	10	Total 10	O 10	0	0

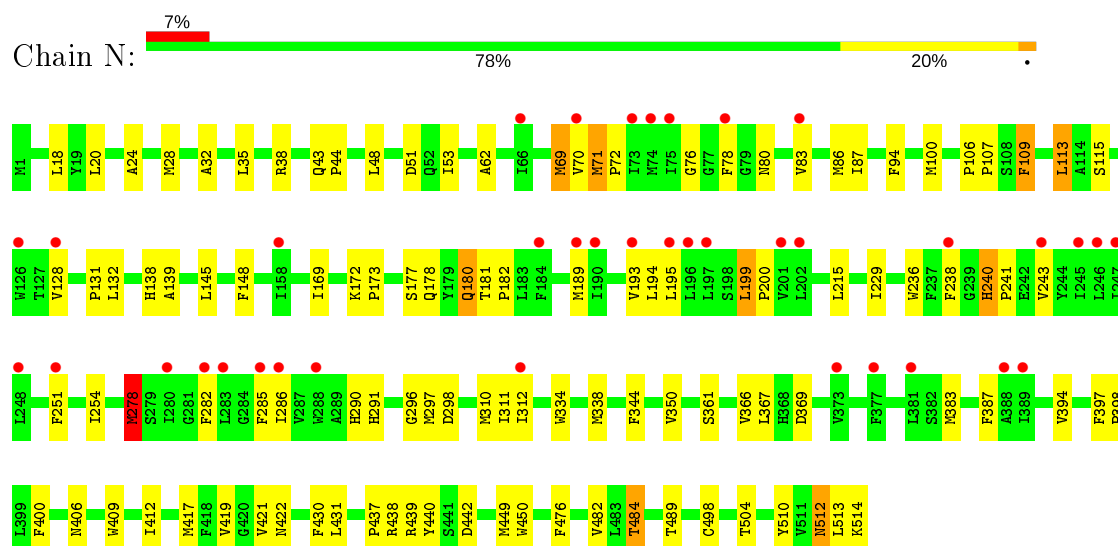
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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.

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

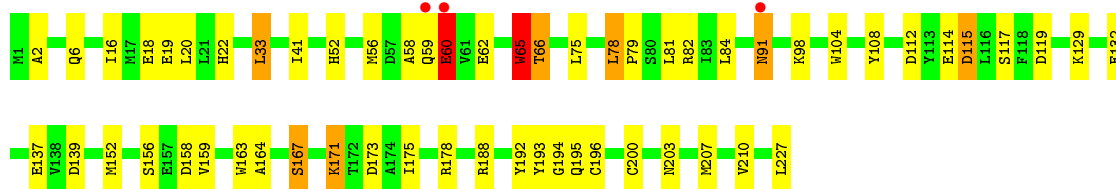


#### • Molecule 1: Cytochrome c oxidase subunit 1

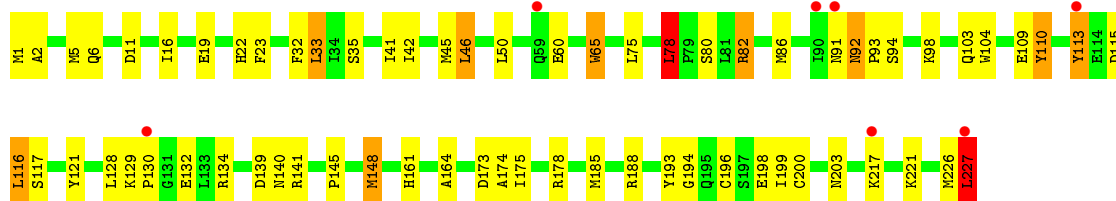


#### • Molecule 2: Cytochrome c oxidase subunit 2

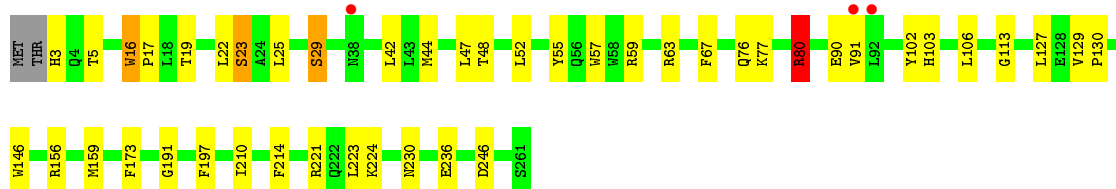
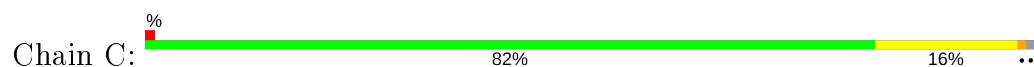




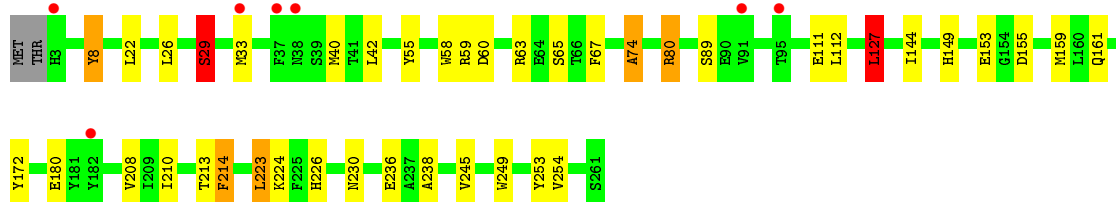
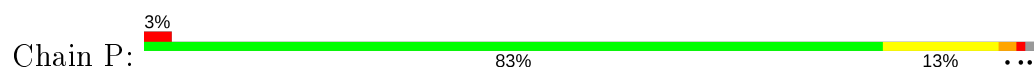
• Molecule 2: Cytochrome c oxidase subunit 2



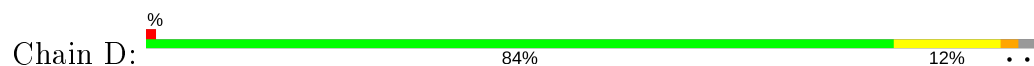
• Molecule 3: Cytochrome c oxidase subunit 3



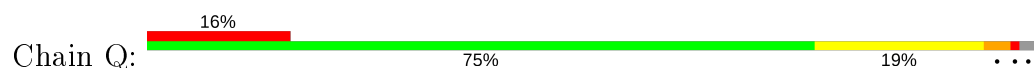
• Molecule 3: Cytochrome c oxidase subunit 3

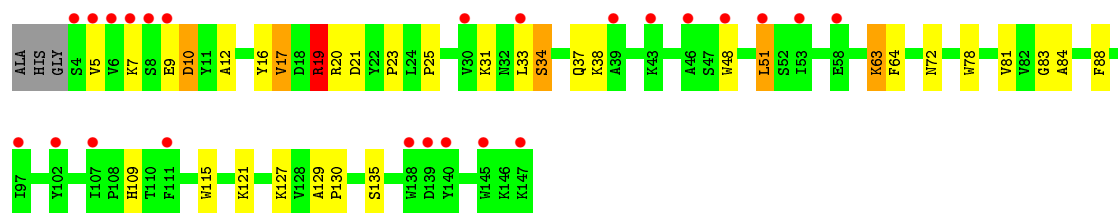


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

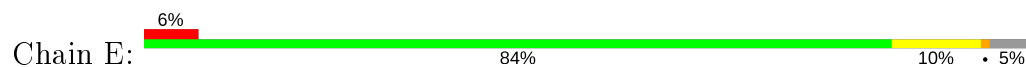


• Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

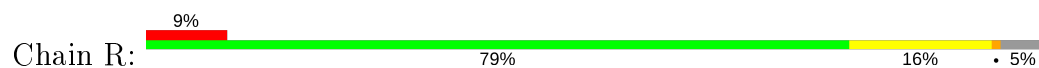




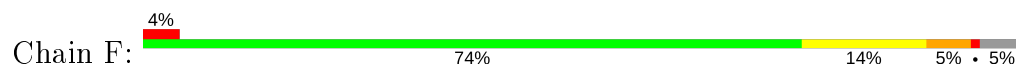
- Molecule 5: Cytochrome c oxidase subunit 5A



- Molecule 5: Cytochrome c oxidase subunit 5A



- Molecule 6: Cytochrome c oxidase subunit 5B



- Molecule 6: Cytochrome c oxidase subunit 5B



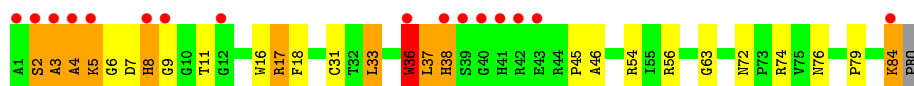
- Molecule 7: Cytochrome c oxidase subunit 6A2



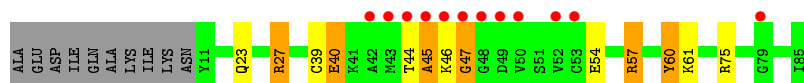
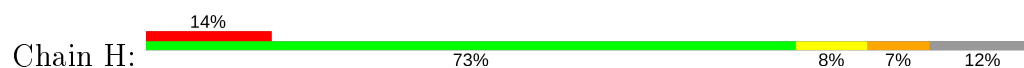
- Molecule 7: Cytochrome c oxidase subunit 6A2



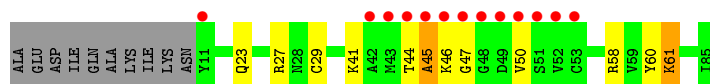
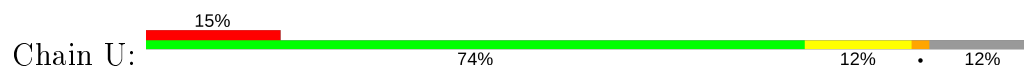




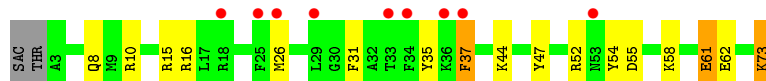
- Molecule 8: Cytochrome c oxidase subunit 6B1



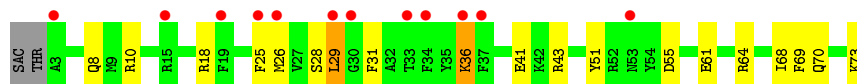
- Molecule 8: Cytochrome c oxidase subunit 6B1



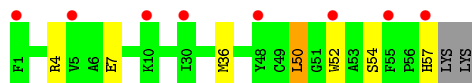
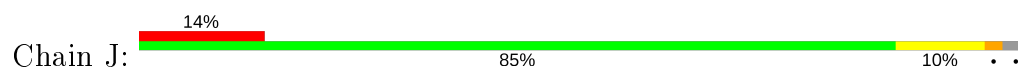
- Molecule 9: Cytochrome c oxidase subunit 6C



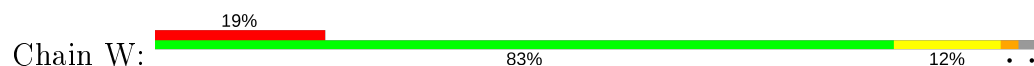
- Molecule 9: Cytochrome c oxidase subunit 6C




- Molecule 10: Cytochrome c oxidase polypeptide 7A1



- Molecule 10: Cytochrome c oxidase polypeptide 7A1




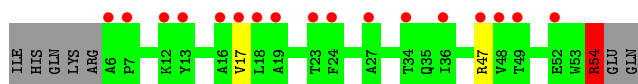
- Molecule 11: Cytochrome c oxidase subunit 7B

Chain K:  79% 9% 13%




- Molecule 11: Cytochrome c oxidase subunit 7B

Chain X:  30% 82% 13%




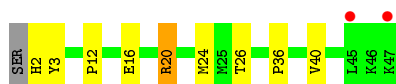
- Molecule 12: Cytochrome c oxidase subunit 7C

Chain L:  4% 79% 17%



- Molecule 12: Cytochrome c oxidase subunit 7C

Chain Y:  4% 79% 17%



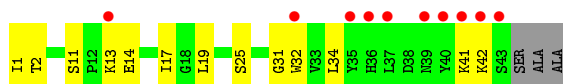
- Molecule 13: Cytochrome c oxidase subunit 8B

Chain M:  13% 67% 20% 7%



- Molecule 13: Cytochrome c oxidase subunit 8B

Chain Z:  22% 65% 28% 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	183.70Å 206.99Å 178.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 1.95 64.10 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-1.95) 96.4 (64.10-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.181 , 0.214 0.196 , 0.226	Depositor DCC
$R_{free}$ test set	16433 reflections (3.48%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.1	Xtriage
Anisotropy	0.394	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 67.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	32113	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.48	26/4156 (0.6%)	1.30	34/5678 (0.6%)
1	N	1.34	13/4156 (0.3%)	1.18	22/5678 (0.4%)
2	B	1.37	10/1860 (0.5%)	1.29	12/2534 (0.5%)
2	O	1.19	9/1860 (0.5%)	1.16	11/2534 (0.4%)
3	C	1.31	8/2197 (0.4%)	1.19	12/3005 (0.4%)
3	P	1.34	13/2197 (0.6%)	1.11	10/3005 (0.3%)
4	D	1.37	5/1229 (0.4%)	1.32	10/1658 (0.6%)
4	Q	1.07	3/1229 (0.2%)	1.08	4/1658 (0.2%)
5	E	1.20	3/860 (0.3%)	1.13	4/1167 (0.3%)
5	R	1.06	0/860	0.99	2/1167 (0.2%)
6	F	1.30	2/733 (0.3%)	1.16	2/996 (0.2%)
6	S	1.28	2/733 (0.3%)	1.29	7/996 (0.7%)
7	G	1.27	2/690 (0.3%)	1.10	3/937 (0.3%)
7	T	1.29	3/690 (0.4%)	1.22	4/937 (0.4%)
8	H	1.27	0/648	1.13	3/877 (0.3%)
8	U	1.03	0/648	0.99	0/877
9	I	1.23	3/598 (0.5%)	1.12	2/792 (0.3%)
9	V	1.09	1/598 (0.2%)	1.00	1/792 (0.1%)
10	J	1.10	0/462	1.04	1/625 (0.2%)
10	W	1.01	0/462	0.94	1/625 (0.2%)
11	K	1.30	1/398 (0.3%)	1.09	0/546
11	X	0.93	0/398	0.97	1/546 (0.2%)
12	L	1.41	2/393 (0.5%)	1.13	1/526 (0.2%)
12	Y	1.19	0/393	0.98	0/526
13	M	1.32	1/345 (0.3%)	1.15	1/470 (0.2%)
13	Z	0.92	0/345	0.95	0/470
All	All	1.29	107/29138 (0.4%)	1.17	148/39622 (0.4%)

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
6	S	0	2

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	S	54	ASN	CB-CG	-10.95	1.25	1.51
1	A	270	TYR	CD1-CE1	9.75	1.53	1.39
4	D	17	VAL	CB-CG1	-9.37	1.33	1.52
1	A	396	TRP	CE3-CZ3	9.08	1.53	1.38
1	A	371	TYR	CD1-CE1	8.87	1.52	1.39
7	T	36	TRP	CB-CG	8.51	1.65	1.50
3	P	29	SER	CB-OG	-8.36	1.31	1.42
1	A	371	TYR	CD2-CE2	8.16	1.51	1.39
3	P	214	PHE	CD1-CE1	7.77	1.54	1.39
2	B	200	CYS	CB-SG	7.66	1.95	1.82
1	A	440	TYR	CE1-CZ	7.55	1.48	1.38
3	C	29	SER	CB-OG	-7.41	1.32	1.42
1	A	393	PHE	CE1-CZ	7.39	1.51	1.37
3	P	253	TYR	CD2-CE2	7.38	1.50	1.39
3	P	172	TYR	CD1-CE1	7.27	1.50	1.39
1	A	494	TRP	CZ3-CH2	7.26	1.51	1.40
7	G	36	TRP	CB-CG	7.19	1.63	1.50
3	P	236	GLU	CG-CD	-6.99	1.41	1.51
2	O	200	CYS	CB-SG	6.93	1.94	1.82
13	M	4	LYS	CB-CG	-6.92	1.33	1.52
7	T	5	LYS	CB-CG	6.85	1.71	1.52
6	F	31	TYR	CE1-CZ	6.78	1.47	1.38
3	P	238	ALA	CA-CB	6.72	1.66	1.52
9	I	61	GLU	CG-CD	-6.68	1.42	1.51
3	C	236	GLU	CG-CD	-6.55	1.42	1.51
1	A	261	TYR	CZ-OH	6.51	1.49	1.37
2	B	19	GLU	CB-CG	-6.50	1.39	1.52
2	O	110	TYR	CD1-CE1	6.43	1.49	1.39
11	K	20	SER	CB-OG	-6.39	1.33	1.42
1	A	260	TYR	CE2-CZ	6.36	1.46	1.38
7	G	5	LYS	CB-CG	6.33	1.69	1.52
2	O	198	GLU	C-O	6.33	1.35	1.23
1	N	298	ASP	CB-CG	6.32	1.65	1.51
3	P	180	GLU	CD-OE1	6.21	1.32	1.25
1	A	474	GLU	CB-CG	6.19	1.64	1.52
4	Q	121	LYS	CE-NZ	6.11	1.64	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	8	TYR	CD1-CE1	6.09	1.48	1.39
3	P	89	SER	CB-OG	6.06	1.50	1.42
5	E	61	PHE	CE2-CZ	6.05	1.48	1.37
2	O	19	GLU	CB-CG	-6.05	1.40	1.52
12	L	35	ALA	CA-CB	6.04	1.65	1.52
12	L	40	VAL	CB-CG2	-5.97	1.40	1.52
1	A	81	TRP	CE3-CZ3	5.95	1.48	1.38
1	A	239	GLY	C-O	5.91	1.33	1.23
2	B	98	LYS	CD-CE	5.88	1.66	1.51
2	B	115	ASP	CB-CG	5.87	1.64	1.51
1	A	242	GLU	CG-CD	5.81	1.60	1.51
1	N	195	LEU	C-O	5.80	1.34	1.23
6	F	71	TRP	CB-CG	5.79	1.60	1.50
3	P	236	GLU	CB-CG	-5.79	1.41	1.52
1	N	78	PHE	CD1-CE1	5.78	1.50	1.39
3	P	74	ALA	CA-CB	5.78	1.64	1.52
1	A	261	TYR	CD1-CE1	5.78	1.48	1.39
1	A	189	MET	CB-CG	5.75	1.69	1.51
5	E	70	VAL	CB-CG2	5.74	1.65	1.52
4	Q	16	TYR	CD1-CE1	5.74	1.48	1.39
9	I	47	TYR	CD1-CE1	5.67	1.47	1.39
5	E	9	GLU	CG-CD	5.64	1.60	1.51
4	D	19	ARG	CZ-NH2	5.62	1.40	1.33
1	A	244	TYR	CD2-CE2	5.60	1.47	1.39
3	C	90	GLU	CB-CG	-5.59	1.41	1.52
4	D	58	GLU	CD-OE1	5.58	1.31	1.25
1	A	323	TRP	CB-CG	5.54	1.60	1.50
1	A	261	TYR	CE2-CZ	5.52	1.45	1.38
2	B	18	GLU	CG-CD	5.51	1.60	1.51
7	T	17	ARG	CD-NE	-5.50	1.37	1.46
1	A	470	PHE	CD1-CE1	5.47	1.50	1.39
1	N	251	PHE	CE2-CZ	5.43	1.47	1.37
1	N	148	PHE	CD1-CE1	5.42	1.50	1.39
3	C	16	TRP	CB-CG	5.40	1.59	1.50
2	O	196	CYS	CB-SG	5.40	1.91	1.82
2	B	156	SER	CA-CB	5.39	1.61	1.52
1	N	94	PHE	CE2-CZ	5.38	1.47	1.37
9	I	54	TYR	CD2-CE2	5.37	1.47	1.39
1	N	193	VAL	CB-CG1	5.35	1.64	1.52
2	O	113	TYR	CD2-CE2	5.35	1.47	1.39
2	O	65	TRP	CB-CG	-5.34	1.40	1.50
1	N	236	TRP	CB-CG	5.34	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	159	VAL	CB-CG2	5.34	1.64	1.52
2	B	192	TYR	CE2-CZ	5.33	1.45	1.38
2	B	167	SER	CB-OG	-5.33	1.35	1.42
3	P	236	GLU	CD-OE1	-5.28	1.19	1.25
1	A	450	TRP	CB-CG	5.27	1.59	1.50
1	A	385	ALA	CA-CB	5.25	1.63	1.52
3	C	57	TRP	CB-CG	5.25	1.59	1.50
3	C	102	TYR	CB-CG	5.24	1.59	1.51
4	D	11	TYR	CB-CG	5.24	1.59	1.51
4	D	58	GLU	CD-OE2	5.23	1.31	1.25
1	N	128	VAL	N-CA	5.22	1.56	1.46
3	C	197	PHE	CE1-CZ	5.20	1.47	1.37
1	A	297	MET	CB-CG	5.19	1.68	1.51
1	N	476	PHE	CD1-CE1	5.19	1.49	1.39
1	N	419	VAL	CA-CB	5.16	1.65	1.54
2	B	163	TRP	CB-CG	5.15	1.59	1.50
1	N	139	ALA	CA-CB	5.14	1.63	1.52
1	A	22	PHE	CD2-CE2	5.12	1.49	1.39
3	C	113	GLY	C-O	-5.10	1.15	1.23
6	S	92	VAL	CB-CG2	-5.09	1.42	1.52
1	A	340	TRP	CE3-CZ3	5.08	1.47	1.38
2	O	35	SER	CB-OG	-5.07	1.35	1.42
1	A	324	LEU	N-CA	5.05	1.56	1.46
9	V	51	TYR	CD2-CE2	5.04	1.47	1.39
4	Q	81	VAL	CB-CG1	5.02	1.63	1.52
3	P	172	TYR	CD2-CE2	5.01	1.46	1.39
1	A	397	PHE	CG-CD1	5.01	1.46	1.38
1	N	83	VAL	CB-CG2	5.00	1.63	1.52
2	O	121	TYR	CB-CG	-5.00	1.44	1.51

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	80	ARG	NE-CZ-NH2	-17.04	111.78	120.30
4	D	20	ARG	NE-CZ-NH2	-16.31	112.14	120.30
4	Q	20	ARG	NE-CZ-NH1	14.03	127.31	120.30
4	D	20	ARG	NE-CZ-NH1	13.62	127.11	120.30
4	D	19	ARG	NE-CZ-NH1	-13.50	113.55	120.30
4	Q	20	ARG	NE-CZ-NH2	-13.39	113.60	120.30
3	C	80	ARG	NE-CZ-NH1	12.82	126.71	120.30
1	A	310	MET	CG-SD-CE	-11.74	81.42	100.20
7	T	17	ARG	NE-CZ-NH2	-10.91	114.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	90	ARG	NE-CZ-NH2	-10.48	115.06	120.30
2	B	188	ARG	NE-CZ-NH2	-10.35	115.12	120.30
4	D	19	ARG	NE-CZ-NH2	9.81	125.20	120.30
1	A	35	LEU	CA-CB-CG	-9.53	93.39	115.30
5	E	90	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	N	71	MET	CG-SD-CE	-9.35	85.24	100.20
1	A	117	MET	CG-SD-CE	-9.28	85.35	100.20
7	T	33	LEU	CA-CB-CG	8.88	135.72	115.30
3	C	156	ARG	NE-CZ-NH1	-8.86	115.87	120.30
1	N	278	MET	CG-SD-CE	-8.28	86.95	100.20
2	O	11	ASP	CB-CG-OD2	8.27	125.75	118.30
1	A	227	ASP	CB-CG-OD2	8.17	125.65	118.30
2	B	139	ASP	CB-CG-OD2	8.06	125.55	118.30
3	P	80	ARG	CG-CD-NE	-7.76	95.51	111.80
1	A	512	ASN	CB-CA-C	-7.70	95.00	110.40
1	N	286	ILE	CG1-CB-CG2	-7.61	94.67	111.40
1	A	278	MET	CG-SD-CE	-7.60	88.05	100.20
1	A	438	ARG	NE-CZ-NH1	-7.51	116.55	120.30
1	A	33	LEU	CB-CG-CD1	-7.47	98.31	111.00
1	A	480	ARG	NE-CZ-NH1	7.43	124.02	120.30
1	A	71	MET	CG-SD-CE	-7.38	88.39	100.20
1	A	442	ASP	CB-CG-OD2	7.28	124.85	118.30
1	N	298	ASP	CB-CG-OD2	7.15	124.73	118.30
12	L	41	ARG	NE-CZ-NH1	7.14	123.87	120.30
9	I	73	LYS	CD-CE-NZ	-7.01	95.58	111.70
1	N	51	ASP	CB-CG-OD2	6.98	124.58	118.30
3	C	29	SER	CB-CA-C	-6.94	96.92	110.10
8	H	27	ARG	NE-CZ-NH1	6.88	123.74	120.30
8	H	75	ARG	NE-CZ-NH1	-6.87	116.86	120.30
1	A	208	MET	CG-SD-CE	6.84	111.14	100.20
3	C	221	ARG	NE-CZ-NH1	-6.82	116.89	120.30
6	S	54	ASN	CB-CA-C	-6.66	97.07	110.40
2	B	171	LYS	CD-CE-NZ	-6.65	96.41	111.70
3	C	80	ARG	CG-CD-NE	-6.62	97.90	111.80
3	P	127	LEU	CA-CB-CG	6.62	130.52	115.30
2	B	173	ASP	CB-CG-OD1	6.58	124.23	118.30
2	O	188	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	227	ASP	CB-CG-OD1	-6.57	112.39	118.30
3	P	214	PHE	CB-CG-CD1	6.52	125.36	120.80
2	B	82	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	N	366	VAL	CG1-CB-CG2	-6.42	100.62	110.90
1	A	96	ARG	NE-CZ-NH2	-6.38	117.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	50	LEU	CB-CG-CD1	-6.32	100.26	111.00
1	A	442	ASP	CB-CG-OD1	-6.28	112.65	118.30
3	C	236	GLU	CA-CB-CG	-6.26	99.62	113.40
6	S	25	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	51	ASP	CB-CG-OD2	6.25	123.92	118.30
9	V	55	ASP	CB-CG-OD1	6.25	123.92	118.30
11	X	54	ARG	NE-CZ-NH1	-6.24	117.18	120.30
2	B	152	MET	CG-SD-CE	6.22	110.15	100.20
1	N	310	MET	CG-SD-CE	-6.22	90.25	100.20
2	B	65	TRP	CB-CA-C	6.21	122.82	110.40
1	N	278	MET	CA-CB-CG	-6.21	102.75	113.30
1	A	278	MET	CA-CB-CG	-6.09	102.95	113.30
3	P	80	ARG	NE-CZ-NH1	-6.08	117.26	120.30
3	C	156	ARG	NE-CZ-NH2	6.05	123.32	120.30
1	N	512	ASN	CB-CA-C	-6.01	98.38	110.40
3	C	214	PHE	CB-CG-CD1	5.98	124.99	120.80
3	P	223	LEU	CB-CG-CD1	-5.97	100.84	111.00
2	O	227	LEU	CB-CG-CD1	-5.94	100.90	111.00
6	S	56	ARG	NE-CZ-NH1	-5.90	117.35	120.30
3	C	214	PHE	CB-CG-CD2	-5.90	116.67	120.80
7	G	8	HIS	N-CA-C	5.88	126.86	111.00
1	A	298	ASP	CB-CG-OD2	5.87	123.58	118.30
1	N	28	MET	CG-SD-CE	5.86	109.58	100.20
9	I	55	ASP	CB-CG-OD2	-5.86	113.03	118.30
2	B	139	ASP	CB-CG-OD1	-5.84	113.04	118.30
3	P	214	PHE	CB-CG-CD2	-5.84	116.71	120.80
1	A	513	LEU	CB-CG-CD1	-5.82	101.11	111.00
6	S	94	HIS	N-CA-C	5.82	126.71	111.00
3	P	127	LEU	CB-CG-CD1	5.79	120.83	111.00
2	B	178	ARG	NE-CZ-NH2	5.78	123.19	120.30
6	S	53	THR	CB-CA-C	-5.77	96.03	111.60
4	D	59	LEU	CB-CG-CD2	-5.76	101.21	111.00
2	B	119	ASP	CB-CG-OD2	5.72	123.45	118.30
1	N	169	ILE	CB-CA-C	-5.70	100.19	111.60
1	N	189	MET	CA-CB-CG	-5.68	103.65	113.30
2	B	112	ASP	CB-CG-OD2	-5.67	113.19	118.30
6	S	65	ASP	CB-CG-OD2	5.65	123.38	118.30
1	A	212	ASP	CB-CG-OD2	5.60	123.34	118.30
4	D	51	LEU	CA-CB-CG	5.60	128.17	115.30
3	C	44	MET	CG-SD-CE	5.59	109.15	100.20
1	A	50	ASP	CB-CG-OD1	5.59	123.33	118.30
1	N	199	LEU	CB-CG-CD1	-5.58	101.51	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	21	ASP	CB-CG-OD2	5.58	123.32	118.30
3	C	47	LEU	CB-CG-CD1	-5.57	101.54	111.00
1	N	498	CYS	CA-CB-SG	-5.56	103.99	114.00
4	Q	19	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	A	407	ASP	CB-CG-OD2	5.56	123.30	118.30
5	R	36	LEU	CB-CG-CD2	-5.54	101.58	111.00
7	G	54	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	N	240	HIS	N-CA-CB	5.52	120.53	110.60
1	A	35	LEU	CB-CG-CD1	5.51	120.37	111.00
2	O	185	MET	CG-SD-CE	5.51	109.02	100.20
4	D	17	VAL	CB-CA-C	-5.51	100.94	111.40
2	O	82	ARG	NE-CZ-NH2	-5.48	117.56	120.30
6	S	45	ASP	CB-CG-OD1	-5.47	113.38	118.30
5	E	21	LYS	CD-CE-NZ	-5.47	99.12	111.70
6	F	18	ARG	NE-CZ-NH2	-5.44	117.58	120.30
7	T	56	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	A	358	LEU	CB-CG-CD2	-5.39	101.83	111.00
3	P	60	ASP	CB-CG-OD1	5.38	123.14	118.30
2	O	173	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	311	ILE	CG1-CB-CG2	-5.34	99.66	111.40
2	O	65	TRP	CB-CA-C	5.33	121.06	110.40
1	N	100	MET	CG-SD-CE	5.32	108.71	100.20
1	N	312	ILE	CG1-CB-CG2	-5.31	99.72	111.40
5	R	40	ASP	CB-CG-OD2	5.31	123.08	118.30
2	B	98	LYS	CD-CE-NZ	-5.31	99.50	111.70
5	E	90	ARG	CG-CD-NE	-5.30	100.66	111.80
1	N	113	LEU	CB-CG-CD2	5.29	120.00	111.00
4	D	13	LEU	CB-CG-CD1	-5.28	102.02	111.00
1	A	495	LEU	CB-CG-CD2	-5.28	102.03	111.00
10	W	50	LEU	CA-CB-CG	5.26	127.41	115.30
7	T	5	LYS	CB-CA-C	5.25	120.91	110.40
1	A	74	MET	CB-CG-SD	-5.23	96.70	112.40
1	A	238	PHE	CD1-CE1-CZ	-5.23	113.82	120.10
10	J	36	MET	CG-SD-CE	-5.22	91.85	100.20
8	H	57	ARG	NE-CZ-NH1	5.18	122.89	120.30
7	G	54	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	366	VAL	CG1-CB-CG2	-5.17	102.62	110.90
1	N	442	ASP	CB-CG-OD2	5.17	122.95	118.30
4	Q	17	VAL	CG1-CB-CG2	-5.15	102.67	110.90
1	N	367	LEU	CB-CG-CD2	-5.14	102.26	111.00
6	F	93	PRO	C-N-CA	5.13	134.52	121.70
2	O	78	LEU	CB-CG-CD1	5.12	119.71	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	29	SER	CB-CA-C	-5.12	100.36	110.10
1	A	431	LEU	CA-CB-CG	-5.08	103.61	115.30
1	A	270	TYR	CG-CD1-CE1	-5.07	117.25	121.30
1	A	369	ASP	CB-CG-OD2	5.07	122.86	118.30
13	M	19	LEU	CB-CG-CD2	-5.07	102.39	111.00
3	P	155	ASP	CB-CG-OD1	5.07	122.86	118.30
2	O	178	ARG	NE-CZ-NH1	5.06	122.83	120.30
2	O	46	LEU	CB-CG-CD1	-5.04	102.42	111.00
1	N	69	MET	CG-SD-CE	5.04	108.26	100.20
1	N	145	LEU	CB-CG-CD2	-5.02	102.47	111.00
1	A	244	TYR	CA-CB-CG	-5.02	103.87	113.40
4	D	125	ASP	CB-CG-OD2	5.02	122.81	118.30
1	A	169	ILE	CB-CA-C	-5.00	101.60	111.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	S	93	PRO	Peptide
6	S	95	GLN	Peptide

## 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	47	0
1	N	4027	0	4001	75	0
2	B	1824	0	1833	28	0
2	O	1824	0	1833	45	0
3	C	2110	0	2027	37	0
3	P	2110	0	2027	32	0
4	D	1195	0	1183	21	0
4	Q	1195	0	1183	27	0
5	E	842	0	838	5	0
5	R	842	0	838	10	0
6	F	717	0	700	16	0
6	S	717	0	700	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	675	0	643	38	0
7	T	675	0	643	45	0
8	H	628	0	580	9	0
8	U	628	0	580	8	0
9	I	585	0	597	13	0
9	V	585	0	597	15	0
10	J	451	0	446	5	0
10	W	451	0	446	6	0
11	K	384	0	366	1	0
11	X	384	0	366	5	0
12	L	380	0	380	11	0
12	Y	380	0	380	10	0
13	M	335	0	352	6	0
13	Z	335	0	352	11	0
14	A	1	0	0	0	0
14	N	1	0	0	0	0
15	A	2	0	0	1	0
15	N	2	0	0	1	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	1	0
17	N	1	0	0	0	0
18	A	120	0	108	11	0
18	N	120	0	108	14	0
19	A	63	0	110	13	0
19	D	63	0	110	9	0
19	L	63	0	110	15	0
19	O	126	0	220	23	0
19	Y	63	0	110	18	0
20	A	102	0	152	8	0
20	C	51	0	76	4	0
20	H	51	0	76	3	0
20	N	153	0	228	12	0
20	P	51	0	76	11	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	29	0	36	2	0
22	C	58	0	70	5	0
22	J	29	0	36	1	0
22	O	29	0	36	0	0
22	P	58	0	71	1	0
22	W	29	0	36	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	C	1	0	0	0	0
23	P	1	0	0	0	0
24	C	53	0	77	7	0
24	G	106	0	154	31	0
24	P	53	0	77	7	0
24	T	106	0	154	30	0
25	C	100	0	156	19	0
25	G	100	0	156	27	0
25	P	100	0	156	24	0
25	T	100	0	156	19	0
26	E	52	0	80	22	0
26	R	52	0	80	15	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	33	0	38	5	0
28	M	33	0	39	0	0
28	P	33	0	40	1	0
28	Z	33	0	38	3	0
29	A	203	0	0	3	0
29	B	131	0	0	2	0
29	C	90	0	0	4	0
29	D	96	0	0	8	0
29	E	62	0	0	0	0
29	F	70	0	0	1	0
29	G	41	0	0	6	0
29	H	46	0	0	2	0
29	I	44	0	0	3	0
29	J	17	0	0	1	0
29	K	22	0	0	2	0
29	L	23	0	0	1	0
29	M	19	0	0	0	0
29	N	196	0	0	3	0
29	O	106	0	0	3	0
29	P	89	0	0	1	0
29	Q	54	0	0	4	0
29	R	52	0	0	0	0
29	S	62	0	0	6	0
29	T	39	0	0	7	0
29	U	39	0	0	2	0
29	V	16	0	0	3	0
29	W	15	0	0	1	0
29	X	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	Y	19	0	0	1	0
29	Z	10	0	0	1	0
All	All	32113	0	31062	673	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 11.

All (673) 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)
24:G:265:PEK:C8	24:G:265:PEK:C7	1.75	1.56
24:G:265:PEK:C9	24:G:265:PEK:C8	1.77	1.55
24:G:265:PEK:C10	24:G:265:PEK:C9	1.81	1.50
1:A:297:MET:SD	1:A:297:MET:CE	2.02	1.48
24:G:265:PEK:H383	25:G:269:CDL:C27	1.46	1.44
1:N:297:MET:CE	1:N:297:MET:SD	2.04	1.44
12:L:20:ARG:NH2	19:L:522:TGL:HC32	1.35	1.37
7:G:5:LYS:HD2	24:G:1263:PEK:C37	1.59	1.33
24:T:1265:PEK:H383	25:T:1269:CDL:C27	1.60	1.28
7:G:5:LYS:CD	24:G:1263:PEK:H371	1.65	1.25
24:G:265:PEK:C38	25:G:269:CDL:C27	2.19	1.21
12:L:20:ARG:HH22	19:L:522:TGL:CC3	1.59	1.15
24:G:265:PEK:H383	25:G:269:CDL:H273	1.26	1.14
7:G:5:LYS:CG	24:G:1263:PEK:H371	1.82	1.10
15:A:520:PER:O1	15:A:520:PER:O2	1.70	1.09
7:T:5:LYS:HD2	24:T:263:PEK:H381	1.28	1.09
3:P:63:ARG:HE	25:P:1270:CDL:HA22	1.13	1.09
2:O:41:ILE:HD13	26:R:1230:PSC:H342	1.35	1.08
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.12	1.08
26:E:230:PSC:H072	9:I:10:ARG:HH21	1.19	1.08
24:P:1264:PEK:H32	24:P:1264:PEK:H71	1.30	1.08
29:N:4407:HOH:O	19:O:1523:TGL:HC32	1.52	1.06
7:T:84:LYS:N	7:T:84:LYS:HD2	1.70	1.06
15:N:520:PER:O2	15:N:520:PER:O1	1.70	1.06
24:T:1265:PEK:C38	25:T:1269:CDL:C27	2.35	1.03
3:C:63:ARG:HE	25:C:270:CDL:HA22	1.19	1.03
25:G:269:CDL:H242	25:G:269:CDL:H542	1.40	1.02
26:R:1230:PSC:O01	26:R:1230:PSC:H212	1.58	1.01
12:L:20:ARG:NH2	19:L:522:TGL:CC3	2.19	1.01
7:T:84:LYS:H	7:T:84:LYS:HD2	1.20	1.01
7:G:5:LYS:HD2	24:G:1263:PEK:H371	1.14	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:116:LEU:HD12	2:O:117:SER:N	1.75	1.01
7:T:2:SER:OG	24:T:263:PEK:H302	1.60	1.01
25:G:269:CDL:C54	25:G:269:CDL:H242	1.91	1.00
20:N:1524:PGV:H221	20:N:1524:PGV:H31	1.40	0.99
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	1.78	0.99
24:T:1265:PEK:C38	25:T:1269:CDL:H272	1.91	0.99
1:N:113:LEU:HD12	19:Y:1522:TGL:H292	1.43	0.99
24:T:1265:PEK:H383	25:T:1269:CDL:H272	1.01	0.99
25:T:1269:CDL:H571	25:T:1269:CDL:H782	1.44	0.99
20:P:1267:PGV:H182	25:P:1270:CDL:H662	1.42	0.98
18:N:515:HEA:C27	18:N:515:HEA:C16	2.41	0.98
24:G:265:PEK:C38	25:G:269:CDL:H272	1.93	0.98
19:Y:1522:TGL:HC22	19:Y:1522:TGL:HC62	1.45	0.98
6:S:95:GLN:HE21	6:S:95:GLN:HA	1.27	0.97
7:T:5:LYS:CD	24:T:263:PEK:H381	1.95	0.97
18:N:515:HEA:H161	18:N:515:HEA:H272	1.47	0.97
7:G:5:LYS:HB3	1:N:278:MET:SD	2.07	0.95
6:S:95:GLN:HG2	29:S:4406:HOH:O	1.63	0.94
24:G:265:PEK:H383	25:G:269:CDL:H271	1.47	0.94
26:E:230:PSC:C07	9:I:10:ARG:HH21	1.80	0.93
25:G:269:CDL:HA21	25:G:269:CDL:H112	1.50	0.91
19:A:521:TGL:H281	19:A:521:TGL:H101	1.51	0.91
7:G:5:LYS:HD2	24:G:1263:PEK:H372	1.54	0.90
18:N:515:HEA:H272	18:N:515:HEA:C16	1.99	0.88
25:P:1270:CDL:OB9	25:P:1270:CDL:H522	1.73	0.88
7:T:84:LYS:H	7:T:84:LYS:CD	1.85	0.88
20:P:1267:PGV:C18	25:P:1270:CDL:H662	2.04	0.88
6:S:85:CYS:SG	6:S:87:THR:HG23	2.14	0.88
7:T:5:LYS:HD2	24:T:263:PEK:C38	2.03	0.87
26:R:1230:PSC:C07	9:V:10:ARG:HH21	1.87	0.87
7:G:5:LYS:HB2	24:G:1263:PEK:H351	1.54	0.86
24:G:265:PEK:H382	25:G:269:CDL:H272	1.55	0.86
24:G:265:PEK:C6	24:G:265:PEK:C8	2.53	0.86
24:T:1265:PEK:C38	25:T:1269:CDL:H273	2.03	0.86
24:P:1264:PEK:HN2	7:T:76:ASN:HD21	1.24	0.85
26:E:230:PSC:H343	26:E:230:PSC:H142	1.57	0.85
1:A:296:GLY:HA2	8:H:23:GLN:OE1	1.77	0.84
7:T:5:LYS:CD	24:T:263:PEK:C38	2.55	0.84
10:W:33:ARG:HG2	22:W:1060:CHD:H151	1.59	0.84
7:T:5:LYS:HB2	24:T:263:PEK:H371	1.60	0.83
19:O:1521:TGL:HB92	19:O:1521:TGL:H281	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:5:LYS:HB2	24:T:263:PEK:C37	2.09	0.82
13:M:39:ASN:O	13:M:43:SER:HB2	1.80	0.82
19:Y:1522:TGL:H231	19:Y:1522:TGL:HA92	1.62	0.81
7:G:38:HIS:CE1	25:G:269:CDL:H111	2.15	0.81
25:T:1269:CDL:H111	25:T:1269:CDL:HA21	1.62	0.81
18:N:515:HEA:H273	18:N:515:HEA:H162	1.60	0.81
20:A:524:PGV:H02	20:A:524:PGV:O14	1.81	0.81
7:G:5:LYS:HG3	24:G:1263:PEK:H371	1.63	0.80
19:O:1521:TGL:H101	19:O:1521:TGL:H281	1.63	0.80
6:S:95:GLN:NE2	6:S:95:GLN:HA	1.96	0.80
3:C:3:HIS:HE1	6:F:96:LEU:CD2	1.93	0.80
1:A:430:PHE:HE1	19:A:521:TGL:HB21	1.46	0.80
19:L:522:TGL:HC62	19:L:522:TGL:CC2	2.10	0.80
19:O:1521:TGL:H101	19:O:1521:TGL:C28	2.12	0.79
24:C:264:PEK:C10	24:C:264:PEK:H161	2.11	0.79
8:H:45:ALA:O	8:H:47:GLY:N	2.14	0.79
7:T:2:SER:OG	24:T:263:PEK:C30	2.29	0.79
7:G:72:ASN:H	7:G:76:ASN:HD22	1.26	0.79
10:J:7:GLU:HG3	29:J:4441:HOH:O	1.83	0.79
9:V:73:LYS:HB2	29:V:4544:HOH:O	1.81	0.79
3:P:224:LYS:CD	25:P:1270:CDL:HB31	2.13	0.78
11:X:54:ARG:HH21	11:X:54:ARG:CG	1.96	0.78
9:I:73:LYS:HB3	29:I:4590:HOH:O	1.84	0.78
7:G:5:LYS:CD	24:G:1263:PEK:C37	2.40	0.78
1:N:400:PHE:HB3	19:Y:1522:TGL:H283	1.66	0.78
6:S:52:ILE:O	6:S:94:HIS:CE1	2.36	0.78
6:F:85:CYS:SG	6:F:87:THR:HG23	2.23	0.78
1:A:472:ILE:HG21	19:L:522:TGL:HA92	1.66	0.78
7:G:84:LYS:H	7:G:84:LYS:CD	1.97	0.78
4:Q:72:ASN:HB3	29:Q:3133:HOH:O	1.83	0.78
29:O:4115:HOH:O	8:U:61:LYS:HD2	1.83	0.78
4:D:34:SER:H	4:D:37:GLN:HE21	1.32	0.77
18:N:515:HEA:HMC1	18:N:515:HEA:HBC1	1.67	0.76
19:O:1523:TGL:H231	19:O:1523:TGL:HA91	1.67	0.76
3:C:3:HIS:HE1	6:F:96:LEU:HD22	1.47	0.76
2:O:226:MET:O	2:O:227:LEU:O	2.03	0.76
4:D:78:TRP:HB3	19:D:523:TGL:HB22	1.68	0.76
20:P:1267:PGV:H182	25:P:1270:CDL:C66	2.15	0.75
1:A:484:THR:HB	13:M:2:THR:OG1	1.86	0.75
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.69	0.75
7:T:31:CYS:SG	25:T:1269:CDL:H551	2.27	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:521:TGL:H322	19:A:521:TGL:HA92	1.68	0.75
24:C:264:PEK:H32	24:C:264:PEK:H71	1.68	0.74
1:N:484:THR:HG22	13:Z:2:THR:OG1	1.87	0.74
24:P:1264:PEK:H161	24:P:1264:PEK:C10	2.16	0.74
3:P:67:PHE:HE1	25:P:1270:CDL:H1	1.51	0.74
3:C:3:HIS:CE1	6:F:96:LEU:HD22	2.22	0.74
4:D:86:MET:HE3	29:K:4663:HOH:O	1.87	0.74
9:V:61:GLU:OE1	9:V:64:ARG:NH2	2.21	0.74
24:T:1265:PEK:H381	25:T:1269:CDL:H273	1.69	0.74
7:G:84:LYS:HD2	7:G:84:LYS:H	1.53	0.74
20:N:1524:PGV:H311	13:Z:19:LEU:HD23	1.67	0.74
3:C:63:ARG:HE	25:C:270:CDL:CA2	2.00	0.73
20:C:267:PGV:H172	25:C:270:CDL:H652	1.69	0.73
4:D:31:LYS:HE2	29:D:4577:HOH:O	1.87	0.73
4:D:31:LYS:NZ	29:D:4577:HOH:O	2.22	0.73
3:C:80:ARG:NH1	24:T:263:PEK:H032	2.04	0.73
7:T:17:ARG:HD3	29:T:3302:HOH:O	1.88	0.73
19:L:522:TGL:HC62	19:L:522:TGL:HC22	1.69	0.73
2:O:226:MET:O	2:O:227:LEU:C	2.28	0.72
2:B:56:MET:HA	26:E:230:PSC:H202	1.71	0.72
4:D:31:LYS:CE	29:D:4577:HOH:O	2.37	0.72
29:N:4424:HOH:O	26:R:1230:PSC:H21	1.90	0.72
19:A:521:TGL:HA82	19:A:521:TGL:H282	1.69	0.72
19:L:522:TGL:HC81	29:L:4545:HOH:O	1.89	0.72
18:N:515:HEA:C27	18:N:515:HEA:H162	2.17	0.72
7:G:38:HIS:HE1	25:G:269:CDL:H111	1.53	0.71
25:G:269:CDL:H332	2:O:78:LEU:HD12	1.73	0.71
10:J:52:TRP:O	10:J:57:HIS:HE1	1.74	0.71
1:N:113:LEU:CD1	19:Y:1522:TGL:H292	2.19	0.71
24:C:264:PEK:H102	24:C:264:PEK:H161	1.70	0.71
19:A:521:TGL:H281	19:A:521:TGL:C10	2.21	0.71
26:E:230:PSC:H212	26:E:230:PSC:H02	1.73	0.70
25:G:269:CDL:H201	1:N:311:ILE:CD1	2.22	0.70
6:S:75:HIS:H	6:S:80:GLN:HE22	1.39	0.70
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.73	0.70
19:O:1521:TGL:CB9	19:O:1521:TGL:H281	2.21	0.70
24:C:264:PEK:H101	24:C:264:PEK:H161	1.74	0.70
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.72	0.70
19:O:1523:TGL:HC21	19:O:1523:TGL:HG11	1.74	0.70
24:P:1264:PEK:H161	24:P:1264:PEK:H101	1.73	0.70
1:N:53:ILE:HD11	12:Y:40:VAL:HG13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:78:TRP:CB	19:D:523:TGL:HB22	2.22	0.69
10:J:4:ARG:HD2	10:J:7:GLU:OE2	1.92	0.69
18:N:515:HEA:H273	18:N:515:HEA:C16	2.17	0.69
2:B:81:LEU:HD12	25:T:1269:CDL:H351	1.74	0.69
3:C:67:PHE:HE1	25:C:270:CDL:H1	1.55	0.69
11:X:54:ARG:NH2	11:X:54:ARG:HG3	1.91	0.69
3:C:63:ARG:NE	25:C:270:CDL:HA22	2.01	0.69
3:P:224:LYS:HD2	25:P:1270:CDL:HB31	1.74	0.69
4:Q:34:SER:O	4:Q:38:LYS:HG3	1.93	0.69
7:T:8:HIS:CE1	24:T:263:PEK:H321	2.28	0.69
19:A:521:TGL:OB1	19:A:521:TGL:HB42	1.91	0.69
26:R:1230:PSC:H071	9:V:10:ARG:HH21	1.58	0.69
10:W:33:ARG:HG2	22:W:1060:CHD:C15	2.22	0.68
24:G:265:PEK:C38	25:G:269:CDL:H273	2.06	0.68
29:G:4754:HOH:O	20:N:1268:PGV:H341	1.91	0.68
7:T:5:LYS:CB	24:T:263:PEK:H371	2.23	0.68
3:C:55:TYR:CE1	25:C:270:CDL:H521	2.28	0.68
20:N:1524:PGV:C22	20:N:1524:PGV:H31	2.19	0.68
24:G:1263:PEK:H222	29:G:4660:HOH:O	1.93	0.68
20:A:522:PGV:H183	24:C:264:PEK:H332	1.74	0.68
7:T:72:ASN:H	7:T:76:ASN:HD22	1.40	0.67
26:R:1230:PSC:O02	26:R:1230:PSC:H032	1.94	0.67
20:N:1524:PGV:H221	20:N:1524:PGV:C3	2.20	0.67
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.76	0.67
25:G:269:CDL:CA2	25:G:269:CDL:H112	2.23	0.66
25:G:269:CDL:H201	1:N:311:ILE:HD11	1.76	0.66
1:A:278:MET:SD	7:T:5:LYS:HB3	2.35	0.66
24:G:265:PEK:C10	24:G:265:PEK:C8	2.73	0.66
7:T:5:LYS:HB2	24:T:263:PEK:H362	1.77	0.66
26:E:230:PSC:H212	26:E:230:PSC:C02	2.26	0.66
3:P:226:HIS:CE1	25:P:1270:CDL:HB32	2.31	0.66
7:T:5:LYS:CG	24:T:263:PEK:H383	2.26	0.66
26:R:1230:PSC:H072	9:V:10:ARG:HH21	1.61	0.65
3:P:63:ARG:HE	25:P:1270:CDL:CA2	2.00	0.65
1:A:430:PHE:CE1	19:A:521:TGL:HB21	2.29	0.65
4:Q:109:HIS:HD2	29:Q:3152:HOH:O	1.79	0.65
19:Y:1522:TGL:CC2	19:Y:1522:TGL:HC62	2.06	0.65
20:N:1524:PGV:H032	20:N:1524:PGV:H22	1.78	0.65
24:C:264:PEK:HN2	7:G:76:ASN:HD21	1.43	0.65
1:A:53:ILE:HD11	12:L:40:VAL:HG13	1.78	0.65
25:C:270:CDL:H661	25:C:270:CDL:H241	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:113:LEU:HD12	19:Y:1522:TGL:C29	2.24	0.65
2:B:129:LYS:HE3	29:B:4594:HOH:O	1.97	0.64
4:D:78:TRP:CA	19:D:523:TGL:HB22	2.27	0.64
25:G:269:CDL:H181	25:G:269:CDL:H511	1.78	0.64
3:P:213:THR:HG21	20:P:1267:PGV:H11	1.78	0.64
7:G:3:ALA:O	7:G:4:ALA:HB2	1.98	0.64
1:A:311:ILE:HD12	25:T:1269:CDL:H201	1.79	0.64
7:G:84:LYS:N	7:G:84:LYS:HD2	2.13	0.64
25:C:270:CDL:H522	25:C:270:CDL:OB9	1.98	0.63
10:J:50:LEU:HD22	10:J:50:LEU:O	1.99	0.63
12:L:20:ARG:HH22	19:L:522:TGL:HC32	0.66	0.63
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.96	0.63
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.34	0.63
25:T:1269:CDL:H571	25:T:1269:CDL:C78	2.25	0.63
1:A:510:TYR:OH	1:A:512:ASN:ND2	2.31	0.63
1:N:177:SER:H	1:N:180:GLN:NE2	1.95	0.63
6:S:94:HIS:CD2	6:S:95:GLN:H	2.16	0.63
20:C:267:PGV:H182	25:C:270:CDL:H671	1.79	0.62
1:N:513:LEU:O	1:N:514:LYS:HB2	1.98	0.62
24:G:265:PEK:C11	24:G:265:PEK:C9	2.75	0.62
3:P:111:GLU:HG3	29:U:4773:HOH:O	1.98	0.62
18:N:516:HEA:HBC1	18:N:516:HEA:HMC1	1.81	0.62
3:P:55:TYR:CE1	25:P:1270:CDL:H521	2.34	0.62
7:T:5:LYS:HB2	24:T:263:PEK:C36	2.29	0.62
6:S:94:HIS:CD2	6:S:95:GLN:N	2.68	0.62
3:C:210:ILE:HG12	20:C:267:PGV:H12	1.81	0.62
1:N:87:ILE:O	1:N:173:PRO:HD3	1.99	0.62
2:O:32:PHE:HE2	19:O:1521:TGL:HA52	1.64	0.62
2:O:116:LEU:HD12	2:O:116:LEU:C	2.20	0.62
19:O:1521:TGL:C10	19:O:1521:TGL:H281	2.28	0.61
2:B:62:GLU:O	2:B:66:THR:HB	1.99	0.61
8:H:54:GLU:OE2	8:H:57:ARG:NH2	2.18	0.61
2:O:116:LEU:HD12	2:O:117:SER:H	1.62	0.61
25:P:1270:CDL:H222	25:P:1270:CDL:H632	1.83	0.61
19:O:1523:TGL:HG31	29:Q:4568:HOH:O	2.00	0.61
1:A:513:LEU:O	1:A:514:LYS:HB2	1.99	0.61
12:L:20:ARG:HH22	19:L:522:TGL:HC62	1.65	0.61
3:P:210:ILE:HD13	20:P:1267:PGV:H301	1.83	0.61
3:P:29:SER:HB3	3:P:42:LEU:HD13	1.81	0.61
25:T:1269:CDL:C11	25:T:1269:CDL:HA21	2.28	0.61
4:D:34:SER:H	4:D:37:GLN:NE2	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:524:PGV:H311	13:M:19:LEU:HD23	1.81	0.61
1:N:482:VAL:HG22	13:Z:1:ILE:HD11	1.83	0.60
1:A:177:SER:H	1:A:180:GLN:HE21	1.49	0.60
2:B:33:LEU:HD13	9:I:31:PHE:CD1	2.37	0.60
26:E:230:PSC:H072	9:I:10:ARG:NH2	2.04	0.60
26:E:230:PSC:H212	26:E:230:PSC:O01	2.01	0.60
17:A:519:NA:NA	29:A:2026:HOH:O	1.73	0.60
7:G:72:ASN:H	7:G:76:ASN:ND2	1.98	0.60
24:P:1264:PEK:H102	24:P:1264:PEK:H161	1.83	0.60
3:P:63:ARG:NE	25:P:1270:CDL:HA22	1.99	0.59
25:G:269:CDL:C63	25:G:269:CDL:H592	2.31	0.59
6:S:26:LYS:HB3	6:S:28:GLN:NE2	2.17	0.59
7:T:5:LYS:HG3	24:T:263:PEK:H383	1.83	0.59
3:C:52:LEU:HD23	25:C:270:CDL:H362	1.84	0.59
25:P:1270:CDL:HB22	25:P:1270:CDL:OA5	2.03	0.59
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.31	0.59
7:G:37:LEU:HD23	7:G:38:HIS:CE1	2.38	0.59
2:O:41:ILE:HD13	26:R:1230:PSC:C34	2.22	0.59
3:C:3:HIS:N	29:C:4573:HOH:O	2.36	0.59
20:N:1524:PGV:H062	29:Z:3153:HOH:O	2.01	0.59
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.38	0.59
24:G:265:PEK:C9	24:G:265:PEK:C7	2.81	0.59
4:D:107:ILE:HB	4:D:108:PRO:CD	2.32	0.59
26:E:230:PSC:H231	26:E:230:PSC:H42	1.84	0.59
19:L:522:TGL:HC41	19:L:522:TGL:OC1	2.02	0.59
1:N:43:GLN:HB2	1:N:44:PRO:HD2	1.85	0.59
12:Y:12:PRO:HG2	19:Y:1522:TGL:HG11	1.84	0.59
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.68	0.58
7:T:5:LYS:CG	24:T:263:PEK:C38	2.81	0.58
2:O:42:ILE:HG21	19:O:1523:TGL:H232	1.84	0.58
12:L:20:ARG:HH12	19:L:522:TGL:HC61	1.68	0.58
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.69	0.58
3:C:80:ARG:HH11	24:T:263:PEK:H032	1.67	0.58
8:H:45:ALA:C	8:H:47:GLY:H	2.05	0.58
7:G:3:ALA:O	7:G:4:ALA:CB	2.51	0.58
7:G:45:PRO:HD2	29:G:2145:HOH:O	2.03	0.58
1:A:281:GLY:C	7:T:4:ALA:HB1	2.25	0.58
1:A:282:PHE:HA	7:T:4:ALA:CB	2.35	0.57
3:C:3:HIS:N	29:C:4600:HOH:O	2.37	0.57
6:F:64:GLU:O	6:F:65:ASP:HB2	2.05	0.57
12:L:14:SER:H	19:L:522:TGL:HC31	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:210:ILE:HG21	20:P:1267:PGV:H282	1.86	0.57
2:B:41:ILE:HD13	26:E:230:PSC:H342	1.87	0.57
19:D:523:TGL:HB42	19:D:523:TGL:HA32	1.87	0.57
4:Q:109:HIS:CD2	29:Q:3152:HOH:O	2.54	0.57
3:C:5:THR:HG22	6:F:96:LEU:HD13	1.87	0.56
7:G:5:LYS:HG3	24:G:1263:PEK:C37	2.32	0.56
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.40	0.56
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.40	0.56
3:C:224:LYS:CD	25:C:270:CDL:HB31	2.36	0.56
1:N:290:HIS:CD2	1:N:291:HIS:CD2	2.93	0.56
7:T:36:TRP:HE1	24:T:1265:PEK:C20	2.19	0.56
9:V:36:LYS:O	9:V:41:GLU:HG2	2.06	0.56
3:C:48:THR:HG23	25:C:270:CDL:H402	1.88	0.55
24:G:1263:PEK:H382	29:G:4355:HOH:O	2.06	0.55
25:P:1270:CDL:HB22	25:P:1270:CDL:PA1	2.46	0.55
7:T:72:ASN:H	7:T:76:ASN:ND2	2.04	0.55
7:T:45:PRO:HD2	29:T:3145:HOH:O	2.05	0.55
2:B:164:ALA:O	2:B:194:GLY:HA3	2.06	0.55
25:G:269:CDL:H601	25:G:269:CDL:H761	1.89	0.55
26:E:230:PSC:C07	9:I:10:ARG:NH2	2.61	0.55
1:N:240:HIS:O	1:N:243:VAL:HG22	2.07	0.55
19:Y:1522:TGL:HC22	19:Y:1522:TGL:CC6	2.28	0.55
1:A:229:ILE:HD11	2:B:175:ILE:HD13	1.88	0.55
6:S:64:GLU:O	6:S:65:ASP:HB2	2.06	0.55
7:T:37:LEU:HD23	7:T:38:HIS:HD1	1.72	0.55
2:B:78:LEU:HD12	25:T:1269:CDL:H352	1.89	0.54
29:A:4231:HOH:O	26:E:230:PSC:H21	2.08	0.54
1:N:430:PHE:CE1	19:O:1521:TGL:HB21	2.43	0.54
1:A:311:ILE:CD1	25:T:1269:CDL:H201	2.38	0.54
19:D:523:TGL:H352	9:I:16:ARG:HH21	1.72	0.54
12:Y:20:ARG:NH2	12:Y:24:MET:CG	2.64	0.54
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.89	0.54
1:N:412:ILE:HD13	4:Q:84:ALA:CB	2.38	0.54
26:R:1230:PSC:H221	26:R:1230:PSC:H42	1.89	0.54
1:N:62:ALA:HB1	18:N:515:HEA:HMD3	1.88	0.54
3:P:254:VAL:HG23	25:T:1269:CDL:H672	1.90	0.54
6:S:25:ARG:HD3	29:S:4659:HOH:O	2.07	0.54
1:N:417:MET:O	1:N:421:VAL:HG22	2.07	0.54
7:G:69:PHE:HZ	28:G:272:DMU:H1	1.72	0.54
1:A:297:MET:CB	1:A:297:MET:CE	2.86	0.53
18:A:515:HEA:HMC1	18:A:515:HEA:HBC1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:P:1270:CDL:C63	25:P:1270:CDL:H222	2.39	0.53
6:S:22:LEU:HD23	6:S:25:ARG:NH1	2.23	0.53
1:N:438:ARG:O	1:N:439:ARG:HB2	2.07	0.53
8:U:45:ALA:O	8:U:47:GLY:N	2.41	0.53
19:A:521:TGL:HC22	29:D:2376:HOH:O	2.08	0.53
25:C:270:CDL:H661	25:C:270:CDL:C24	2.38	0.53
1:A:112:LEU:HG	29:A:2073:HOH:O	2.08	0.53
2:O:145:PRO:HB2	2:O:148:MET:HG3	1.91	0.53
19:A:521:TGL:CA9	19:A:521:TGL:H322	2.37	0.53
18:A:515:HEA:H122	18:A:515:HEA:HHC	1.89	0.53
4:D:78:TRP:HA	19:D:523:TGL:HB22	1.90	0.53
5:E:12:ASP:OD1	5:E:44:GLU:HG3	2.08	0.53
20:A:524:PGV:H152	20:A:524:PGV:C32	2.39	0.52
4:D:31:LYS:NZ	29:D:4344:HOH:O	2.40	0.52
4:D:86:MET:CE	29:K:4663:HOH:O	2.51	0.52
28:G:272:DMU:O1	28:G:272:DMU:H29	2.09	0.52
7:G:5:LYS:HD2	24:G:1263:PEK:C38	2.36	0.52
1:A:177:SER:H	1:A:180:GLN:NE2	2.06	0.52
26:E:230:PSC:C06	9:I:10:ARG:HE	2.22	0.52
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.92	0.52
2:O:129:LYS:O	2:O:132:GLU:HB2	2.09	0.52
3:P:112:LEU:CD2	29:T:3156:HOH:O	2.57	0.52
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.90	0.52
1:A:514:LYS:OXT	6:F:37:LYS:HE2	2.09	0.52
1:N:172:LYS:NZ	1:N:178:GLN:HE22	2.07	0.52
19:O:1523:TGL:HC21	19:O:1523:TGL:CG1	2.40	0.52
9:V:18:ARG:HG3	29:V:3367:HOH:O	2.08	0.52
19:Y:1522:TGL:OA1	19:Y:1522:TGL:H171	2.10	0.52
26:E:230:PSC:H343	26:E:230:PSC:C14	2.36	0.52
1:N:430:PHE:HE1	19:O:1521:TGL:HB21	1.75	0.52
3:P:213:THR:CG2	20:P:1267:PGV:H11	2.39	0.52
3:C:59:ARG:HG3	25:C:270:CDL:H512	1.92	0.52
9:I:58:LYS:O	9:I:62:GLU:HG3	2.10	0.52
2:O:139:ASP:OD2	2:O:140:ASN:N	2.41	0.52
2:O:128:LEU:HD22	2:O:132:GLU:HB3	1.92	0.51
19:O:1523:TGL:H121	19:O:1523:TGL:HB81	1.92	0.51
2:O:221:LYS:NZ	29:O:4469:HOH:O	2.43	0.51
2:B:132:GLU:HB3	2:B:137:GLU:HG3	1.92	0.51
8:H:27:ARG:NH1	29:H:2296:HOH:O	2.43	0.51
24:P:1264:PEK:H32	24:P:1264:PEK:C7	2.19	0.51
2:O:41:ILE:CD1	26:R:1230:PSC:H342	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:37:LEU:HD23	7:T:38:HIS:ND1	2.25	0.51
20:A:524:PGV:H152	20:A:524:PGV:H322	1.92	0.51
1:N:199:LEU:N	1:N:200:PRO:CD	2.74	0.51
4:D:58:GLU:HG3	4:D:58:GLU:O	2.10	0.51
25:G:269:CDL:H752	1:N:282:PHE:HZ	1.76	0.51
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.93	0.51
24:C:264:PEK:H102	24:C:264:PEK:C16	2.40	0.50
25:G:269:CDL:H632	25:G:269:CDL:H592	1.92	0.50
6:S:94:HIS:CG	6:S:95:GLN:H	2.24	0.50
12:Y:24:MET:SD	19:Y:1522:TGL:H162	2.51	0.50
19:Y:1522:TGL:H311	29:Y:4350:HOH:O	2.10	0.50
2:O:32:PHE:CE2	19:O:1521:TGL:HA52	2.46	0.50
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.08	0.50
6:S:22:LEU:CD2	6:S:25:ARG:NH1	2.75	0.50
8:U:27:ARG:NH1	29:U:3296:HOH:O	2.43	0.50
1:N:20:LEU:HB3	19:Y:1522:TGL:H221	1.93	0.50
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.94	0.50
11:X:54:ARG:NH2	11:X:54:ARG:CG	2.65	0.50
9:V:25:PHE:O	9:V:28:SER:HB2	2.11	0.49
19:O:1521:TGL:H101	19:O:1521:TGL:H283	1.90	0.49
4:Q:33:LEU:HD22	4:Q:37:GLN:HB3	1.94	0.49
2:B:59:GLN:C	2:B:60:GLU:HG3	2.33	0.49
1:A:28:MET:CE	18:A:515:HEA:H271	2.41	0.49
12:L:20:ARG:HH22	19:L:522:TGL:CC6	2.25	0.49
2:O:23:PHE:CZ	2:O:80:SER:HB2	2.48	0.49
4:Q:48:TRP:HA	4:Q:51:LEU:HD22	1.94	0.49
1:A:37:ILE:HG21	18:A:515:HEA:CMA	2.43	0.49
7:G:2:SER:O	24:G:1263:PEK:H322	2.13	0.49
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.95	0.49
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.76	0.49
1:N:383:MET:O	1:N:387:PHE:HB2	2.12	0.48
2:O:113:TYR:HD1	8:U:58:ARG:HH22	1.61	0.48
28:G:272:DMU:C10	28:G:272:DMU:H29	2.43	0.48
2:O:116:LEU:CD2	2:O:226:MET:HG2	2.43	0.48
1:A:47:LEU:O	13:M:41:LYS:HD2	2.14	0.48
18:N:516:HEA:CBC	18:N:516:HEA:HMC1	2.42	0.48
6:S:43:LYS:HE3	29:S:3347:HOH:O	2.13	0.48
6:S:52:ILE:O	6:S:94:HIS:HE1	1.91	0.48
7:T:36:TRP:HD1	29:T:4758:HOH:O	1.96	0.48
20:A:524:PGV:O02	20:A:524:PGV:P	2.72	0.48
2:B:66:THR:HG21	22:B:1086:CHD:H3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:84:LYS:N	7:G:84:LYS:CD	2.72	0.48
1:N:172:LYS:HZ2	1:N:178:GLN:HE22	1.59	0.48
1:N:48:LEU:HB2	29:N:3109:HOH:O	2.14	0.48
2:O:128:LEU:HD11	2:O:134:ARG:HA	1.96	0.48
6:S:26:LYS:HB3	6:S:28:GLN:HE22	1.79	0.48
6:S:95:GLN:CA	6:S:95:GLN:HE21	2.14	0.48
3:P:67:PHE:CE1	25:P:1270:CDL:H1	2.40	0.48
9:I:35:TYR:C	9:I:37:PHE:H	2.17	0.48
10:J:50:LEU:HD22	10:J:54:SER:HG	1.79	0.48
7:T:36:TRP:HE1	24:T:1265:PEK:H201	1.79	0.48
1:A:87:ILE:O	1:A:173:PRO:HD3	2.13	0.48
26:E:230:PSC:H232	26:E:230:PSC:H201	1.51	0.48
1:N:422:ASN:OD1	19:O:1521:TGL:H262	2.14	0.48
3:C:246:ASP:HB2	29:C:4215:HOH:O	2.13	0.48
25:G:269:CDL:H571	25:G:269:CDL:H782	1.96	0.48
5:E:11:PHE:CB	26:E:230:PSC:H073	2.44	0.47
3:C:106:LEU:HD13	20:H:268:PGV:H22	1.95	0.47
6:S:10:GLU:OE2	6:S:25:ARG:NH1	2.47	0.47
1:A:198:SER:HB2	1:A:238:PHE:HA	1.96	0.47
1:A:282:PHE:CA	7:T:4:ALA:HB3	2.41	0.47
2:B:59:GLN:O	2:B:60:GLU:HG3	2.14	0.47
2:O:1:FME:HCN	2:O:193:TYR:HB2	1.96	0.47
26:R:1230:PSC:H071	9:V:10:ARG:NH2	2.28	0.47
5:E:82:TYR:HB3	5:E:83:PRO:HD3	1.96	0.47
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.14	0.47
1:A:281:GLY:O	7:T:4:ALA:HB1	2.15	0.47
2:B:114:GLU:HG3	2:B:227:LEU:HD11	1.96	0.47
4:Q:33:LEU:HA	4:Q:37:GLN:NE2	2.29	0.47
3:C:210:ILE:HD13	20:C:267:PGV:H301	1.97	0.47
1:A:431:LEU:HD21	1:A:450:TRP:HB2	1.96	0.47
7:G:2:SER:OG	24:G:1263:PEK:H291	2.14	0.47
22:C:271:CHD:H212	22:C:271:CHD:H12	1.97	0.47
7:G:45:PRO:CD	29:G:2145:HOH:O	2.62	0.47
18:N:515:HEA:H261	18:N:515:HEA:H172	1.36	0.47
3:P:254:VAL:CG2	25:T:1269:CDL:H672	2.45	0.47
1:A:25:TRP:CE3	19:L:522:TGL:HB91	2.49	0.47
2:B:52:HIS:CE1	26:E:230:PSC:H211	2.49	0.47
5:E:8:ASP:HA	26:E:230:PSC:H071	1.95	0.47
6:F:94:HIS:HB3	6:F:95:GLN:NE2	2.30	0.47
1:N:24:ALA:HA	18:N:515:HEA:H22	1.96	0.47
4:Q:23:PRO:HD2	5:R:34:ASN:OD1	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:30:ILE:O	10:W:34:VAL:HG23	2.15	0.47
20:P:1267:PGV:H182	25:P:1270:CDL:C67	2.45	0.46
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.80	0.46
2:O:164:ALA:O	2:O:194:GLY:HA3	2.15	0.46
2:B:65:TRP:HZ3	26:E:230:PSC:H322	1.79	0.46
4:D:127:LYS:HD2	29:I:2384:HOH:O	2.14	0.46
7:G:69:PHE:CZ	28:G:272:DMU:H1	2.50	0.46
4:Q:63:LYS:HG2	4:Q:64:PHE:CE1	2.51	0.46
25:P:1270:CDL:H362	25:P:1270:CDL:H411	1.97	0.46
10:W:52:TRP:O	10:W:57:HIS:HE1	1.98	0.46
18:A:515:HEA:H11	18:A:515:HEA:HMB1	1.76	0.46
19:A:521:TGL:HA91	19:A:521:TGL:H241	1.96	0.46
8:H:60:TYR:C	8:H:60:TYR:CD1	2.89	0.46
4:Q:7:LYS:O	4:Q:10:ASP:HB2	2.16	0.46
13:Z:31:GLY:C	28:Z:1526:DMU:H1	2.36	0.46
4:D:40:LEU:CD2	4:D:58:GLU:HG2	2.46	0.46
7:G:37:LEU:HD21	25:G:269:CDL:H341	1.98	0.46
1:N:177:SER:H	1:N:180:GLN:HE21	1.60	0.46
1:N:172:LYS:HD2	1:N:181:THR:CG2	2.46	0.46
28:P:1272:DMU:H40	7:T:63:GLY:H	1.80	0.46
4:Q:83:GLY:HA3	11:X:17:VAL:HG12	1.97	0.46
12:Y:2:HIS:ND1	12:Y:3:TYR:N	2.61	0.46
4:D:107:ILE:HD12	4:D:111:PHE:CD1	2.51	0.46
6:F:26:LYS:HE3	29:F:4627:HOH:O	2.16	0.46
25:G:269:CDL:H201	1:N:311:ILE:HD12	1.96	0.46
19:O:1521:TGL:H241	19:O:1521:TGL:H322	1.98	0.46
7:T:79:PRO:HD2	29:T:3129:HOH:O	2.16	0.46
7:G:84:LYS:CE	7:G:84:LYS:H	2.28	0.46
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.97	0.46
1:N:412:ILE:HD13	4:Q:84:ALA:HB3	1.96	0.46
1:N:514:LYS:HE2	29:S:3332:HOH:O	2.15	0.46
3:C:3:HIS:CE1	6:F:96:LEU:CD2	2.83	0.46
1:N:350:VAL:HG13	19:O:1521:TGL:HB81	1.98	0.46
4:Q:88:PHE:HZ	13:Z:19:LEU:HD21	1.80	0.46
6:S:94:HIS:CG	6:S:95:GLN:N	2.82	0.46
1:N:113:LEU:CD1	19:Y:1522:TGL:C29	2.92	0.46
4:D:109:HIS:HD2	29:D:2152:HOH:O	1.99	0.45
1:N:510:TYR:OH	1:N:512:ASN:ND2	2.42	0.45
2:O:33:LEU:HD13	9:V:31:PHE:CD1	2.52	0.45
6:S:94:HIS:HD2	6:S:95:GLN:N	2.13	0.45
1:N:131:PRO:O	1:N:132:LEU:C	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:PHE:CE1	19:A:521:TGL:CB2	2.97	0.45
5:R:11:PHE:HB3	26:R:1230:PSC:H073	1.98	0.45
5:R:67:ILE:O	5:R:70:VAL:HG12	2.16	0.45
20:N:1524:PGV:H152	20:N:1524:PGV:H321	1.97	0.45
1:N:254:ILE:HD12	1:N:254:ILE:HG23	1.60	0.45
2:B:78:LEU:CB	2:B:79:PRO:CD	2.95	0.45
22:J:60:CHD:H112	22:J:60:CHD:H12A	1.44	0.45
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.82	0.45
2:O:130:PRO:HA	4:Q:115:TRP:CH2	2.52	0.45
22:P:1271:CHD:H112	22:P:1271:CHD:H12A	1.51	0.45
25:T:1269:CDL:H562	25:T:1269:CDL:H762	1.98	0.45
9:V:73:LYS:HD2	9:V:73:LYS:HA	1.64	0.45
26:R:1230:PSC:H212	26:R:1230:PSC:C1	2.45	0.45
7:T:2:SER:CB	24:T:263:PEK:H302	2.43	0.45
1:N:215:LEU:HD11	24:P:1264:PEK:H271	1.98	0.45
2:B:2:ALA:HA	2:B:6:GLN:OE1	2.16	0.45
22:C:525:CHD:H112	22:C:525:CHD:H12A	1.56	0.45
18:N:515:HEA:H122	18:N:515:HEA:HHC	1.99	0.45
3:P:22:LEU:O	3:P:26:LEU:HG	2.17	0.45
1:A:297:MET:CE	1:A:297:MET:HB2	2.47	0.45
22:B:1086:CHD:H12A	22:B:1086:CHD:H112	1.68	0.45
26:E:230:PSC:H061	9:I:10:ARG:HE	1.80	0.45
4:D:107:ILE:HG21	4:D:107:ILE:HD13	1.75	0.44
3:P:226:HIS:HE1	25:P:1270:CDL:HB32	1.81	0.44
24:T:263:PEK:H5	24:T:263:PEK:H21	1.83	0.44
7:T:3:ALA:O	7:T:4:ALA:HB2	2.17	0.44
12:L:13:PHE:HB3	19:L:522:TGL:HG12	2.00	0.44
1:N:69:MET:HE3	1:N:70:VAL:HG23	1.99	0.44
2:O:22:HIS:CE1	9:V:43:ARG:HG2	2.53	0.44
1:N:172:LYS:NZ	1:N:178:GLN:NE2	2.65	0.44
1:N:489:THR:HA	6:S:71:TRP:O	2.17	0.44
5:R:90:ARG:HB3	5:R:91:PRO:HD3	1.99	0.44
9:V:68:ILE:HD11	9:V:69:PHE:CZ	2.53	0.44
1:A:513:LEU:HD23	1:A:513:LEU:HA	1.58	0.44
3:C:22:LEU:HA	3:C:22:LEU:HD23	1.83	0.44
25:C:270:CDL:HB21	25:C:270:CDL:PA1	2.57	0.44
8:H:44:THR:O	8:H:45:ALA:O	2.36	0.44
1:N:229:ILE:HD11	2:O:175:ILE:HD13	2.00	0.44
3:P:58:TRP:CG	20:P:1267:PGV:H41	2.52	0.44
4:Q:17:VAL:O	4:Q:25:PRO:HG3	2.18	0.44
20:A:524:PGV:C02	20:A:524:PGV:O14	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:224:LYS:HD2	25:C:270:CDL:HB31	1.98	0.44
6:S:55:LYS:HA	6:S:74:LEU:O	2.18	0.44
1:A:309:THR:HG22	18:A:516:HEA:HMB2	1.99	0.44
18:A:516:HEA:HMC1	18:A:516:HEA:HBC1	2.00	0.44
6:F:76:LYS:HD2	6:F:93:PRO:HG3	2.00	0.44
24:G:1263:PEK:O13	3:P:80:ARG:HD2	2.17	0.44
25:T:1269:CDL:H561	25:T:1269:CDL:H592	1.26	0.44
4:Q:88:PHE:CZ	13:Z:19:LEU:HD21	2.53	0.44
4:D:31:LYS:HG2	29:D:4601:HOH:O	2.18	0.43
9:I:52:ARG:NH1	29:I:4726:HOH:O	2.51	0.43
1:N:439:ARG:HD3	2:O:199:ILE:HB	2.00	0.43
19:O:1521:TGL:H251	19:O:1521:TGL:H222	1.44	0.43
1:N:449:MET:SD	2:O:5:MET:HG2	2.58	0.43
2:B:22:HIS:CE1	9:I:44:LYS:HG3	2.53	0.43
25:C:270:CDL:H242	25:C:270:CDL:H642	2.00	0.43
29:B:2353:HOH:O	19:D:523:TGL:HC61	2.18	0.43
6:F:92:VAL:O	6:F:92:VAL:HG23	2.17	0.43
7:G:83:GLU:HG2	7:G:84:LYS:HZ2	1.83	0.43
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.19	0.43
5:R:11:PHE:CB	26:R:1230:PSC:H073	2.48	0.43
1:A:299:VAL:CG2	2:B:84:LEU:HG	2.48	0.43
24:G:265:PEK:H361	25:G:269:CDL:H273	2.00	0.43
19:O:1523:TGL:HB22	4:Q:78:TRP:HA	2.01	0.43
13:M:37:LEU:HD23	13:M:37:LEU:HA	1.59	0.43
1:N:240:HIS:O	1:N:241:PRO:C	2.55	0.43
1:N:71:MET:HB2	1:N:72:PRO:HD3	2.00	0.43
7:T:17:ARG:CD	29:T:3302:HOH:O	2.58	0.43
19:A:521:TGL:H121	19:A:521:TGL:H292	1.79	0.43
2:O:92:ASN:HA	2:O:93:PRO:HD2	1.60	0.43
3:P:55:TYR:HE1	25:P:1270:CDL:H521	1.81	0.43
12:Y:20:ARG:HH21	19:Y:1522:TGL:HC32	1.84	0.43
1:A:383:MET:O	1:A:387:PHE:HB2	2.17	0.43
1:A:440:TYR:OH	2:B:195:GLN:HB3	2.19	0.43
3:C:91:VAL:HG22	24:T:263:PEK:H132	2.01	0.43
2:O:98:LYS:HB2	2:O:109:GLU:HB2	2.01	0.43
3:P:249:TRP:HD1	29:P:3171:HOH:O	2.00	0.43
10:W:40:LEU:HD12	22:W:1060:CHD:H183	2.01	0.43
22:W:1060:CHD:H232	22:W:1060:CHD:H211	1.69	0.43
13:Z:11:SER:OG	13:Z:14:GLU:HG3	2.19	0.43
24:G:265:PEK:H361	25:G:269:CDL:C27	2.49	0.43
20:H:268:PGV:H202	20:H:268:PGV:H231	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:31:LYS:HE3	6:S:83:PRO:O	2.18	0.43
13:Z:32:TRP:N	28:Z:1526:DMU:H1	2.34	0.43
1:N:406:ASN:HD21	20:N:1524:PGV:C2	2.32	0.43
18:N:515:HEA:HAD1	18:N:515:HEA:HHA	1.79	0.43
2:O:161:HIS:HB2	2:O:174:ALA:HB3	2.00	0.43
20:P:1267:PGV:H12	20:P:1267:PGV:C16	2.45	0.43
6:S:87:THR:HG21	29:S:4604:HOH:O	2.19	0.43
18:A:515:HEA:C16	18:A:515:HEA:H272	2.48	0.43
3:C:146:TRP:CE2	7:G:17:ARG:HG3	2.54	0.43
5:R:99:SER:HB2	5:R:104:LEU:HD21	2.01	0.43
3:C:19:THR:O	3:C:23:SER:HB3	2.19	0.42
29:O:3250:HOH:O	4:Q:129:ALA:HB2	2.18	0.42
7:G:63:GLY:HA2	28:G:272:DMU:H34	2.01	0.42
2:O:116:LEU:HD21	2:O:226:MET:HG2	2.01	0.42
2:O:82:ARG:HH11	2:O:86:MET:CE	2.32	0.42
2:O:113:TYR:HD1	8:U:58:ARG:NH2	2.17	0.42
2:B:108:TYR:O	2:B:117:SER:HA	2.18	0.42
1:N:290:HIS:HD2	1:N:291:HIS:CD2	2.35	0.42
8:U:50:VAL:CG1	8:U:50:VAL:O	2.68	0.42
26:E:230:PSC:H221	26:E:230:PSC:H251	1.70	0.42
1:N:18:LEU:CD2	19:Y:1522:TGL:HB21	2.49	0.42
25:P:1270:CDL:H612	25:P:1270:CDL:H641	1.75	0.42
3:P:8:TYR:CE1	3:P:74:ALA:HB1	2.54	0.42
24:T:263:PEK:H361	24:T:263:PEK:H332	1.61	0.42
19:A:521:TGL:OB1	19:A:521:TGL:CB4	2.53	0.42
10:W:1:PHE:N	29:W:4539:HOH:O	2.52	0.42
13:Z:17:ILE:HG21	13:Z:17:ILE:HD13	1.73	0.42
20:N:1524:PGV:H92	4:Q:84:ALA:HB2	2.01	0.42
1:N:86:MET:HB3	1:N:182:PRO:HG2	2.02	0.42
8:U:50:VAL:O	8:U:50:VAL:HG12	2.20	0.42
4:D:20:ARG:HG3	29:D:4139:HOH:O	2.19	0.42
2:O:16:ILE:HD13	2:O:16:ILE:HA	1.94	0.42
2:O:41:ILE:O	2:O:45:MET:HG2	2.20	0.42
18:A:515:HEA:HAD1	18:A:515:HEA:HHA	1.73	0.42
1:N:513:LEU:HD23	1:N:513:LEU:HA	1.93	0.42
5:R:8:ASP:HA	26:R:1230:PSC:H071	2.02	0.42
3:C:76:GLN:O	3:C:80:ARG:HG3	2.20	0.42
5:E:23:ASP:N	5:E:23:ASP:OD2	2.48	0.42
1:A:334:TRP:HB2	19:D:523:TGL:HG11	2.01	0.41
3:C:191:GLY:HA3	29:G:2156:HOH:O	2.18	0.41
22:C:525:CHD:H42	3:P:127:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:208:VAL:HG22	3:P:245:VAL:CG1	2.51	0.41
1:A:240:HIS:HB3	1:A:241:PRO:HD3	2.02	0.41
2:B:20:LEU:HA	2:B:20:LEU:HD23	1.85	0.41
22:C:271:CHD:H12A	22:C:271:CHD:H112	1.52	0.41
1:N:69:MET:CE	1:N:70:VAL:CG2	2.98	0.41
5:R:25:ASP:OD1	5:R:28:GLU:HG3	2.20	0.41
6:S:95:GLN:CG	29:S:4406:HOH:O	2.41	0.41
7:T:37:LEU:HD23	7:T:38:HIS:CE1	2.56	0.41
25:C:270:CDL:H861	25:C:270:CDL:H831	1.92	0.41
1:N:409:TRP:CE2	20:N:1524:PGV:H61	2.55	0.41
1:A:207:THR:O	1:A:211:THR:HG23	2.19	0.41
3:C:246:ASP:HB2	29:C:4076:HOH:O	2.20	0.41
11:K:24:PHE:O	11:K:28:VAL:HG12	2.21	0.41
3:P:144:ILE:HD13	3:P:144:ILE:HG21	1.80	0.41
2:B:91:ASN:C	2:B:91:ASN:HD22	2.24	0.41
3:C:103:HIS:ND1	22:C:525:CHD:O26	2.54	0.41
6:F:53:THR:HB	6:F:54:ASN:H	1.66	0.41
20:H:268:PGV:H52	20:H:268:PGV:H21	1.94	0.41
1:N:35:LEU:HB3	28:Z:1526:DMU:H24	2.03	0.41
25:C:270:CDL:PA1	25:C:270:CDL:CB2	3.09	0.41
26:E:230:PSC:H042	26:E:230:PSC:H062	1.67	0.41
2:O:16:ILE:HG23	2:O:16:ILE:HD12	1.82	0.41
3:P:65:SER:HB2	20:P:1267:PGV:H041	2.03	0.41
4:Q:130:PRO:HA	4:Q:135:SER:HB2	2.02	0.41
4:Q:33:LEU:HA	4:Q:37:GLN:HE21	1.84	0.41
3:C:129:VAL:N	3:C:130:PRO:CD	2.84	0.41
1:N:437:PRO:HG2	1:N:440:TYR:CE1	2.55	0.41
19:O:1523:TGL:CG3	19:O:1523:TGL:OB1	2.68	0.41
9:V:29:LEU:HD12	9:V:29:LEU:HA	1.79	0.41
6:F:64:GLU:O	6:F:65:ASP:CB	2.69	0.41
1:N:109:PHE:HB3	19:Y:1522:TGL:H122	2.03	0.41
3:P:224:LYS:CE	25:P:1270:CDL:HB31	2.49	0.41
3:C:16:TRP:N	3:C:17:PRO:CD	2.84	0.41
4:Q:127:LYS:HD2	29:V:3384:HOH:O	2.20	0.41
1:A:37:ILE:HG21	18:A:515:HEA:HMA	2.02	0.41
20:A:522:PGV:H42	20:A:522:PGV:H251	2.02	0.41
2:O:103:GLN:HB3	2:O:104:TRP:CE2	2.55	0.41
2:O:2:ALA:HA	2:O:6:GLN:OE1	2.21	0.41
4:Q:34:SER:N	4:Q:37:GLN:HE21	2.19	0.41
7:T:5:LYS:CB	24:T:263:PEK:C37	2.89	0.41
1:N:106:PRO:N	1:N:107:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:46:ALA:HB1	29:T:4681:HOH:O	2.21	0.41
2:O:141:ARG:HG3	9:V:70:GLN:NE2	2.36	0.41
1:N:431:LEU:HD21	1:N:450:TRP:HB2	2.03	0.40
1:N:69:MET:CE	1:N:70:VAL:HG23	2.51	0.40
1:N:76:GLY:O	1:N:80:ASN:HB2	2.21	0.40
2:O:139:ASP:N	2:O:139:ASP:OD2	2.52	0.40
5:R:65:VAL:HG13	5:R:101:PRO:HG3	2.03	0.40
1:A:181:THR:HA	1:A:182:PRO:HD3	1.94	0.40
1:A:311:ILE:HD13	1:A:311:ILE:HG21	1.85	0.40
25:G:269:CDL:C53	25:G:269:CDL:H242	2.47	0.40
7:G:7:ASP:HA	1:N:178:GLN:HG2	2.03	0.40
1:N:344:PHE:C	1:N:344:PHE:CD1	2.95	0.40
7:T:8:HIS:O	7:T:9:GLY:C	2.60	0.40
3:C:173:PHE:CD2	3:C:173:PHE:C	2.94	0.40
12:L:6:GLY:O	12:L:7:PRO:C	2.59	0.40
3:P:59:ARG:HG3	25:P:1270:CDL:H512	2.03	0.40
2:B:193:TYR:CD1	2:B:210:VAL:HG22	2.57	0.40
2:B:58:ALA:O	2:B:62:GLU:HG3	2.21	0.40
19:D:523:TGL:HB92	19:D:523:TGL:H121	1.47	0.40
8:H:23:GLN:HG3	29:H:4130:HOH:O	2.21	0.40
13:M:4:LYS:HB2	13:M:5:PRO:HD2	2.03	0.40
3:P:149:HIS:O	3:P:153:GLU:HG3	2.22	0.40
4:Q:12:ALA:HA	6:S:73:TRP:CD1	2.56	0.40
19:Y:1522:TGL:CC2	19:Y:1522:TGL:CC6	2.82	0.40
18:A:515:HEA:C12	18:A:515:HEA:HHC	2.51	0.40
8:H:39:CYS:O	8:H:40:GLU:C	2.58	0.40
20:N:1524:PGV:H02	20:N:1524:PGV:O14	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	512/514 (100%)	495 (97%)	17 (3%)	0	100	100
1	N	512/514 (100%)	490 (96%)	22 (4%)	0	100	100
2	B	225/227 (99%)	216 (96%)	8 (4%)	1 (0%)	34	22
2	O	225/227 (99%)	214 (95%)	10 (4%)	1 (0%)	34	22
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%)	137 (96%)	5 (4%)	0	100	100
4	Q	142/147 (97%)	129 (91%)	12 (8%)	1 (1%)	22	11
5	E	102/109 (94%)	101 (99%)	1 (1%)	0	100	100
5	R	102/109 (94%)	102 (100%)	0	0	100	100
6	F	91/98 (93%)	87 (96%)	2 (2%)	2 (2%)	6	1
6	S	91/98 (93%)	85 (93%)	5 (6%)	1 (1%)	14	5
7	G	81/85 (95%)	69 (85%)	7 (9%)	5 (6%)	1	0
7	T	81/85 (95%)	66 (82%)	10 (12%)	5 (6%)	1	0
8	H	73/85 (86%)	69 (94%)	1 (1%)	3 (4%)	3	0
8	U	73/85 (86%)	66 (90%)	5 (7%)	2 (3%)	5	1
9	I	69/73 (94%)	66 (96%)	3 (4%)	0	100	100
9	V	69/73 (94%)	67 (97%)	2 (3%)	0	100	100
10	J	55/59 (93%)	55 (100%)	0	0	100	100
10	W	55/59 (93%)	55 (100%)	0	0	100	100
11	K	47/56 (84%)	47 (100%)	0	0	100	100
11	X	47/56 (84%)	46 (98%)	1 (2%)	0	100	100
12	L	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/47 (94%)	42 (96%)	2 (4%)	0	100	100
13	M	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
13	Z	41/46 (89%)	40 (98%)	0	1 (2%)	6	1
All	All	3478/3614 (96%)	3328 (96%)	128 (4%)	22 (1%)	25	14

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	GLU
6	F	95	GLN
7	G	4	ALA

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Mol	Chain	Res	Type
7	G	7	ASP
7	G	8	HIS
8	H	45	ALA
8	H	46	LYS
6	S	94	HIS
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
8	U	45	ALA
6	F	94	HIS
8	H	47	GLY
8	U	46	LYS
13	Z	41	LYS
7	G	6	GLY
7	G	37	LEU
4	Q	34	SER
7	T	3	ALA
7	T	6	GLY
2	O	92	ASN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	426/426 (100%)	415 (97%)	11 (3%)	46	36
1	N	426/426 (100%)	413 (97%)	13 (3%)	40	28
2	B	210/210 (100%)	198 (94%)	12 (6%)	20	9
2	O	210/210 (100%)	197 (94%)	13 (6%)	18	7
3	C	224/226 (99%)	217 (97%)	7 (3%)	40	28
3	P	224/226 (99%)	215 (96%)	9 (4%)	31	19
4	D	128/129 (99%)	127 (99%)	1 (1%)	81	80
4	Q	128/129 (99%)	121 (94%)	7 (6%)	21	9
5	E	91/95 (96%)	90 (99%)	1 (1%)	73	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	R	91/95 (96%)	88 (97%)	3 (3%)	38	26
6	F	79/81 (98%)	73 (92%)	6 (8%)	13	4
6	S	79/81 (98%)	73 (92%)	6 (8%)	13	4
7	G	67/68 (98%)	58 (87%)	9 (13%)	4	0
7	T	67/68 (98%)	58 (87%)	9 (13%)	4	0
8	H	67/75 (89%)	64 (96%)	3 (4%)	27	15
8	U	67/75 (89%)	62 (92%)	5 (8%)	13	4
9	I	56/57 (98%)	51 (91%)	5 (9%)	9	2
9	V	56/57 (98%)	52 (93%)	4 (7%)	14	5
10	J	48/50 (96%)	47 (98%)	1 (2%)	53	46
10	W	48/50 (96%)	47 (98%)	1 (2%)	53	46
11	K	39/46 (85%)	37 (95%)	2 (5%)	24	11
11	X	39/46 (85%)	37 (95%)	2 (5%)	24	11
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	36
12	Y	39/40 (98%)	37 (95%)	2 (5%)	24	11
13	M	37/38 (97%)	31 (84%)	6 (16%)	2	0
13	Z	37/38 (97%)	34 (92%)	3 (8%)	11	3
All	All	3022/3082 (98%)	2880 (95%)	142 (5%)	26	13

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	38	ARG
1	A	109	PHE
1	A	115	SER
1	A	138	HIS
1	A	180	GLN
1	A	238	PHE
1	A	278	MET
1	A	338	MET
1	A	369	ASP
1	A	504	THR
2	B	16	ILE
2	B	33	LEU
2	B	60	GLU

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Mol	Chain	Res	Type
2	B	65	TRP
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	115	ASP
2	B	158	ASP
2	B	167	SER
2	B	171	LYS
3	C	23	SER
3	C	77	LYS
3	C	80	ARG
3	C	127	LEU
3	C	159	MET
3	C	223	LEU
3	C	230	ASN
4	D	51	LEU
5	E	90	ARG
6	F	37	LYS
6	F	48	LEU
6	F	53	THR
6	F	78	GLU
6	F	95	GLN
6	F	96	LEU
7	G	2	SER
7	G	17	ARG
7	G	18	PHE
7	G	33	LEU
7	G	36	TRP
7	G	43	GLU
7	G	54	ARG
7	G	74	ARG
7	G	84	LYS
8	H	40	GLU
8	H	60	TYR
8	H	61	LYS
9	I	8	GLN
9	I	15	ARG
9	I	26	MET
9	I	37	PHE
9	I	61	GLU
10	J	50	LEU

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Mol	Chain	Res	Type
11	K	47	ARG
11	K	54	ARG
12	L	46	LYS
13	M	4	LYS
13	M	13	LYS
13	M	34	LEU
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	278	MET
1	N	338	MET
1	N	361	SER
1	N	369	ASP
1	N	394	VAL
1	N	484	THR
1	N	504	THR
2	O	33	LEU
2	O	60	GLU
2	O	65	TRP
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	94	SER
2	O	110	TYR
2	O	115	ASP
2	O	116	LEU
2	O	148	MET
2	O	217	LYS
2	O	227	LEU
3	P	29	SER
3	P	33	MET
3	P	40	MET
3	P	127	LEU
3	P	159	MET
3	P	161	GLN
3	P	214	PHE

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Mol	Chain	Res	Type
3	P	223	LEU
3	P	230	ASN
4	Q	5	VAL
4	Q	9	GLU
4	Q	10	ASP
4	Q	19	ARG
4	Q	31	LYS
4	Q	51	LEU
4	Q	63	LYS
5	R	79	LYS
5	R	90	ARG
5	R	108	LYS
6	S	37	LYS
6	S	48	LEU
6	S	53	THR
6	S	87	THR
6	S	94	HIS
6	S	95	GLN
7	T	2	SER
7	T	18	PHE
7	T	33	LEU
7	T	36	TRP
7	T	37	LEU
7	T	38	HIS
7	T	54	ARG
7	T	74	ARG
7	T	84	LYS
8	U	29	CYS
8	U	41	LYS
8	U	44	THR
8	U	60	TYR
8	U	61	LYS
9	V	8	GLN
9	V	26	MET
9	V	29	LEU
9	V	36	LYS
10	W	50	LEU
11	X	47	ARG
11	X	54	ARG
12	Y	16	GLU
12	Y	20	ARG
13	Z	13	LYS

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

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

Mol	Chain	Res	Type
1	A	4	ASN
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	10	GLN
2	B	22	HIS
2	B	91	ASN
2	B	181	GLN
3	C	3	HIS
3	C	68	GLN
3	C	149	HIS
4	D	37	GLN
4	D	101	HIS
4	D	109	HIS
5	E	94	ASN
7	G	34	ASN
7	G	38	HIS
7	G	76	ASN
9	I	8	GLN
10	J	29	ASN
10	J	57	HIS
11	K	35	GLN
1	N	178	GLN
1	N	180	GLN
1	N	413	HIS
1	N	512	ASN
2	O	10	GLN
2	O	22	HIS
2	O	195	GLN
3	P	68	GLN
3	P	76	GLN
3	P	149	HIS
3	P	161	GLN
4	Q	32	ASN
4	Q	37	GLN
4	Q	101	HIS

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Mol	Chain	Res	Type
5	R	94	ASN
6	S	28	GLN
6	S	80	GLN
6	S	94	HIS
6	S	95	GLN
7	T	76	ASN
10	W	29	ASN
10	W	57	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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$
2	FME	O	1	2	8,9,10	0.94	1 (12%)	7,9,11	5.69	4 (57%)
1	FME	N	1	1	8,9,10	0.86	0	7,9,11	6.19	4 (57%)
2	FME	B	1	2	8,9,10	1.90	3 (37%)	7,9,11	6.74	3 (42%)
7	TPO	G	11	7	8,10,11	2.15	3 (37%)	10,14,16	2.24	4 (40%)
1	FME	A	1	1	8,9,10	0.96	1 (12%)	7,9,11	4.97	3 (42%)
7	TPO	T	11	7	8,10,11	2.01	5 (62%)	10,14,16	1.94	2 (20%)

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	11	TPO	P-O1P	4.01	1.63	1.50
2	B	1	FME	O1-CN	-3.67	1.11	1.22
7	T	11	TPO	P-O1P	3.33	1.61	1.50
7	G	11	TPO	P-O2P	2.34	1.63	1.54
2	B	1	FME	CB-CG	2.34	1.60	1.51
2	B	1	FME	CG-SD	-2.32	1.69	1.81
1	A	1	FME	O1-CN	-2.29	1.15	1.22
7	G	11	TPO	P-OG1	2.23	1.63	1.59
7	T	11	TPO	P-O3P	2.17	1.63	1.54
2	O	1	FME	O1-CN	-2.10	1.16	1.22
7	T	11	TPO	P-OG1	2.06	1.63	1.59
7	T	11	TPO	CG2-CB	2.06	1.56	1.51
7	T	11	TPO	P-O2P	2.03	1.62	1.54

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-16.38	97.64	122.82
1	N	1	FME	CA-N-CN	-15.33	99.25	122.82
2	O	1	FME	CA-N-CN	-13.71	101.73	122.82
1	A	1	FME	CA-N-CN	-12.21	104.05	122.82
2	B	1	FME	O1-CN-N	5.27	139.14	125.27
7	T	11	TPO	CG2-CB-CA	4.91	122.86	113.16
1	N	1	FME	CE-SD-CG	4.82	116.95	100.40
7	G	11	TPO	CG2-CB-CA	4.67	122.37	113.16
2	O	1	FME	CG-CB-CA	-4.28	101.06	112.95
1	A	1	FME	CE-SD-CG	4.25	114.99	100.40
2	B	1	FME	CB-CG-SD	-3.72	93.50	113.48
7	G	11	TPO	O2P-P-OG1	3.48	121.61	105.99
2	O	1	FME	C-CA-N	3.29	115.66	109.73
7	T	11	TPO	O-C-CA	-2.49	118.25	124.78
1	A	1	FME	O-C-CA	-2.30	118.75	124.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	1	FME	O1-CN-N	2.23	131.15	125.27
2	O	1	FME	CE-SD-CG	2.18	107.88	100.40
7	G	11	TPO	OG1-P-O1P	-2.13	101.19	109.39
7	G	11	TPO	O-C-CA	-2.08	119.31	124.78
1	N	1	FME	O-C-CA	-2.02	119.49	124.78

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	O	1	FME	O1-CN-N-CA
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
2	B	1	FME	O1-CN-N-CA
7	G	11	TPO	N-CA-CB-CG2
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	C-CA-CB-CG2
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
7	T	11	TPO	O-C-CA-CB
2	O	1	FME	CB-CG-SD-CE
7	T	11	TPO	CB-OG1-P-O3P
1	N	1	FME	CB-CG-SD-CE
1	N	1	FME	C-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
7	G	11	TPO	O-C-CA-CB

There are no ring outliers.

3 monomers are involved in 3 short contacts:

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

## 5.5 Carbohydrates

There are no carbohydrates in this entry.



## 5.6 Ligand geometry ⓘ

Of 56 ligands modelled in this entry, 2 are unknown and 8 are monoatomic - leaving 46 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
24	PEK	G	265	-	52,52,52	1.79	5 (9%)	55,57,57	1.38	6 (10%)
28	DMU	P	1272	-	34,34,34	1.32	3 (8%)	45,45,45	3.09	22 (48%)
22	CHD	O	229	-	29,32,32	1.39	5 (17%)	48,51,51	5.68	36 (75%)
18	HEA	A	515	1	44,67,67	1.35	6 (13%)	37,103,103	2.50	18 (48%)
25	CDL	G	269	-	99,99,99	1.49	13 (13%)	105,111,111	1.52	17 (16%)
15	PER	A	520	18,14	0,1,1	0.00	-	-		
19	TGL	A	521	-	62,62,62	1.22	7 (11%)	65,65,65	2.01	12 (18%)
28	DMU	Z	1526	-	34,34,34	1.11	3 (8%)	45,45,45	3.33	23 (51%)
22	CHD	W	1060	-	29,32,32	0.70	0	48,51,51	5.20	35 (72%)
19	TGL	L	522	-	62,62,62	1.60	7 (11%)	65,65,65	1.95	18 (27%)
21	CUA	B	228	2	0,1,1	0.00	-	-		
26	PSC	E	230	-	51,51,51	1.32	3 (5%)	57,59,59	1.15	5 (8%)
22	CHD	B	1086	-	29,32,32	1.30	4 (13%)	48,51,51	5.83	35 (72%)
28	DMU	M	526	-	34,34,34	0.94	1 (2%)	45,45,45	3.20	23 (51%)
25	CDL	P	1270	-	99,99,99	1.42	13 (13%)	105,111,111	1.47	14 (13%)
20	PGV	H	268	-	50,50,50	1.34	2 (4%)	53,56,56	1.50	8 (15%)
24	PEK	P	1264	-	52,52,52	1.02	4 (7%)	55,57,57	1.77	10 (18%)
24	PEK	C	264	-	52,52,52	0.98	3 (5%)	55,57,57	1.50	12 (21%)
25	CDL	T	1269	-	99,99,99	1.39	12 (12%)	105,111,111	1.42	17 (16%)
20	PGV	N	1268	-	50,50,50	1.22	3 (6%)	53,56,56	1.46	6 (11%)
22	CHD	J	60	-	29,32,32	0.78	0	48,51,51	5.05	37 (77%)
18	HEA	N	515	1	44,67,67	1.16	4 (9%)	37,103,103	2.32	10 (27%)
18	HEA	N	516	1,15	44,67,67	1.20	5 (11%)	37,103,103	2.51	13 (35%)
26	PSC	R	1230	-	51,51,51	1.20	3 (5%)	57,59,59	1.20	5 (8%)
20	PGV	N	1266	-	50,50,50	0.89	2 (4%)	53,56,56	1.58	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	TGL	O	1523	-	62,62,62	1.41	6 (9%)	65,65,65	1.44	10 (15%)
22	CHD	C	271	-	29,32,32	1.17	2 (6%)	48,51,51	5.44	34 (70%)
15	PER	N	520	18,14	0,1,1	0.00	-	-		
24	PEK	T	1265	-	52,52,52	1.23	2 (3%)	55,57,57	1.38	6 (10%)
19	TGL	D	523	-	62,62,62	1.60	7 (11%)	65,65,65	1.61	16 (24%)
18	HEA	A	516	1,15	44,67,67	1.47	6 (13%)	37,103,103	2.19	10 (27%)
19	TGL	O	1521	-	62,62,62	1.33	6 (9%)	65,65,65	1.56	12 (18%)
22	CHD	P	1525	-	29,32,32	1.41	2 (6%)	48,51,51	5.76	39 (81%)
24	PEK	G	1263	-	52,52,52	1.17	2 (3%)	55,57,57	1.33	5 (9%)
20	PGV	A	524	-	50,50,50	1.23	3 (6%)	53,56,56	1.60	10 (18%)
22	CHD	P	1271	-	29,32,32	0.86	1 (3%)	48,51,51	5.43	31 (64%)
20	PGV	C	267	-	50,50,50	0.97	2 (4%)	53,56,56	1.29	5 (9%)
24	PEK	T	263	-	52,52,52	1.20	2 (3%)	55,57,57	1.39	7 (12%)
28	DMU	G	272	-	34,34,34	1.32	4 (11%)	45,45,45	3.47	24 (53%)
22	CHD	C	525	-	29,32,32	1.67	6 (20%)	48,51,51	5.64	39 (81%)
20	PGV	P	1267	-	50,50,50	0.90	2 (4%)	53,56,56	1.45	10 (18%)
19	TGL	Y	1522	-	62,62,62	1.54	6 (9%)	65,65,65	1.62	17 (26%)
21	CUA	O	228	2	0,1,1	0.00	-	-		
20	PGV	N	1524	-	50,50,50	1.07	2 (4%)	53,56,56	1.53	6 (11%)
20	PGV	A	522	-	50,50,50	1.09	3 (6%)	53,56,56	1.50	7 (13%)
25	CDL	C	270	-	99,99,99	1.39	14 (14%)	105,111,111	1.59	16 (15%)

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
24	PEK	G	265	-	-	30/56/56/56	-
22	CHD	O	229	-	-	0/7/74/74	0/4/4/4
18	HEA	A	515	1	3/3/7/16	4/24/76/76	-
25	CDL	G	269	-	-	66/110/110/110	-
22	CHD	P	1271	-	1/1/12/12	2/7/74/74	0/4/4/4
24	PEK	T	263	-	-	28/56/56/56	-
19	TGL	A	521	-	-	32/65/65/65	-
28	DMU	Z	1526	-	5/5/10/10	11/19/59/59	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CHD	W	1060	-	2/2/12/12	4/7/74/74	0/4/4/4
19	TGL	L	522	-	-	34/65/65/65	-
24	PEK	P	1264	-	-	19/56/56/56	-
22	CHD	B	1086	-	1/1/12/12	0/7/74/74	0/4/4/4
28	DMU	M	526	-	4/4/10/10	10/19/59/59	0/2/2/2
25	CDL	P	1270	-	-	62/110/110/110	-
20	PGV	H	268	-	-	35/55/55/55	-
26	PSC	E	230	-	-	38/55/55/55	-
24	PEK	C	264	-	-	21/56/56/56	-
25	CDL	T	1269	-	-	59/110/110/110	-
20	PGV	N	1268	-	-	27/55/55/55	-
22	CHD	J	60	-	2/2/12/12	4/7/74/74	0/4/4/4
18	HEA	N	515	1	3/3/7/16	3/24/76/76	-
18	HEA	N	516	1,15	3/3/7/16	2/24/76/76	-
26	PSC	R	1230	-	-	30/55/55/55	-
20	PGV	N	1266	-	-	15/55/55/55	-
19	TGL	O	1523	-	-	31/65/65/65	-
22	CHD	C	271	-	1/1/12/12	4/7/74/74	0/4/4/4
24	PEK	T	1265	-	-	33/56/56/56	-
19	TGL	D	523	-	-	34/65/65/65	-
18	HEA	A	516	1,15	3/3/7/16	1/24/76/76	-
19	TGL	O	1521	-	-	32/65/65/65	-
22	CHD	P	1525	-	-	2/7/74/74	0/4/4/4
24	PEK	G	1263	-	-	31/56/56/56	-
20	PGV	A	524	-	-	28/55/55/55	-
20	PGV	C	267	-	-	13/55/55/55	-
28	DMU	P	1272	-	4/4/10/10	10/19/59/59	0/2/2/2
28	DMU	G	272	-	5/5/10/10	10/19/59/59	0/2/2/2
22	CHD	C	525	-	-	0/7/74/74	0/4/4/4
20	PGV	P	1267	-	-	15/55/55/55	-
19	TGL	Y	1522	-	-	40/65/65/65	-
20	PGV	N	1524	-	-	33/55/55/55	-
20	PGV	A	522	-	-	16/55/55/55	-
25	CDL	C	270	-	-	65/110/110/110	-

All (186) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	265	PEK	C9-C8	7.82	1.77	1.31
19	L	522	TGL	OG2-CB1	6.61	1.52	1.34
19	Y	1522	TGL	OG2-CB1	6.57	1.52	1.34
19	D	523	TGL	OG1-CA1	6.45	1.52	1.33
20	H	268	PGV	O01-C1	6.43	1.52	1.34
25	G	269	CDL	OB6-CB5	6.06	1.51	1.34
24	T	1265	PEK	O01-C1	5.93	1.51	1.34
24	G	1263	PEK	O03-C21	5.58	1.49	1.33
25	C	270	CDL	OA8-CA7	5.55	1.49	1.33
25	G	269	CDL	OA6-CA5	5.52	1.49	1.34
20	N	1268	PGV	O01-C1	5.49	1.49	1.34
25	P	1270	CDL	OA8-CA7	5.42	1.49	1.33
19	O	1523	TGL	OG2-CB1	5.38	1.49	1.34
24	T	263	PEK	O03-C21	5.34	1.48	1.33
26	E	230	PSC	O01-C1	5.25	1.49	1.34
28	P	1272	DMU	O16-C6	5.22	1.49	1.40
19	O	1523	TGL	OG1-CA1	5.21	1.48	1.33
19	L	522	TGL	OG1-CA1	5.20	1.48	1.33
24	G	265	PEK	O01-C1	5.17	1.48	1.34
19	L	522	TGL	OG3-CC1	5.14	1.48	1.33
20	A	524	PGV	O03-C19	5.05	1.48	1.33
19	Y	1522	TGL	OG3-CC1	5.02	1.48	1.33
19	Y	1522	TGL	OG1-CA1	5.02	1.48	1.33
19	O	1521	TGL	OG2-CB1	5.02	1.48	1.34
20	H	268	PGV	O03-C19	4.97	1.47	1.33
26	E	230	PSC	O03-C19	4.95	1.47	1.33
25	T	1269	CDL	OB6-CB5	4.94	1.48	1.34
25	T	1269	CDL	OA6-CA5	4.89	1.48	1.34
19	D	523	TGL	OB1-CB1	4.88	1.37	1.22
24	G	265	PEK	O03-C21	4.86	1.47	1.33
24	T	1265	PEK	O03-C21	4.85	1.47	1.33
28	G	272	DMU	O16-C6	4.82	1.48	1.40
24	T	263	PEK	O01-C1	4.81	1.47	1.34
19	O	1521	TGL	OG1-CA1	4.80	1.47	1.33
25	G	269	CDL	OB8-CB7	4.77	1.47	1.33
25	P	1270	CDL	OB8-CB7	4.76	1.47	1.33
19	O	1523	TGL	OG3-CC1	4.73	1.47	1.33
25	T	1269	CDL	OB8-CB7	4.62	1.46	1.33
19	D	523	TGL	OG3-CC1	4.56	1.46	1.33
25	G	269	CDL	OA8-CA7	4.53	1.46	1.33
25	P	1270	CDL	OA6-CA5	4.53	1.47	1.34
20	N	1524	PGV	O03-C19	4.52	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	270	CDL	OA6-CA5	4.51	1.47	1.34
26	R	1230	PSC	O01-C1	4.50	1.47	1.34
19	D	523	TGL	OG2-CB1	4.45	1.46	1.34
20	A	524	PGV	O01-C1	4.40	1.46	1.34
22	P	1525	CHD	C13-C14	-4.38	1.48	1.55
24	G	265	PEK	C10-C9	4.30	1.81	1.51
19	A	521	TGL	OG1-CA1	4.30	1.45	1.33
20	N	1268	PGV	O03-C19	4.23	1.45	1.33
18	A	516	HEA	CMD-C2D	4.21	1.61	1.51
19	A	521	TGL	OG2-CB1	4.21	1.46	1.34
22	C	525	CHD	C13-C12	-4.19	1.48	1.54
18	A	515	HEA	O11-C11	4.18	1.52	1.42
25	P	1270	CDL	OB6-CB5	4.17	1.46	1.34
20	N	1524	PGV	O01-C1	4.15	1.46	1.34
24	P	1264	PEK	O03-C01	-4.05	1.35	1.45
26	R	1230	PSC	O03-C19	4.03	1.45	1.33
25	T	1269	CDL	OA8-CA7	4.02	1.45	1.33
24	G	1263	PEK	O01-C1	4.00	1.45	1.34
19	O	1521	TGL	OG3-CC1	3.99	1.45	1.33
24	C	264	PEK	O01-C1	3.97	1.45	1.34
28	Z	1526	DMU	C3-C4	-3.97	1.42	1.52
26	E	230	PSC	C13-C12	3.91	1.54	1.31
20	A	522	PGV	O01-C1	3.88	1.45	1.34
20	A	522	PGV	O03-C19	3.87	1.44	1.33
19	L	522	TGL	C20-CA9	-3.85	1.30	1.51
20	N	1266	PGV	O01-C1	3.80	1.45	1.34
26	R	1230	PSC	C13-C12	3.78	1.53	1.31
25	C	270	CDL	OB8-CB7	3.75	1.44	1.33
25	T	1269	CDL	C59-C58	-3.60	1.31	1.51
25	G	269	CDL	C59-C58	-3.56	1.31	1.51
19	O	1521	TGL	C10-CB9	-3.50	1.32	1.51
24	P	1264	PEK	O01-C1	3.47	1.44	1.34
19	A	521	TGL	OG3-CC1	3.46	1.43	1.33
20	C	267	PGV	O01-C1	3.43	1.44	1.34
25	T	1269	CDL	C62-C61	-3.40	1.32	1.51
19	Y	1522	TGL	C20-CA9	-3.40	1.32	1.51
24	G	265	PEK	C7-C8	3.40	1.75	1.51
25	C	270	CDL	C79-C78	-3.33	1.32	1.51
25	C	270	CDL	C59-C58	-3.33	1.32	1.51
19	Y	1522	TGL	C10-CB9	-3.32	1.32	1.51
19	L	522	TGL	C10-CB9	-3.32	1.32	1.51
25	P	1270	CDL	C59-C58	-3.28	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	N	515	HEA	C3A-C2A	3.26	1.44	1.40
18	N	515	HEA	CMD-C2D	3.20	1.59	1.51
25	G	269	CDL	C19-C18	-3.19	1.33	1.51
20	P	1267	PGV	O03-C19	3.18	1.42	1.33
25	T	1269	CDL	C42-C41	-3.18	1.33	1.51
25	C	270	CDL	C39-C38	-3.18	1.33	1.51
18	A	516	HEA	C18-C19	3.17	1.40	1.33
25	C	270	CDL	C62-C61	-3.17	1.33	1.51
18	N	516	HEA	O11-C11	3.12	1.49	1.42
25	C	270	CDL	C82-C81	-3.07	1.34	1.51
24	C	264	PEK	O03-C21	3.04	1.42	1.33
25	P	1270	CDL	C22-C21	-3.04	1.34	1.51
25	G	269	CDL	C22-C21	-3.03	1.34	1.51
18	A	516	HEA	CAD-C3D	3.03	1.56	1.52
19	O	1523	TGL	C10-CB9	-3.01	1.34	1.51
19	A	521	TGL	C10-CB9	-3.01	1.34	1.51
25	P	1270	CDL	C19-C18	-3.00	1.34	1.51
25	P	1270	CDL	C79-C78	-2.99	1.34	1.51
22	C	525	CHD	C13-C14	-2.99	1.50	1.55
25	G	269	CDL	C42-C41	-2.98	1.34	1.51
19	O	1521	TGL	C20-CA9	-2.96	1.35	1.51
20	N	1266	PGV	O03-C19	2.93	1.41	1.33
22	C	525	CHD	C6-C7	-2.93	1.47	1.52
25	G	269	CDL	C62-C61	-2.93	1.35	1.51
19	O	1523	TGL	C20-CA9	-2.93	1.35	1.51
19	O	1523	TGL	C15-CC9	-2.91	1.35	1.51
25	C	270	CDL	C22-C21	-2.90	1.35	1.51
25	C	270	CDL	C19-C18	-2.89	1.35	1.51
25	P	1270	CDL	C39-C38	-2.86	1.35	1.51
19	A	521	TGL	C20-CA9	-2.86	1.35	1.51
18	A	515	HEA	C1C-CHC	2.85	1.48	1.41
25	T	1269	CDL	C19-C18	-2.84	1.35	1.51
25	P	1270	CDL	C62-C61	-2.84	1.35	1.51
20	C	267	PGV	O03-C19	2.82	1.41	1.33
22	C	271	CHD	C10-C5	-2.80	1.50	1.55
25	T	1269	CDL	C82-C81	-2.79	1.35	1.51
25	C	270	CDL	OB6-CB5	2.79	1.42	1.34
25	P	1270	CDL	C82-C81	-2.79	1.35	1.51
18	A	516	HEA	O11-C11	2.79	1.49	1.42
20	P	1267	PGV	O01-C1	2.79	1.42	1.34
18	N	516	HEA	C18-C19	2.78	1.39	1.33
19	Y	1522	TGL	C15-CC9	-2.77	1.36	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	270	CDL	C42-C41	-2.72	1.36	1.51
19	D	523	TGL	C10-CB9	-2.72	1.36	1.51
19	O	1521	TGL	C15-CC9	-2.69	1.36	1.51
25	G	269	CDL	C79-C78	-2.69	1.36	1.51
25	T	1269	CDL	C39-C38	-2.69	1.36	1.51
25	G	269	CDL	C39-C38	-2.68	1.36	1.51
25	T	1269	CDL	C79-C78	-2.68	1.36	1.51
22	B	1086	CHD	C11-C12	2.68	1.57	1.53
19	D	523	TGL	C15-CC9	-2.68	1.36	1.51
22	O	229	CHD	C1-C10	-2.68	1.49	1.54
19	D	523	TGL	C20-CA9	-2.67	1.36	1.51
25	G	269	CDL	C82-C81	-2.64	1.36	1.51
22	O	229	CHD	C13-C12	-2.62	1.50	1.54
19	L	522	TGL	C15-CC9	-2.61	1.36	1.51
22	C	525	CHD	C1-C10	-2.59	1.49	1.54
22	B	1086	CHD	C10-C5	-2.59	1.51	1.55
20	A	524	PGV	C2-C1	-2.59	1.43	1.50
25	T	1269	CDL	C22-C21	-2.58	1.37	1.51
28	M	526	DMU	C3-C4	-2.56	1.46	1.52
18	N	516	HEA	C4C-CHD	2.55	1.48	1.41
19	A	521	TGL	C15-CC9	-2.54	1.37	1.51
18	A	515	HEA	C3C-C2C	2.53	1.43	1.40
22	O	229	CHD	C18-C13	-2.51	1.50	1.54
22	C	525	CHD	C18-C13	2.50	1.58	1.54
22	P	1525	CHD	C10-C5	-2.50	1.51	1.55
22	C	525	CHD	C10-C5	-2.50	1.51	1.55
25	P	1270	CDL	C42-C41	-2.47	1.37	1.51
25	C	270	CDL	OB6-CB4	-2.45	1.40	1.46
18	A	516	HEA	C1C-CHC	2.45	1.47	1.41
28	Z	1526	DMU	O1-C10	2.43	1.48	1.41
22	B	1086	CHD	C11-C9	-2.43	1.49	1.53
18	A	516	HEA	C3C-CAC	2.41	1.52	1.47
25	P	1270	CDL	PB2-OB2	2.40	1.69	1.59
24	P	1264	PEK	O03-C21	2.40	1.40	1.33
22	O	229	CHD	C1-C2	-2.37	1.48	1.53
18	A	515	HEA	C4D-ND	2.34	1.41	1.36
22	O	229	CHD	C10-C5	-2.34	1.51	1.55
19	L	522	TGL	CG3-CG2	2.33	1.57	1.50
28	G	272	DMU	C3-C4	-2.30	1.46	1.52
28	P	1272	DMU	C3-C4	-2.30	1.46	1.52
28	G	272	DMU	O1-C10	2.29	1.47	1.41
20	A	522	PGV	P-O14	-2.28	1.44	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	P	1264	PEK	C2-C1	2.27	1.57	1.50
19	A	521	TGL	OC1-CC1	-2.27	1.15	1.22
18	N	515	HEA	O11-C11	2.27	1.48	1.42
18	N	515	HEA	C3B-C11	-2.24	1.51	1.52
22	C	271	CHD	C20-C17	2.24	1.58	1.54
24	C	264	PEK	O03-C01	-2.22	1.40	1.45
28	Z	1526	DMU	O16-C6	2.20	1.44	1.40
22	B	1086	CHD	C13-C12	-2.14	1.51	1.54
18	N	516	HEA	C17-C18	2.12	1.57	1.50
25	C	270	CDL	PA1-OA5	2.10	1.67	1.59
18	A	515	HEA	CMB-C2B	2.08	1.56	1.51
25	G	269	CDL	C71-CB7	2.08	1.56	1.50
28	P	1272	DMU	O1-C10	2.07	1.47	1.41
28	G	272	DMU	C2-C1	2.04	1.57	1.52
18	N	516	HEA	C1B-NB	-2.03	1.32	1.36
22	P	1271	CHD	C20-C17	2.02	1.57	1.54
18	A	515	HEA	C3B-C11	-2.01	1.51	1.52
20	N	1268	PGV	P-O11	2.01	1.67	1.59

All (693) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1086	CHD	C18-C13-C12	-15.14	93.65	109.07
22	P	1271	CHD	C10-C9-C8	14.20	127.07	111.82
22	O	229	CHD	C6-C5-C10	14.18	127.72	112.66
22	W	1060	CHD	C10-C9-C8	14.10	126.96	111.82
22	B	1086	CHD	C6-C5-C10	13.91	127.42	112.66
22	C	525	CHD	C1-C10-C5	13.42	127.62	107.77
22	P	1525	CHD	C6-C5-C10	13.02	126.48	112.66
22	P	1525	CHD	C1-C10-C5	12.80	126.71	107.77
22	J	60	CHD	C10-C9-C8	12.50	125.24	111.82
22	C	525	CHD	C6-C5-C10	12.44	125.87	112.66
22	C	271	CHD	C10-C9-C8	12.34	125.07	111.82
22	P	1271	CHD	C18-C13-C12	-11.92	96.93	109.07
22	P	1525	CHD	C18-C13-C12	-11.76	97.09	109.07
22	B	1086	CHD	C17-C13-C12	11.48	128.15	117.67
22	O	229	CHD	C1-C10-C5	11.42	124.66	107.77
22	C	525	CHD	C18-C13-C12	-11.35	97.51	109.07
22	P	1525	CHD	C14-C13-C12	10.91	117.56	107.40
22	C	525	CHD	C4-C3-C2	10.89	123.56	110.55
22	O	229	CHD	C10-C9-C8	10.59	123.20	111.82
22	B	1086	CHD	C1-C10-C5	10.59	123.44	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	525	CHD	C10-C9-C8	10.55	123.14	111.82
22	O	229	CHD	C19-C10-C9	-10.41	96.84	111.18
22	C	525	CHD	C19-C10-C9	-10.25	97.06	111.18
22	C	525	CHD	C17-C13-C12	10.24	127.02	117.67
22	B	1086	CHD	C19-C10-C9	-10.20	97.13	111.18
22	P	1525	CHD	C17-C13-C12	10.03	126.82	117.67
22	B	1086	CHD	C10-C9-C8	10.03	122.59	111.82
22	P	1525	CHD	C10-C9-C8	9.91	122.46	111.82
22	P	1525	CHD	C4-C3-C2	9.73	122.17	110.55
22	B	1086	CHD	C6-C7-C8	9.68	121.81	111.48
22	C	271	CHD	C18-C13-C12	-9.44	99.46	109.07
22	O	229	CHD	C17-C13-C14	9.23	109.40	100.09
22	O	229	CHD	C14-C13-C12	9.18	115.95	107.40
22	P	1525	CHD	C15-C14-C13	9.13	112.50	103.55
22	P	1271	CHD	C6-C5-C10	8.96	122.17	112.66
22	C	271	CHD	C21-C20-C22	-8.93	96.37	110.36
22	O	229	CHD	C17-C13-C12	8.79	125.69	117.67
22	C	271	CHD	C14-C13-C12	8.76	115.56	107.40
22	B	1086	CHD	C14-C13-C12	8.74	115.54	107.40
22	P	1271	CHD	C17-C13-C12	8.69	125.60	117.67
22	P	1271	CHD	C19-C10-C9	-8.61	99.32	111.18
22	O	229	CHD	C18-C13-C12	-8.60	100.31	109.07
22	O	229	CHD	C6-C5-C4	-8.54	101.35	111.19
22	P	1271	CHD	C1-C2-C3	8.50	121.37	110.47
22	J	60	CHD	C1-C10-C5	8.47	120.30	107.77
22	C	271	CHD	C17-C13-C12	8.37	125.30	117.67
22	B	1086	CHD	C9-C11-C12	8.35	125.33	114.30
22	W	1060	CHD	C13-C17-C20	8.33	129.44	119.50
19	A	521	TGL	CG2-OG2-CB1	8.20	137.99	117.79
22	W	1060	CHD	C17-C13-C12	8.20	125.15	117.67
22	W	1060	CHD	C1-C10-C5	8.18	119.87	107.77
22	C	271	CHD	C16-C17-C20	8.17	124.79	112.15
22	C	271	CHD	C6-C5-C10	8.14	121.30	112.66
22	C	271	CHD	C18-C13-C17	-8.08	98.56	111.21
22	O	229	CHD	C18-C13-C17	-8.07	98.58	111.21
22	B	1086	CHD	C1-C2-C3	8.06	120.81	110.47
18	A	516	HEA	C13-C12-C11	-7.99	102.35	114.35
22	P	1271	CHD	C1-C10-C5	7.93	119.49	107.77
22	C	271	CHD	C19-C10-C9	-7.91	100.29	111.18
22	W	1060	CHD	C6-C7-C8	7.88	119.89	111.48
28	G	272	DMU	O16-C6-C1	7.84	120.55	108.30
22	J	60	CHD	C4-C3-C2	7.82	119.89	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	P	1272	DMU	O1-C9-C8	7.79	123.83	109.69
22	C	271	CHD	C1-C10-C5	7.78	119.28	107.77
28	G	272	DMU	C18-O16-C6	7.62	126.48	113.84
20	N	1524	PGV	O01-C1-C2	7.51	127.69	111.50
22	O	229	CHD	O12-C12-C13	-7.51	98.34	111.03
28	M	526	DMU	O1-C9-C8	7.48	123.27	109.69
22	C	271	CHD	C4-C3-C2	7.36	119.34	110.55
22	J	60	CHD	C6-C7-C8	7.34	119.32	111.48
22	P	1271	CHD	C6-C7-C8	7.31	119.28	111.48
22	C	271	CHD	C6-C7-C8	7.31	119.28	111.48
28	M	526	DMU	O1-C10-C5	7.25	125.69	110.35
18	N	515	HEA	C27-C19-C20	7.24	127.44	115.27
22	J	60	CHD	C14-C13-C12	7.18	114.08	107.40
22	P	1525	CHD	C5-C4-C3	7.14	123.25	112.76
28	M	526	DMU	O5-C6-C1	7.10	125.38	110.35
22	P	1525	CHD	C19-C10-C9	-7.10	101.40	111.18
22	W	1060	CHD	C5-C6-C7	7.08	122.28	114.46
22	W	1060	CHD	C4-C3-C2	7.05	118.97	110.55
22	J	60	CHD	C13-C17-C20	7.05	127.91	119.50
22	C	271	CHD	C15-C14-C8	6.97	128.08	118.33
22	C	525	CHD	O12-C12-C13	-6.91	99.34	111.03
28	G	272	DMU	O1-C9-C8	6.90	122.22	109.69
22	J	60	CHD	C17-C13-C12	6.89	123.95	117.67
22	J	60	CHD	C5-C6-C7	6.87	122.04	114.46
22	P	1271	CHD	C16-C17-C13	6.84	110.26	103.55
22	C	525	CHD	C13-C17-C20	6.80	127.61	119.50
22	W	1060	CHD	C1-C2-C3	6.79	119.18	110.47
19	A	521	TGL	OG2-CB1-CB2	6.74	126.02	111.50
22	P	1271	CHD	C4-C3-C2	6.72	118.57	110.55
28	G	272	DMU	O5-C4-C57	6.71	123.11	106.44
22	C	525	CHD	C15-C14-C13	6.70	110.13	103.55
22	O	229	CHD	C9-C8-C7	6.64	119.81	111.88
22	C	271	CHD	C15-C14-C13	6.63	110.06	103.55
28	Z	1526	DMU	O5-C6-C1	6.63	124.38	110.35
22	P	1271	CHD	C15-C14-C8	6.58	127.53	118.33
22	W	1060	CHD	C5-C4-C3	6.56	122.40	112.76
22	C	525	CHD	C14-C13-C12	6.56	113.51	107.40
22	W	1060	CHD	C11-C12-C13	6.54	117.96	111.24
24	P	1264	PEK	C2-C3-C4	6.53	124.87	113.23
22	P	1271	CHD	O12-C12-C13	-6.53	99.99	111.03
22	O	229	CHD	C5-C4-C3	6.53	122.34	112.76
28	Z	1526	DMU	C8-C7-C5	6.53	122.22	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1086	CHD	C17-C13-C14	6.52	106.67	100.09
22	W	1060	CHD	C14-C13-C12	6.52	113.47	107.40
20	N	1268	PGV	O03-C19-C20	6.50	132.32	111.91
28	Z	1526	DMU	O1-C9-C8	6.49	121.48	109.69
22	C	271	CHD	O7-C7-C6	-6.48	93.87	109.94
28	Z	1526	DMU	O5-C4-C57	6.46	122.50	106.44
22	C	525	CHD	C6-C5-C4	-6.46	103.75	111.19
28	Z	1526	DMU	O1-C10-C5	6.44	123.98	110.35
22	J	60	CHD	C6-C5-C10	6.42	119.47	112.66
22	B	1086	CHD	C11-C9-C10	6.40	120.33	113.73
22	O	229	CHD	C18-C13-C14	-6.39	101.20	111.21
28	G	272	DMU	O1-C10-C5	6.36	123.81	110.35
22	B	1086	CHD	C5-C4-C3	6.36	122.10	112.76
22	O	229	CHD	C4-C3-C2	6.34	118.12	110.55
28	P	1272	DMU	O16-C6-C1	6.32	118.18	108.30
22	C	525	CHD	C9-C8-C7	6.32	119.43	111.88
22	P	1271	CHD	C4-C5-C10	6.31	119.36	112.66
22	W	1060	CHD	C6-C5-C10	6.31	119.36	112.66
22	P	1271	CHD	C5-C6-C7	6.29	121.40	114.46
22	P	1271	CHD	C16-C17-C20	6.28	121.86	112.15
22	J	60	CHD	C1-C2-C3	6.25	118.49	110.47
22	P	1271	CHD	C11-C9-C8	6.24	120.01	110.88
22	J	60	CHD	C5-C4-C3	6.24	121.92	112.76
22	W	1060	CHD	C9-C11-C12	6.23	122.53	114.30
22	J	60	CHD	C16-C17-C13	6.22	109.65	103.55
22	P	1525	CHD	C11-C9-C8	6.20	119.95	110.88
22	O	229	CHD	C1-C2-C3	6.19	118.42	110.47
22	P	1525	CHD	C18-C13-C17	-6.14	101.59	111.21
24	T	263	PEK	O01-C1-C2	6.12	124.70	111.50
22	C	271	CHD	C11-C9-C8	6.12	119.83	110.88
22	J	60	CHD	C16-C17-C20	6.12	121.62	112.15
22	P	1271	CHD	C11-C12-C13	6.08	117.49	111.24
22	J	60	CHD	C18-C13-C12	-6.08	102.88	109.07
28	Z	1526	DMU	O1-C9-C11	6.03	121.44	106.44
22	J	60	CHD	C11-C9-C8	6.01	119.67	110.88
22	W	1060	CHD	C16-C17-C13	6.00	109.44	103.55
28	Z	1526	DMU	O16-C6-C1	5.99	117.66	108.30
22	C	525	CHD	C11-C12-C13	5.99	117.39	111.24
22	P	1525	CHD	C9-C8-C7	5.96	119.00	111.88
22	C	271	CHD	C5-C6-C7	5.94	121.02	114.46
20	N	1266	PGV	O03-C19-C20	5.88	130.37	111.91
18	N	516	HEA	OMA-CMA-C3A	-5.84	112.19	124.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	P	1272	DMU	O5-C4-C3	5.83	122.05	109.75
22	C	271	CHD	C11-C12-C13	5.76	117.16	111.24
22	B	1086	CHD	C6-C5-C4	-5.75	104.57	111.19
22	C	271	CHD	C5-C4-C3	5.72	121.16	112.76
19	L	522	TGL	CG2-OG2-CB1	5.71	131.86	117.79
25	G	269	CDL	OB6-CB5-C51	5.66	123.70	111.50
25	P	1270	CDL	OA6-CA5-C11	5.63	123.64	111.50
22	P	1271	CHD	O7-C7-C6	-5.63	95.98	109.94
25	T	1269	CDL	OB6-CB5-C51	5.60	123.56	111.50
28	Z	1526	DMU	O7-C10-C5	-5.59	93.61	108.10
22	P	1271	CHD	C6-C5-C4	-5.58	104.76	111.19
22	C	271	CHD	C1-C2-C3	5.57	117.61	110.47
22	J	60	CHD	C14-C8-C7	5.56	119.19	111.81
22	J	60	CHD	C15-C14-C13	5.55	109.00	103.55
22	O	229	CHD	C9-C11-C12	5.55	121.63	114.30
22	B	1086	CHD	C4-C3-C2	5.51	117.13	110.55
18	A	515	HEA	C4B-C3B-C2B	-5.49	103.03	106.87
25	G	269	CDL	OA6-CA5-C11	5.49	123.33	111.50
22	P	1271	CHD	C14-C13-C12	5.49	112.51	107.40
22	J	60	CHD	O12-C12-C11	-5.47	97.97	109.12
22	P	1525	CHD	C17-C13-C14	5.47	105.61	100.09
28	P	1272	DMU	O1-C10-C5	5.46	121.91	110.35
20	N	1266	PGV	O03-C19-O04	-5.45	109.85	123.59
22	C	271	CHD	C2-C1-C10	5.44	122.11	112.78
22	J	60	CHD	C2-C1-C10	5.43	122.10	112.78
22	W	1060	CHD	C1-C10-C9	-5.43	102.82	111.35
22	W	1060	CHD	C18-C13-C12	-5.43	103.54	109.07
28	P	1272	DMU	C8-C7-C5	5.43	120.30	110.82
19	L	522	TGL	OG3-CC1-CC2	5.41	128.90	111.91
22	W	1060	CHD	C15-C14-C13	5.40	108.85	103.55
28	G	272	DMU	O5-C4-C3	5.40	121.13	109.75
22	P	1271	CHD	C15-C14-C13	5.39	108.84	103.55
22	P	1271	CHD	C5-C4-C3	5.38	120.66	112.76
22	W	1060	CHD	C15-C14-C8	5.36	125.82	118.33
25	C	270	CDL	CB4-OB6-CB5	-5.34	104.64	117.79
28	P	1272	DMU	O5-C4-C57	5.33	119.69	106.44
24	T	1265	PEK	O01-C1-C2	5.33	122.99	111.50
28	M	526	DMU	C2-C3-C4	5.33	123.14	110.93
22	O	229	CHD	C11-C9-C8	5.33	118.67	110.88
22	B	1086	CHD	O12-C12-C11	-5.31	98.31	109.12
22	C	525	CHD	C17-C13-C14	5.30	105.44	100.09
22	J	60	CHD	C1-C10-C9	-5.29	103.04	111.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	1086	CHD	C18-C13-C17	-5.29	102.94	111.21
18	A	515	HEA	C16-C17-C18	5.29	129.25	111.88
22	O	229	CHD	C15-C14-C8	5.27	125.70	118.33
22	J	60	CHD	C15-C14-C8	5.26	125.69	118.33
18	N	515	HEA	OMA-CMA-C3A	-5.25	113.48	124.91
22	W	1060	CHD	C2-C1-C10	5.24	121.77	112.78
24	G	1263	PEK	O01-C1-C2	5.24	122.78	111.50
22	W	1060	CHD	C14-C8-C7	5.23	118.74	111.81
28	G	272	DMU	O1-C9-C11	5.21	119.38	106.44
22	P	1525	CHD	C13-C17-C20	5.18	125.68	119.50
19	Y	1522	TGL	OG2-CB1-CB2	5.15	122.59	111.50
22	O	229	CHD	C11-C12-C13	5.12	116.50	111.24
22	C	271	CHD	C16-C17-C13	5.11	108.56	103.55
28	G	272	DMU	C8-C7-C5	5.11	119.74	110.82
28	Z	1526	DMU	O5-C4-C3	5.11	120.52	109.75
20	H	268	PGV	O01-C1-C2	5.07	122.44	111.50
28	M	526	DMU	O7-C10-C5	-5.07	94.97	108.10
28	M	526	DMU	O5-C4-C3	5.06	120.42	109.75
22	W	1060	CHD	C13-C14-C8	5.02	121.15	114.74
19	O	1521	TGL	CG2-OG2-CB1	5.02	130.15	117.79
28	Z	1526	DMU	C2-C3-C4	4.96	122.30	110.93
22	P	1525	CHD	C6-C5-C4	-4.95	105.50	111.19
22	W	1060	CHD	C16-C17-C20	4.94	119.79	112.15
18	A	515	HEA	C20-C21-C22	-4.93	95.69	111.88
22	W	1060	CHD	O12-C12-C11	-4.92	99.09	109.12
20	H	268	PGV	O03-C19-C20	4.89	127.25	111.91
22	C	271	CHD	O12-C12-C13	-4.88	102.78	111.03
22	P	1525	CHD	C18-C13-C14	-4.86	103.60	111.21
22	C	525	CHD	C5-C4-C3	4.79	119.79	112.76
22	J	60	CHD	C11-C12-C13	4.79	116.16	111.24
22	P	1525	CHD	O12-C12-C13	-4.79	102.94	111.03
25	C	270	CDL	OA6-CA5-C11	4.78	121.81	111.50
28	G	272	DMU	C2-C3-C4	4.78	121.88	110.93
22	W	1060	CHD	C4-C5-C10	4.77	117.73	112.66
19	L	522	TGL	OG3-CC1-OC1	-4.76	111.58	123.59
18	N	515	HEA	C27-C19-C18	-4.74	111.51	123.68
22	J	60	CHD	C9-C11-C12	4.74	120.56	114.30
22	C	525	CHD	C5-C6-C7	4.71	119.66	114.46
18	N	516	HEA	C4B-C3B-C2B	-4.71	103.58	106.87
22	W	1060	CHD	C19-C10-C5	-4.69	102.40	110.36
18	N	516	HEA	O11-C11-C3B	-4.63	98.65	112.00
18	N	516	HEA	CAA-CBA-CGA	-4.62	104.92	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	G	272	DMU	O5-C6-C1	4.61	120.11	110.35
28	G	272	DMU	C6-C1-C2	4.59	119.56	110.00
18	A	515	HEA	C27-C19-C18	-4.55	112.00	123.68
22	J	60	CHD	C19-C10-C5	-4.53	102.68	110.36
25	C	270	CDL	OB8-CB7-OB9	-4.52	112.18	123.59
28	M	526	DMU	C8-C7-C5	4.52	118.71	110.82
22	J	60	CHD	C9-C10-C5	4.51	114.91	108.58
22	P	1525	CHD	C16-C17-C20	4.51	119.12	112.15
28	M	526	DMU	O5-C4-C57	4.48	117.57	106.44
20	A	524	PGV	C02-O01-C1	4.47	128.79	117.79
22	P	1525	CHD	C23-C22-C20	-4.47	108.70	114.72
22	C	271	CHD	C4-C5-C10	4.46	117.39	112.66
22	P	1271	CHD	C13-C17-C20	4.45	124.81	119.50
19	O	1523	TGL	OG2-CB1-CB2	4.45	121.08	111.50
25	P	1270	CDL	OB8-CB7-C71	4.44	125.84	111.91
22	W	1060	CHD	C11-C9-C8	4.43	117.36	110.88
19	D	523	TGL	OG2-CB1-CB2	-4.43	101.96	111.50
24	P	1264	PEK	O01-C1-O02	-4.41	113.03	123.70
22	P	1525	CHD	O12-C12-C11	-4.40	100.17	109.12
22	C	525	CHD	C4-C5-C10	-4.39	107.99	112.66
28	P	1272	DMU	C6-C1-C2	4.39	119.14	110.00
22	P	1525	CHD	C11-C12-C13	4.39	115.75	111.24
22	P	1525	CHD	C22-C20-C17	-4.37	101.25	110.28
24	G	265	PEK	O03-C21-C22	4.37	125.64	111.91
18	N	516	HEA	CBD-CAD-C3D	4.37	120.55	112.49
22	J	60	CHD	C4-C5-C10	4.36	117.29	112.66
25	C	270	CDL	OB8-CB7-C71	4.35	125.57	111.91
25	G	269	CDL	CB6-CB4-CB3	-4.35	101.51	111.79
22	J	60	CHD	C22-C20-C17	4.34	119.26	110.28
22	B	1086	CHD	C15-C14-C13	4.34	107.81	103.55
28	M	526	DMU	C7-C8-C9	4.34	117.97	110.24
19	A	521	TGL	OG1-CA1-CA2	4.30	125.42	111.91
22	O	229	CHD	C16-C17-C20	4.30	118.80	112.15
18	N	516	HEA	CMB-C2B-C1B	-4.30	121.86	128.46
22	C	525	CHD	C18-C13-C14	-4.29	104.50	111.21
22	C	525	CHD	C1-C10-C9	-4.29	104.61	111.35
19	A	521	TGL	OG3-CC1-OC1	-4.29	112.77	123.59
22	P	1525	CHD	O7-C7-C6	-4.25	99.39	109.94
19	D	523	TGL	OG1-CA1-CA2	4.25	125.25	111.91
22	J	60	CHD	C18-C13-C14	-4.24	104.57	111.21
28	G	272	DMU	O7-C3-C2	4.24	118.55	107.28
28	G	272	DMU	C7-C8-C9	4.22	117.76	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	W	1060	CHD	C6-C5-C4	-4.21	106.34	111.19
22	B	1086	CHD	C14-C8-C9	4.18	115.45	109.71
24	G	265	PEK	O01-C1-C2	4.18	120.51	111.50
19	D	523	TGL	CG1-OG1-CA1	4.18	132.59	117.12
28	P	1272	DMU	C6-O5-C4	4.18	121.89	113.69
22	P	1271	CHD	C9-C11-C12	4.17	119.81	114.30
22	C	271	CHD	C9-C11-C12	4.17	119.81	114.30
22	C	271	CHD	C17-C13-C14	4.16	104.28	100.09
18	N	516	HEA	C13-C12-C11	-4.16	108.11	114.35
24	T	1265	PEK	O03-C21-C22	4.15	124.93	111.91
22	C	525	CHD	C14-C8-C9	4.12	115.37	109.71
22	W	1060	CHD	C18-C13-C14	-4.12	104.76	111.21
26	E	230	PSC	O01-C1-C2	4.12	120.38	111.50
28	P	1272	DMU	C18-O16-C6	4.12	120.66	113.84
22	B	1086	CHD	O7-C7-C6	-4.09	99.79	109.94
19	O	1521	TGL	OG2-CB1-CB2	4.04	120.21	111.50
22	W	1060	CHD	C18-C13-C17	-4.04	104.89	111.21
28	P	1272	DMU	O1-C9-C11	4.03	116.45	106.44
18	A	516	HEA	C20-C19-C18	-3.99	113.04	121.12
28	M	526	DMU	O3-C5-C7	3.99	119.57	110.35
28	P	1272	DMU	O5-C6-C1	3.98	118.78	110.35
22	W	1060	CHD	C22-C20-C17	3.98	118.51	110.28
22	P	1271	CHD	O12-C12-C11	-3.97	101.04	109.12
22	O	229	CHD	C13-C17-C20	3.97	124.23	119.50
20	A	524	PGV	C4-C3-C2	-3.96	98.95	113.19
22	J	60	CHD	C19-C10-C9	-3.96	105.73	111.18
20	A	522	PGV	O03-C01-C02	3.94	119.91	108.43
25	T	1269	CDL	OA6-CA5-C11	3.92	119.95	111.50
19	O	1521	TGL	OG1-CA1-CA2	3.90	124.15	111.91
28	Z	1526	DMU	C7-C8-C9	3.90	117.19	110.24
18	A	515	HEA	C27-C19-C20	3.89	121.81	115.27
22	B	1086	CHD	O7-C7-C8	-3.88	100.76	109.43
22	P	1525	CHD	C6-C7-C8	3.87	115.61	111.48
22	C	525	CHD	C9-C11-C12	3.86	119.40	114.30
22	O	229	CHD	C14-C8-C9	3.86	115.00	109.71
22	W	1060	CHD	O7-C7-C6	-3.85	100.38	109.94
19	A	521	TGL	CB7-CB6-CB5	-3.85	94.88	114.42
28	P	1272	DMU	C1-C2-C3	3.84	118.44	109.68
20	N	1268	PGV	C03-C02-C01	-3.83	102.73	111.79
22	C	525	CHD	O7-C7-C6	-3.82	100.46	109.94
28	M	526	DMU	O1-C9-C11	3.82	115.93	106.44
19	O	1521	TGL	CG3-OG3-CC1	3.81	131.25	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	1525	CHD	C1-C10-C9	-3.80	105.37	111.35
24	G	1263	PEK	O01-C1-O02	-3.80	114.51	123.70
28	P	1272	DMU	C2-C3-C4	3.80	119.64	110.93
24	G	1263	PEK	O03-C21-C22	3.80	123.82	111.91
22	P	1525	CHD	C2-C1-C10	3.79	119.28	112.78
20	A	522	PGV	O03-C19-O04	-3.75	114.13	123.59
20	A	522	PGV	O03-C19-C20	3.74	123.63	111.91
19	O	1523	TGL	OG3-CC1-CC2	3.73	123.62	111.91
28	Z	1526	DMU	O7-C3-C2	3.72	117.18	107.28
28	G	272	DMU	C6-O5-C4	3.72	120.99	113.69
22	P	1525	CHD	C4-C5-C10	-3.72	108.71	112.66
22	B	1086	CHD	C16-C17-C13	3.71	107.19	103.55
22	C	271	CHD	C6-C5-C4	-3.71	106.92	111.19
20	P	1267	PGV	C8-C9-C10	-3.70	97.68	113.79
24	P	1264	PEK	O03-C01-C02	-3.69	97.69	108.43
24	G	265	PEK	O03-C21-O04	-3.68	114.30	123.59
22	P	1525	CHD	O7-C7-C8	-3.68	101.20	109.43
22	W	1060	CHD	C9-C10-C5	3.67	113.73	108.58
22	O	229	CHD	O7-C7-C8	-3.66	101.24	109.43
22	P	1271	CHD	C18-C13-C17	-3.65	105.50	111.21
20	A	524	PGV	O03-C19-C20	3.65	123.35	111.91
25	P	1270	CDL	C53-C52-C51	-3.63	100.14	113.19
22	J	60	CHD	C17-C13-C14	3.61	103.74	100.09
28	P	1272	DMU	C10-C5-C7	3.61	117.52	110.00
24	C	264	PEK	O03-C01-C02	-3.61	97.93	108.43
18	A	516	HEA	C12-C13-C14	-3.60	102.73	112.23
22	B	1086	CHD	O12-C12-C13	-3.60	104.95	111.03
22	B	1086	CHD	C18-C13-C14	-3.60	105.58	111.21
24	C	264	PEK	C24-C23-C22	-3.60	100.27	113.19
22	C	525	CHD	C2-C1-C10	3.59	118.94	112.78
18	N	515	HEA	C16-C17-C18	3.58	123.65	111.88
24	P	1264	PEK	O01-C1-C2	3.56	119.17	111.50
20	N	1524	PGV	O01-C1-O02	-3.54	115.14	123.70
26	R	1230	PSC	O01-C1-C2	3.54	119.12	111.50
22	P	1271	CHD	C17-C13-C14	3.52	103.65	100.09
18	A	516	HEA	C1B-C2B-C3B	-3.52	104.55	107.00
22	J	60	CHD	O7-C7-C6	-3.52	101.22	109.94
22	B	1086	CHD	C16-C17-C20	3.50	117.56	112.15
22	C	271	CHD	C23-C22-C20	3.50	119.44	114.72
22	P	1271	CHD	C2-C1-C10	3.50	118.78	112.78
19	A	521	TGL	OG1-CA1-OA1	-3.47	114.84	123.59
18	N	515	HEA	C12-C11-C3B	3.47	121.65	112.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	1525	CHD	C14-C8-C9	3.46	114.47	109.71
22	P	1525	CHD	C19-C10-C5	-3.46	104.49	110.36
24	T	1265	PEK	O03-C21-O04	-3.46	114.87	123.59
22	P	1525	CHD	C13-C14-C8	3.44	119.13	114.74
28	Z	1526	DMU	C6-O5-C4	3.44	120.44	113.69
18	N	516	HEA	CAD-CBD-CGD	-3.44	106.90	112.67
22	C	271	CHD	C14-C8-C9	3.43	114.42	109.71
22	O	229	CHD	C6-C7-C8	3.43	115.14	111.48
22	J	60	CHD	C18-C13-C17	-3.43	105.85	111.21
19	Y	1522	TGL	CG2-OG2-CB1	3.42	126.22	117.79
20	A	524	PGV	O02-C1-C2	-3.41	110.43	123.73
20	A	522	PGV	O01-C1-C2	3.40	118.84	111.50
28	Z	1526	DMU	C1-C2-C3	3.39	117.43	109.68
19	Y	1522	TGL	OG1-CA1-CA2	3.39	122.54	111.91
25	G	269	CDL	OB8-CB7-OB9	-3.38	115.06	123.59
20	N	1524	PGV	O03-C19-C20	3.38	122.52	111.91
22	B	1086	CHD	C22-C23-C24	-3.35	106.38	113.59
28	P	1272	DMU	C10-O1-C9	3.33	120.23	113.69
26	R	1230	PSC	O03-C19-C20	3.33	122.36	111.91
20	C	267	PGV	O03-C19-O04	-3.33	115.20	123.59
25	C	270	CDL	C53-C52-C51	-3.32	101.27	113.19
19	O	1523	TGL	OG3-CC1-OC1	-3.30	115.26	123.59
28	Z	1526	DMU	C10-O1-C9	3.30	120.17	113.69
20	N	1268	PGV	O03-C19-O04	-3.30	115.26	123.59
28	P	1272	DMU	C7-C8-C9	3.30	116.12	110.24
22	C	525	CHD	O3-C3-C4	3.30	116.42	109.85
22	C	525	CHD	C11-C9-C8	3.30	115.70	110.88
20	C	267	PGV	C27-C26-C25	-3.30	97.69	114.42
22	C	525	CHD	C11-C9-C10	3.29	117.12	113.73
25	T	1269	CDL	CB2-C1-CA2	-3.28	103.14	112.79
20	N	1266	PGV	O03-C01-C02	3.28	117.97	108.43
20	A	522	PGV	O01-C1-O02	-3.27	115.79	123.70
28	G	272	DMU	C10-C5-C7	3.27	116.81	110.00
20	P	1267	PGV	C27-C26-C25	-3.24	97.97	114.42
22	B	1086	CHD	C11-C9-C8	3.23	115.61	110.88
24	T	263	PEK	O01-C1-O02	-3.23	115.90	123.70
22	C	525	CHD	C18-C13-C17	-3.23	106.16	111.21
24	P	1264	PEK	C30-C29-C28	-3.22	98.08	114.42
28	M	526	DMU	C11-C9-C8	3.21	120.53	113.00
28	M	526	DMU	C18-O16-C6	3.21	119.16	113.84
19	O	1521	TGL	OG3-CC1-CC2	3.21	121.97	111.91
19	Y	1522	TGL	CG3-OG3-CC1	3.20	128.97	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	524	PGV	O01-C1-O02	3.20	131.43	123.70
22	O	229	CHD	C2-C1-C10	3.19	118.25	112.78
22	B	1086	CHD	C9-C8-C7	3.19	115.69	111.88
18	N	516	HEA	C26-C15-C16	3.18	120.63	115.27
22	W	1060	CHD	C14-C8-C9	3.18	114.07	109.71
19	L	522	TGL	OG1-CA1-CA2	3.17	121.87	111.91
22	C	271	CHD	C22-C23-C24	3.17	120.39	113.59
22	C	525	CHD	C22-C23-C24	-3.15	106.81	113.59
22	O	229	CHD	C5-C6-C7	3.15	117.94	114.46
18	N	515	HEA	C1B-C2B-C3B	-3.15	104.81	107.00
20	A	524	PGV	C8-C9-C10	-3.14	100.09	113.79
18	A	515	HEA	C25-C23-C24	3.14	121.55	114.60
18	A	516	HEA	C27-C19-C20	3.14	120.55	115.27
19	L	522	TGL	OG3-CG3-CG2	3.14	117.57	108.43
18	A	515	HEA	CAD-C3D-C2D	3.13	136.24	127.25
20	P	1267	PGV	C02-O01-C1	3.13	125.50	117.79
20	P	1267	PGV	O03-C19-O04	-3.13	115.70	123.59
22	J	60	CHD	C6-C5-C4	-3.13	107.59	111.19
22	P	1525	CHD	C15-C16-C17	3.12	111.33	105.13
25	T	1269	CDL	C83-C82-C81	3.12	130.27	114.42
22	C	525	CHD	O12-C12-C11	-3.12	102.77	109.12
24	G	1263	PEK	O03-C01-C02	3.12	117.50	108.43
22	C	525	CHD	C13-C14-C8	3.11	118.71	114.74
28	M	526	DMU	C31-C28-C25	-3.11	98.64	114.42
19	L	522	TGL	CB4-CB3-CB2	-3.10	102.03	113.19
19	A	521	TGL	OG3-CC1-CC2	3.10	121.63	111.91
19	Y	1522	TGL	OG3-CC1-OC1	-3.08	115.81	123.59
28	G	272	DMU	O5-C6-O16	3.08	117.26	109.97
19	O	1523	TGL	CG3-CG2-CG1	-3.06	104.55	111.79
28	M	526	DMU	C1-C2-C3	3.06	116.66	109.68
19	D	523	TGL	C10-CB9-CB8	3.06	129.95	114.42
22	P	1271	CHD	C21-C20-C17	3.05	117.59	112.92
25	C	270	CDL	O1-C1-CB2	3.05	120.25	109.56
22	P	1525	CHD	C5-C6-C7	3.04	117.81	114.46
22	C	525	CHD	C19-C10-C5	-3.04	105.21	110.36
20	C	267	PGV	O14-P-O13	3.02	127.19	112.24
19	L	522	TGL	CA4-CA3-CA2	-3.02	102.32	113.19
22	C	525	CHD	C15-C16-C17	3.02	111.13	105.13
22	W	1060	CHD	C17-C13-C14	3.02	103.14	100.09
19	L	522	TGL	CC3-CC2-CC1	3.02	124.59	113.62
25	C	270	CDL	OB6-CB5-C51	3.01	117.99	111.50
19	D	523	TGL	CB3-CB2-CB1	3.01	124.57	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	515	HEA	C17-C18-C19	-3.00	120.45	127.66
19	A	521	TGL	OB1-CB1-CB2	-2.98	112.11	123.73
28	M	526	DMU	C57-C4-C3	2.97	121.96	113.33
20	A	524	PGV	O01-C1-C2	2.97	117.90	111.50
19	Y	1522	TGL	OG3-CC1-CC2	2.96	121.21	111.91
28	M	526	DMU	C6-C1-C2	2.95	116.15	110.00
28	Z	1526	DMU	O3-C5-C7	2.93	117.11	110.35
20	N	1268	PGV	O01-C1-C2	2.93	117.81	111.50
22	C	271	CHD	O12-C12-C11	-2.92	103.17	109.12
22	P	1525	CHD	C9-C11-C12	2.92	118.16	114.30
28	G	272	DMU	C10-O1-C9	2.92	119.41	113.69
25	T	1269	CDL	OB8-CB6-CB4	2.91	116.91	108.43
26	E	230	PSC	C02-O01-C1	2.91	124.95	117.79
19	O	1523	TGL	OG1-CG1-CG2	2.91	116.90	108.43
22	O	229	CHD	O12-C12-C11	-2.90	103.21	109.12
20	N	1268	PGV	O04-C19-C20	-2.90	112.41	123.73
19	D	523	TGL	CG3-OG3-CC1	2.90	127.86	117.12
19	A	521	TGL	CA3-CA2-CA1	-2.89	103.11	113.62
19	D	523	TGL	OG2-CB1-OB1	2.89	130.69	123.70
20	P	1267	PGV	C4-C3-C2	-2.89	102.81	113.19
19	D	523	TGL	C21-C20-CA9	2.88	129.07	114.42
18	N	516	HEA	CMB-C2B-C3B	2.88	130.34	124.69
19	O	1523	TGL	OG1-CA1-CA2	2.88	120.96	111.91
19	D	523	TGL	CG2-OG2-CB1	2.88	124.88	117.79
24	G	265	PEK	C10-C9-C8	-2.88	99.30	123.57
28	M	526	DMU	O49-C1-C2	2.87	116.99	110.35
22	B	1086	CHD	C23-C22-C20	2.87	118.59	114.72
28	P	1272	DMU	C11-C9-C8	2.86	119.71	113.00
25	C	270	CDL	OB6-CB5-OB7	-2.86	116.79	123.70
24	T	263	PEK	O03-C01-C02	2.86	116.75	108.43
28	G	272	DMU	C1-C2-C3	2.86	116.20	109.68
18	A	515	HEA	CMB-C2B-C1B	2.85	132.84	128.46
24	C	264	PEK	C02-O01-C1	2.84	124.79	117.79
19	L	522	TGL	OG1-CG1-CG2	2.84	116.69	108.43
24	C	264	PEK	O01-C1-O02	-2.84	116.85	123.70
25	G	269	CDL	OA8-CA7-C31	2.83	120.79	111.91
24	G	265	PEK	C8-C7-C6	-2.82	98.16	112.02
26	E	230	PSC	O03-C19-C20	2.81	120.74	111.91
20	A	524	PGV	O01-C02-C03	2.81	118.58	108.40
20	H	268	PGV	O04-C19-C20	-2.81	112.78	123.73
18	A	515	HEA	C12-C11-C3B	2.80	119.90	112.56
19	L	522	TGL	OG2-CB1-CB2	2.79	117.52	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L	522	TGL	C22-C21-C20	-2.79	100.27	114.42
22	C	525	CHD	C21-C20-C22	-2.79	106.00	110.36
19	L	522	TGL	C26-C25-C24	-2.78	100.33	114.42
25	C	270	CDL	C73-C72-C71	-2.77	103.22	113.19
18	N	516	HEA	CAD-C3D-C2D	-2.77	119.28	127.25
28	Z	1526	DMU	O5-C6-O16	2.76	116.51	109.97
18	A	515	HEA	OMA-CMA-C3A	-2.75	118.91	124.91
28	M	526	DMU	C10-C5-C7	2.75	115.72	110.00
19	Y	1522	TGL	CB3-CB2-CB1	2.75	123.60	113.62
28	G	272	DMU	O7-C3-C4	2.74	116.97	109.45
18	A	515	HEA	C26-C15-C16	2.73	119.86	115.27
22	O	229	CHD	C1-C10-C9	-2.73	107.07	111.35
20	P	1267	PGV	O03-C19-C20	2.73	120.46	111.91
22	C	271	CHD	C14-C8-C7	2.73	115.42	111.81
25	P	1270	CDL	OB8-CB7-OB9	-2.72	116.72	123.59
20	C	267	PGV	O06-C06-C05	-2.72	97.17	110.20
19	O	1523	TGL	CG3-OG3-CC1	2.71	127.17	117.12
22	C	271	CHD	C19-C10-C5	-2.71	105.76	110.36
22	B	1086	CHD	C1-C10-C9	-2.71	107.09	111.35
28	Z	1526	DMU	C22-C19-C18	-2.71	101.50	113.49
24	T	263	PEK	C14-C13-C12	2.70	125.32	112.02
24	C	264	PEK	O11-P-O14	-2.69	98.58	109.07
18	A	515	HEA	C17-C18-C19	-2.67	121.22	127.66
18	A	516	HEA	C17-C18-C19	2.67	134.09	127.66
22	O	229	CHD	C11-C9-C10	2.66	116.47	113.73
24	C	264	PEK	C25-C24-C23	-2.65	100.96	114.42
19	Y	1522	TGL	OG1-CG1-CG2	2.65	116.15	108.43
20	N	1524	PGV	C02-O01-C1	2.65	124.31	117.79
28	M	526	DMU	O5-C6-O16	2.63	116.21	109.97
25	G	269	CDL	C40-C39-C38	2.63	127.77	114.42
22	B	1086	CHD	C2-C1-C10	2.63	117.29	112.78
25	C	270	CDL	OA8-CA6-CA4	2.61	116.04	108.43
19	L	522	TGL	OG2-CG2-CG3	2.60	117.83	108.40
28	Z	1526	DMU	C18-O16-C6	2.59	118.14	113.84
20	N	1266	PGV	O14-P-O11	2.59	119.76	107.75
25	T	1269	CDL	OA6-CA5-OA7	-2.58	117.47	123.70
19	Y	1522	TGL	CC3-CC2-CC1	2.57	122.97	113.62
25	T	1269	CDL	C40-C39-C38	2.57	127.47	114.42
25	G	269	CDL	C58-C57-C56	-2.57	101.39	114.42
20	N	1266	PGV	O01-C1-C2	2.57	117.03	111.50
25	P	1270	CDL	OA6-CA5-OA7	-2.57	117.50	123.70
19	L	522	TGL	CA5-CA4-CA3	-2.56	101.41	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	P	1272	DMU	O61-C57-C4	2.56	120.08	111.29
19	O	1521	TGL	CG1-OG1-CA1	2.55	126.57	117.12
18	N	516	HEA	CMC-C2C-C1C	-2.54	124.56	128.46
28	M	526	DMU	O16-C18-C19	-2.53	100.71	109.56
22	P	1525	CHD	C22-C23-C24	-2.52	108.16	113.59
20	N	1524	PGV	O03-C19-O04	-2.52	117.23	123.59
19	O	1521	TGL	OG3-CG3-CG2	2.52	115.76	108.43
18	N	515	HEA	CMC-C2C-C3C	2.52	129.39	124.68
25	T	1269	CDL	OA8-CA7-C31	2.51	119.80	111.91
22	B	1086	CHD	O3-C3-C4	2.51	114.85	109.85
28	P	1272	DMU	O3-C5-C10	-2.51	103.95	110.05
28	G	272	DMU	O61-C57-C4	2.51	119.89	111.29
25	G	269	CDL	C39-C38-C37	2.50	127.12	114.42
26	R	1230	PSC	C29-C28-C27	-2.49	101.80	114.42
22	O	229	CHD	C14-C8-C7	2.48	115.10	111.81
18	A	515	HEA	C20-C19-C18	2.48	126.14	121.12
19	L	522	TGL	CA3-CA2-CA1	-2.48	104.59	113.62
25	T	1269	CDL	OB4-PB2-OB3	2.48	124.52	112.24
25	P	1270	CDL	CA6-OA8-CA7	2.48	126.31	117.12
19	L	522	TGL	OB1-CB1-CB2	-2.48	114.05	123.73
19	L	522	TGL	CA7-CA6-CA5	-2.48	101.86	114.42
25	P	1270	CDL	OB2-PB2-OB3	2.47	118.74	109.07
28	G	272	DMU	O3-C5-C10	-2.47	104.04	110.05
24	P	1264	PEK	C24-C23-C22	-2.47	104.30	113.19
18	A	515	HEA	C17-C16-C15	2.47	121.10	112.98
24	T	263	PEK	O03-C21-C22	2.47	119.65	111.91
20	P	1267	PGV	O01-C02-C03	-2.46	99.48	108.40
25	C	270	CDL	C42-C41-C40	2.46	126.93	114.42
24	P	1264	PEK	C02-O01-C1	2.45	123.83	117.79
20	P	1267	PGV	O01-C1-C2	2.45	116.78	111.50
24	C	264	PEK	C2-C3-C4	2.45	117.60	113.23
24	C	264	PEK	O13-P-O14	2.45	124.36	112.24
28	Z	1526	DMU	C28-C25-C22	-2.44	102.03	114.42
20	A	524	PGV	O03-C19-O04	-2.44	117.43	123.59
25	T	1269	CDL	OA8-CA7-OA9	-2.44	117.44	123.59
18	A	516	HEA	O11-C11-C3B	-2.44	104.97	112.00
19	O	1523	TGL	C24-C23-C22	2.43	126.78	114.42
25	P	1270	CDL	OB6-CB4-CB6	2.43	117.20	108.40
22	P	1271	CHD	C22-C23-C24	-2.43	108.37	113.59
22	J	60	CHD	C9-C8-C7	2.42	114.77	111.88
22	C	525	CHD	C23-C22-C20	-2.41	111.48	114.72
22	J	60	CHD	O12-C12-C13	-2.40	106.96	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	264	PEK	O01-C1-C2	2.40	116.68	111.50
19	O	1521	TGL	OG1-CA1-OA1	-2.40	117.54	123.59
22	O	229	CHD	C13-C14-C8	2.40	117.80	114.74
24	T	1265	PEK	C03-C02-C01	-2.39	106.12	111.79
24	G	1263	PEK	C01-O03-C21	2.39	125.98	117.12
25	T	1269	CDL	OB6-CB5-OB7	-2.39	117.92	123.70
25	G	269	CDL	CA6-OA8-CA7	2.39	125.97	117.12
18	A	515	HEA	C12-C13-C14	-2.39	105.93	112.23
22	J	60	CHD	O7-C7-C8	-2.38	104.10	109.43
25	P	1270	CDL	C42-C41-C40	2.38	126.50	114.42
19	O	1521	TGL	CB7-CB6-CB5	-2.37	102.38	114.42
22	C	525	CHD	O7-C7-C8	-2.36	104.15	109.43
28	M	526	DMU	O55-C2-C1	2.36	115.79	110.35
20	N	1268	PGV	C02-O01-C1	2.35	123.58	117.79
24	T	263	PEK	C2-C3-C4	2.35	117.42	113.23
25	P	1270	CDL	C79-C78-C77	2.34	126.31	114.42
22	C	271	CHD	C9-C10-C5	2.34	111.87	108.58
19	A	521	TGL	OG2-CG2-CG1	2.34	116.87	108.40
22	O	229	CHD	O3-C3-C2	2.34	116.11	110.16
25	G	269	CDL	C43-C42-C41	2.34	126.28	114.42
25	P	1270	CDL	O1-C1-CA2	-2.33	101.37	109.56
22	P	1525	CHD	O3-C3-C4	2.33	114.49	109.85
19	A	521	TGL	CG3-OG3-CC1	2.33	125.74	117.12
25	P	1270	CDL	C39-C38-C37	2.33	126.23	114.42
19	Y	1522	TGL	C15-CC9-CC8	2.33	126.23	114.42
20	H	268	PGV	O14-P-O13	2.32	123.73	112.24
28	Z	1526	DMU	C6-C1-C2	2.32	114.84	110.00
25	G	269	CDL	CB4-OB6-CB5	2.32	123.51	117.79
18	A	515	HEA	C3C-C4C-NC	2.32	112.21	109.21
18	A	516	HEA	C3C-C4C-NC	-2.31	106.22	109.21
20	H	268	PGV	O01-C02-C03	2.31	116.76	108.40
19	A	521	TGL	C15-CC9-CC8	2.31	126.14	114.42
28	G	272	DMU	C11-C9-C8	2.30	118.38	113.00
19	Y	1522	TGL	C26-C25-C24	-2.30	102.77	114.42
25	G	269	CDL	C80-C79-C78	2.29	126.07	114.42
18	N	515	HEA	C17-C16-C15	-2.29	105.43	112.98
18	A	515	HEA	CBA-CAA-C2A	2.29	116.70	112.48
18	N	515	HEA	C13-C12-C11	2.29	117.79	114.35
24	P	1264	PEK	C03-C02-C01	-2.29	106.38	111.79
19	O	1523	TGL	C21-C20-CA9	2.29	126.03	114.42
22	P	1525	CHD	C21-C20-C22	2.28	113.93	110.36
19	Y	1522	TGL	C24-C23-C22	-2.27	102.88	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	T	1269	CDL	C82-C81-C80	2.27	125.96	114.42
24	C	264	PEK	C26-C25-C24	-2.27	102.92	114.42
25	P	1270	CDL	OA8-CA7-C31	2.27	119.02	111.91
25	C	270	CDL	O1-C1-CA2	-2.26	101.62	109.56
28	M	526	DMU	O4-C7-C8	2.26	115.58	110.35
28	P	1272	DMU	O7-C10-O1	2.26	116.99	110.67
22	J	60	CHD	O3-C3-C2	-2.26	104.41	110.16
25	T	1269	CDL	C19-C18-C17	2.26	125.88	114.42
25	C	270	CDL	OA8-CA7-C31	2.25	118.97	111.91
19	D	523	TGL	C16-C15-CC9	2.25	125.83	114.42
25	G	269	CDL	OB7-CB5-C51	-2.24	114.98	123.73
22	B	1086	CHD	C13-C17-C20	2.24	122.17	119.50
19	O	1521	TGL	OB1-CB1-CB2	-2.23	115.05	123.73
25	C	270	CDL	OB6-CB4-CB3	-2.22	100.36	108.40
19	D	523	TGL	OG1-CG1-CG2	2.22	114.90	108.43
20	N	1266	PGV	O01-C1-O02	-2.22	118.34	123.70
24	T	263	PEK	C01-O03-C21	2.22	125.34	117.12
19	O	1523	TGL	OG1-CA1-OA1	-2.22	118.00	123.59
24	C	264	PEK	C32-C31-C30	-2.21	103.21	114.42
19	Y	1522	TGL	CA9-CA8-CA7	-2.21	103.22	114.42
19	L	522	TGL	C15-CC9-CC8	2.21	125.62	114.42
26	E	230	PSC	C08-N-C06	2.20	114.63	108.97
20	A	522	PGV	C01-O03-C19	-2.19	109.00	117.12
24	T	1265	PEK	C33-C32-C31	-2.19	103.32	114.42
24	P	1264	PEK	C26-C25-C24	-2.18	103.33	114.42
20	H	268	PGV	C3-C2-C1	2.18	121.56	113.62
25	G	269	CDL	C72-C71-CB7	2.18	121.56	113.62
22	W	1060	CHD	O3-C3-C2	-2.18	104.62	110.16
19	D	523	TGL	CC3-CC2-CC1	-2.18	105.71	113.62
19	O	1521	TGL	C15-CC9-CC8	2.17	125.46	114.42
19	Y	1522	TGL	OG2-CG2-CG3	2.17	116.25	108.40
28	P	1272	DMU	O16-C18-C19	2.16	117.14	109.56
25	T	1269	CDL	CB6-OB8-CB7	2.16	125.12	117.12
24	T	1265	PEK	C35-C34-C33	-2.16	103.47	114.42
20	H	268	PGV	O02-C1-C2	-2.16	115.32	123.73
18	A	516	HEA	C3A-C4A-NA	-2.15	106.89	110.94
22	C	525	CHD	C19-C10-C1	2.14	111.72	108.26
20	P	1267	PGV	O01-C1-O02	-2.14	118.52	123.70
22	B	1086	CHD	C5-C6-C7	-2.14	112.10	114.46
19	D	523	TGL	C20-CA9-CA8	2.14	125.28	114.42
19	Y	1522	TGL	OG1-CA1-OA1	-2.14	118.20	123.59
25	C	270	CDL	CA6-OA8-CA7	2.14	125.03	117.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	C	525	CHD	C6-C7-C8	2.13	113.76	111.48
28	P	1272	DMU	O7-C3-C2	2.13	112.95	107.28
25	T	1269	CDL	C20-C19-C18	2.13	125.23	114.42
20	H	268	PGV	O12-P-O13	-2.13	100.75	109.07
25	T	1269	CDL	C80-C79-C78	2.13	125.23	114.42
28	G	272	DMU	O4-C7-C5	2.13	115.27	110.35
24	C	264	PEK	O04-C21-C22	2.13	132.03	123.73
19	O	1521	TGL	C16-C15-CC9	2.12	125.21	114.42
19	D	523	TGL	C15-CC9-CC8	2.12	125.21	114.42
24	P	1264	PEK	C01-O03-C21	2.12	124.98	117.12
25	P	1270	CDL	C62-C61-C60	2.12	125.19	114.42
22	O	229	CHD	C4-C5-C10	-2.12	110.41	112.66
22	B	1086	CHD	C19-C10-C5	-2.10	106.80	110.36
25	T	1269	CDL	OB2-PB2-OB3	-2.10	100.86	109.07
18	N	516	HEA	C12-C13-C14	-2.10	106.69	112.23
20	C	267	PGV	O01-C02-C03	-2.10	100.80	108.40
26	R	1230	PSC	C07-N-C06	-2.09	103.60	108.97
25	G	269	CDL	C79-C78-C77	2.09	125.01	114.42
20	A	522	PGV	C21-C20-C19	-2.08	106.04	113.62
26	E	230	PSC	C27-C26-C25	-2.08	103.89	114.42
28	Z	1526	DMU	C31-C28-C25	-2.08	103.89	114.42
28	G	272	DMU	O7-C10-O1	2.08	116.47	110.67
18	A	516	HEA	CMC-C2C-C1C	-2.07	125.28	128.46
20	P	1267	PGV	O06-C06-C05	-2.06	100.31	110.20
20	N	1266	PGV	C01-O03-C19	-2.06	109.50	117.12
19	Y	1522	TGL	OB1-CB1-CB2	-2.06	115.71	123.73
19	D	523	TGL	OG3-CC1-OC1	-2.05	118.41	123.59
25	G	269	CDL	OA6-CA5-OA7	-2.05	118.74	123.70
28	Z	1526	DMU	C10-C5-C7	2.05	114.27	110.00
24	G	265	PEK	C7-C8-C9	-2.05	106.27	123.57
22	P	1271	CHD	C16-C15-C14	2.05	109.19	105.13
26	R	1230	PSC	O01-C1-O02	-2.05	118.75	123.70
20	A	524	PGV	C01-O03-C19	2.05	124.70	117.12
22	C	525	CHD	C15-C14-C8	2.05	121.19	118.33
19	Y	1522	TGL	CB4-CB3-CB2	-2.04	105.85	113.19
25	C	270	CDL	C19-C18-C17	2.04	124.79	114.42
18	A	515	HEA	CMB-C2B-C3B	-2.03	120.71	124.69
25	G	269	CDL	OB8-CB7-C71	2.03	118.27	111.91
19	D	523	TGL	OG1-CA1-OA1	-2.03	118.48	123.59
22	O	229	CHD	C15-C16-C17	2.02	109.13	105.13
22	O	229	CHD	O7-C7-C6	-2.02	104.94	109.94
20	N	1524	PGV	O01-C02-C03	2.00	115.65	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	1525	CHD	C14-C8-C7	2.00	114.46	111.81

All (37) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
28	P	1272	DMU	C2
28	P	1272	DMU	C4
28	P	1272	DMU	C9
28	P	1272	DMU	C5
18	A	515	HEA	ND
18	A	515	HEA	NA
18	A	515	HEA	NB
28	Z	1526	DMU	C2
28	Z	1526	DMU	C4
28	Z	1526	DMU	C6
28	Z	1526	DMU	C9
28	Z	1526	DMU	C5
22	W	1060	CHD	C17
22	W	1060	CHD	C9
22	B	1086	CHD	C9
28	M	526	DMU	C2
28	M	526	DMU	C4
28	M	526	DMU	C9
28	M	526	DMU	C5
22	J	60	CHD	C17
22	J	60	CHD	C9
18	N	515	HEA	ND
18	N	515	HEA	NA
18	N	515	HEA	NB
18	N	516	HEA	ND
18	N	516	HEA	NA
18	N	516	HEA	NB
22	C	271	CHD	C9
18	A	516	HEA	ND
18	A	516	HEA	NA
18	A	516	HEA	NB
22	P	1271	CHD	C9
28	G	272	DMU	C2
28	G	272	DMU	C4
28	G	272	DMU	C9
28	G	272	DMU	C6
28	G	272	DMU	C5

All (934) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	G	265	PEK	C03-O11-P-O13
24	G	265	PEK	C03-O11-P-O14
24	G	265	PEK	O12-C04-C05-N
24	G	265	PEK	C5-C6-C7-C8
28	P	1272	DMU	C1-C6-O16-C18
28	P	1272	DMU	O5-C6-O16-C18
28	Z	1526	DMU	O5-C6-O16-C18
28	Z	1526	DMU	C19-C18-O16-C6
25	G	269	CDL	CA2-C1-CB2-OB2
25	G	269	CDL	CA3-OA5-PA1-OA4
25	G	269	CDL	C1-CB2-OB2-PB2
25	G	269	CDL	CB2-OB2-PB2-OB5
25	G	269	CDL	CB3-OB5-PB2-OB3
22	W	1060	CHD	C16-C17-C20-C21
24	T	263	PEK	C03-O11-P-O12
24	T	263	PEK	C03-O11-P-O13
24	T	263	PEK	C03-O11-P-O14
24	T	263	PEK	O12-C04-C05-N
24	T	263	PEK	C2-C3-C4-C5
19	A	521	TGL	CB2-CB1-OG2-CG2
19	A	521	TGL	OB1-CB1-OG2-CG2
24	P	1264	PEK	C7-C8-C9-C10
25	P	1270	CDL	CA2-OA2-PA1-OA3
25	P	1270	CDL	C11-CA5-OA6-CA4
25	P	1270	CDL	CB2-OB2-PB2-OB3
25	P	1270	CDL	OB7-CB5-OB6-CB4
20	H	268	PGV	C03-O11-P-O13
20	H	268	PGV	C2-C1-O01-C02
24	C	264	PEK	C11-C10-C9-C8
24	C	264	PEK	C11-C12-C13-C14
24	C	264	PEK	C13-C14-C15-C16
25	T	1269	CDL	CA2-C1-CB2-OB2
25	T	1269	CDL	C1-CB2-OB2-PB2
25	T	1269	CDL	CB3-OB5-PB2-OB4
20	N	1268	PGV	C03-O11-P-O13
20	N	1268	PGV	O01-C02-C03-O11
20	N	1268	PGV	C02-C03-O11-P
18	N	515	HEA	C16-C17-C18-C19
18	N	516	HEA	O11-C11-C12-C13
26	R	1230	PSC	C04-O12-P-O14
26	R	1230	PSC	C10-C11-C12-C13
22	C	271	CHD	C20-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
24	T	1265	PEK	C03-O11-P-O12
24	T	1265	PEK	C03-O11-P-O14
24	T	1265	PEK	C04-O12-P-O11
24	T	1265	PEK	C04-O12-P-O13
24	T	1265	PEK	C04-O12-P-O14
24	T	1265	PEK	O01-C02-C03-O11
24	T	1265	PEK	O12-C04-C05-N
24	T	1265	PEK	C2-C1-O01-C02
24	T	1265	PEK	C9-C10-C11-C12
19	D	523	TGL	OG1-CG1-CG2-OG2
26	E	230	PSC	C03-O11-P-O14
26	E	230	PSC	C11-C10-C9-C8
24	G	1263	PEK	C03-O11-P-O13
24	G	1263	PEK	O03-C01-C02-O01
24	G	1263	PEK	O12-C04-C05-N
24	G	1263	PEK	C13-C14-C15-C16
20	A	524	PGV	C02-C03-O11-P
20	A	524	PGV	O12-C04-C05-C06
20	A	524	PGV	O04-C19-O03-C01
20	A	524	PGV	C20-C19-O03-C01
28	G	272	DMU	O5-C6-O16-C18
19	Y	1522	TGL	CB2-CB1-OG2-CG2
20	N	1524	PGV	C02-C03-O11-P
20	N	1524	PGV	C04-C05-C06-O06
20	N	1524	PGV	O02-C1-O01-C02
20	N	1524	PGV	C2-C1-O01-C02
20	N	1524	PGV	C20-C19-O03-C01
25	C	270	CDL	CB2-C1-CA2-OA2
25	C	270	CDL	CA2-OA2-PA1-OA3
25	C	270	CDL	CA4-CA3-OA5-PA1
25	C	270	CDL	C11-CA5-OA6-CA4
25	C	270	CDL	CB2-OB2-PB2-OB3
25	C	270	CDL	CB3-OB5-PB2-OB3
20	N	1524	PGV	O04-C19-O03-C01
26	E	230	PSC	C02-C01-O03-C19
19	O	1523	TGL	OC1-CC1-OG3-CG3
19	D	523	TGL	OC1-CC1-OG3-CG3
22	W	1060	CHD	C16-C17-C20-C22
25	P	1270	CDL	OA7-CA5-OA6-CA4
24	T	1265	PEK	O02-C1-O01-C02
20	A	524	PGV	O02-C1-O01-C02
19	Y	1522	TGL	OB1-CB1-OG2-CG2

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Mol	Chain	Res	Type	Atoms
25	C	270	CDL	OA7-CA5-OA6-CA4
26	R	1230	PSC	C20-C19-O03-C01
19	O	1523	TGL	CC2-CC1-OG3-CG3
19	D	523	TGL	CC2-CC1-OG3-CG3
26	E	230	PSC	C20-C19-O03-C01
28	M	526	DMU	O5-C4-C57-O61
25	P	1270	CDL	C51-CB5-OB6-CB4
22	J	60	CHD	C16-C17-C20-C22
19	L	522	TGL	CA2-CA1-OG1-CG1
28	G	272	DMU	O6-C11-C9-O1
24	G	265	PEK	C10-C11-C12-C13
24	G	265	PEK	C13-C14-C15-C16
24	T	263	PEK	C4-C5-C6-C7
24	T	263	PEK	C7-C8-C9-C10
24	P	1264	PEK	C10-C11-C12-C13
24	C	264	PEK	C7-C8-C9-C10
24	C	264	PEK	C10-C11-C12-C13
26	R	1230	PSC	C11-C12-C13-C14
24	T	1265	PEK	C13-C14-C15-C16
26	E	230	PSC	C11-C12-C13-C14
26	E	230	PSC	C22-C23-C24-C25
19	L	522	TGL	C20-C21-C22-C23
25	G	269	CDL	OA7-CA5-OA6-CA4
20	H	268	PGV	O02-C1-O01-C02
19	L	522	TGL	OA1-CA1-OG1-CG1
26	R	1230	PSC	O04-C19-O03-C01
20	H	268	PGV	C6-C7-C8-C9
19	Y	1522	TGL	CC3-CC4-CC5-CC6
28	Z	1526	DMU	O5-C4-C57-O61
28	Z	1526	DMU	O6-C11-C9-O1
25	T	1269	CDL	C56-C57-C58-C59
25	G	269	CDL	O1-C1-CB2-OB2
25	P	1270	CDL	O1-C1-CB2-OB2
20	N	1524	PGV	O12-C04-C05-O05
26	E	230	PSC	O04-C19-O03-C01
25	G	269	CDL	C11-CA5-OA6-CA4
20	A	524	PGV	C2-C1-O01-C02
19	O	1521	TGL	CA9-C20-C21-C22
24	T	263	PEK	C33-C34-C35-C36
20	H	268	PGV	C20-C21-C22-C23
25	T	1269	CDL	C22-C23-C24-C25
24	T	1265	PEK	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
24	G	265	PEK	C28-C29-C30-C31
19	L	522	TGL	CC3-CC4-CC5-CC6
26	E	230	PSC	C20-C21-C22-C23
25	P	1270	CDL	C82-C83-C84-C85
25	T	1269	CDL	C15-C16-C17-C18
25	C	270	CDL	C83-C84-C85-C86
18	N	515	HEA	C26-C15-C16-C17
18	N	515	HEA	C14-C15-C16-C17
19	Y	1522	TGL	CC1-CC2-CC3-CC4
25	T	1269	CDL	C73-C74-C75-C76
19	D	523	TGL	CB9-C10-C11-C12
19	A	521	TGL	CA9-C20-C21-C22
19	Y	1522	TGL	CA2-CA1-OG1-CG1
19	L	522	TGL	CC1-CC2-CC3-CC4
28	M	526	DMU	C19-C22-C25-C28
25	G	269	CDL	C15-C16-C17-C18
25	P	1270	CDL	CB2-C1-CA2-OA2
25	P	1270	CDL	CA2-C1-CB2-OB2
20	N	1524	PGV	O12-C04-C05-C06
19	Y	1522	TGL	OA1-CA1-OG1-CG1
19	O	1521	TGL	C22-C23-C24-C25
25	T	1269	CDL	C71-CB7-OB8-CB6
19	O	1521	TGL	CC2-CC1-OG3-CG3
22	J	60	CHD	C13-C17-C20-C22
25	C	270	CDL	CB7-C71-C72-C73
28	P	1272	DMU	O6-C11-C9-O1
22	C	271	CHD	C17-C20-C22-C23
28	M	526	DMU	O6-C11-C9-C8
25	G	269	CDL	O1-C1-CA2-OA2
25	T	1269	CDL	O1-C1-CB2-OB2
25	G	269	CDL	CA5-C11-C12-C13
28	G	272	DMU	C1-C6-O16-C18
24	T	263	PEK	O03-C01-C02-O01
25	G	269	CDL	C59-C60-C61-C62
28	P	1272	DMU	C3-C4-C57-O61
20	A	524	PGV	C19-C20-C21-C22
25	G	269	CDL	CA7-C31-C32-C33
20	H	268	PGV	C1-C2-C3-C4
24	G	1263	PEK	C21-C22-C23-C24
19	Y	1522	TGL	CB1-CB2-CB3-CB4
20	C	267	PGV	C10-C11-C12-C13
20	A	522	PGV	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	G	269	CDL	C60-C61-C62-C63
22	P	1271	CHD	C13-C17-C20-C21
25	P	1270	CDL	CB7-C71-C72-C73
25	T	1269	CDL	CA7-C31-C32-C33
26	R	1230	PSC	C1-C2-C3-C4
19	O	1523	TGL	CB1-CB2-CB3-CB4
20	N	1524	PGV	C19-C20-C21-C22
19	A	521	TGL	C12-C13-C14-C29
26	E	230	PSC	C04-C05-N-C08
24	G	265	PEK	C1-C2-C3-C4
25	P	1270	CDL	CA7-C31-C32-C33
24	C	264	PEK	C1-C2-C3-C4
22	J	60	CHD	C16-C17-C20-C21
22	W	1060	CHD	C13-C17-C20-C21
22	J	60	CHD	C13-C17-C20-C21
22	W	1060	CHD	C13-C17-C20-C22
22	C	271	CHD	C21-C20-C22-C23
25	G	269	CDL	C39-C40-C41-C42
25	P	1270	CDL	C61-C62-C63-C64
25	T	1269	CDL	OB9-CB7-OB8-CB6
19	O	1521	TGL	OC1-CC1-OG3-CG3
18	A	515	HEA	C15-C16-C17-C18
28	M	526	DMU	O6-C11-C9-O1
20	N	1268	PGV	O12-C04-C05-O05
20	A	524	PGV	O12-C04-C05-O05
25	C	270	CDL	O1-C1-CA2-OA2
20	P	1267	PGV	C12-C13-C14-C15
20	N	1268	PGV	C1-C2-C3-C4
20	P	1267	PGV	C1-C2-C3-C4
24	P	1264	PEK	C13-C14-C15-C16
24	G	1263	PEK	C10-C11-C12-C13
28	P	1272	DMU	O16-C18-C19-C22
24	G	265	PEK	C03-O11-P-O12
25	G	269	CDL	CB3-OB5-PB2-OB2
25	P	1270	CDL	CA2-OA2-PA1-OA5
25	P	1270	CDL	CA3-OA5-PA1-OA2
25	P	1270	CDL	CB2-OB2-PB2-OB5
25	T	1269	CDL	CB3-OB5-PB2-OB2
26	R	1230	PSC	C04-O12-P-O11
26	E	230	PSC	C04-O12-P-O11
24	G	1263	PEK	C03-O11-P-O12
24	G	1263	PEK	C04-O12-P-O11

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Mol	Chain	Res	Type	Atoms
20	N	1524	PGV	C04-O12-P-O11
25	C	270	CDL	CA2-OA2-PA1-OA5
25	C	270	CDL	CA3-OA5-PA1-OA2
25	C	270	CDL	CB2-OB2-PB2-OB5
25	C	270	CDL	CB3-OB5-PB2-OB2
20	N	1268	PGV	O12-C04-C05-C06
26	R	1230	PSC	C04-C05-N-C06
26	R	1230	PSC	C04-C05-N-C08
28	G	272	DMU	C3-C4-C57-O61
24	T	263	PEK	C22-C21-O03-C01
19	O	1523	TGL	CA9-C20-C21-C22
24	T	1265	PEK	C15-C16-C17-C18
20	A	522	PGV	C19-C20-C21-C22
25	G	269	CDL	C56-C57-C58-C59
26	E	230	PSC	C24-C25-C26-C27
24	G	1263	PEK	C31-C32-C33-C34
28	G	272	DMU	O5-C4-C57-O61
25	G	269	CDL	C75-C76-C77-C78
19	L	522	TGL	CA5-CA6-CA7-CA8
25	P	1270	CDL	C62-C63-C64-C65
20	N	1266	PGV	C6-C7-C8-C9
20	N	1266	PGV	C7-C8-C9-C10
19	D	523	TGL	C16-C15-CC9-CC8
19	O	1521	TGL	CB9-C10-C11-C12
25	C	270	CDL	C38-C39-C40-C41
24	G	265	PEK	C22-C21-O03-C01
28	Z	1526	DMU	C25-C28-C31-C34
25	G	269	CDL	C36-C37-C38-C39
25	P	1270	CDL	C36-C37-C38-C39
20	H	268	PGV	C28-C29-C30-C31
20	N	1268	PGV	C6-C7-C8-C9
26	R	1230	PSC	C24-C25-C26-C27
19	O	1523	TGL	C15-C16-C17-C18
24	T	1265	PEK	C29-C30-C31-C32
19	O	1521	TGL	CC5-CC6-CC7-CC8
20	C	267	PGV	C7-C8-C9-C10
28	G	272	DMU	C28-C31-C34-C37
19	Y	1522	TGL	C22-C23-C24-C25
25	C	270	CDL	C39-C40-C41-C42
25	C	270	CDL	C58-C59-C60-C61
25	C	270	CDL	C61-C62-C63-C64
19	A	521	TGL	CG1-CG2-OG2-CB1

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Mol	Chain	Res	Type	Atoms
26	E	230	PSC	C19-C20-C21-C22
25	G	269	CDL	C22-C23-C24-C25
19	L	522	TGL	CC6-CC7-CC8-CC9
24	P	1264	PEK	C23-C24-C25-C26
25	P	1270	CDL	C77-C78-C79-C80
19	Y	1522	TGL	CC6-CC7-CC8-CC9
19	Y	1522	TGL	C19-C33-C34-C35
20	N	1524	PGV	C2-C3-C4-C5
20	H	268	PGV	C02-C03-O11-P
24	T	263	PEK	O04-C21-O03-C01
20	N	1268	PGV	C10-C11-C12-C13
20	A	524	PGV	C10-C11-C12-C13
19	A	521	TGL	C13-C14-C29-C30
19	A	521	TGL	C21-C22-C23-C24
19	L	522	TGL	C16-C15-CC9-CC8
25	P	1270	CDL	C37-C38-C39-C40
20	H	268	PGV	C24-C25-C26-C27
20	N	1268	PGV	C13-C14-C15-C16
20	N	1268	PGV	C22-C23-C24-C25
25	P	1270	CDL	O1-C1-CA2-OA2
28	Z	1526	DMU	O16-C18-C19-C22
25	G	269	CDL	C38-C39-C40-C41
19	L	522	TGL	CC4-CC5-CC6-CC7
25	C	270	CDL	C16-C17-C18-C19
26	E	230	PSC	C1-C2-C3-C4
19	O	1523	TGL	OG1-CG1-CG2-OG2
25	G	269	CDL	C77-C78-C79-C80
19	A	521	TGL	C20-C21-C22-C23
24	P	1264	PEK	C31-C32-C33-C34
25	T	1269	CDL	C31-C32-C33-C34
25	T	1269	CDL	C82-C83-C84-C85
26	R	1230	PSC	C21-C22-C23-C24
19	O	1523	TGL	CA4-CA5-CA6-CA7
19	O	1523	TGL	CC4-CC5-CC6-CC7
19	D	523	TGL	C11-C10-CB9-CB8
25	C	270	CDL	C57-C58-C59-C60
25	G	269	CDL	C80-C81-C82-C83
25	P	1270	CDL	C63-C64-C65-C66
24	G	1263	PEK	C27-C28-C29-C30
24	T	263	PEK	C16-C17-C18-C19
25	P	1270	CDL	C12-C13-C14-C15
25	P	1270	CDL	C53-C54-C55-C56

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Mol	Chain	Res	Type	Atoms
25	T	1269	CDL	C18-C19-C20-C21
25	T	1269	CDL	C75-C76-C77-C78
20	N	1268	PGV	C23-C24-C25-C26
19	O	1523	TGL	CC9-C15-C16-C17
24	T	1265	PEK	C16-C17-C18-C19
19	O	1521	TGL	CA4-CA5-CA6-CA7
19	O	1521	TGL	C10-C11-C12-C13
19	O	1521	TGL	C18-C19-C33-C34
20	N	1524	PGV	C24-C25-C26-C27
25	C	270	CDL	C11-C12-C13-C14
25	C	270	CDL	C52-C53-C54-C55
25	T	1269	CDL	C38-C39-C40-C41
20	A	524	PGV	C26-C27-C28-C29
19	Y	1522	TGL	CB4-CB5-CB6-CB7
19	Y	1522	TGL	C21-C22-C23-C24
20	A	524	PGV	C04-C05-C06-O06
25	T	1269	CDL	C11-CA5-OA6-CA4
25	G	269	CDL	C55-C56-C57-C58
20	H	268	PGV	C4-C5-C6-C7
25	T	1269	CDL	C36-C37-C38-C39
19	Y	1522	TGL	CB9-C10-C11-C12
19	Y	1522	TGL	C18-C19-C33-C34
20	N	1524	PGV	C3-C4-C5-C6
25	C	270	CDL	C71-C72-C73-C74
25	G	269	CDL	C16-C17-C18-C19
25	P	1270	CDL	C42-C43-C44-C45
20	N	1268	PGV	C24-C25-C26-C27
19	O	1523	TGL	CC2-CC3-CC4-CC5
24	T	1265	PEK	C33-C34-C35-C36
19	O	1521	TGL	C16-C17-C18-C19
25	C	270	CDL	C72-C73-C74-C75
26	R	1230	PSC	C04-C05-N-C07
28	M	526	DMU	O5-C6-O16-C18
26	E	230	PSC	C01-C02-C03-O11
24	G	265	PEK	C24-C25-C26-C27
28	P	1272	DMU	C31-C34-C37-C40
25	G	269	CDL	C42-C43-C44-C45
24	P	1264	PEK	C24-C25-C26-C27
25	T	1269	CDL	C11-C12-C13-C14
25	T	1269	CDL	C61-C62-C63-C64
19	O	1523	TGL	CB9-C10-C11-C12
19	D	523	TGL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
19	O	1521	TGL	C17-C18-C19-C33
19	O	1521	TGL	C14-C29-C30-C31
25	C	270	CDL	C17-C18-C19-C20
25	P	1270	CDL	C73-C74-C75-C76
25	P	1270	CDL	C81-C82-C83-C84
25	T	1269	CDL	C60-C61-C62-C63
24	G	1263	PEK	C25-C26-C27-C28
19	D	523	TGL	CB1-CB2-CB3-CB4
19	O	1521	TGL	CA1-CA2-CA3-CA4
20	N	1524	PGV	C1-C2-C3-C4
25	G	269	CDL	C18-C19-C20-C21
25	G	269	CDL	C21-C22-C23-C24
19	A	521	TGL	C24-C25-C26-C27
20	N	1266	PGV	C5-C6-C7-C8
19	O	1523	TGL	CC5-CC6-CC7-CC8
24	G	1263	PEK	C29-C30-C31-C32
19	A	521	TGL	CC5-CC6-CC7-CC8
25	P	1270	CDL	C74-C75-C76-C77
19	D	523	TGL	C21-C20-CA9-CA8
20	A	524	PGV	C14-C15-C16-C17
25	G	269	CDL	C73-C74-C75-C76
25	P	1270	CDL	C16-C17-C18-C19
25	T	1269	CDL	C55-C56-C57-C58
26	R	1230	PSC	C5-C6-C7-C8
19	Y	1522	TGL	C11-C10-CB9-CB8
25	T	1269	CDL	CB7-C71-C72-C73
19	L	522	TGL	C21-C22-C23-C24
25	T	1269	CDL	OA7-CA5-OA6-CA4
24	T	1265	PEK	C25-C26-C27-C28
20	A	524	PGV	C25-C26-C27-C28
19	Y	1522	TGL	C16-C17-C18-C19
20	H	268	PGV	C19-C20-C21-C22
24	T	263	PEK	C29-C30-C31-C32
20	P	1267	PGV	C22-C23-C24-C25
25	C	270	CDL	C51-CB5-OB6-CB4
25	G	269	CDL	C33-C34-C35-C36
24	C	264	PEK	C27-C28-C29-C30
19	O	1523	TGL	C11-C12-C13-C14
20	P	1267	PGV	C24-C25-C26-C27
19	Y	1522	TGL	C23-C24-C25-C26
22	P	1525	CHD	C13-C17-C20-C21
20	N	1524	PGV	O05-C05-C06-O06

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Mol	Chain	Res	Type	Atoms
19	O	1523	TGL	CA6-CA7-CA8-CA9
19	O	1523	TGL	C16-C15-CC9-CC8
19	D	523	TGL	C17-C18-C19-C33
25	C	270	CDL	C53-C54-C55-C56
24	G	265	PEK	C2-C3-C4-C5
24	P	1264	PEK	C15-C16-C17-C18
20	N	1268	PGV	C12-C13-C14-C15
24	T	1265	PEK	C2-C3-C4-C5
25	P	1270	CDL	C64-C65-C66-C67
24	T	1265	PEK	C34-C35-C36-C37
20	P	1267	PGV	C28-C29-C30-C31
25	C	270	CDL	C36-C37-C38-C39
25	G	269	CDL	C62-C63-C64-C65
25	T	1269	CDL	C59-C60-C61-C62
26	E	230	PSC	C5-C6-C7-C8
19	Y	1522	TGL	C14-C29-C30-C31
24	G	265	PEK	O04-C21-O03-C01
19	O	1523	TGL	C21-C20-CA9-CA8
20	A	522	PGV	C23-C24-C25-C26
25	C	270	CDL	C35-C36-C37-C38
25	C	270	CDL	OB7-CB5-OB6-CB4
24	P	1264	PEK	C26-C27-C28-C29
19	Y	1522	TGL	CB5-CB6-CB7-CB8
19	Y	1522	TGL	C24-C25-C26-C27
20	C	267	PGV	C1-C2-C3-C4
24	C	264	PEK	C25-C26-C27-C28
28	M	526	DMU	C25-C28-C31-C34
26	R	1230	PSC	C29-C30-C31-C32
26	E	230	PSC	C26-C27-C28-C29
19	O	1521	TGL	C25-C26-C27-C28
19	Y	1522	TGL	CC9-C15-C16-C17
25	C	270	CDL	C21-C22-C23-C24
19	A	521	TGL	CA1-CA2-CA3-CA4
25	G	269	CDL	C71-C72-C73-C74
19	A	521	TGL	CB3-CB4-CB5-CB6
19	D	523	TGL	C15-C16-C17-C18
24	C	264	PEK	C28-C29-C30-C31
20	N	1266	PGV	C23-C24-C25-C26
24	T	1265	PEK	C7-C8-C9-C10
24	G	1263	PEK	C4-C5-C6-C7
24	C	264	PEK	C3-C4-C5-C6
19	L	522	TGL	C17-C18-C19-C33

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Mol	Chain	Res	Type	Atoms
20	H	268	PGV	C30-C31-C32-C33
28	G	272	DMU	C31-C34-C37-C40
26	E	230	PSC	C13-C14-C15-C16
19	L	522	TGL	OB1-CB1-OG2-CG2
25	T	1269	CDL	CB5-C51-C52-C53
19	A	521	TGL	CC2-CC1-OG3-CG3
20	N	1268	PGV	C31-C32-C33-C34
25	G	269	CDL	C20-C21-C22-C23
19	A	521	TGL	CC4-CC5-CC6-CC7
19	O	1521	TGL	CC4-CC5-CC6-CC7
19	O	1521	TGL	CB1-CB2-CB3-CB4
19	A	521	TGL	CA7-CA8-CA9-C20
19	A	521	TGL	C21-C20-CA9-CA8
25	T	1269	CDL	C57-C58-C59-C60
25	T	1269	CDL	C71-C72-C73-C74
20	A	522	PGV	C26-C27-C28-C29
19	A	521	TGL	C16-C15-CC9-CC8
20	N	1268	PGV	C14-C15-C16-C17
20	N	1266	PGV	C29-C30-C31-C32
19	D	523	TGL	CA6-CA7-CA8-CA9
25	T	1269	CDL	C40-C41-C42-C43
19	Y	1522	TGL	CC4-CC5-CC6-CC7
25	C	270	CDL	C56-C57-C58-C59
25	C	270	CDL	C79-C80-C81-C82
19	L	522	TGL	CB2-CB1-OG2-CG2
19	D	523	TGL	CB2-CB1-OG2-CG2
19	O	1521	TGL	CB2-CB1-OG2-CG2
20	H	268	PGV	O01-C02-C03-O11
19	L	522	TGL	C11-C12-C13-C14
25	T	1269	CDL	O1-C1-CA2-OA2
19	O	1521	TGL	OB1-CB1-OG2-CG2
20	H	268	PGV	O03-C01-C02-O01
19	A	521	TGL	CA5-CA6-CA7-CA8
26	R	1230	PSC	C26-C27-C28-C29
25	P	1270	CDL	C71-C72-C73-C74
19	O	1523	TGL	CA5-CA6-CA7-CA8
24	G	1263	PEK	C22-C23-C24-C25
20	A	524	PGV	C21-C22-C23-C24
24	P	1264	PEK	C1-C2-C3-C4
25	G	269	CDL	C78-C79-C80-C81
20	C	267	PGV	C29-C30-C31-C32
26	R	1230	PSC	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
20	C	267	PGV	C20-C21-C22-C23
20	N	1524	PGV	C22-C23-C24-C25
24	C	264	PEK	C23-C24-C25-C26
19	D	523	TGL	CB2-CB3-CB4-CB5
20	H	268	PGV	C13-C14-C15-C16
19	O	1523	TGL	CC6-CC7-CC8-CC9
19	A	521	TGL	OC1-CC1-OG3-CG3
19	D	523	TGL	OB1-CB1-OG2-CG2
24	G	265	PEK	C30-C31-C32-C33
19	A	521	TGL	CC7-CC8-CC9-C15
25	C	270	CDL	C42-C43-C44-C45
25	T	1269	CDL	CA3-OA5-PA1-OA2
26	E	230	PSC	C03-O11-P-O12
26	E	230	PSC	C27-C28-C29-C30
25	P	1270	CDL	OA5-CA3-CA4-CA6
20	H	268	PGV	C01-C02-C03-O11
20	N	1268	PGV	C01-C02-C03-O11
24	T	1265	PEK	C01-C02-C03-O11
25	C	270	CDL	OA5-CA3-CA4-CA6
19	Y	1522	TGL	C15-C16-C17-C18
20	N	1524	PGV	C30-C31-C32-C33
25	C	270	CDL	C78-C79-C80-C81
28	M	526	DMU	O16-C18-C19-C22
20	P	1267	PGV	C7-C8-C9-C10
25	P	1270	CDL	C51-C52-C53-C54
19	O	1523	TGL	C18-C19-C33-C34
28	G	272	DMU	C25-C28-C31-C34
20	N	1524	PGV	C12-C13-C14-C15
25	C	270	CDL	CB5-C51-C52-C53
28	Z	1526	DMU	C22-C25-C28-C31
19	O	1523	TGL	C14-C29-C30-C31
18	A	515	HEA	C27-C19-C20-C21
25	T	1269	CDL	C72-C73-C74-C75
19	O	1521	TGL	C16-C15-CC9-CC8
19	L	522	TGL	CC2-CC3-CC4-CC5
20	N	1524	PGV	C5-C6-C7-C8
25	G	269	CDL	CB7-C71-C72-C73
19	A	521	TGL	C16-C17-C18-C19
25	G	269	CDL	CA3-CA4-CA6-OA8
25	G	269	CDL	C58-C59-C60-C61
25	G	269	CDL	C74-C75-C76-C77
24	T	263	PEK	O03-C01-C02-C03

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Mol	Chain	Res	Type	Atoms
19	L	522	TGL	C21-C20-CA9-CA8
19	O	1523	TGL	OG1-CG1-CG2-CG3
19	D	523	TGL	OG1-CG1-CG2-CG3
24	G	1263	PEK	O03-C01-C02-C03
20	P	1267	PGV	C15-C16-C17-C18
24	T	1265	PEK	C4-C5-C6-C7
20	P	1267	PGV	C10-C11-C12-C13
19	O	1523	TGL	CC7-CC8-CC9-C15
19	O	1521	TGL	CB4-CB5-CB6-CB7
28	Z	1526	DMU	C34-C37-C40-C43
20	N	1266	PGV	C31-C32-C33-C34
25	G	269	CDL	C32-C31-CA7-OA8
20	N	1268	PGV	C19-C20-C21-C22
24	G	265	PEK	C35-C36-C37-C38
24	T	263	PEK	C26-C27-C28-C29
24	P	1264	PEK	C3-C4-C5-C6
20	A	522	PGV	C31-C32-C33-C34
24	C	264	PEK	C15-C16-C17-C18
19	D	523	TGL	C16-C17-C18-C19
25	G	269	CDL	C61-C62-C63-C64
24	T	1265	PEK	C22-C21-O03-C01
25	G	269	CDL	C35-C36-C37-C38
25	C	270	CDL	C18-C19-C20-C21
24	P	1264	PEK	C25-C26-C27-C28
24	C	264	PEK	C17-C18-C19-C20
25	T	1269	CDL	C24-C25-C26-C27
26	R	1230	PSC	C03-C02-O01-C1
19	O	1523	TGL	CG3-CG2-OG2-CB1
19	D	523	TGL	CG3-CG2-OG2-CB1
26	E	230	PSC	C03-C02-O01-C1
20	A	524	PGV	C03-C02-O01-C1
25	G	269	CDL	C17-C18-C19-C20
26	R	1230	PSC	C31-C32-C33-C34
24	T	1265	PEK	C30-C31-C32-C33
20	A	522	PGV	C5-C6-C7-C8
20	H	268	PGV	C15-C16-C17-C18
25	T	1269	CDL	C34-C35-C36-C37
19	D	523	TGL	CA5-CA6-CA7-CA8
20	C	267	PGV	C31-C32-C33-C34
20	P	1267	PGV	C25-C26-C27-C28
19	Y	1522	TGL	C17-C18-C19-C33
20	N	1524	PGV	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	L	522	TGL	OG2-CB1-CB2-CB3
26	E	230	PSC	C04-C05-N-C07
26	E	230	PSC	C3-C4-C5-C6
26	E	230	PSC	C31-C32-C33-C34
20	C	267	PGV	C24-C25-C26-C27
25	C	270	CDL	C82-C83-C84-C85
20	A	524	PGV	C28-C29-C30-C31
22	C	271	CHD	C13-C17-C20-C22
20	A	522	PGV	C24-C25-C26-C27
20	H	268	PGV	C11-C10-C9-C8
24	P	1264	PEK	C35-C36-C37-C38
25	G	269	CDL	OA6-CA4-CA6-OA8
25	G	269	CDL	OB6-CB4-CB6-OB8
25	P	1270	CDL	OB6-CB4-CB6-OB8
25	C	270	CDL	OA6-CA4-CA6-OA8
19	A	521	TGL	CA4-CA5-CA6-CA7
20	A	524	PGV	C24-C25-C26-C27
25	C	270	CDL	C37-C38-C39-C40
19	L	522	TGL	CB7-CB8-CB9-C10
19	O	1521	TGL	C20-C21-C22-C23
19	Y	1522	TGL	CA9-C20-C21-C22
28	M	526	DMU	C34-C37-C40-C43
19	O	1523	TGL	CA7-CA8-CA9-C20
25	P	1270	CDL	C57-C58-C59-C60
20	H	268	PGV	C25-C26-C27-C28
19	L	522	TGL	C13-C14-C29-C30
25	P	1270	CDL	C13-C14-C15-C16
25	G	269	CDL	OA5-CA3-CA4-CA6
25	T	1269	CDL	OA5-CA3-CA4-CA6
26	R	1230	PSC	C28-C29-C30-C31
20	N	1524	PGV	C28-C29-C30-C31
24	G	1263	PEK	C26-C27-C28-C29
18	A	515	HEA	C16-C17-C18-C19
25	P	1270	CDL	C24-C25-C26-C27
26	R	1230	PSC	C2-C3-C4-C5
25	C	270	CDL	C1-CA2-OA2-PA1
25	P	1270	CDL	C72-C73-C74-C75
28	P	1272	DMU	C19-C18-O16-C6
19	O	1521	TGL	CB6-CB7-CB8-CB9
19	L	522	TGL	C22-C23-C24-C25
25	P	1270	CDL	C59-C60-C61-C62
19	D	523	TGL	CA4-CA5-CA6-CA7

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Mol	Chain	Res	Type	Atoms
25	G	269	CDL	C34-C35-C36-C37
25	G	269	CDL	C52-C53-C54-C55
20	H	268	PGV	C23-C24-C25-C26
20	N	1524	PGV	C20-C21-C22-C23
25	P	1270	CDL	CB3-CB4-CB6-OB8
26	R	1230	PSC	O03-C01-C02-C03
26	E	230	PSC	O03-C01-C02-C03
25	C	270	CDL	CA3-CA4-CA6-OA8
25	C	270	CDL	CB3-CB4-CB6-OB8
24	G	265	PEK	C4-C5-C6-C7
20	H	268	PGV	C10-C11-C12-C13
20	N	1524	PGV	C31-C32-C33-C34
25	C	270	CDL	C84-C85-C86-C87
25	G	269	CDL	C31-C32-C33-C34
20	H	268	PGV	C21-C22-C23-C24
24	G	265	PEK	C11-C10-C9-C8
24	G	265	PEK	C9-C10-C11-C12
24	T	263	PEK	C6-C7-C8-C9
24	T	263	PEK	C11-C12-C13-C14
24	T	263	PEK	C12-C13-C14-C15
24	P	1264	PEK	C11-C10-C9-C8
24	P	1264	PEK	C9-C10-C11-C12
20	H	268	PGV	C03-O11-P-O12
24	C	264	PEK	C9-C10-C11-C12
24	C	264	PEK	C12-C13-C14-C15
26	R	1230	PSC	C9-C10-C11-C12
24	T	1265	PEK	C5-C6-C7-C8
24	T	1265	PEK	C6-C7-C8-C9
24	G	1263	PEK	C9-C10-C11-C12
24	G	1263	PEK	C11-C12-C13-C14
24	T	1265	PEK	O04-C21-O03-C01
19	L	522	TGL	C11-C10-CB9-CB8
20	N	1524	PGV	C26-C27-C28-C29
24	T	263	PEK	O01-C02-C03-O11
25	C	270	CDL	OA5-CA3-CA4-OA6
24	P	1264	PEK	C17-C18-C19-C20
25	P	1270	CDL	C52-C53-C54-C55
19	A	521	TGL	CB9-C10-C11-C12
25	C	270	CDL	C54-C55-C56-C57
19	D	523	TGL	OG2-CB1-CB2-CB3
19	L	522	TGL	OG2-CG2-CG3-OG3
28	P	1272	DMU	C28-C31-C34-C37

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Mol	Chain	Res	Type	Atoms
20	A	524	PGV	C31-C32-C33-C34
19	O	1521	TGL	CC7-CC8-CC9-C15
19	A	521	TGL	C14-C29-C30-C31
20	H	268	PGV	C5-C6-C7-C8
19	Y	1522	TGL	C11-C12-C13-C14
25	P	1270	CDL	CA4-CA3-OA5-PA1
24	G	1263	PEK	C02-C03-O11-P
20	C	267	PGV	C02-C03-O11-P
20	P	1267	PGV	C13-C14-C15-C16
26	E	230	PSC	C04-C05-N-C06
26	E	230	PSC	C29-C30-C31-C32
19	L	522	TGL	OG1-CA1-CA2-CA3
25	P	1270	CDL	C84-C85-C86-C87
19	D	523	TGL	C13-C14-C29-C30
26	R	1230	PSC	C27-C28-C29-C30
28	M	526	DMU	C22-C25-C28-C31
19	D	523	TGL	CC6-CC7-CC8-CC9
28	Z	1526	DMU	C19-C22-C25-C28
19	A	521	TGL	CB6-CB7-CB8-CB9
20	H	268	PGV	C27-C28-C29-C30
25	T	1269	CDL	OB5-CB3-CB4-CB6
20	N	1524	PGV	C01-C02-C03-O11
19	D	523	TGL	OG1-CA1-CA2-CA3
20	C	267	PGV	C12-C13-C14-C15
20	A	522	PGV	C11-C10-C9-C8
24	T	263	PEK	C25-C26-C27-C28
19	O	1521	TGL	C19-C33-C34-C35
25	G	269	CDL	C54-C55-C56-C57
19	L	522	TGL	C12-C13-C14-C29
20	H	268	PGV	C20-C19-O03-C01
24	G	265	PEK	C26-C27-C28-C29
25	C	270	CDL	C40-C41-C42-C43
20	H	268	PGV	C22-C23-C24-C25
24	G	1263	PEK	C16-C17-C18-C19
20	P	1267	PGV	C14-C15-C16-C17
20	A	524	PGV	C11-C10-C9-C8
20	N	1268	PGV	C05-C04-O12-P
19	Y	1522	TGL	CG1-CG2-CG3-OG3
25	C	270	CDL	C59-C60-C61-C62
25	P	1270	CDL	OB5-CB3-CB4-OB6
28	P	1272	DMU	C34-C37-C40-C43
20	N	1268	PGV	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	N	1266	PGV	C25-C26-C27-C28
20	P	1267	PGV	C31-C32-C33-C34
20	C	267	PGV	C28-C29-C30-C31
28	P	1272	DMU	O6-C11-C9-C8
20	A	524	PGV	O05-C05-C06-O06
24	G	265	PEK	C25-C26-C27-C28
20	A	524	PGV	C7-C8-C9-C10
26	R	1230	PSC	O02-C1-O01-C02
19	O	1521	TGL	C23-C24-C25-C26
20	N	1268	PGV	C3-C4-C5-C6
19	D	523	TGL	C18-C19-C33-C34
24	G	265	PEK	C29-C30-C31-C32
26	E	230	PSC	C6-C7-C8-C9
20	A	524	PGV	C04-O12-P-O11
25	T	1269	CDL	CA4-CA3-OA5-PA1
20	H	268	PGV	O04-C19-O03-C01
25	G	269	CDL	CA3-OA5-PA1-OA3
25	G	269	CDL	CB3-OB5-PB2-OB4
25	P	1270	CDL	CA2-OA2-PA1-OA4
25	P	1270	CDL	CA3-OA5-PA1-OA3
25	P	1270	CDL	CB2-OB2-PB2-OB4
20	H	268	PGV	C03-O11-P-O14
25	T	1269	CDL	CA2-OA2-PA1-OA3
25	T	1269	CDL	CA2-OA2-PA1-OA4
25	T	1269	CDL	CA3-OA5-PA1-OA3
25	T	1269	CDL	CA3-OA5-PA1-OA4
26	R	1230	PSC	C04-O12-P-O13
26	E	230	PSC	C03-O11-P-O13
26	E	230	PSC	C04-O12-P-O13
24	G	1263	PEK	C04-O12-P-O13
24	G	1263	PEK	C04-O12-P-O14
20	N	1524	PGV	C03-O11-P-O13
20	N	1524	PGV	C04-O12-P-O13
25	C	270	CDL	CA2-OA2-PA1-OA4
25	C	270	CDL	CA3-OA5-PA1-OA3
25	C	270	CDL	CB2-OB2-PB2-OB4
25	C	270	CDL	CB3-OB5-PB2-OB4
24	T	263	PEK	C01-C02-C03-O11
19	Y	1522	TGL	CA5-CA6-CA7-CA8
28	G	272	DMU	C34-C37-C40-C43
24	T	263	PEK	C32-C33-C34-C35
19	L	522	TGL	CC7-CC8-CC9-C15

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Mol	Chain	Res	Type	Atoms
25	P	1270	CDL	C43-C44-C45-C46
25	P	1270	CDL	C83-C84-C85-C86
24	T	263	PEK	C28-C29-C30-C31
19	O	1521	TGL	CA3-CA4-CA5-CA6
24	G	1263	PEK	C32-C33-C34-C35
19	L	522	TGL	C10-C11-C12-C13
25	P	1270	CDL	C31-C32-C33-C34
25	T	1269	CDL	OA5-CA3-CA4-OA6
26	E	230	PSC	O01-C02-C03-O11
25	C	270	CDL	C34-C35-C36-C37
19	D	523	TGL	CC7-CC8-CC9-C15
19	Y	1522	TGL	CB7-CB8-CB9-C10
26	E	230	PSC	O01-C1-C2-C3
25	G	269	CDL	CB3-CB4-CB6-OB8
19	L	522	TGL	CG1-CG2-CG3-OG3
26	R	1230	PSC	O12-C04-C05-N
26	E	230	PSC	O12-C04-C05-N
25	C	270	CDL	OB6-CB4-CB6-OB8
19	O	1521	TGL	C12-C13-C14-C29
19	Y	1522	TGL	CA4-CA5-CA6-CA7
24	C	264	PEK	C34-C35-C36-C37
25	G	269	CDL	CB4-CB3-OB5-PB2
20	P	1267	PGV	C02-C03-O11-P
20	A	522	PGV	C7-C8-C9-C10
19	L	522	TGL	CB6-CB7-CB8-CB9
25	T	1269	CDL	C14-C15-C16-C17
28	G	272	DMU	C5-C10-O7-C3
24	G	265	PEK	C23-C24-C25-C26
20	N	1524	PGV	C11-C12-C13-C14
25	G	269	CDL	C32-C33-C34-C35
20	N	1266	PGV	C26-C27-C28-C29
20	A	522	PGV	O03-C19-C20-C21
20	N	1266	PGV	C10-C11-C12-C13
25	G	269	CDL	C23-C24-C25-C26
24	T	1265	PEK	C14-C15-C16-C17
25	T	1269	CDL	C80-C81-C82-C83
25	G	269	CDL	C14-C15-C16-C17
25	G	269	CDL	C76-C77-C78-C79
25	T	1269	CDL	C20-C21-C22-C23
19	O	1521	TGL	CG1-CG2-OG2-CB1
25	G	269	CDL	OB7-CB5-OB6-CB4
20	N	1268	PGV	O02-C1-O01-C02

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Mol	Chain	Res	Type	Atoms
19	A	521	TGL	CA6-CA7-CA8-CA9
25	C	270	CDL	C1-CB2-OB2-PB2
25	P	1270	CDL	OA5-CA3-CA4-OA6
19	Y	1522	TGL	OG2-CB1-CB2-CB3
20	N	1268	PGV	C15-C16-C17-C18
24	G	1263	PEK	C17-C18-C19-C20
25	T	1269	CDL	C44-C45-C46-C47
26	R	1230	PSC	C2-C1-O01-C02
20	N	1266	PGV	C9-C10-C11-C12
24	C	264	PEK	C24-C25-C26-C27
20	A	522	PGV	C29-C30-C31-C32
24	G	265	PEK	C04-O12-P-O11
25	G	269	CDL	CA3-OA5-PA1-OA2
25	P	1270	CDL	CB3-OB5-PB2-OB2
20	H	268	PGV	C04-O12-P-O11
25	T	1269	CDL	CB2-OB2-PB2-OB5
20	N	1268	PGV	C04-O12-P-O11
26	R	1230	PSC	C03-O11-P-O12
20	N	1524	PGV	C03-O11-P-O12
25	G	269	CDL	C53-C54-C55-C56
19	Y	1522	TGL	CC2-CC1-OG3-CG3
25	P	1270	CDL	CA3-CA4-CA6-OA8
24	T	1265	PEK	O03-C01-C02-C03
25	G	269	CDL	C12-C13-C14-C15
20	H	268	PGV	C2-C3-C4-C5
25	G	269	CDL	C40-C41-C42-C43
25	G	269	CDL	C57-C58-C59-C60
25	C	270	CDL	C51-C52-C53-C54
20	A	524	PGV	O01-C1-C2-C3
24	G	265	PEK	C17-C18-C19-C20
19	Y	1522	TGL	C16-C15-CC9-CC8
25	G	269	CDL	C51-CB5-OB6-CB4
20	P	1267	PGV	C23-C24-C25-C26
24	C	264	PEK	C2-C3-C4-C5
19	O	1523	TGL	C22-C23-C24-C25
25	G	269	CDL	C32-C31-CA7-OA9
25	T	1269	CDL	C31-CA7-OA8-CA6
25	P	1270	CDL	C1-CA2-OA2-PA1
25	C	270	CDL	C60-C61-C62-C63
19	L	522	TGL	C29-C30-C31-C32
20	C	267	PGV	C30-C31-C32-C33
20	N	1266	PGV	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
20	A	522	PGV	C12-C13-C14-C15
24	T	263	PEK	O01-C1-C2-C3
25	T	1269	CDL	C37-C38-C39-C40
25	P	1270	CDL	C19-C20-C21-C22
19	Y	1522	TGL	OC1-CC1-OG3-CG3
20	A	522	PGV	C28-C29-C30-C31
19	O	1523	TGL	C12-C13-C14-C29
25	T	1269	CDL	C16-C17-C18-C19
25	C	270	CDL	C43-C44-C45-C46
19	Y	1522	TGL	C33-C34-C35-C36
19	D	523	TGL	C29-C30-C31-C32
20	N	1268	PGV	C29-C30-C31-C32
20	H	268	PGV	O03-C01-C02-C03
20	N	1268	PGV	C9-C10-C11-C12
20	A	524	PGV	C11-C12-C13-C14
19	L	522	TGL	CA6-CA7-CA8-CA9
19	O	1523	TGL	CB2-CB3-CB4-CB5
19	D	523	TGL	CA2-CA3-CA4-CA5
20	P	1267	PGV	C29-C30-C31-C32
20	N	1524	PGV	C03-C02-O01-C1
20	N	1266	PGV	O03-C19-C20-C21
20	N	1266	PGV	C20-C21-C22-C23
24	P	1264	PEK	C14-C15-C16-C17
20	A	522	PGV	C9-C10-C11-C12
25	T	1269	CDL	OA9-CA7-OA8-CA6
24	G	265	PEK	C6-C7-C8-C9
24	T	263	PEK	C9-C10-C11-C12
24	G	1263	PEK	C11-C10-C9-C8
24	G	1263	PEK	C12-C13-C14-C15
20	N	1268	PGV	C25-C26-C27-C28
24	G	1263	PEK	C01-C02-C03-O11
24	G	1263	PEK	C33-C34-C35-C36
25	T	1269	CDL	C77-C78-C79-C80
24	T	1265	PEK	C22-C23-C24-C25
19	O	1521	TGL	C11-C10-CB9-CB8
28	Z	1526	DMU	C28-C31-C34-C37
25	P	1270	CDL	C11-C12-C13-C14
20	N	1524	PGV	C25-C26-C27-C28
24	G	265	PEK	C7-C8-C9-C10
24	T	1265	PEK	C10-C11-C12-C13
20	A	522	PGV	C11-C12-C13-C14
25	T	1269	CDL	C54-C55-C56-C57

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Mol	Chain	Res	Type	Atoms
24	T	263	PEK	C22-C23-C24-C25
20	C	267	PGV	C13-C14-C15-C16
20	A	524	PGV	C9-C10-C11-C12
25	T	1269	CDL	C79-C80-C81-C82
26	E	230	PSC	C28-C29-C30-C31
25	P	1270	CDL	C58-C59-C60-C61
26	E	230	PSC	C7-C8-C9-C10
19	Y	1522	TGL	OG1-CA1-CA2-CA3
19	O	1521	TGL	CB3-CB4-CB5-CB6
20	A	522	PGV	C4-C5-C6-C7
19	Y	1522	TGL	CB6-CB7-CB8-CB9
19	A	521	TGL	C18-C19-C33-C34
19	L	522	TGL	C16-C17-C18-C19
20	H	268	PGV	C12-C13-C14-C15
19	Y	1522	TGL	OG2-CG2-CG3-OG3
20	N	1524	PGV	O01-C1-C2-C3
24	T	263	PEK	C3-C4-C5-C6
24	G	265	PEK	O02-C1-O01-C02
26	R	1230	PSC	O03-C19-C20-C21
20	A	524	PGV	C2-C3-C4-C5
19	L	522	TGL	OA1-CA1-CA2-CA3
18	A	515	HEA	C18-C19-C20-C21
26	E	230	PSC	C4-C5-C6-C7
24	G	265	PEK	C3-C4-C5-C6
20	A	524	PGV	C12-C13-C14-C15
24	G	1263	PEK	O01-C02-C03-O11
24	C	264	PEK	O01-C1-C2-C3
25	G	269	CDL	C83-C84-C85-C86
20	A	524	PGV	C15-C16-C17-C18
25	C	270	CDL	C41-C42-C43-C44
25	T	1269	CDL	C42-C43-C44-C45
24	P	1264	PEK	O01-C1-C2-C3
19	D	523	TGL	OG3-CC1-CC2-CC3
24	G	265	PEK	C14-C15-C16-C17
24	T	1265	PEK	C3-C4-C5-C6
25	T	1269	CDL	C35-C36-C37-C38
25	P	1270	CDL	C52-C51-CB5-OB6
24	T	263	PEK	C15-C16-C17-C18
24	G	1263	PEK	C15-C16-C17-C18
26	E	230	PSC	C21-C22-C23-C24
19	O	1521	TGL	OG1-CG1-CG2-OG2
22	P	1525	CHD	C13-C17-C20-C22

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Mol	Chain	Res	Type	Atoms
19	O	1523	TGL	CB5-CB6-CB7-CB8
26	E	230	PSC	O03-C19-C20-C21
25	C	270	CDL	C12-C11-CA5-OA6
25	P	1270	CDL	C12-C11-CA5-OA6
20	N	1266	PGV	C11-C10-C9-C8
19	Y	1522	TGL	C29-C30-C31-C32
19	D	523	TGL	OA1-CA1-CA2-CA3
20	N	1268	PGV	C2-C1-O01-C02
25	P	1270	CDL	C52-C51-CB5-OB7
19	O	1523	TGL	C17-C18-C19-C33
19	L	522	TGL	OB1-CB1-CB2-CB3
20	N	1524	PGV	O02-C1-C2-C3
19	A	521	TGL	CB2-CB3-CB4-CB5
19	O	1523	TGL	C23-C24-C25-C26
19	O	1521	TGL	C21-C22-C23-C24
19	D	523	TGL	CC5-CC6-CC7-CC8
25	P	1270	CDL	C14-C15-C16-C17
19	A	521	TGL	C29-C30-C31-C32
24	P	1264	PEK	C16-C17-C18-C19
25	P	1270	CDL	C12-C11-CA5-OA7
25	C	270	CDL	C44-C45-C46-C47
24	P	1264	PEK	O02-C1-C2-C3
26	R	1230	PSC	O04-C19-C20-C21
25	C	270	CDL	C12-C11-CA5-OA7
25	T	1269	CDL	C81-C82-C83-C84
24	G	265	PEK	C04-O12-P-O14
20	H	268	PGV	C04-O12-P-O13
25	T	1269	CDL	CB2-OB2-PB2-OB3
20	N	1266	PGV	C04-O12-P-O13
25	C	270	CDL	C81-C82-C83-C84
19	D	523	TGL	OC1-CC1-CC2-CC3
19	Y	1522	TGL	C21-C20-CA9-CA8
24	C	264	PEK	O02-C1-C2-C3
26	E	230	PSC	O04-C19-C20-C21
22	P	1271	CHD	C16-C17-C20-C22
18	N	516	HEA	C26-C15-C16-C17
18	A	516	HEA	C26-C15-C16-C17
19	A	521	TGL	CB5-CB6-CB7-CB8
20	H	268	PGV	C31-C32-C33-C34
24	C	264	PEK	C22-C23-C24-C25
19	D	523	TGL	OB1-CB1-CB2-CB3
19	L	522	TGL	CB4-CB5-CB6-CB7

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Mol	Chain	Res	Type	Atoms
19	D	523	TGL	CC3-CC4-CC5-CC6
20	C	267	PGV	C05-C04-O12-P
19	A	521	TGL	CA2-CA3-CA4-CA5
25	C	270	CDL	C75-C76-C77-C78
19	O	1523	TGL	OG1-CA1-CA2-CA3
24	T	1265	PEK	O01-C1-C2-C3
24	G	1263	PEK	C30-C31-C32-C33
28	M	526	DMU	C28-C31-C34-C37
19	A	521	TGL	OG3-CC1-CC2-CC3
28	Z	1526	DMU	C31-C34-C37-C40

There are no ring outliers.

40 monomers are involved in 344 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	G	265	PEK	16	0
28	P	1272	DMU	1	0
18	A	515	HEA	9	0
25	G	269	CDL	27	0
15	A	520	PER	1	0
19	A	521	TGL	13	0
28	Z	1526	DMU	3	0
22	W	1060	CHD	4	0
19	L	522	TGL	15	0
26	E	230	PSC	22	0
22	B	1086	CHD	2	0
25	P	1270	CDL	24	0
20	H	268	PGV	3	0
24	P	1264	PEK	7	0
24	C	264	PEK	7	0
25	T	1269	CDL	19	0
20	N	1268	PGV	1	0
22	J	60	CHD	1	0
18	N	515	HEA	12	0
18	N	516	HEA	2	0
26	R	1230	PSC	15	0
19	O	1523	TGL	9	0
22	C	271	CHD	2	0
15	N	520	PER	1	0
24	T	1265	PEK	8	0
19	D	523	TGL	9	0
18	A	516	HEA	2	0

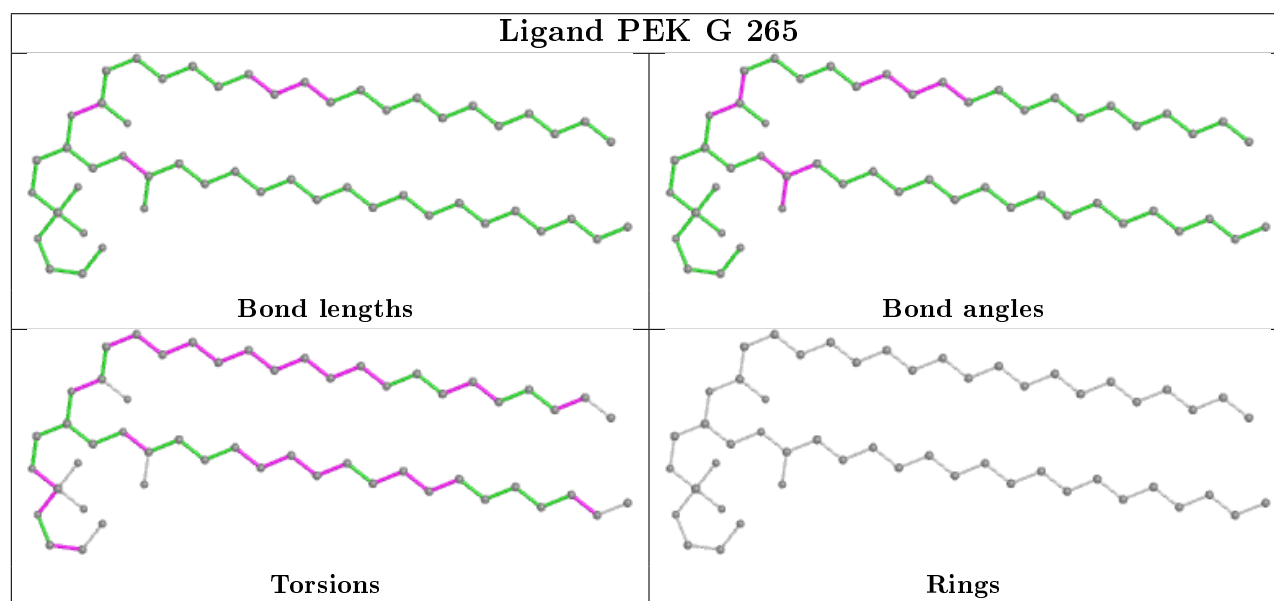
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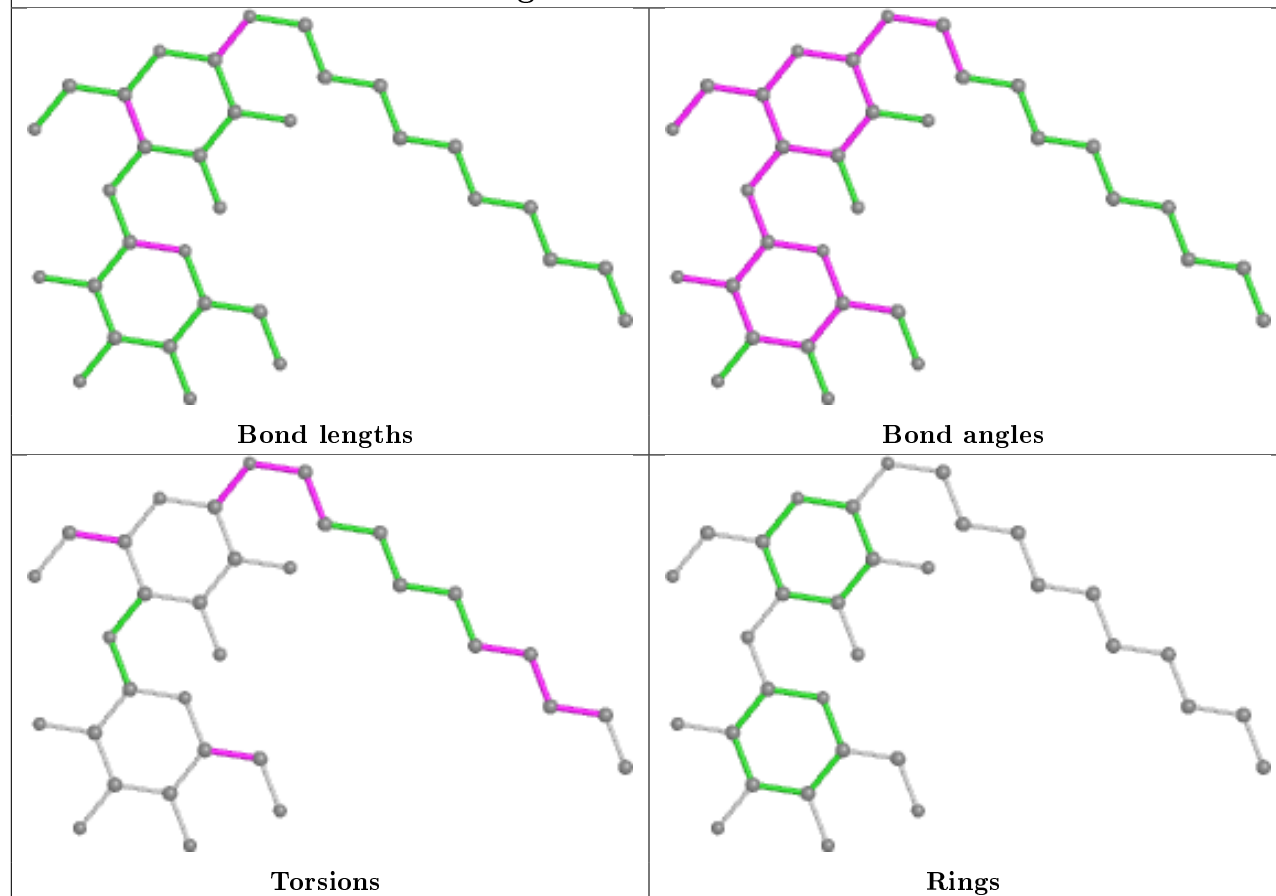
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	O	1521	TGL	14	0
24	G	1263	PEK	15	0
20	A	524	PGV	6	0
22	P	1271	CHD	1	0
20	C	267	PGV	4	0
24	T	263	PEK	22	0
28	G	272	DMU	5	0
22	C	525	CHD	3	0
20	P	1267	PGV	11	0
19	Y	1522	TGL	18	0
20	N	1524	PGV	11	0
20	A	522	PGV	2	0
25	C	270	CDL	19	0

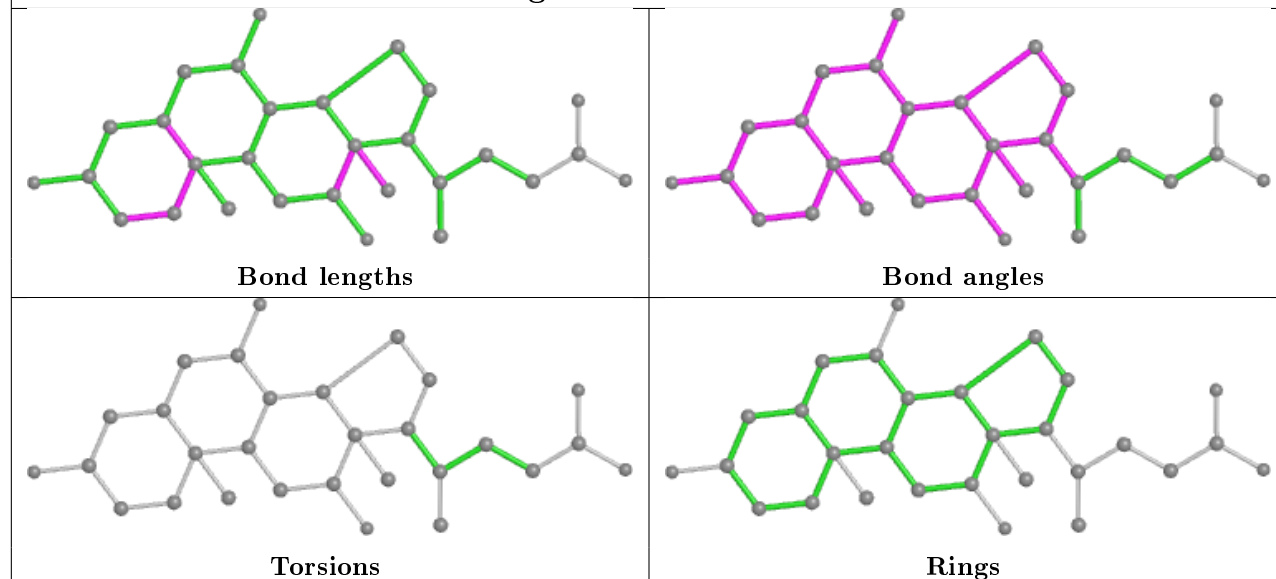
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

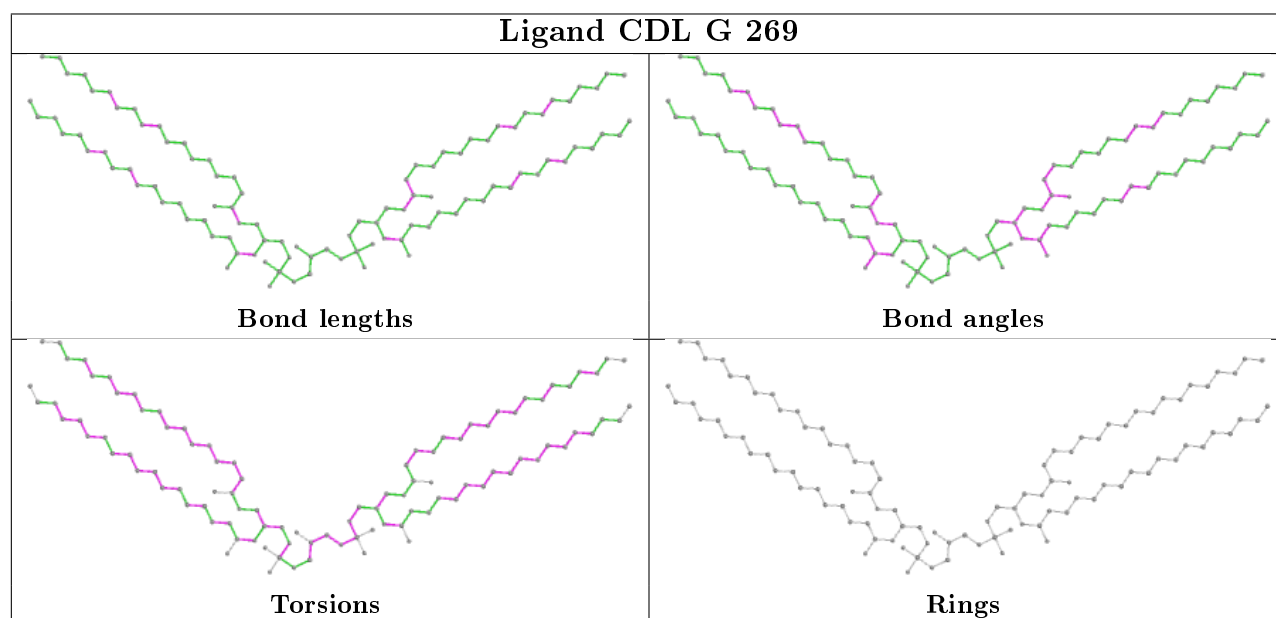
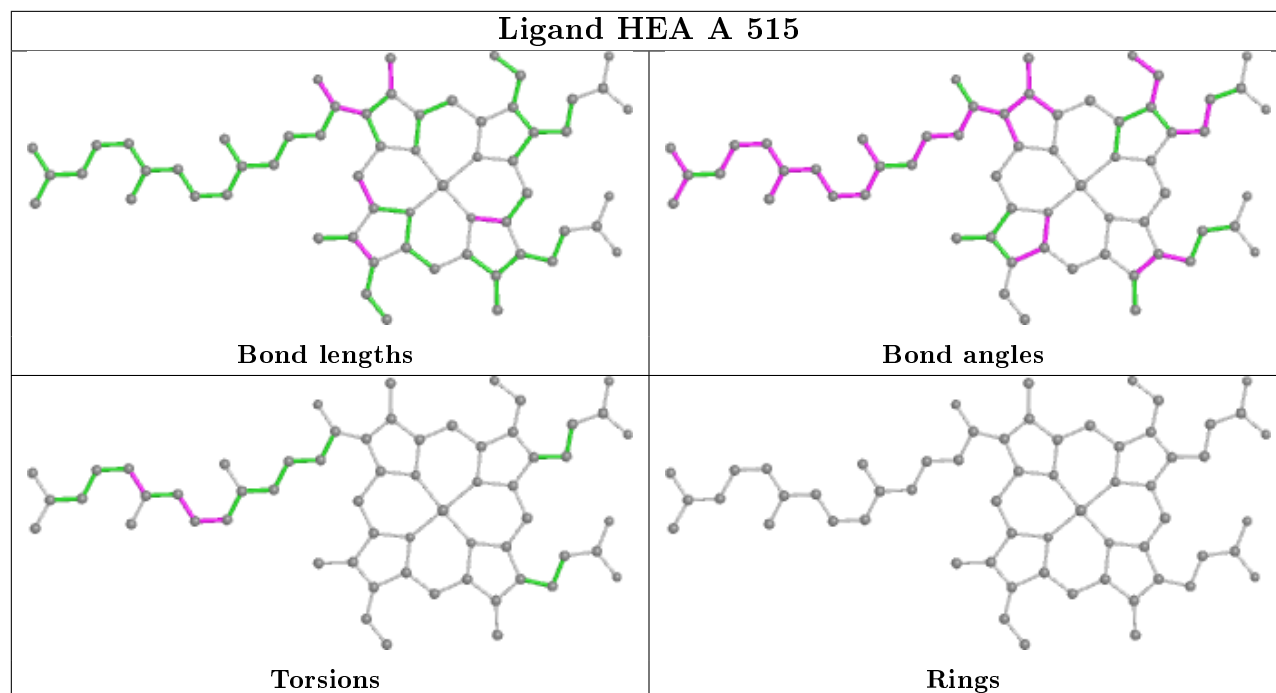


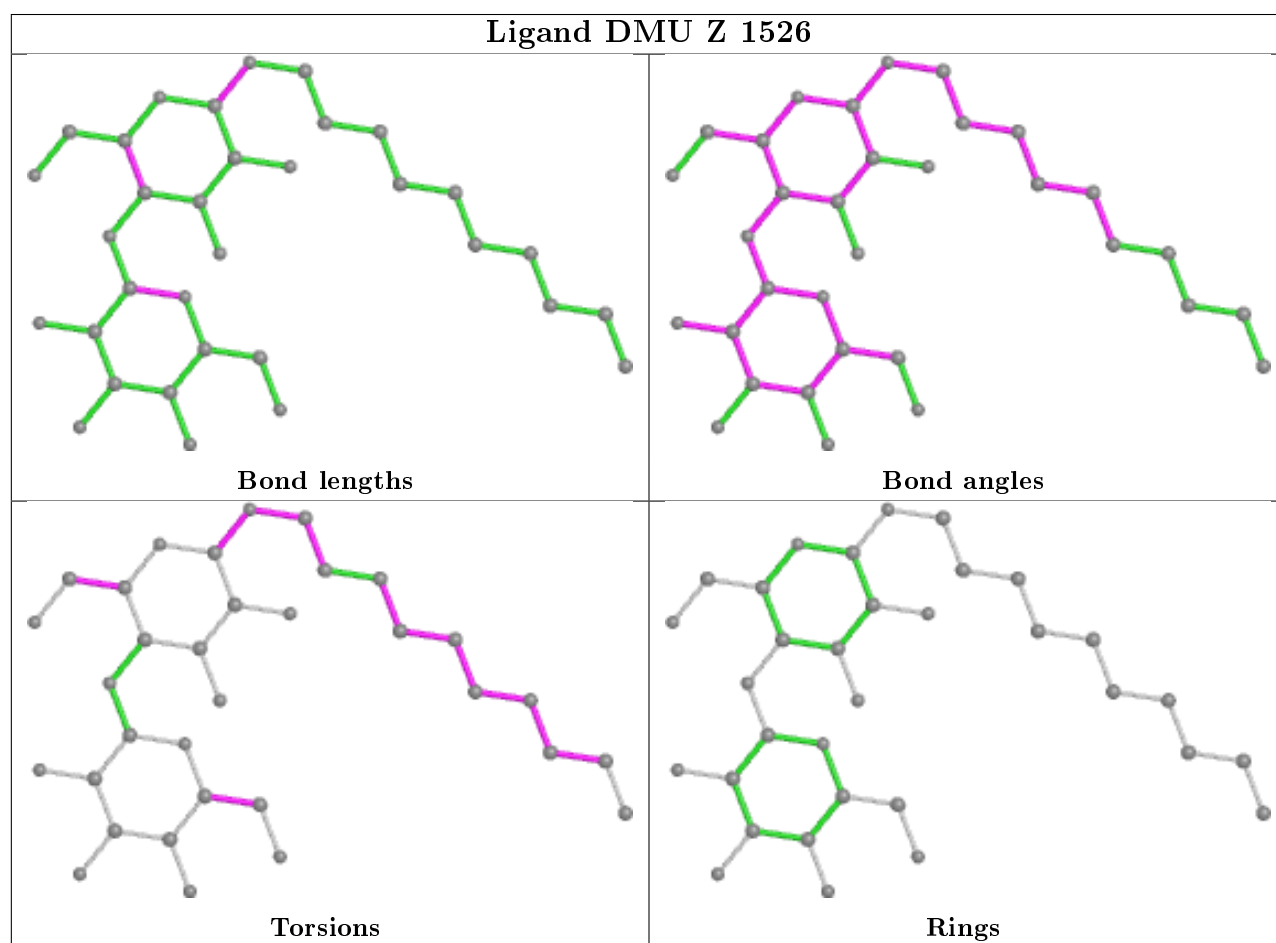
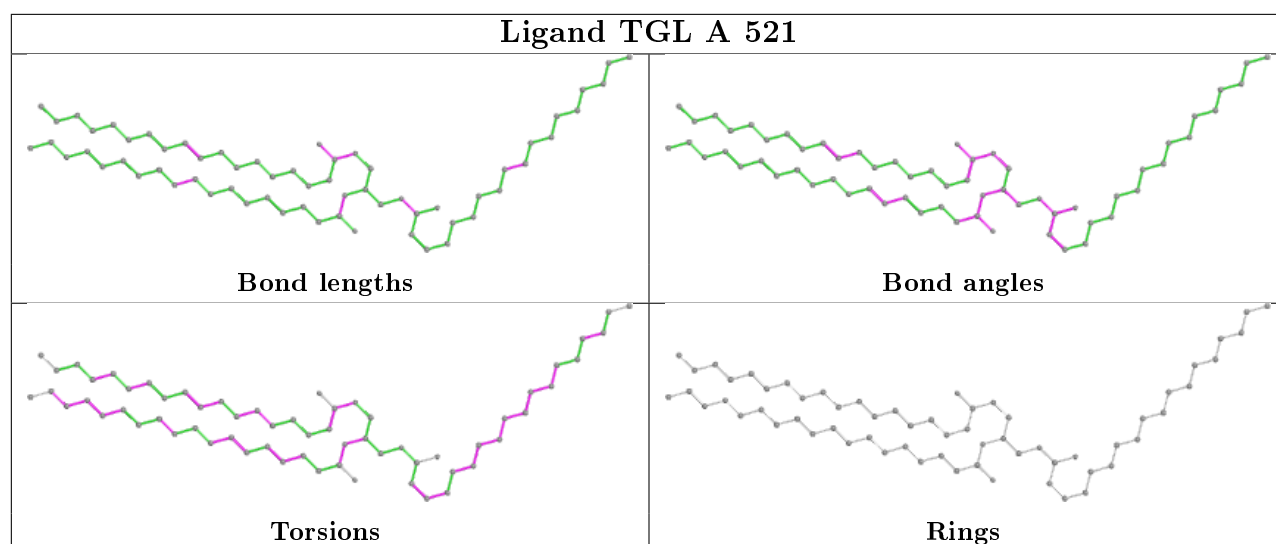
## Ligand DMU P 1272

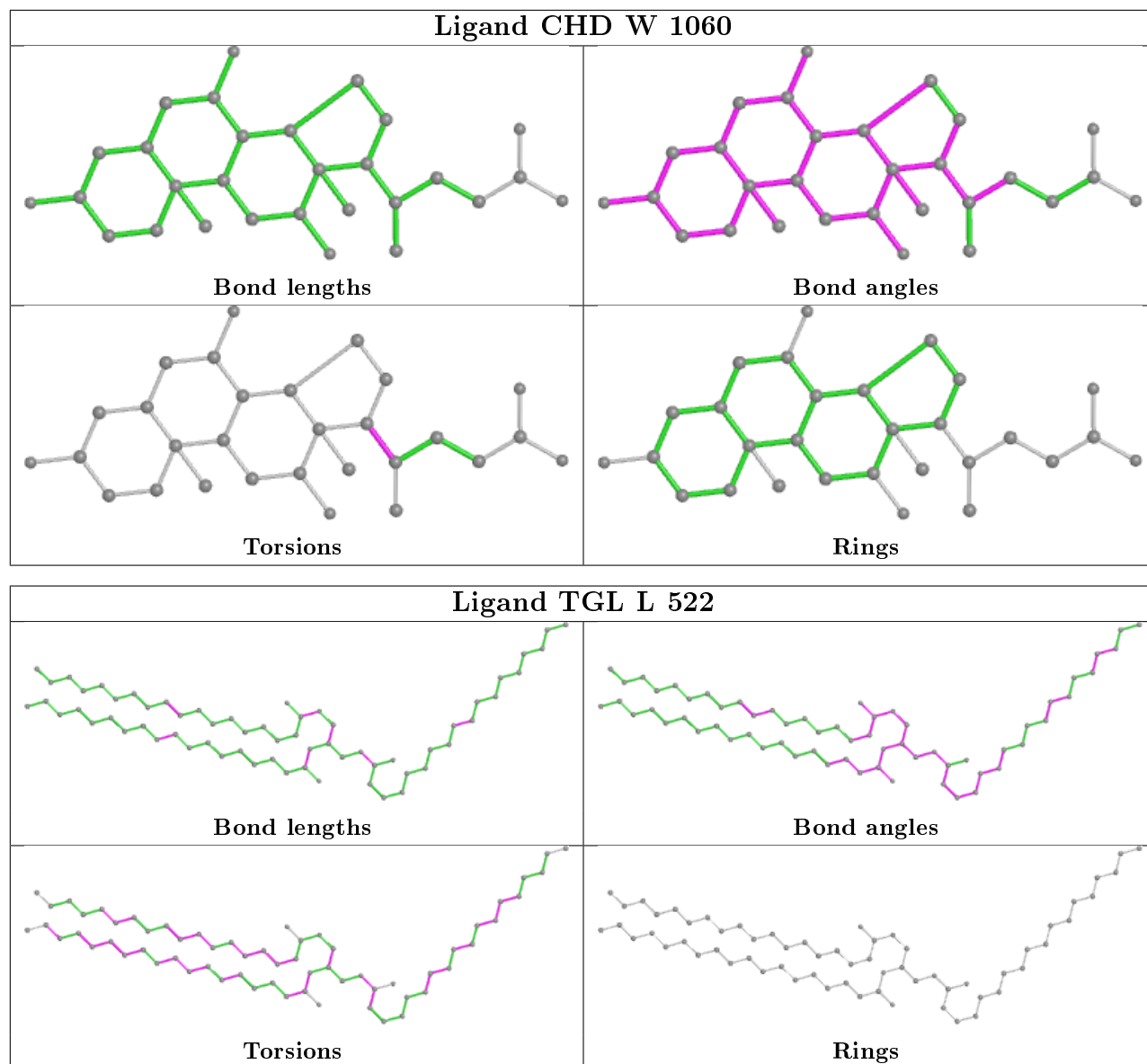


## Ligand CHD O 229

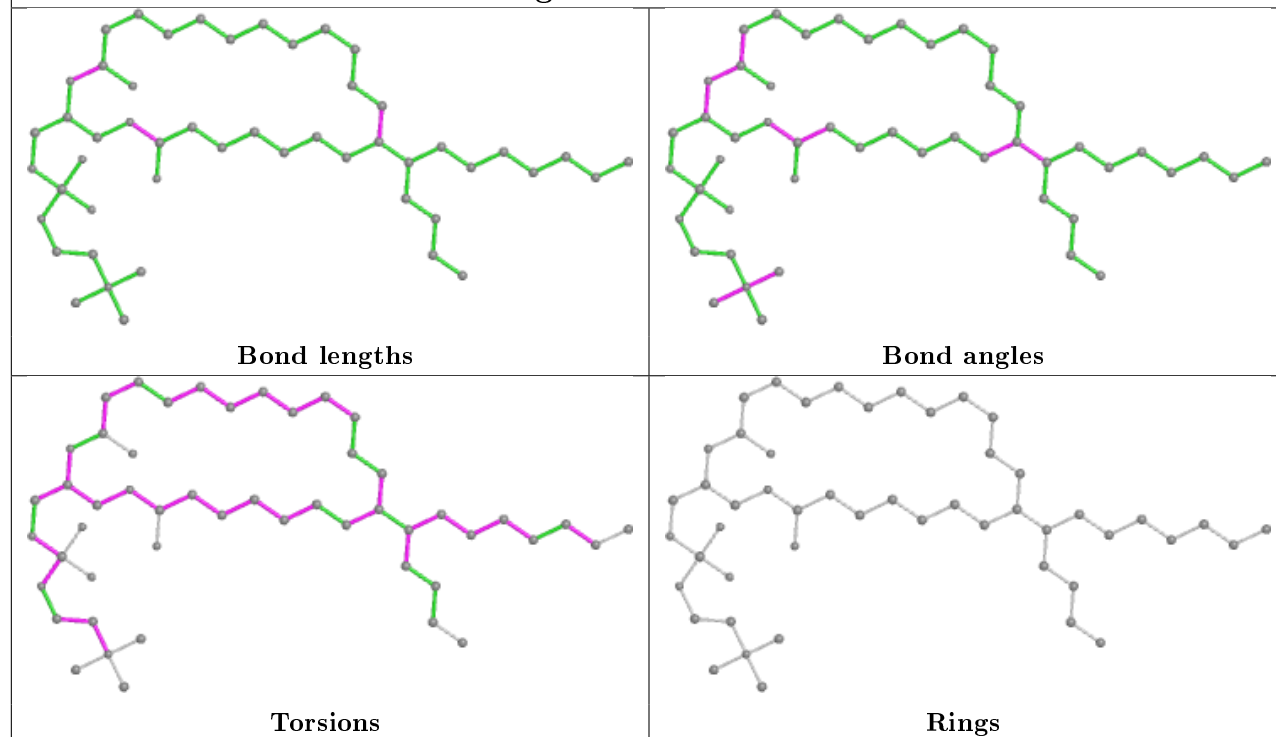




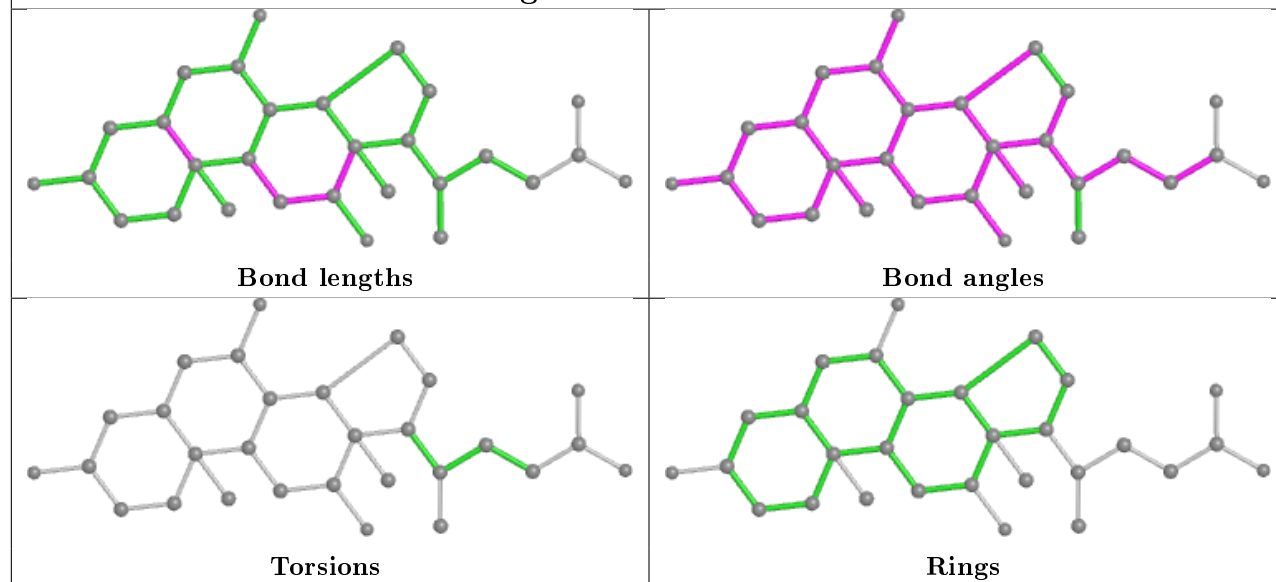


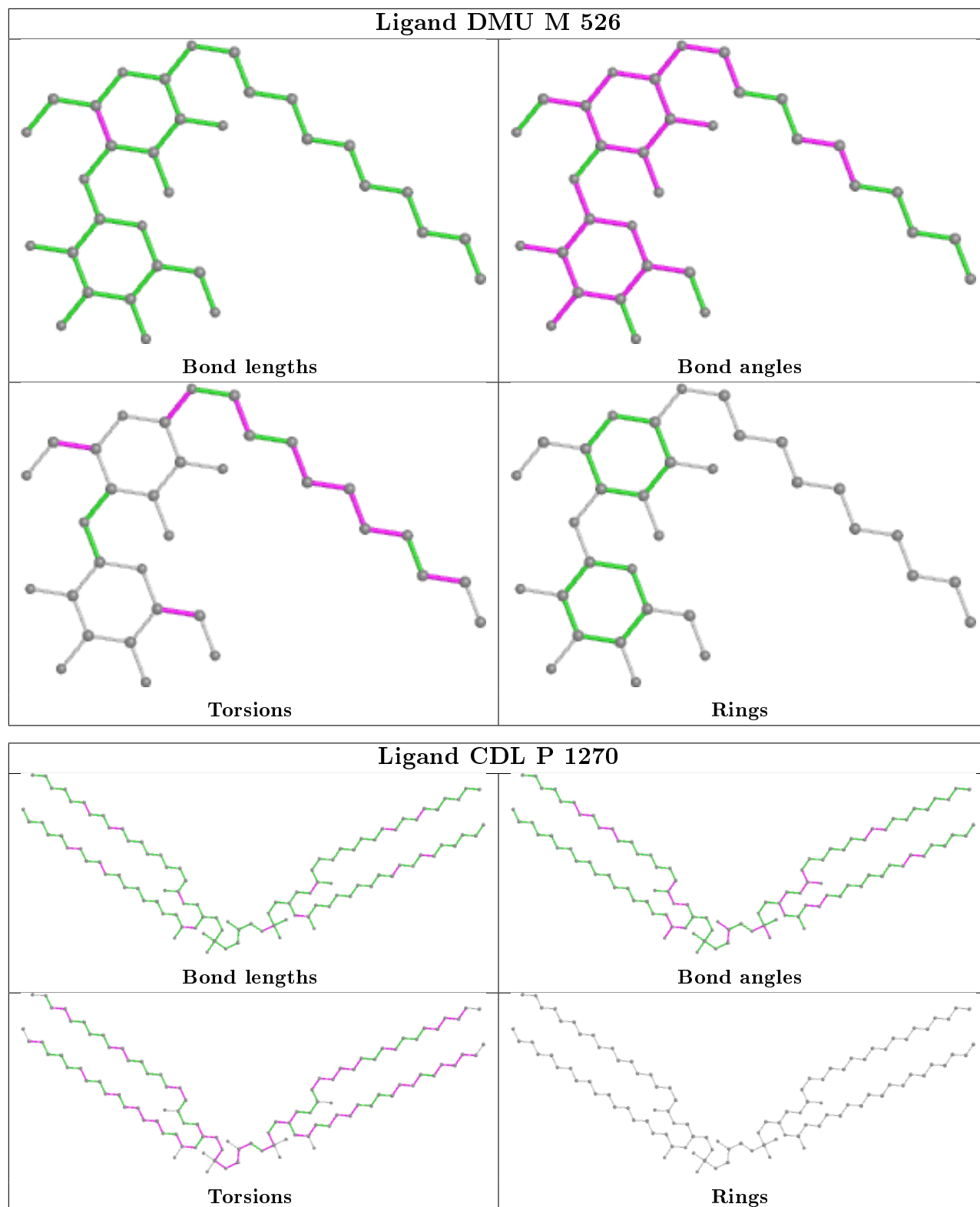


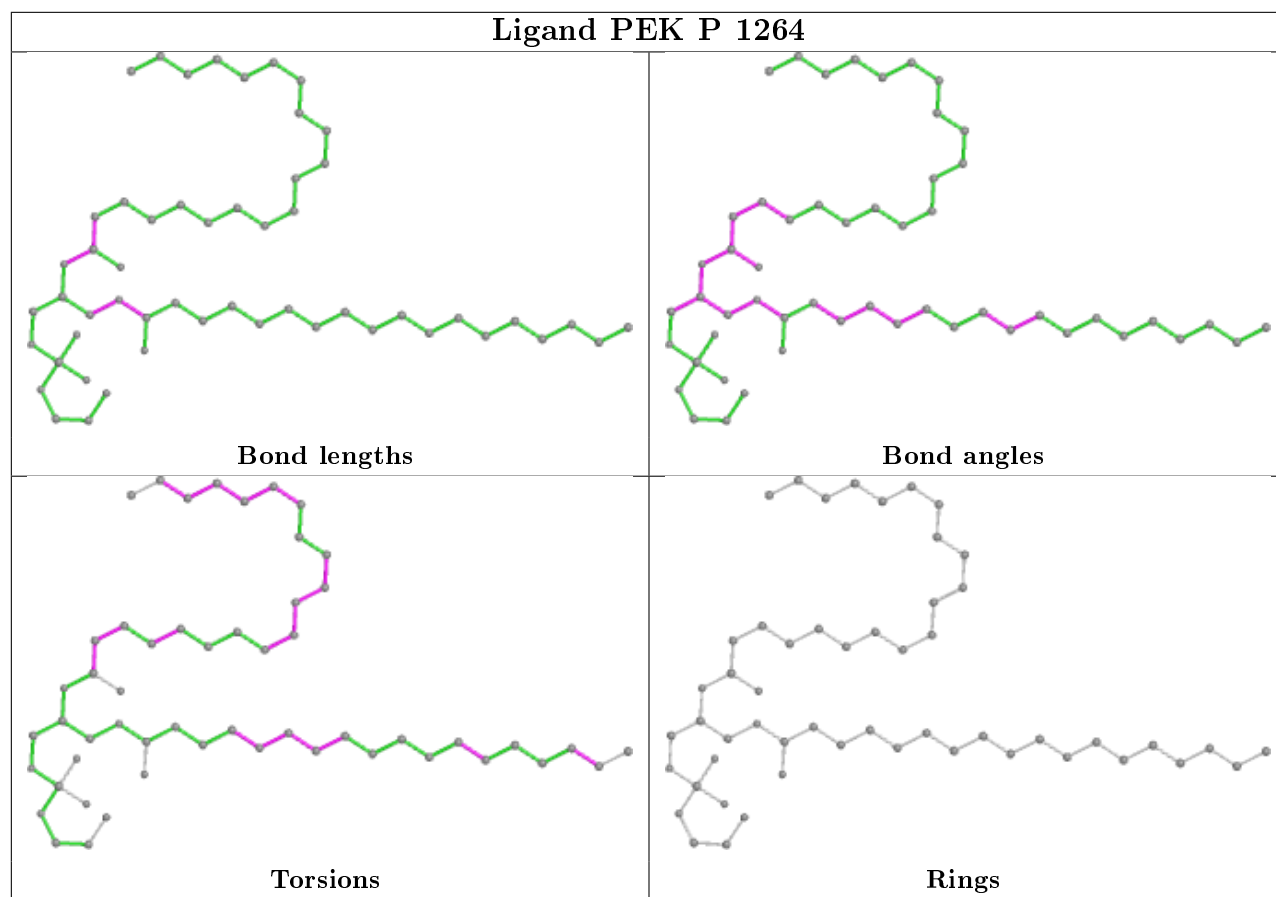
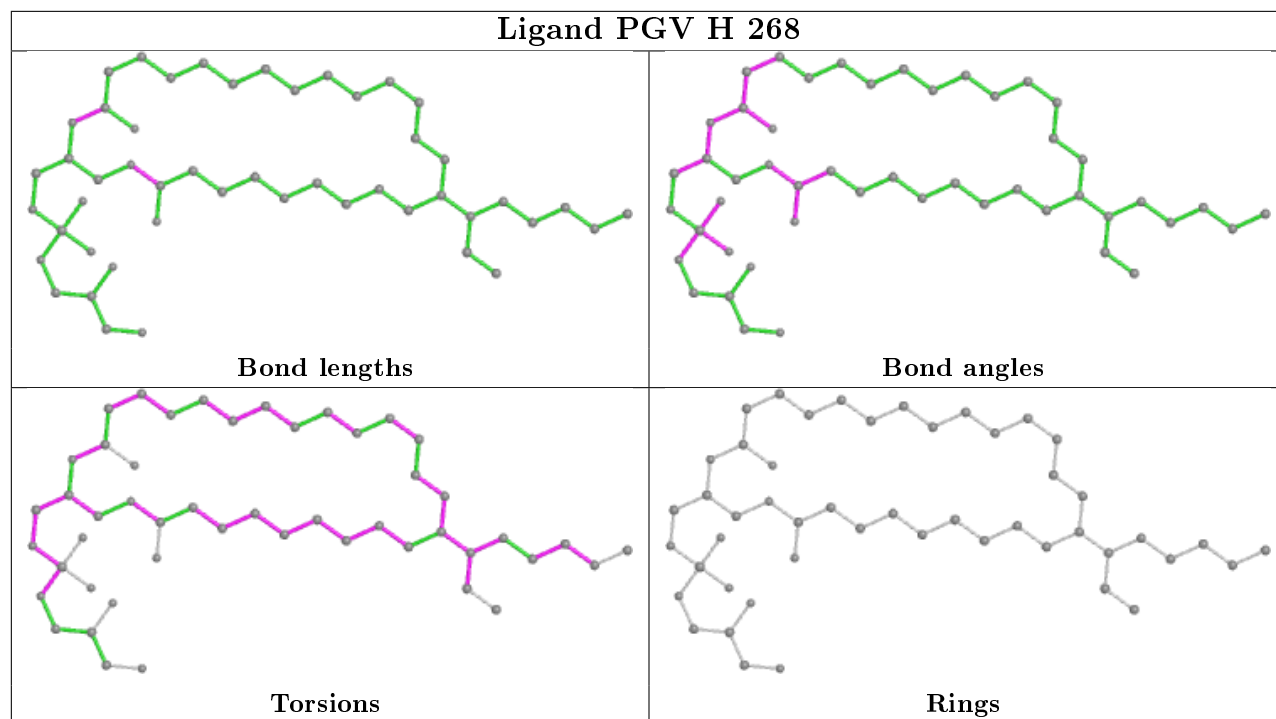
## Ligand PSC E 230



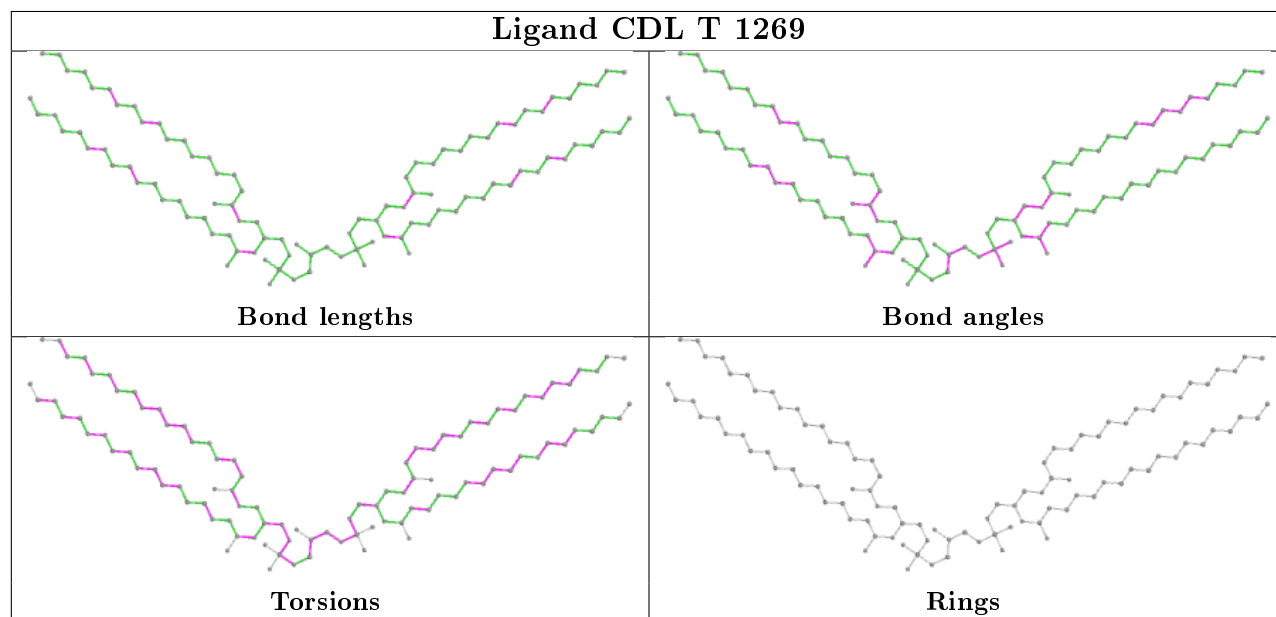
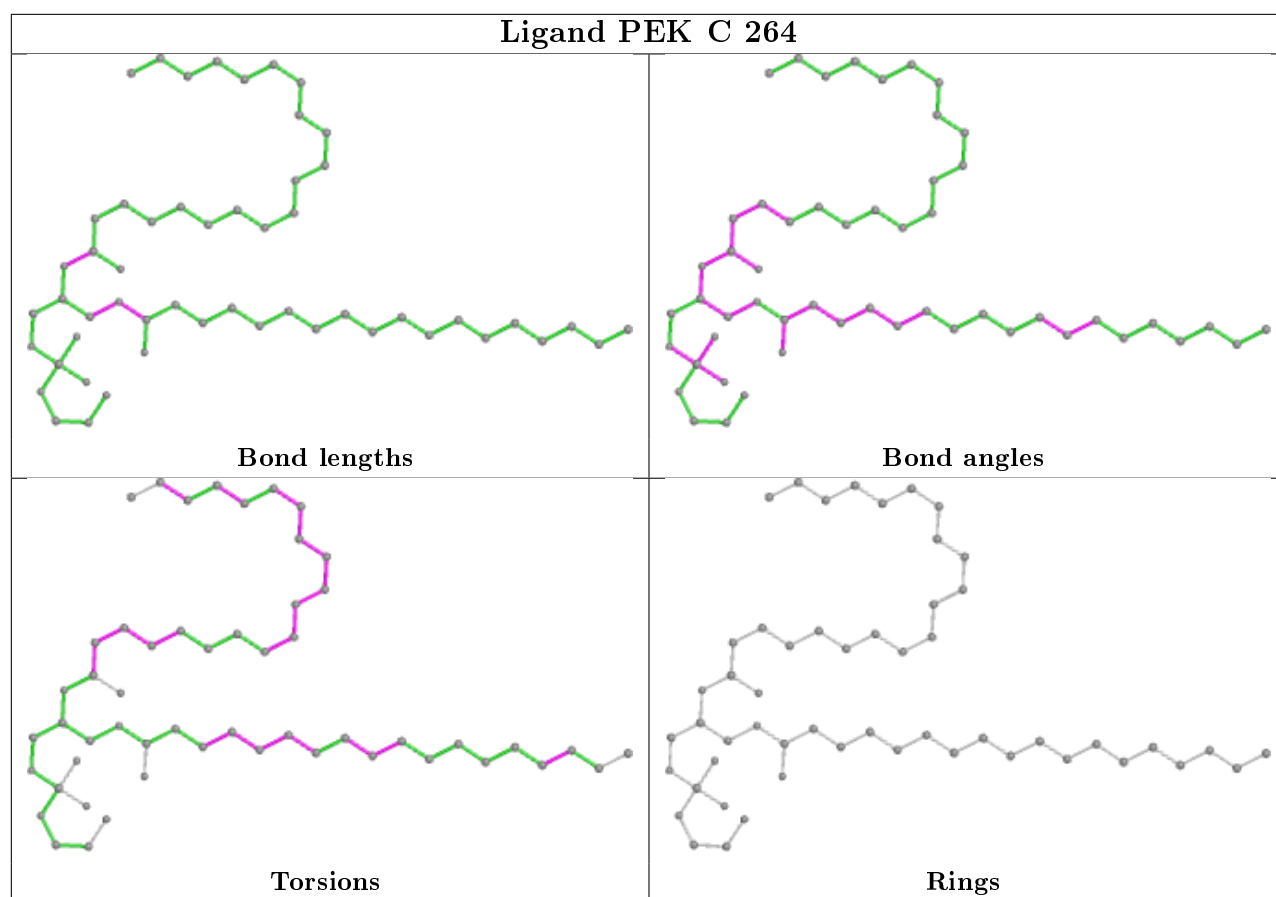
## Ligand CHD B 1086



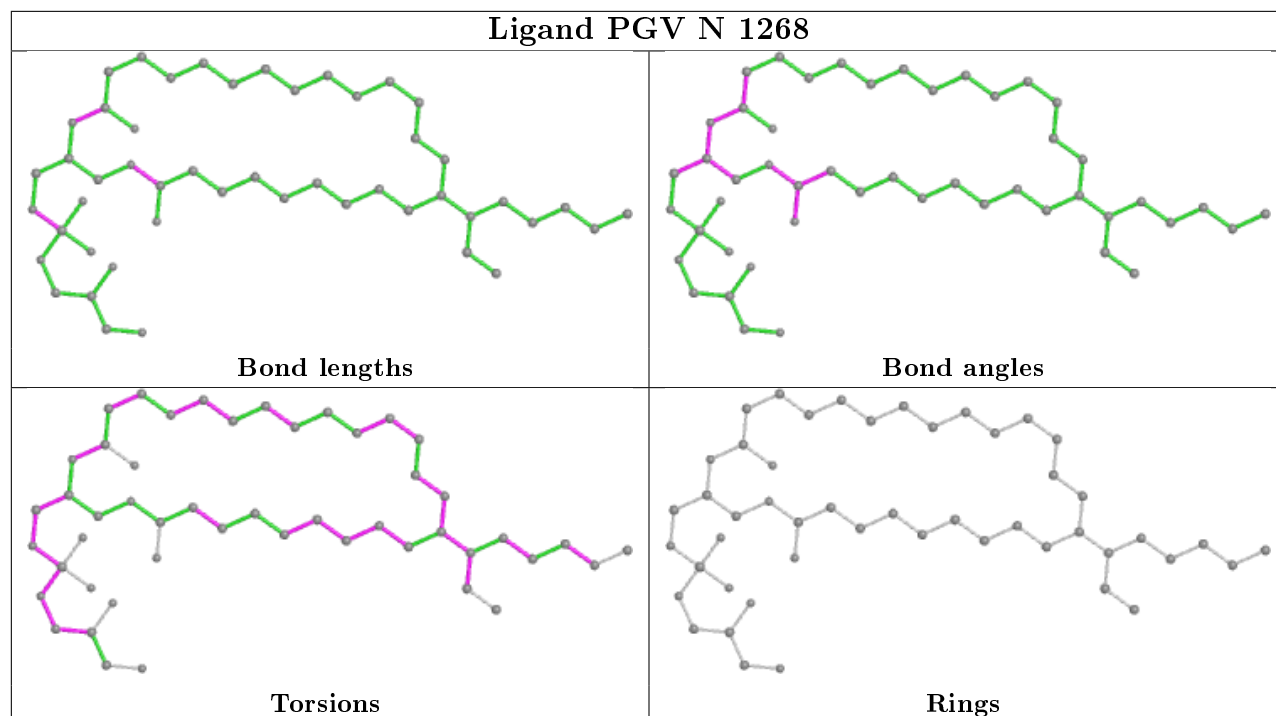




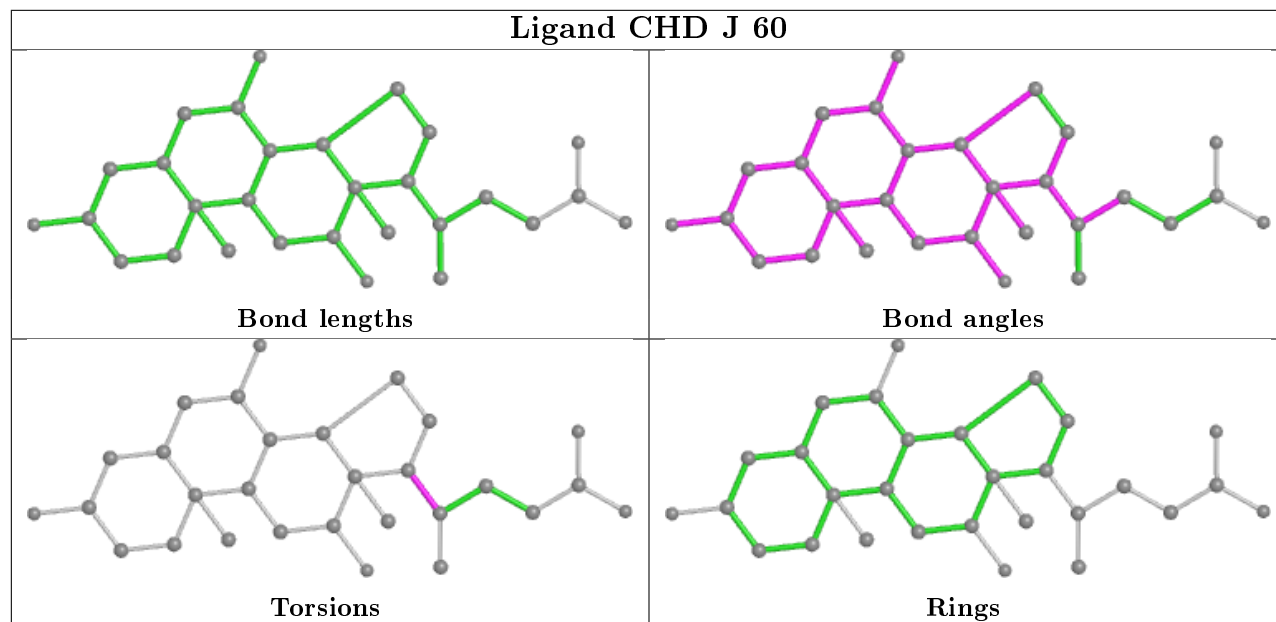


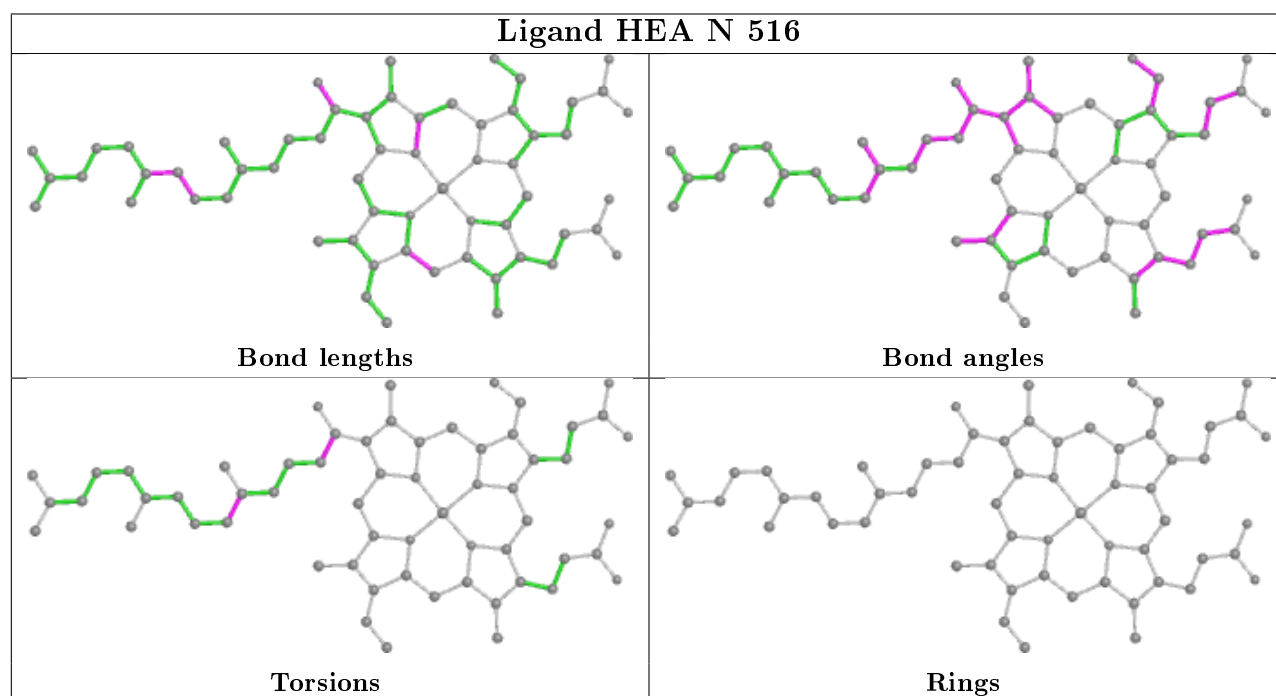
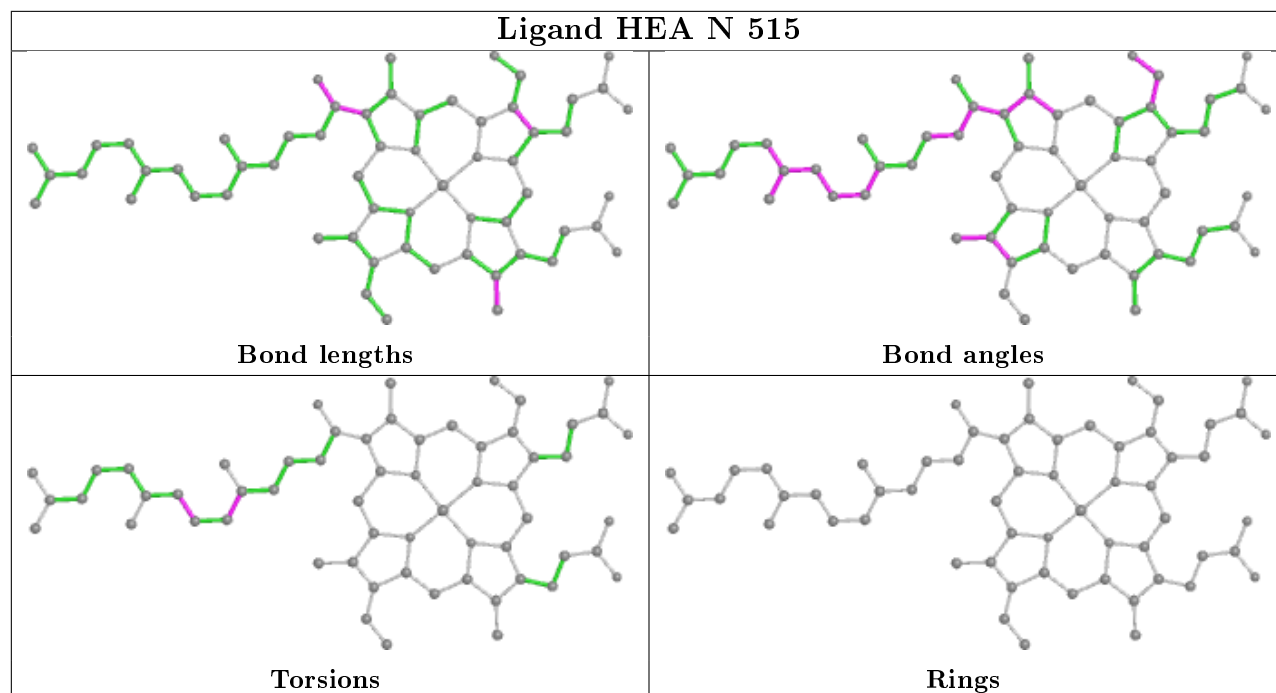


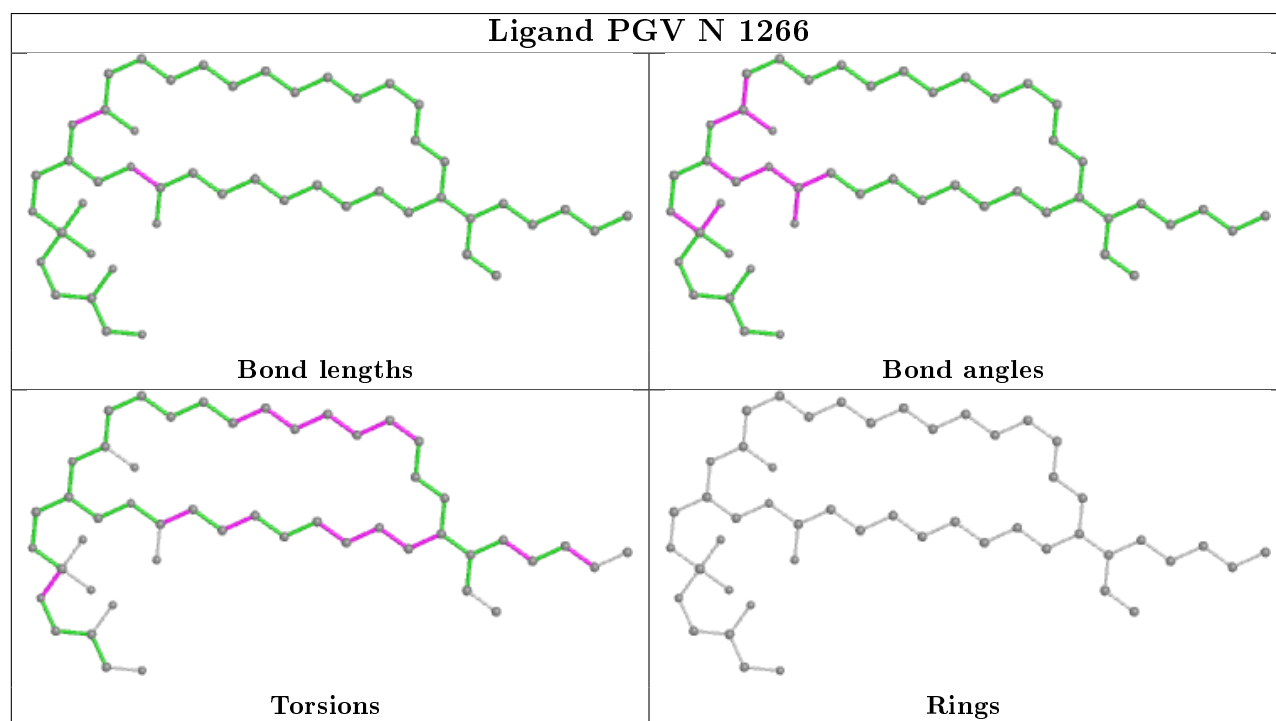
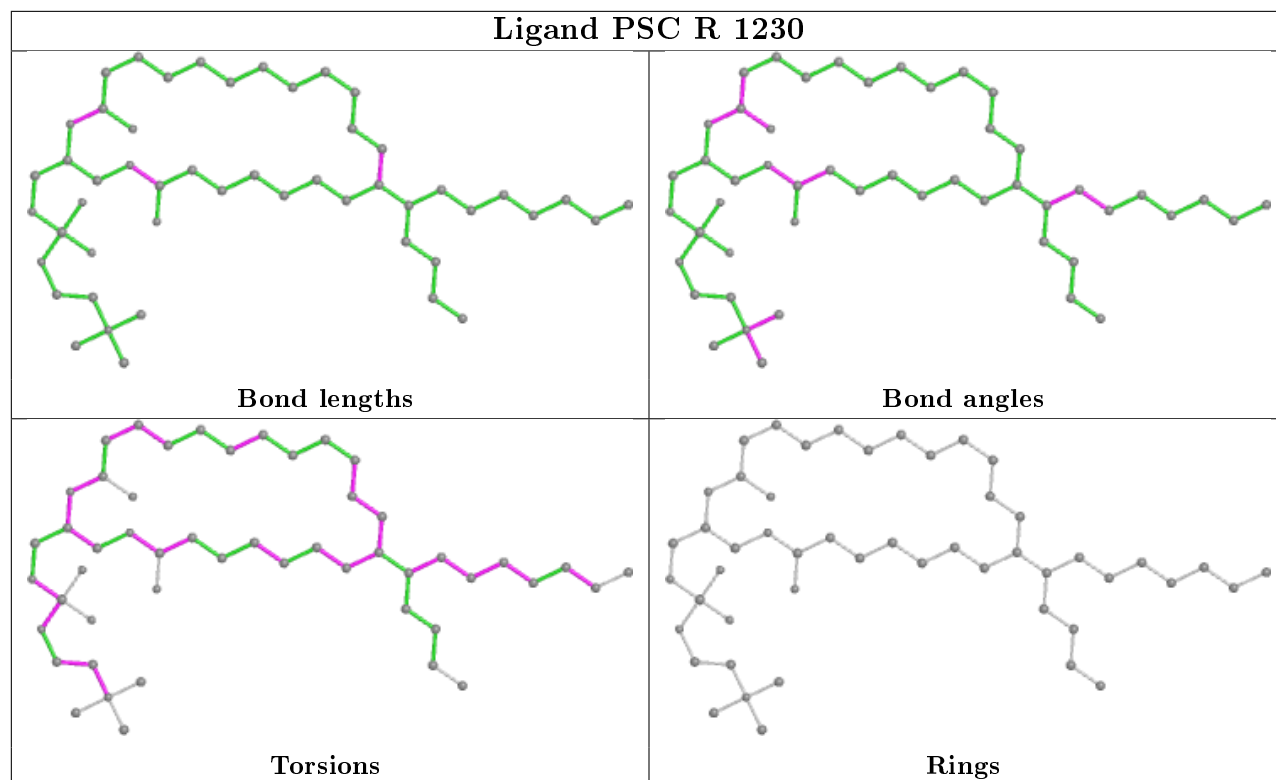
## Ligand PGV N 1268

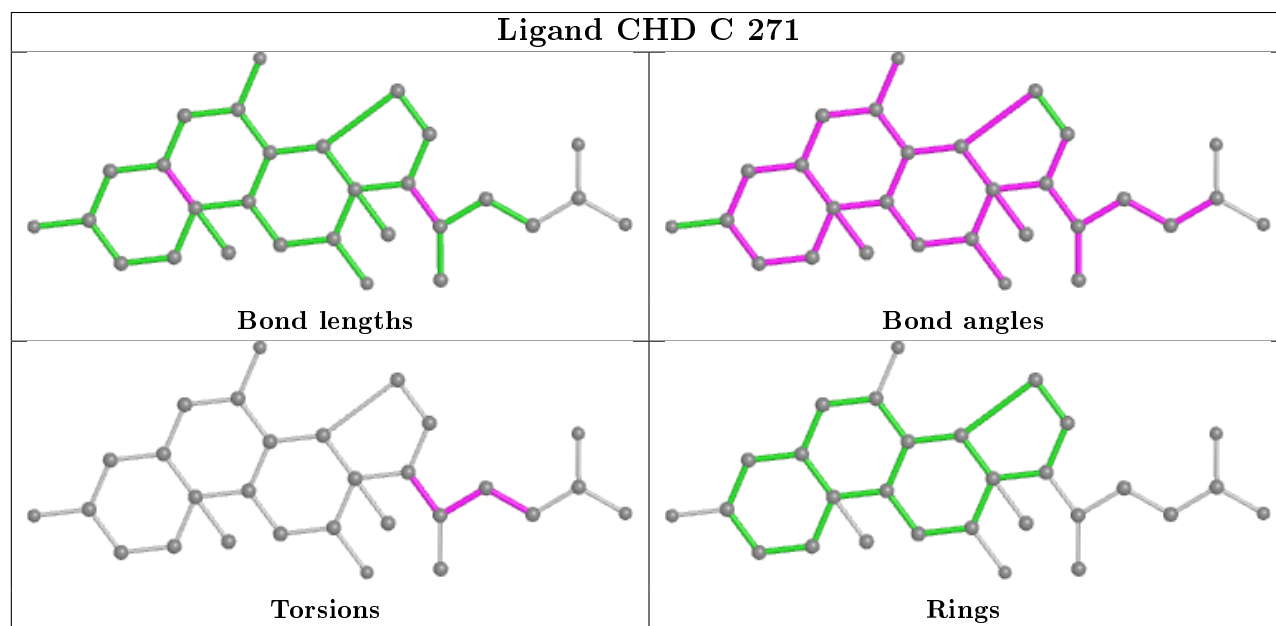
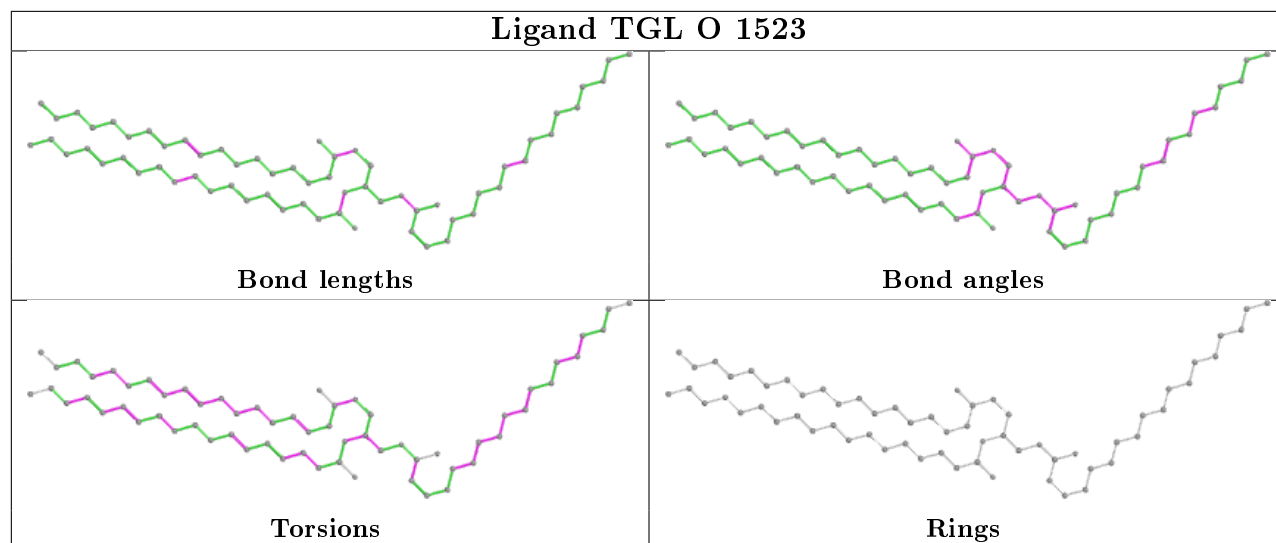


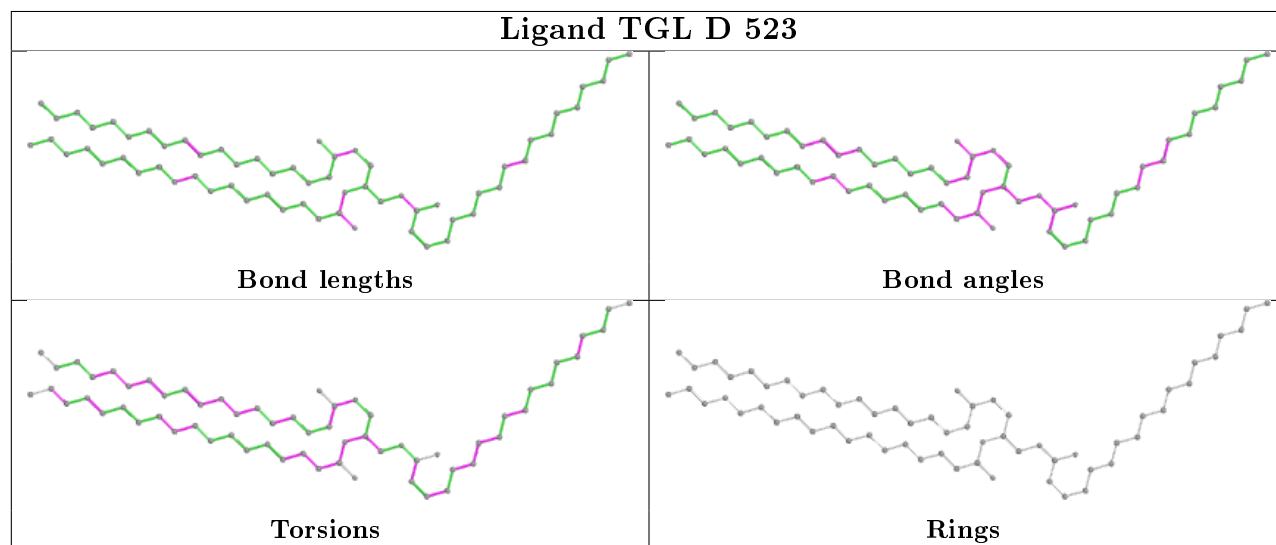
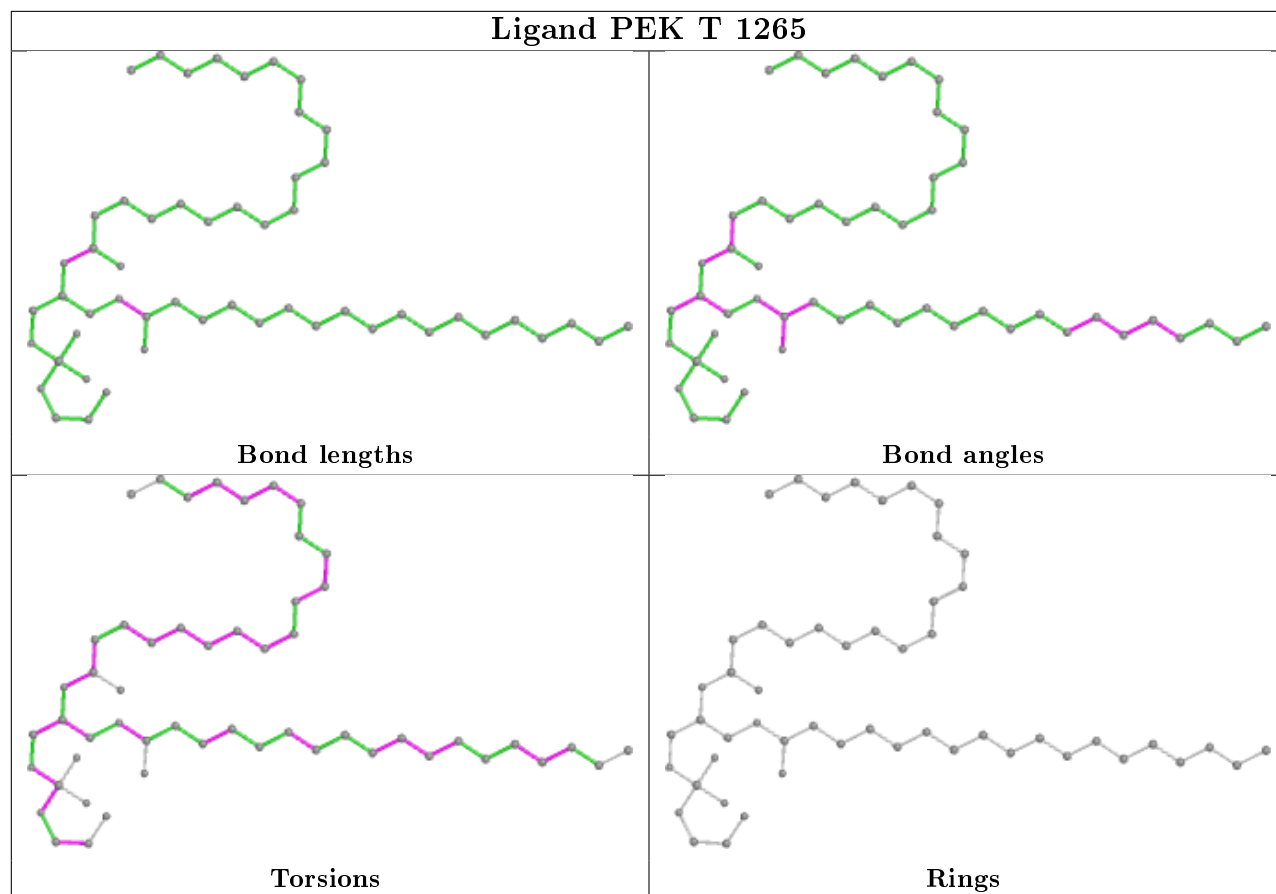
## Ligand CHD J 60

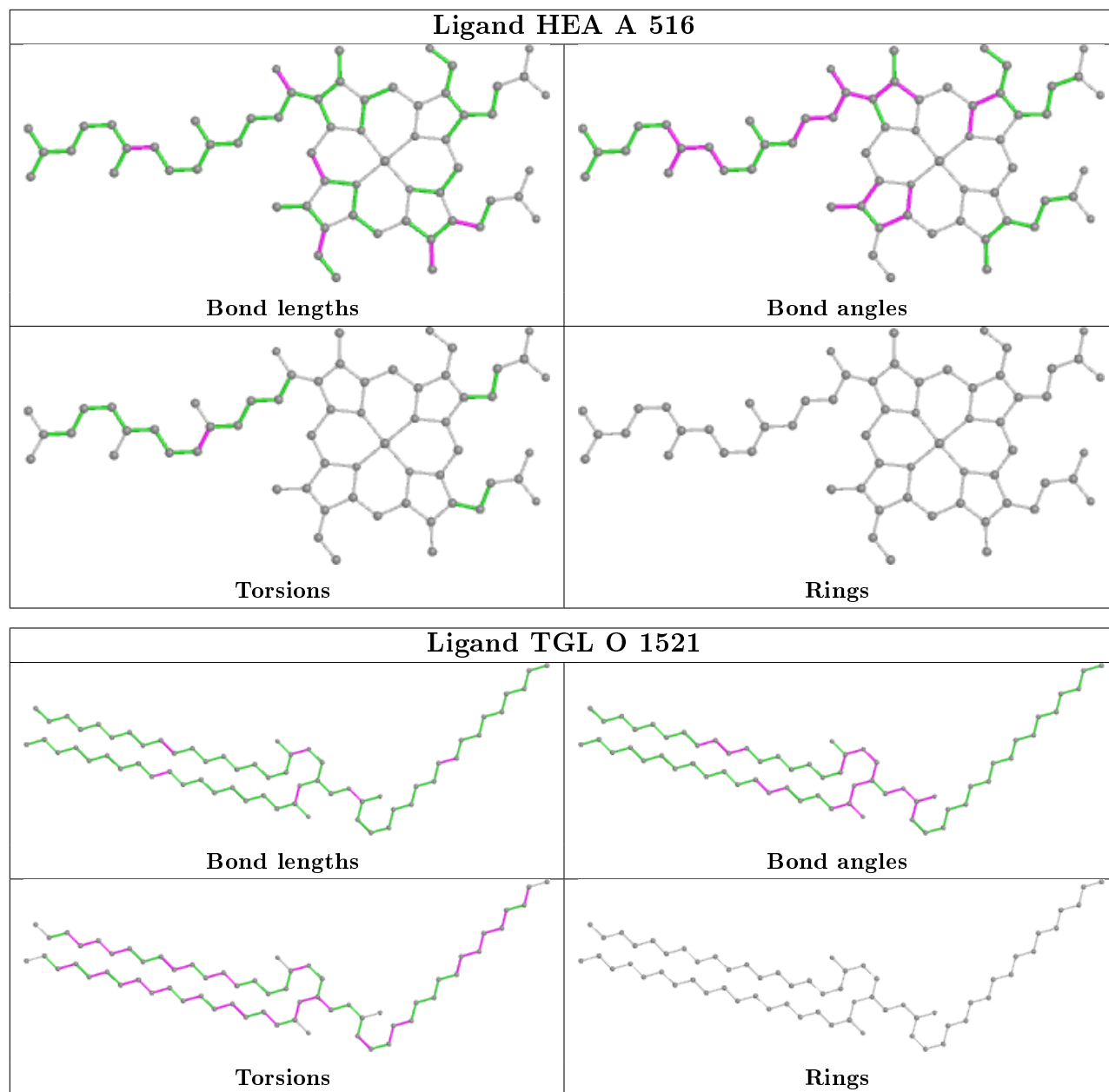




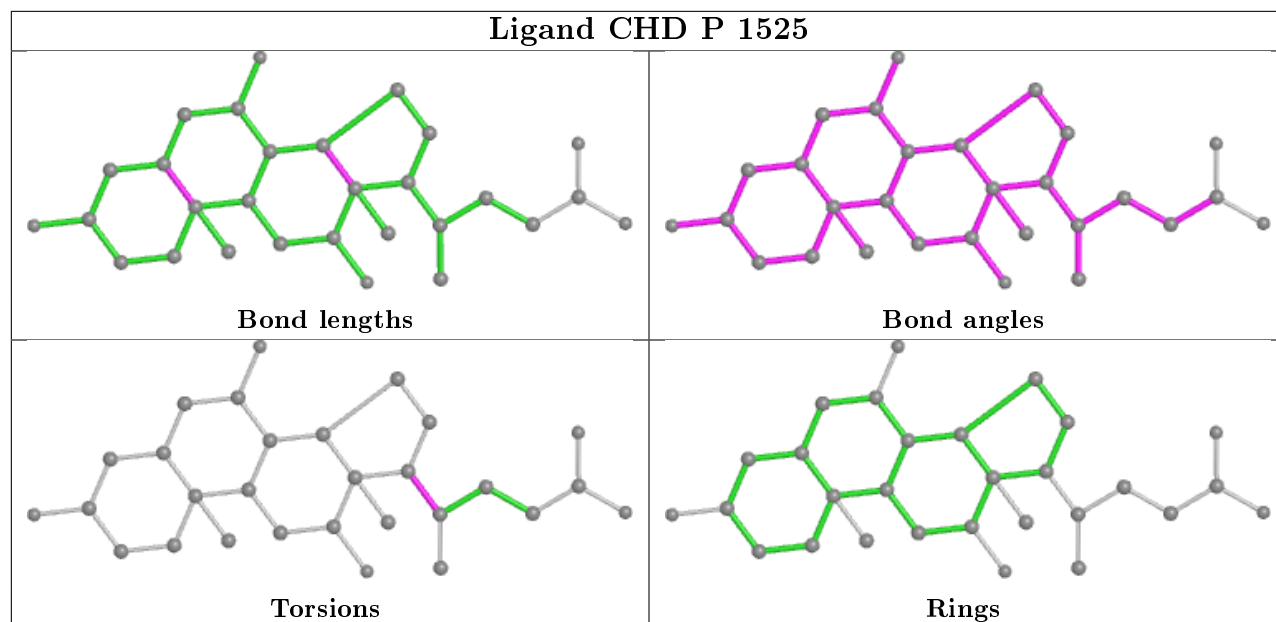




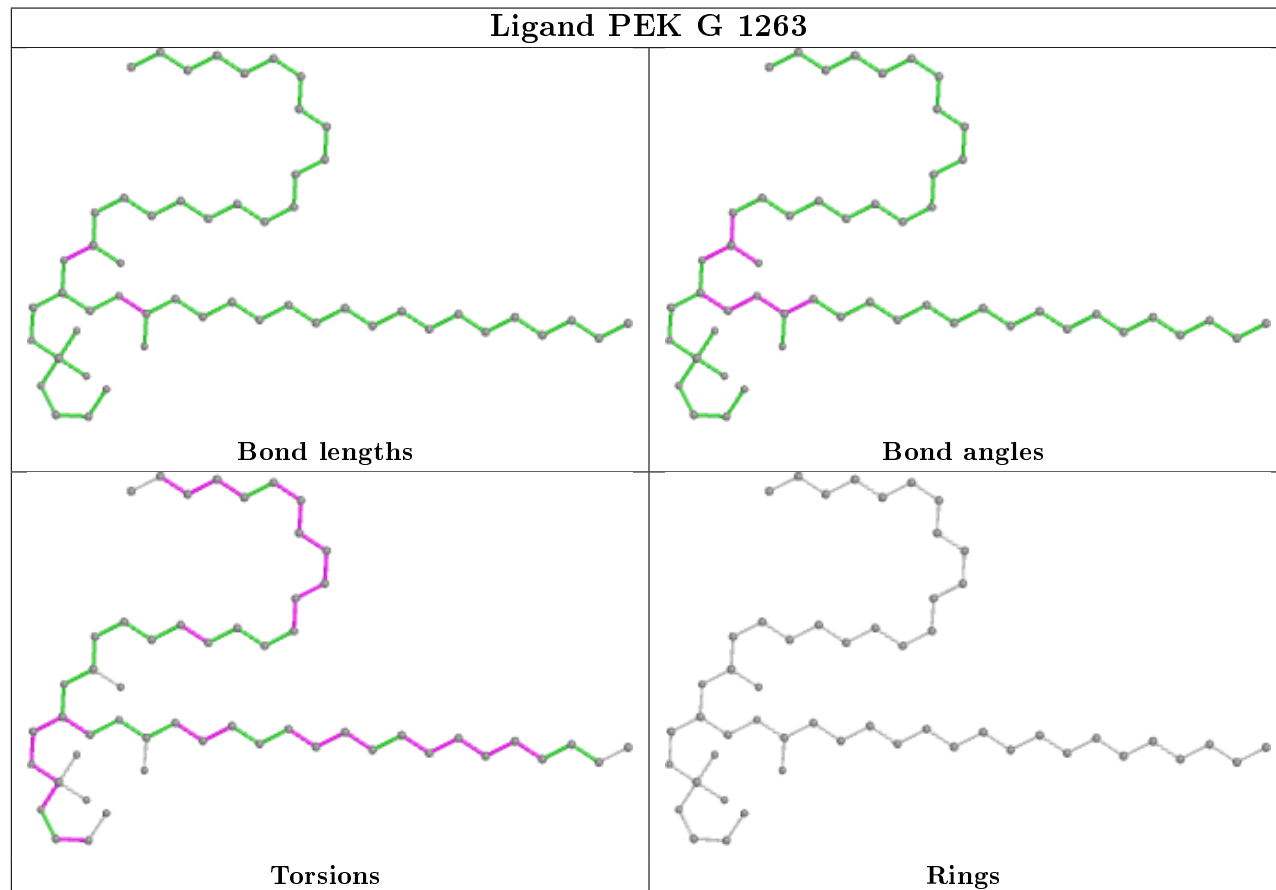




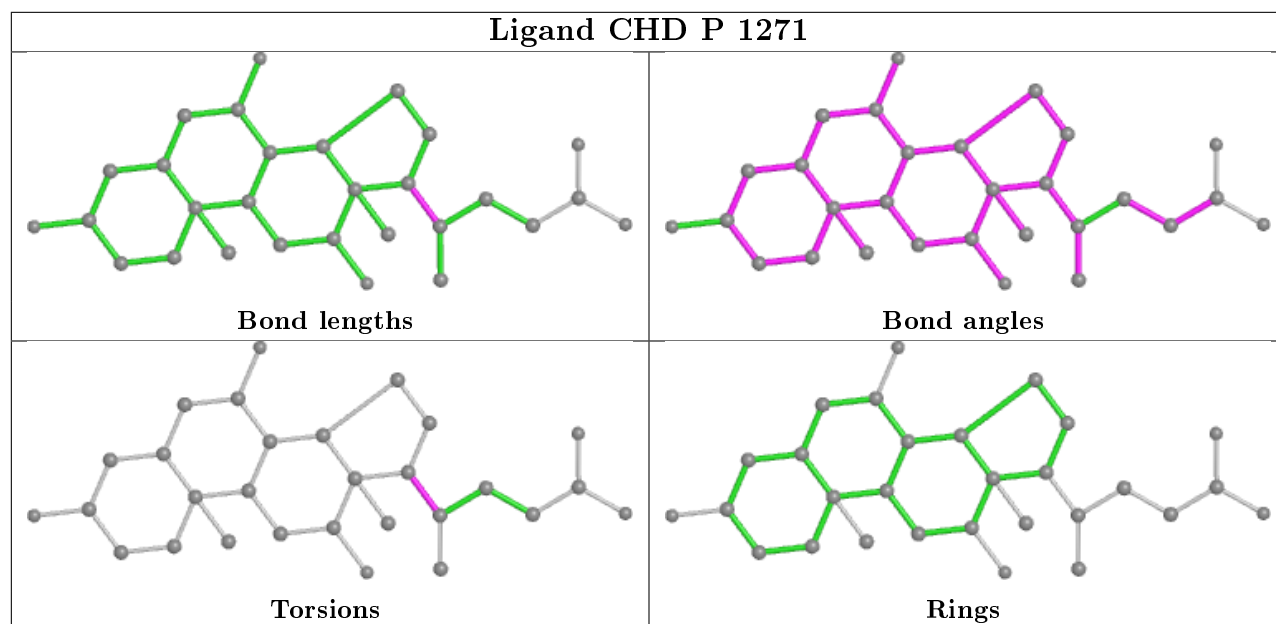
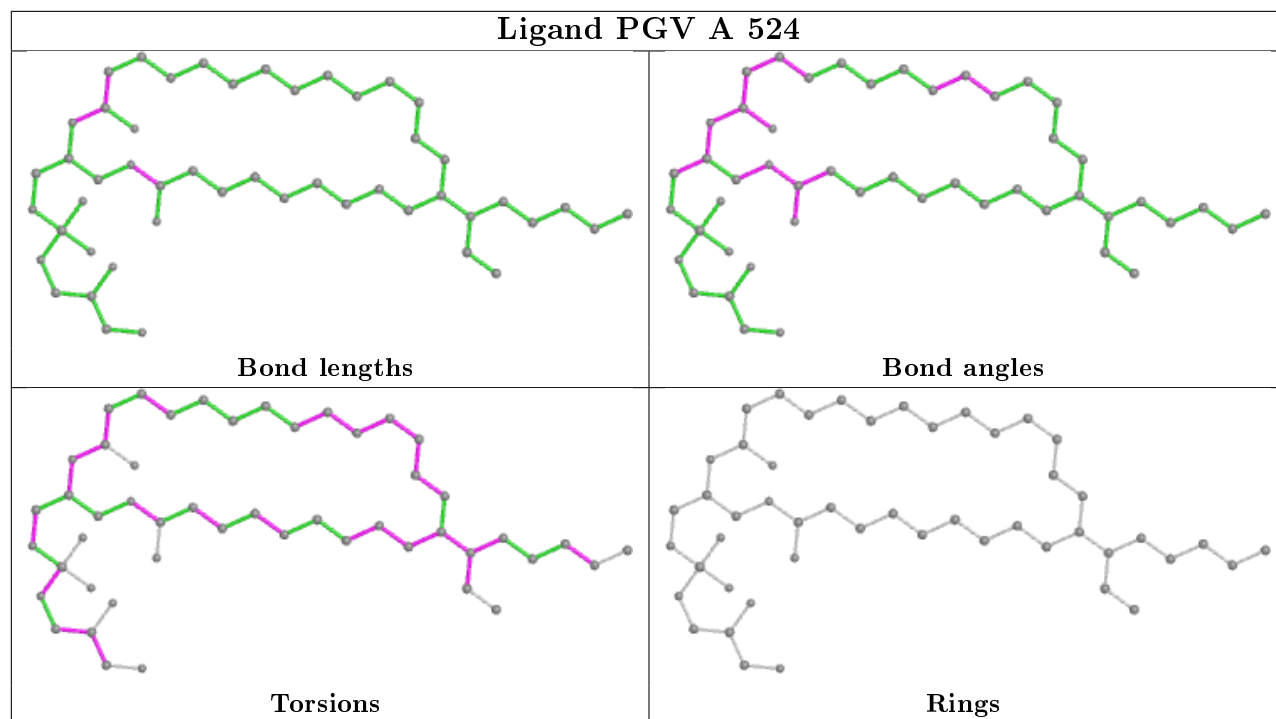
## Ligand CHD P 1525

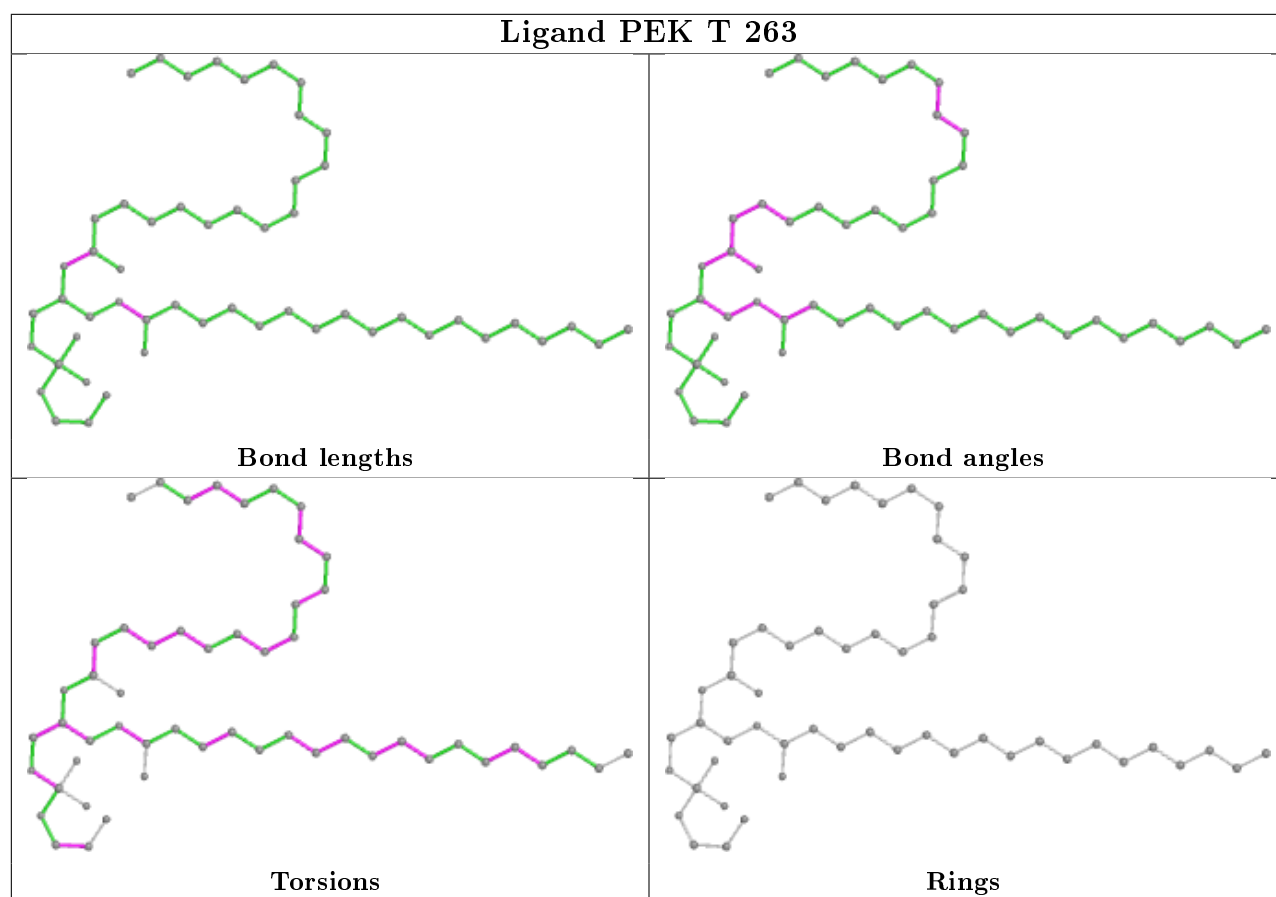
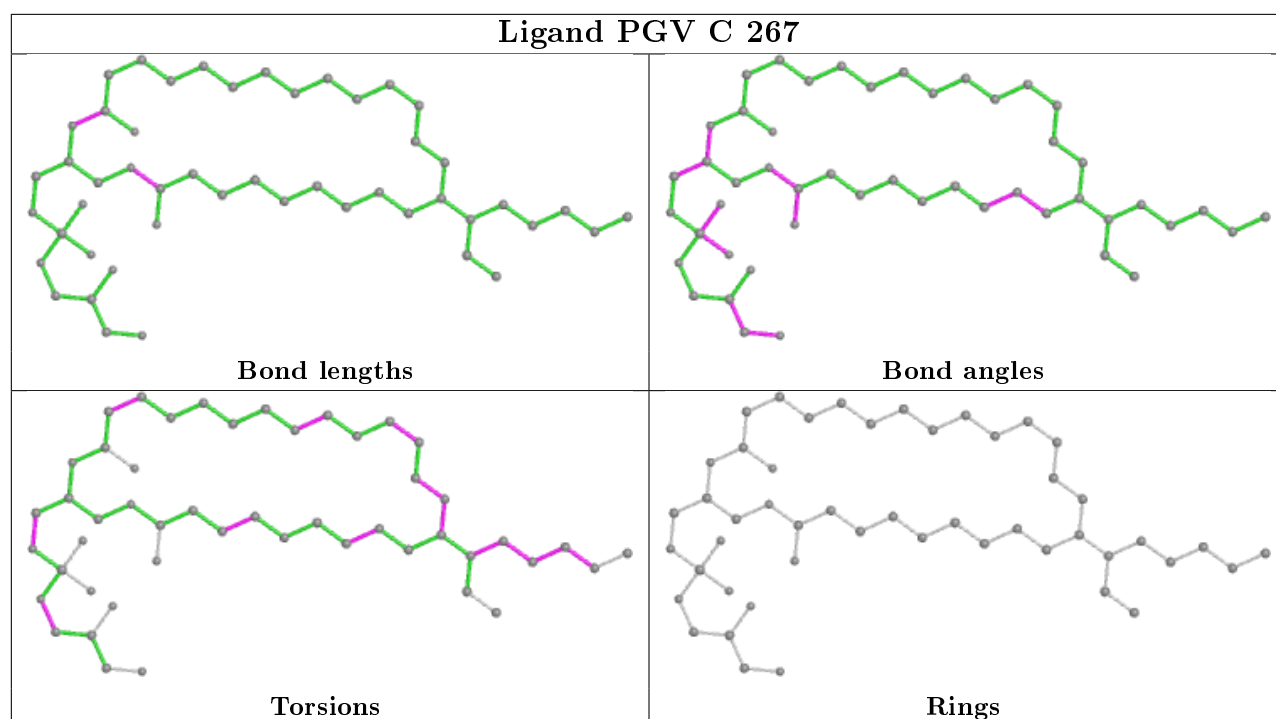


## Ligand PEK G 1263

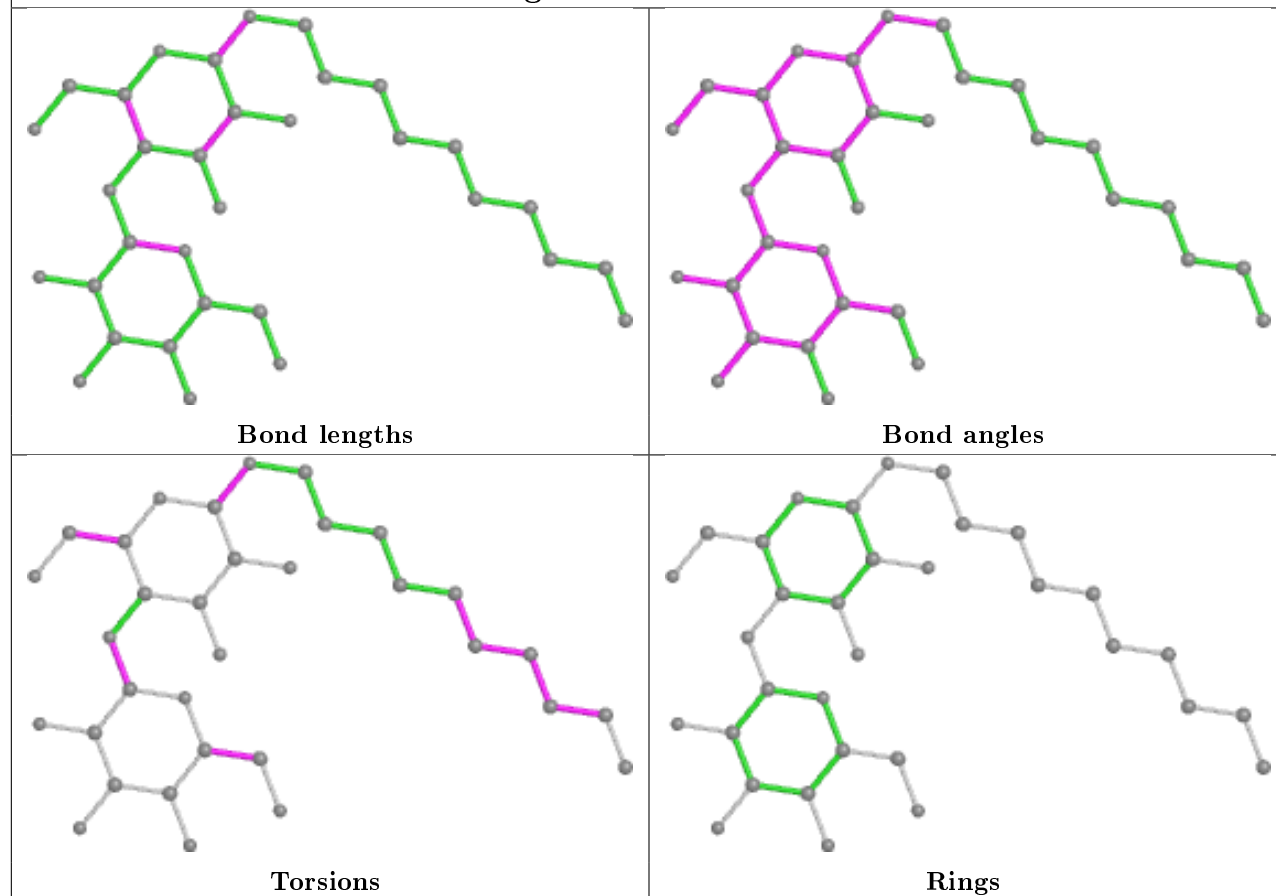




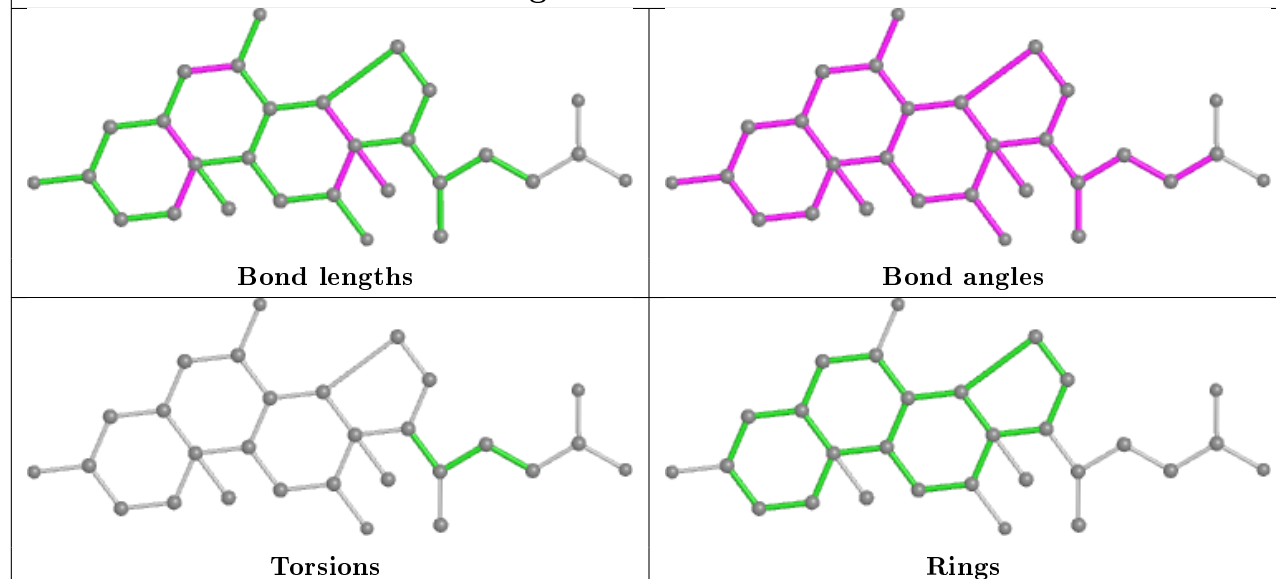


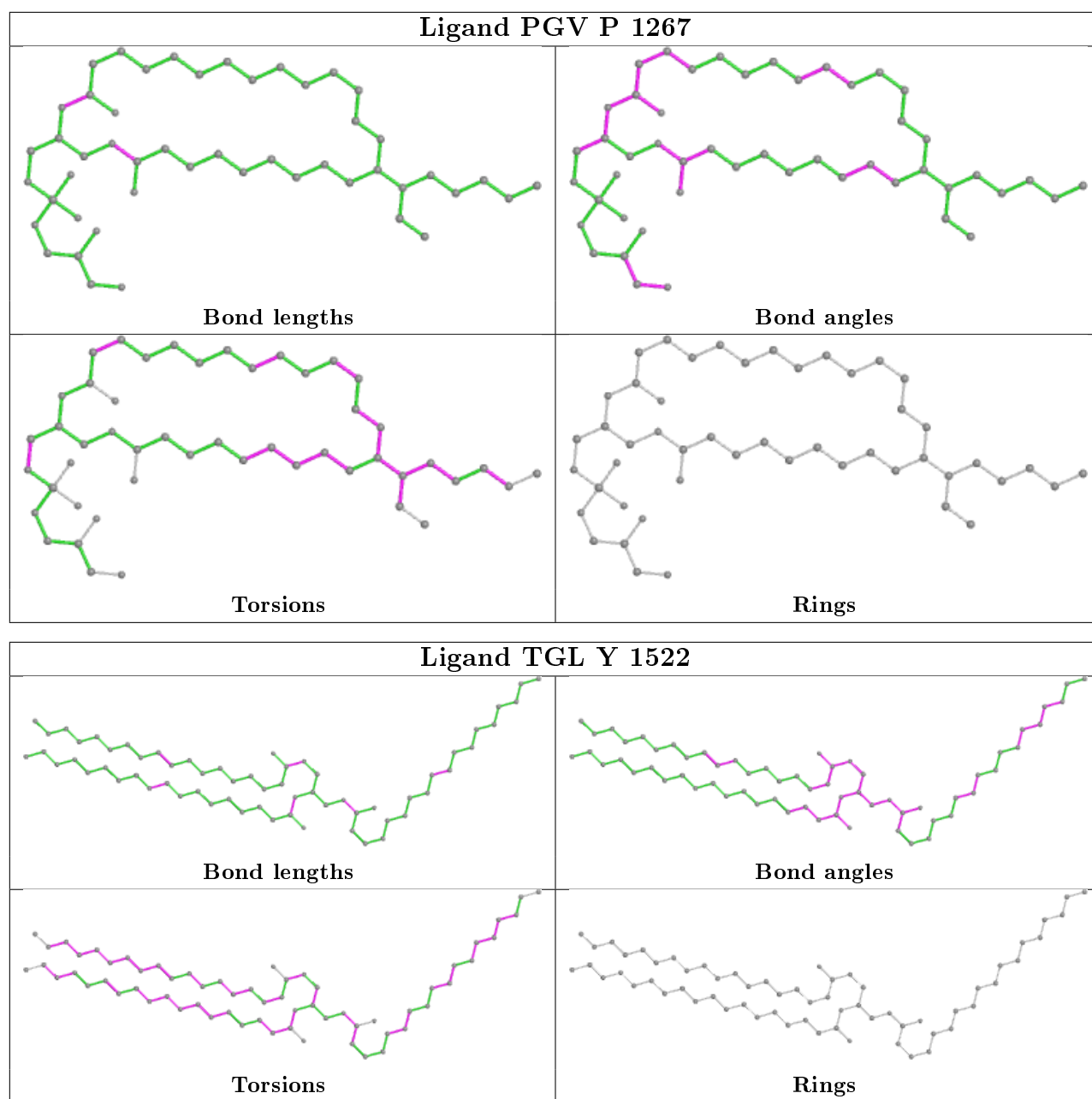


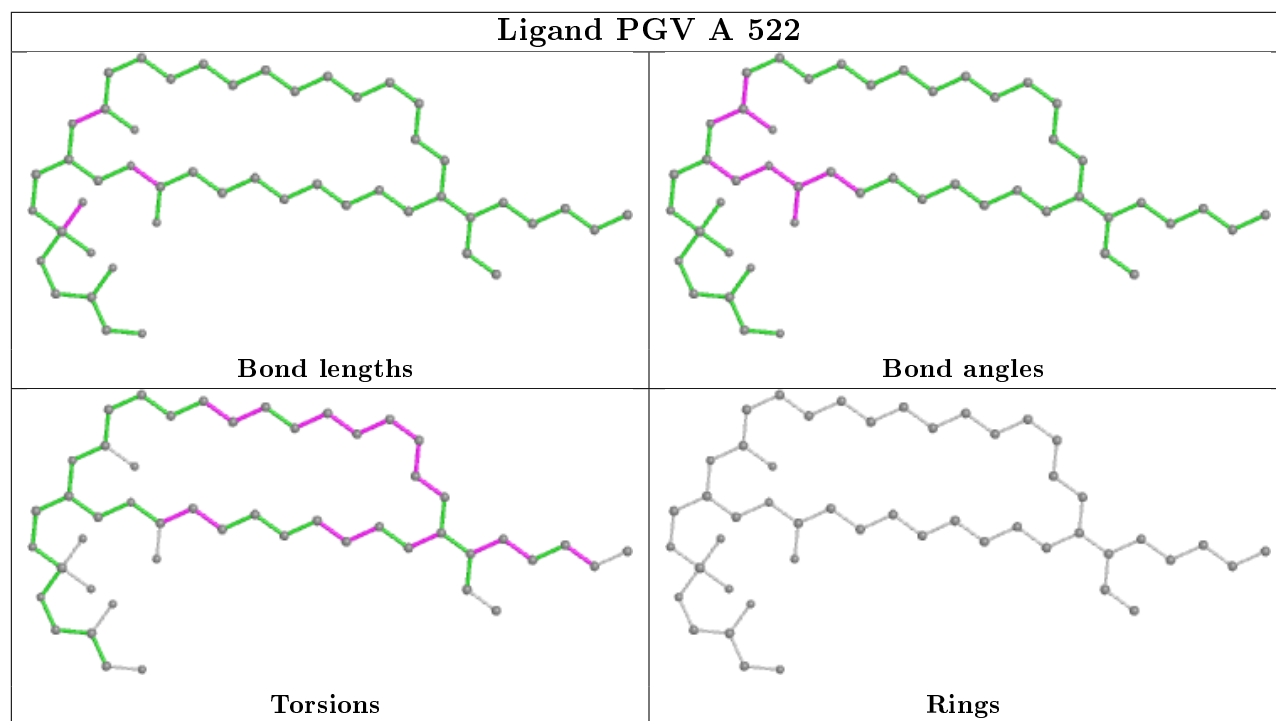
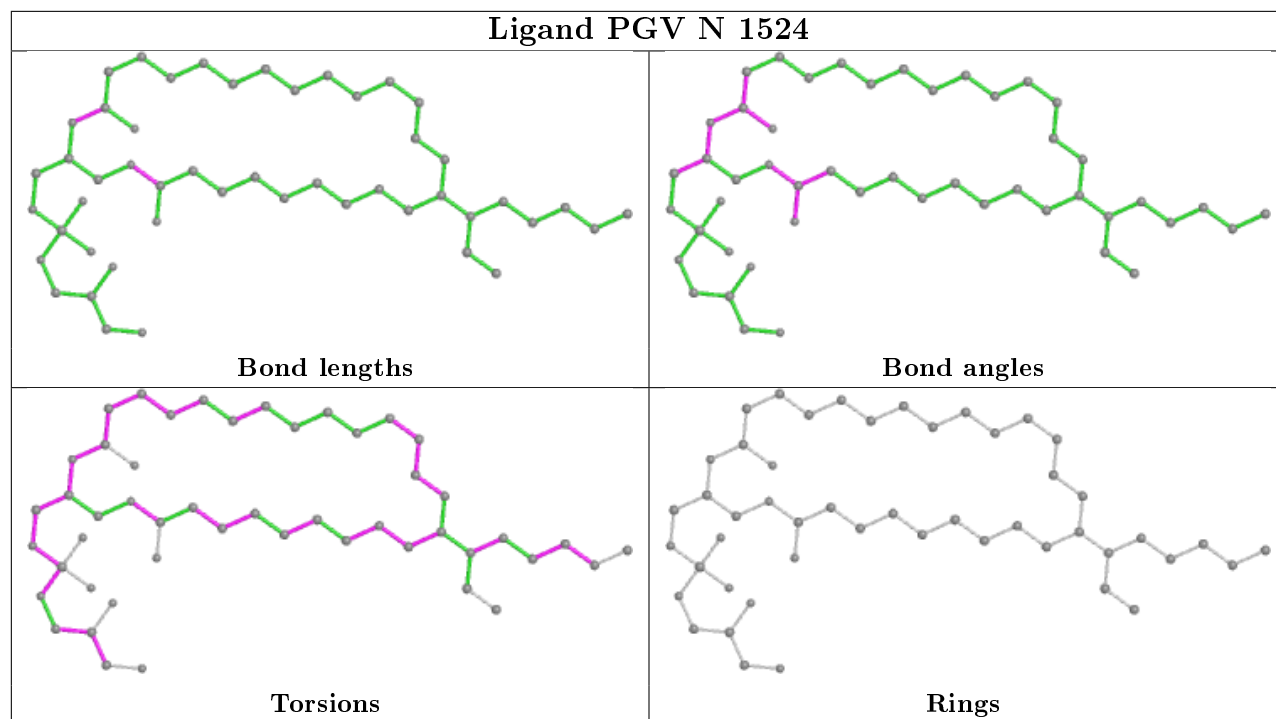
## Ligand DMU G 272

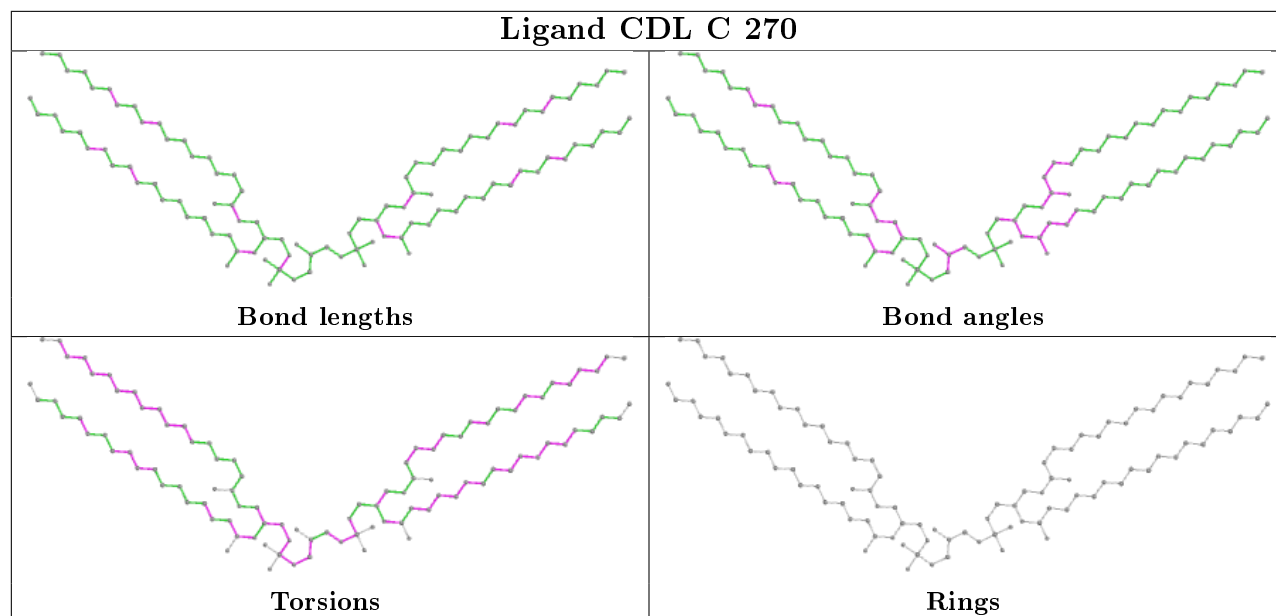


## Ligand CHD C 525









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	513/514 (99%)	0.71	51 (9%) 7 12	23, 29, 37, 63	0
1	N	513/514 (99%)	0.50	38 (7%) 14 22	27, 34, 43, 64	0
2	B	226/227 (99%)	-0.13	3 (1%) 77 83	24, 34, 56, 82	0
2	O	226/227 (99%)	-0.00	7 (3%) 49 58	30, 40, 63, 82	0
3	C	259/261 (99%)	-0.19	3 (1%) 79 84	25, 32, 44, 61	0
3	P	259/261 (99%)	-0.05	7 (2%) 54 63	28, 35, 47, 64	0
4	D	144/147 (97%)	-0.26	2 (1%) 75 82	29, 35, 50, 65	0
4	Q	144/147 (97%)	1.15	24 (16%) 1 2	36, 50, 70, 109	0
5	E	104/109 (95%)	0.20	7 (6%) 17 26	29, 35, 54, 70	0
5	R	104/109 (95%)	0.75	10 (9%) 8 13	32, 41, 57, 75	0
6	F	93/98 (94%)	0.24	4 (4%) 35 45	29, 38, 56, 93	0
6	S	93/98 (94%)	0.25	4 (4%) 35 45	32, 40, 62, 87	0
7	G	83/85 (97%)	0.85	16 (19%) 1 1	29, 38, 93, 99	0
7	T	83/85 (97%)	1.10	16 (19%) 1 1	30, 42, 90, 104	0
8	H	75/85 (88%)	0.62	12 (16%) 1 2	30, 41, 77, 83	0
8	U	75/85 (88%)	0.81	13 (17%) 1 2	36, 46, 80, 86	0
9	I	71/73 (97%)	0.68	9 (12%) 3 6	31, 41, 65, 71	0
9	V	71/73 (97%)	1.19	12 (16%) 1 2	36, 51, 66, 75	0
10	J	57/59 (96%)	0.44	8 (14%) 2 4	32, 41, 58, 73	0
10	W	57/59 (96%)	0.82	11 (19%) 1 1	36, 45, 62, 78	0
11	K	49/56 (87%)	-0.04	0 100 100	32, 38, 49, 58	0
11	X	49/56 (87%)	1.54	17 (34%) 0 0	42, 47, 62, 69	0
12	L	46/47 (97%)	-0.09	2 (4%) 35 45	30, 35, 54, 79	0
12	Y	46/47 (97%)	0.02	2 (4%) 35 45	34, 42, 62, 82	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	0.48	6 (13%) 2 4	29, 35, 87, 107	0
13	Z	43/46 (93%)	0.97	10 (23%) 0 0	37, 44, 96, 112	0
All	All	3526/3614 (97%)	0.40	294 (8%) 11 17	23, 36, 61, 112	0

All (294) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	18.9
6	F	96	LEU	12.7
4	Q	5	VAL	11.9
4	Q	4	SER	11.6
13	Z	43	SER	9.9
6	F	95	GLN	8.4
13	M	43	SER	8.3
13	Z	40	TYR	8.2
4	Q	8	SER	7.7
8	H	45	ALA	7.5
7	T	36	TRP	7.4
9	I	37	PHE	6.7
7	G	2	SER	6.7
6	S	96	LEU	6.6
7	G	1	ALA	6.6
13	Z	42	LYS	6.5
9	V	37	PHE	5.9
7	T	42	ARG	5.8
13	M	42	LYS	5.7
10	W	52	TRP	5.5
7	T	1	ALA	5.5
6	F	94	HIS	5.5
2	O	113	TYR	5.4
6	S	94	HIS	5.3
8	H	43	MET	5.2
13	M	40	TYR	5.1
8	U	44	THR	5.1
11	X	13	TYR	5.1
8	U	42	ALA	5.0
9	V	36	LYS	5.0
7	T	3	ALA	4.9
4	Q	147	LYS	4.9
8	U	49	ASP	4.9
5	R	109	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
8	H	47	GLY	4.8
13	Z	39	ASN	4.8
8	U	45	ALA	4.7
7	T	8	HIS	4.7
4	Q	48	TRP	4.7
7	G	42	ARG	4.6
7	G	5	LYS	4.6
7	T	40	GLY	4.6
7	T	4	ALA	4.5
6	S	93	PRO	4.5
10	W	57	HIS	4.5
8	U	48	GLY	4.4
7	T	5	LYS	4.4
4	Q	53	ILE	4.4
8	H	44	THR	4.4
8	H	50	VAL	4.3
9	I	25	PHE	4.3
11	X	7	PRO	4.3
13	Z	37	LEU	4.2
8	H	46	LYS	4.2
7	G	84	LYS	4.2
7	T	84	LYS	4.2
9	I	29	LEU	4.2
7	T	2	SER	4.1
9	I	26	MET	4.0
7	G	3	ALA	3.9
11	X	19	ALA	3.9
7	T	39	SER	3.9
7	G	36	TRP	3.9
12	Y	45	LEU	3.8
4	Q	7	LYS	3.8
10	J	1	PHE	3.8
9	V	53	ASN	3.8
8	H	48	GLY	3.7
7	G	4	ALA	3.7
8	U	47	GLY	3.7
13	Z	35	TYR	3.7
4	Q	51	LEU	3.7
5	R	96	LEU	3.7
9	I	33	THR	3.6
11	X	23	THR	3.6
8	U	50	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
4	Q	138	TRP	3.6
9	V	34	PHE	3.6
13	Z	32	TRP	3.6
7	T	41	HIS	3.5
5	E	11	PHE	3.5
1	A	389	ILE	3.5
9	V	33	THR	3.5
1	A	202	LEU	3.5
1	N	246	LEU	3.5
11	X	16	ALA	3.5
10	W	1	PHE	3.5
7	G	40	GLY	3.5
1	N	282	PHE	3.5
11	X	6	ALA	3.4
9	I	36	LYS	3.4
10	J	52	TRP	3.4
7	G	9	GLY	3.4
13	M	41	LYS	3.4
1	A	75	ILE	3.4
9	V	30	GLY	3.3
7	G	41	HIS	3.3
2	O	91	ASN	3.3
10	W	55	PHE	3.3
8	U	46	LYS	3.3
1	N	193	VAL	3.3
1	A	66	ILE	3.3
8	U	52	VAL	3.3
12	Y	47	LYS	3.3
6	S	95	GLN	3.2
7	T	9	GLY	3.2
11	X	27	ALA	3.2
5	R	89	LEU	3.2
10	W	26	ALA	3.2
1	A	201	VAL	3.1
12	L	47	LYS	3.1
4	Q	140	TYR	3.1
10	W	4	ARG	3.1
1	A	385	ALA	3.1
1	N	126	TRP	3.1
1	A	246	LEU	3.1
4	Q	43	LYS	3.1
1	N	66	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	N	73	ILE	3.1
4	Q	58	GLU	3.1
1	N	78	PHE	3.1
1	A	126	TRP	3.0
1	A	247	ILE	3.0
8	H	49	ASP	3.0
10	W	56	PRO	3.0
5	E	109	VAL	3.0
1	A	195	LEU	3.0
10	W	48	TYR	3.0
1	N	197	LEU	3.0
4	Q	46	ALA	3.0
1	A	380	VAL	3.0
4	Q	30	VAL	3.0
5	R	93	LEU	2.9
11	X	36	ILE	2.9
1	A	193	VAL	2.9
1	N	201	VAL	2.9
11	X	18	LEU	2.9
1	N	389	ILE	2.9
1	A	235	PHE	2.9
13	M	39	ASN	2.9
7	T	43	GLU	2.9
3	C	38	ASN	2.9
1	A	243	VAL	2.9
2	B	59	GLN	2.9
1	A	73	ILE	2.9
8	U	11	TYR	2.9
1	N	70	VAL	2.9
1	N	283	LEU	2.9
4	Q	107	ILE	2.9
10	J	30	ILE	2.9
4	Q	102	TYR	2.8
9	V	3	ALA	2.8
1	N	285	PHE	2.8
1	A	188	VAL	2.8
3	P	3	HIS	2.8
8	H	42	ALA	2.8
1	A	197	LEU	2.8
9	V	29	LEU	2.8
1	A	396	TRP	2.8
8	U	43	MET	2.8

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Mol	Chain	Res	Type	RSRZ
11	X	24	PHE	2.7
1	N	195	LEU	2.7
11	X	47	ARG	2.7
1	N	238	PHE	2.7
1	N	388	ALA	2.7
1	A	248	LEU	2.7
1	N	247	ILE	2.7
5	R	24	ILE	2.7
7	G	8	HIS	2.7
1	A	250	GLY	2.7
1	N	251	PHE	2.6
7	T	12	GLY	2.6
1	A	203	ALA	2.6
10	J	48	TYR	2.6
5	R	52	LEU	2.6
1	A	60	ALA	2.6
1	N	128	VAL	2.6
9	V	25	PHE	2.6
11	X	17	VAL	2.6
1	A	67	PHE	2.5
1	N	245	ILE	2.5
13	Z	41	LYS	2.5
1	A	237	PHE	2.5
5	E	19	PHE	2.5
1	N	202	LEU	2.5
5	E	7	THR	2.5
4	D	4	SER	2.5
9	I	34	PHE	2.5
3	C	92	LEU	2.5
1	A	199	LEU	2.5
9	V	19	PHE	2.5
2	O	90	ILE	2.4
10	W	30	ILE	2.4
3	P	38	ASN	2.4
10	W	18	LEU	2.4
2	O	217	LYS	2.4
5	R	97	GLY	2.4
3	P	91	VAL	2.4
1	A	161	ALA	2.4
4	D	147	LYS	2.4
1	A	20	LEU	2.4
1	A	377	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	N	184	PHE	2.3
3	P	37	PHE	2.3
11	X	12	LYS	2.3
10	J	5	VAL	2.3
1	A	192	ALA	2.3
4	Q	33	LEU	2.3
4	Q	39	ALA	2.3
5	R	51	ALA	2.3
4	Q	111	PHE	2.3
10	J	55	PHE	2.3
1	A	284	GLY	2.3
1	N	196	LEU	2.3
1	N	381	LEU	2.3
7	G	37	LEU	2.3
5	E	9	GLU	2.3
12	L	2	HIS	2.3
1	N	83	VAL	2.3
1	A	245	ILE	2.3
8	H	53	CYS	2.3
2	O	59	GLN	2.3
1	A	74	MET	2.3
1	N	190	ILE	2.3
6	F	43	LYS	2.3
13	M	38	ASP	2.3
13	Z	36	HIS	2.3
1	A	70	VAL	2.2
3	C	91	VAL	2.2
1	N	158	ILE	2.2
1	A	150	LEU	2.2
1	N	74	MET	2.2
4	Q	145	TRP	2.2
1	A	249	PRO	2.2
9	V	26	MET	2.2
1	A	63	PHE	2.2
1	N	377	PHE	2.2
5	R	11	PHE	2.2
11	X	34	THR	2.2
10	J	57	HIS	2.2
9	I	53	ASN	2.2
1	A	381	LEU	2.2
1	N	248	LEU	2.2
1	N	288	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
7	G	43	GLU	2.2
3	P	182	TYR	2.2
1	A	62	ALA	2.2
1	A	498	CYS	2.2
1	A	391	GLY	2.2
7	G	6	GLY	2.2
1	N	75	ILE	2.2
7	T	38	HIS	2.2
11	X	49	THR	2.2
5	E	6	GLU	2.2
4	Q	139	ASP	2.2
11	X	52	GLU	2.1
1	A	384	GLY	2.1
1	A	388	ALA	2.1
1	A	373	VAL	2.1
1	N	373	VAL	2.1
2	O	130	PRO	2.1
8	H	52	VAL	2.1
8	U	53	CYS	2.1
9	I	18	ARG	2.1
1	A	65	MET	2.1
8	U	51	SER	2.1
11	X	48	VAL	2.1
3	P	33	MET	2.1
4	Q	97	ILE	2.1
5	E	96	LEU	2.1
8	H	79	GLY	2.1
4	Q	9	GLU	2.1
1	A	350	VAL	2.1
1	N	189	MET	2.1
1	N	243	VAL	2.1
3	P	95	THR	2.1
9	V	15	ARG	2.1
1	A	153	ALA	2.1
2	B	91	ASN	2.1
13	Z	13	LYS	2.1
1	N	280	ILE	2.1
1	N	312	ILE	2.1
5	R	68	LEU	2.1
1	A	281	GLY	2.1
1	A	124	THR	2.0
1	A	236	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
7	G	10	GLY	2.0
1	N	286	ILE	2.0
2	O	227	LEU	2.0
10	W	27	THR	2.0
1	A	78	PHE	2.0
1	A	285	PHE	2.0
10	J	10	LYS	2.0
2	B	60	GLU	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
7	TPO	T	11	11/12	0.56	0.24	71,78,95,96	0
7	TPO	G	11	11/12	0.61	0.26	71,78,96,97	0
1	FME	A	1	10/11	0.93	0.12	48,51,72,78	0
1	FME	N	1	10/11	0.94	0.16	47,49,70,71	0
2	FME	B	1	10/11	0.96	0.12	32,33,40,58	0
2	FME	O	1	10/11	0.96	0.11	39,40,48,52	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
28	DMU	G	272	33/33	0.51	0.34	65,94,105,105	0
28	DMU	P	1272	33/33	0.55	0.36	80,103,111,112	0
24	PEK	T	263	53/53	0.58	0.37	55,95,117,119	0
24	PEK	G	1263	53/53	0.60	0.34	60,95,118,119	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
25	CDL	G	269	100/100	0.61	0.30	64,87,115,118	0
24	PEK	G	265	53/53	0.63	0.28	45,82,114,116	0
26	PSC	E	230	52/52	0.64	0.37	58,99,125,127	0
26	PSC	R	1230	52/52	0.65	0.31	43,96,122,124	0
24	PEK	T	1265	53/53	0.67	0.29	44,79,110,112	0
19	TGL	Y	1522	63/63	0.67	0.29	45,72,86,88	0
20	PGV	H	268	51/51	0.69	0.34	59,84,110,112	0
25	CDL	T	1269	100/100	0.69	0.26	61,84,108,111	0
23	UNX	C	262	1/1	0.71	0.47	28,28,28,28	0
22	CHD	W	1060	29/29	0.72	0.38	87,91,96,97	0
20	PGV	N	1268	51/51	0.72	0.33	67,91,112,114	0
25	CDL	P	1270	100/100	0.75	0.30	41,85,115,120	0
19	TGL	O	1523	63/63	0.77	0.20	54,76,89,94	0
22	CHD	J	60	29/29	0.79	0.29	77,83,93,94	0
19	TGL	L	522	63/63	0.79	0.25	38,59,77,79	0
19	TGL	D	523	63/63	0.80	0.19	44,63,81,82	0
20	PGV	A	524	51/51	0.80	0.26	33,74,105,108	0
20	PGV	N	1524	51/51	0.80	0.30	41,75,113,114	0
19	TGL	O	1521	63/63	0.82	0.21	53,77,88,89	0
25	CDL	C	270	100/100	0.82	0.31	41,84,118,119	0
28	DMU	Z	1526	33/33	0.86	0.22	39,54,67,69	0
19	TGL	A	521	63/63	0.87	0.18	48,69,84,89	0
23	UNX	P	1262	1/1	0.87	0.47	22,22,22,22	0
28	DMU	M	526	33/33	0.91	0.13	39,47,65,67	0
17	NA	A	519	1/1	0.92	0.12	42,42,42,42	0
17	NA	N	1519	1/1	0.92	0.20	45,45,45,45	0
22	CHD	C	271	29/29	0.94	0.15	46,51,53,55	0
22	CHD	P	1271	29/29	0.94	0.15	48,53,56,58	0
24	PEK	P	1264	53/53	0.95	0.12	29,48,75,78	0
20	PGV	C	267	51/51	0.96	0.12	25,36,67,70	0
22	CHD	O	229	29/29	0.96	0.10	23,31,37,37	0
24	PEK	C	264	53/53	0.96	0.12	29,47,73,75	0
22	CHD	C	525	29/29	0.96	0.15	28,33,40,45	0
20	PGV	P	1267	51/51	0.96	0.12	28,40,72,79	0
22	CHD	P	1525	29/29	0.96	0.16	29,36,42,44	0
16	MG	N	1518	1/1	0.96	0.13	34,34,34,34	0
22	CHD	B	1086	29/29	0.96	0.08	26,30,37,47	0
20	PGV	N	1266	51/51	0.97	0.12	31,42,67,71	0
21	CUA	O	228	2/2	0.97	0.11	36,36,36,37	0
15	PER	A	520	2/2	0.97	0.18	25,25,25,32	0
20	PGV	A	522	51/51	0.97	0.13	25,39,65,66	0
15	PER	N	520	2/2	0.97	0.17	31,31,31,34	0

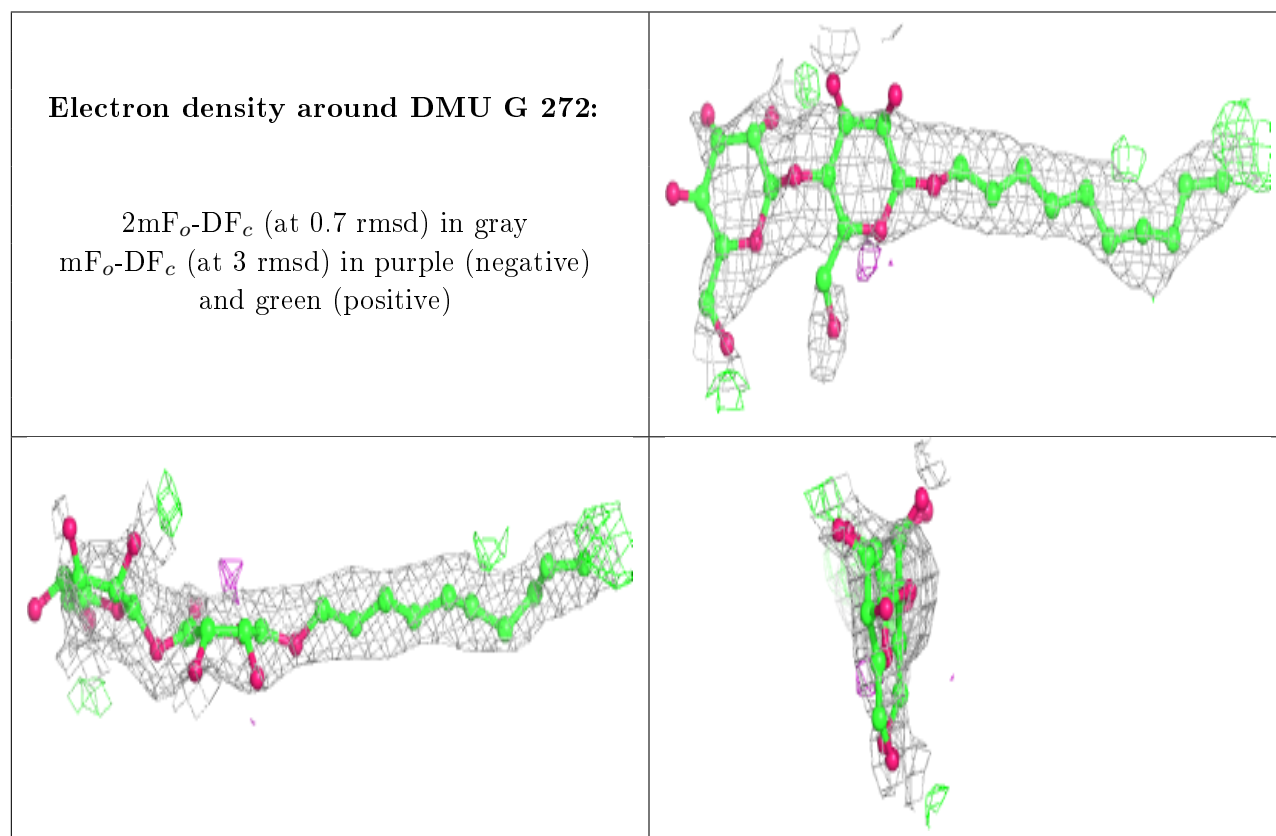
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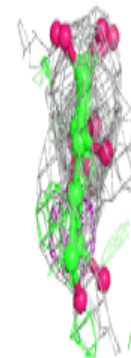
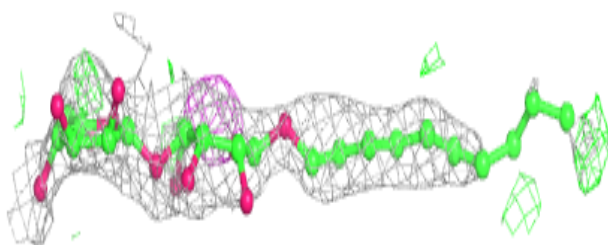
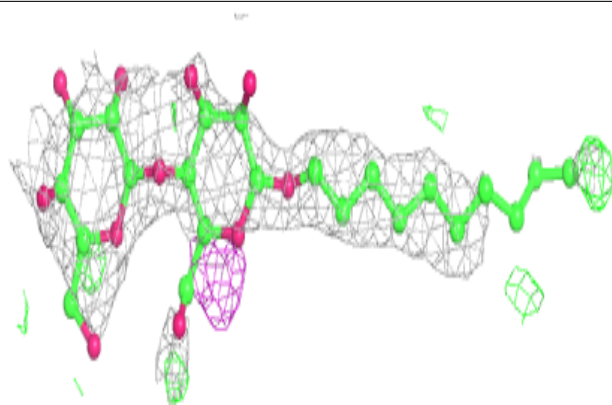
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
18	HEA	N	516	60/60	0.98	0.18	26,32,39,41	0
18	HEA	N	515	60/60	0.98	0.17	23,32,51,54	0
14	CU	N	517	1/1	0.99	0.16	32,32,32,32	0
16	MG	A	518	1/1	0.99	0.15	27,27,27,27	0
21	CUA	B	228	2/2	0.99	0.14	27,27,27,30	0
18	HEA	A	516	60/60	0.99	0.15	20,26,33,36	0
27	ZN	S	99	1/1	0.99	0.09	38,38,38,38	0
18	HEA	A	515	60/60	0.99	0.17	19,26,50,53	0
14	CU	A	517	1/1	1.00	0.15	29,29,29,29	0
27	ZN	F	99	1/1	1.00	0.09	34,34,34,34	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



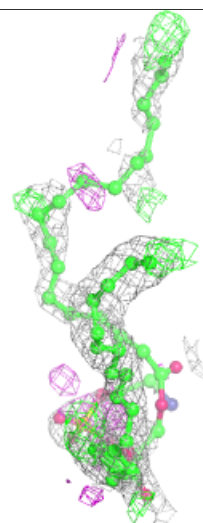
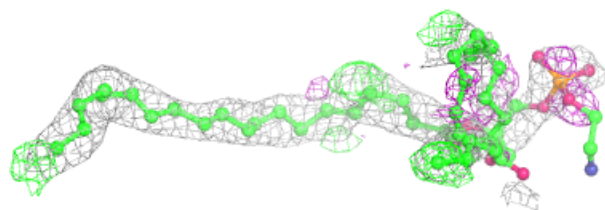
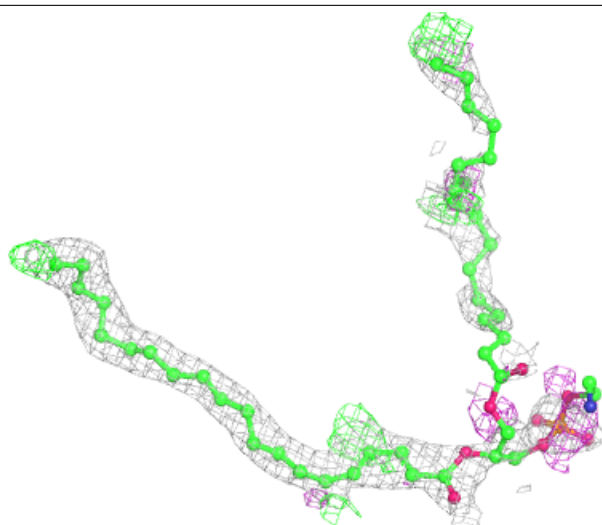
**Electron density around DMU P 1272:**

$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



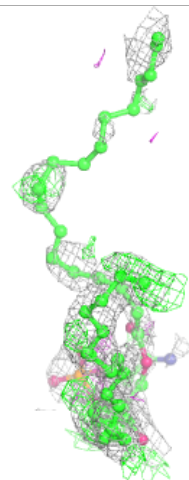
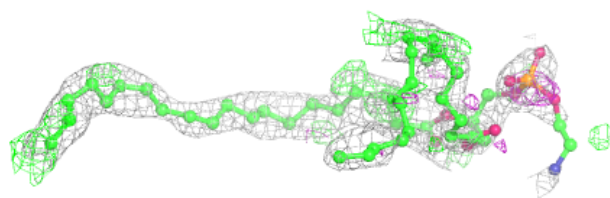
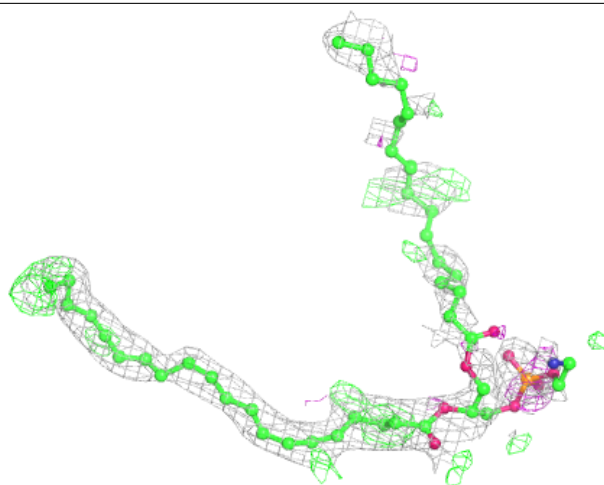
**Electron density around PEK T 263:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



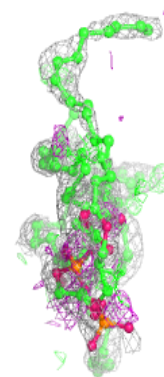
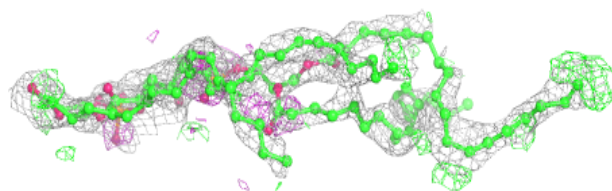
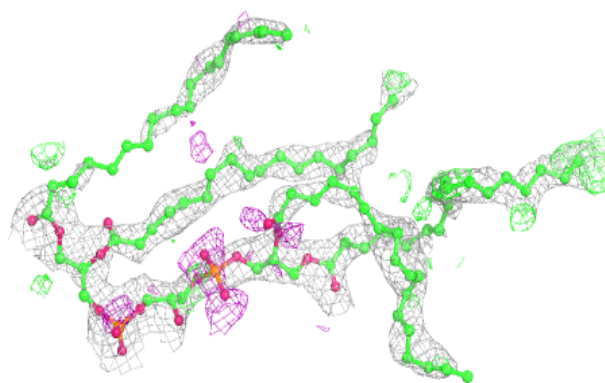
**Electron density around PEK G 1263:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

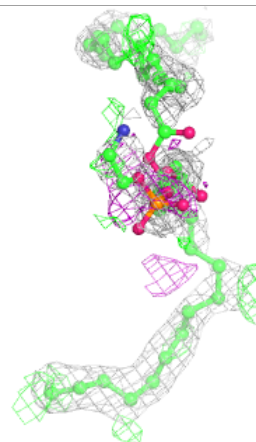
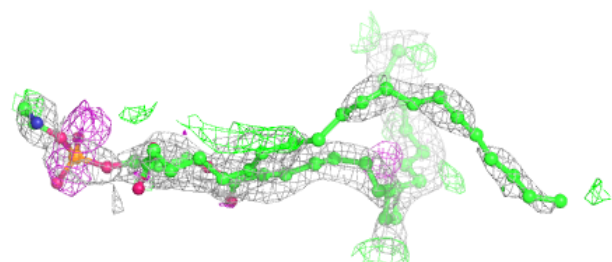
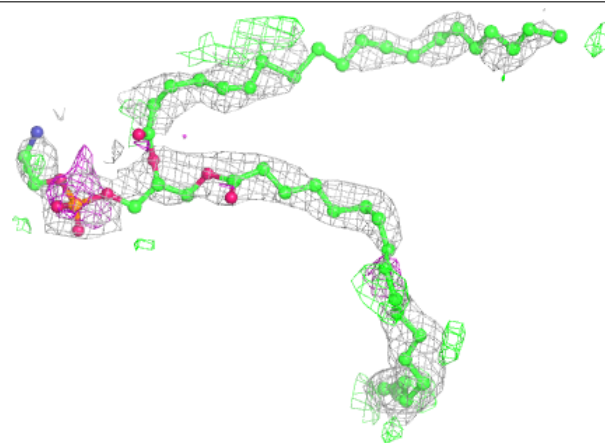


**Electron density around CDL G 269:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

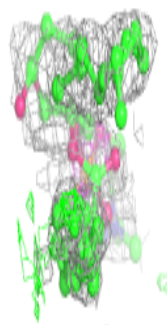
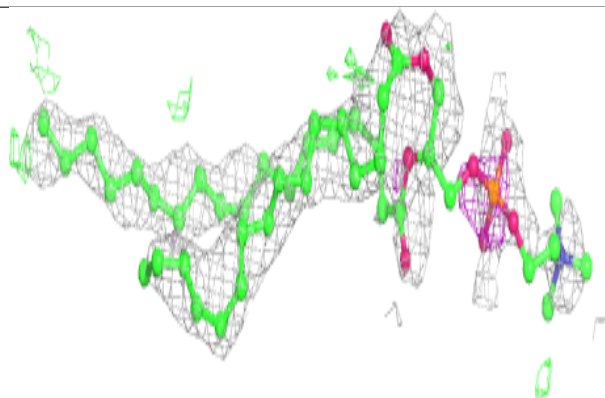
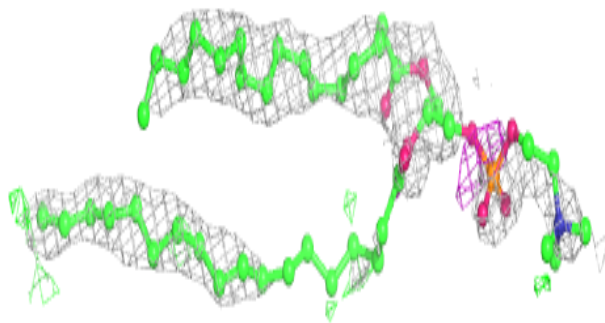
**Electron density around PEK G 265:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

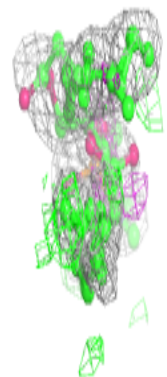
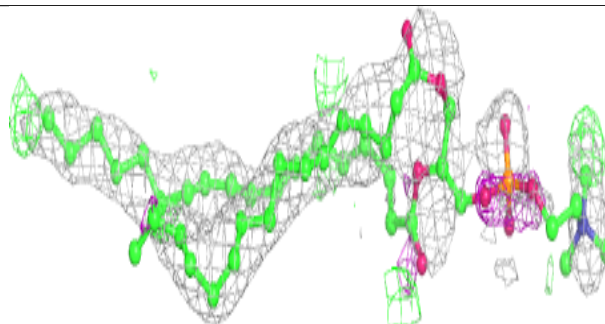
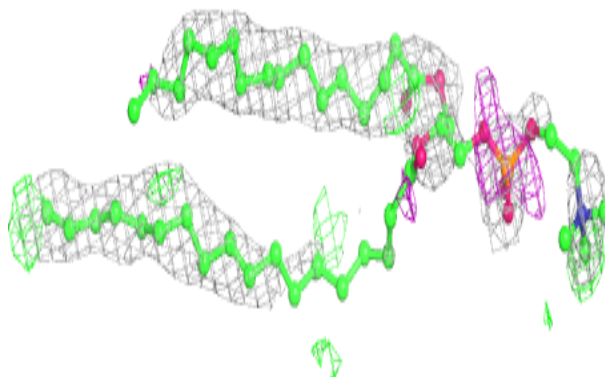


**Electron density around PSC E 230:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

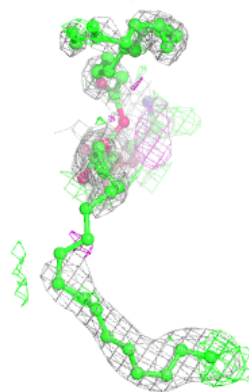
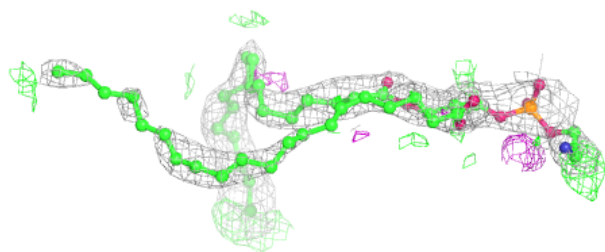
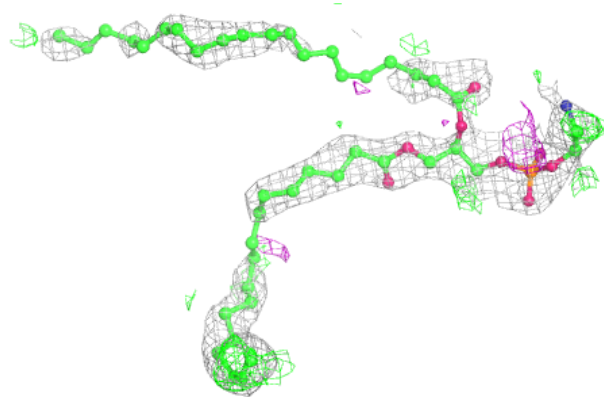
**Electron density around PSC R 1230:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

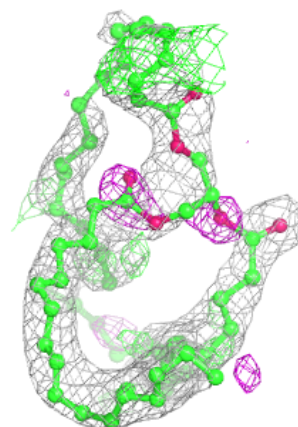
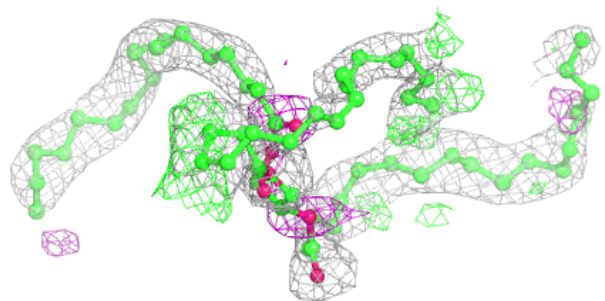
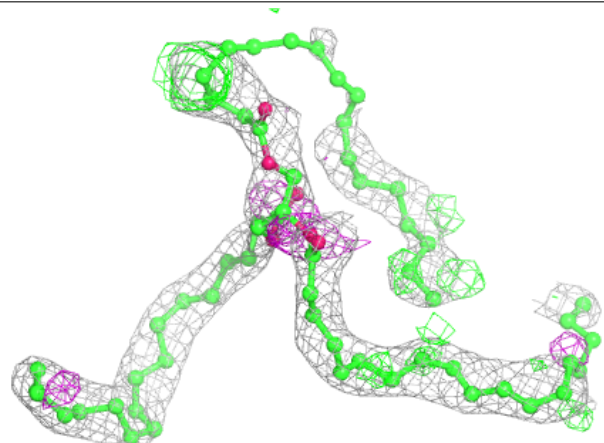


**Electron density around PEK T 1265:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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and green (positive)

**Electron density around TGL Y 1522:**

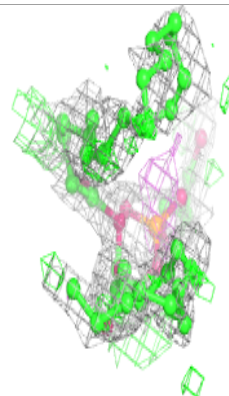
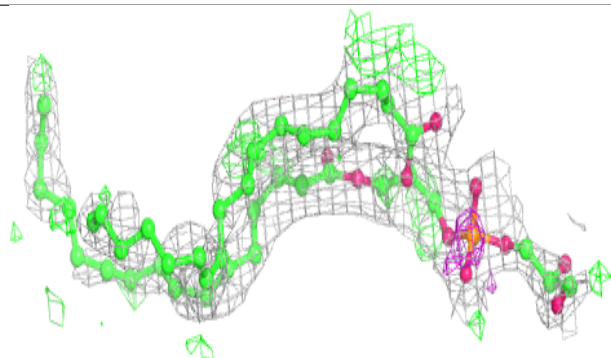
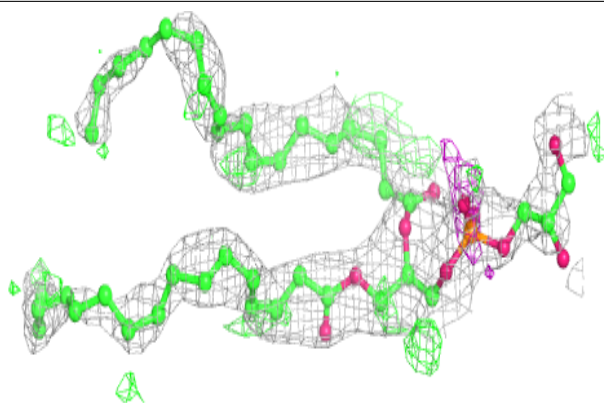
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and green (positive)



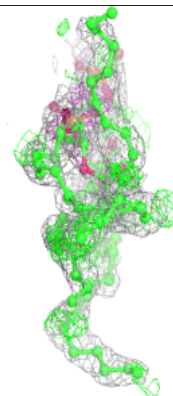
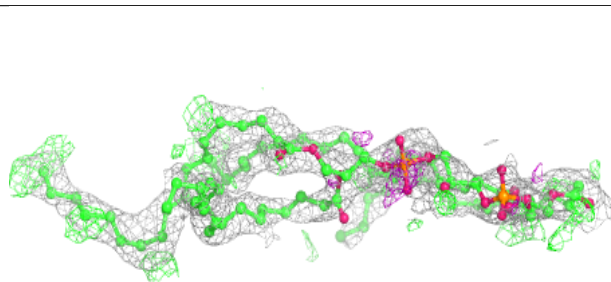
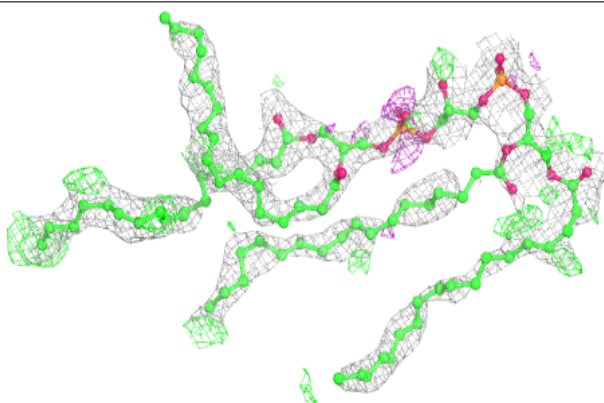


**Electron density around PGV H 268:**

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and green (positive)

**Electron density around CDL T 1269:**

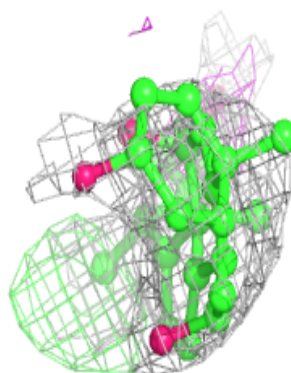
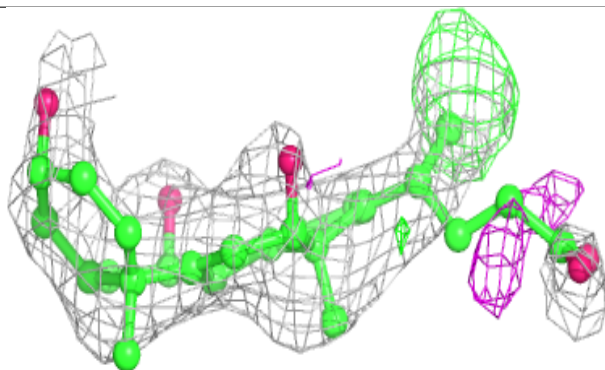
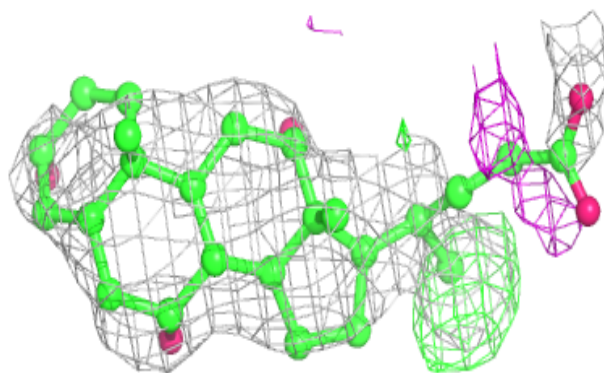
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



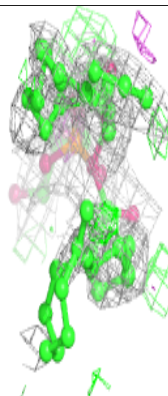
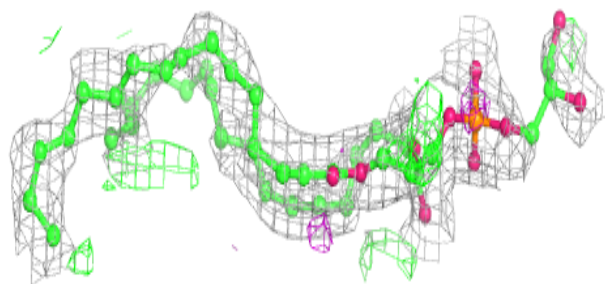
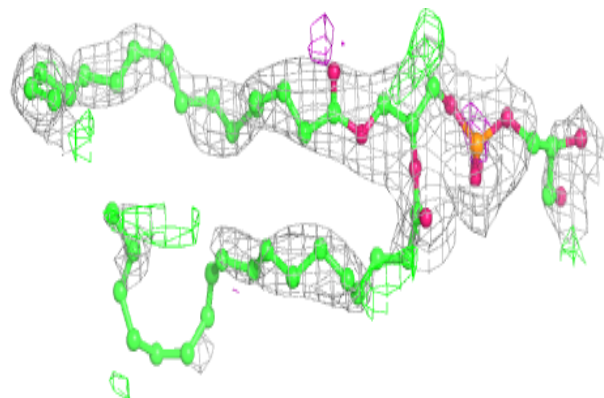


**Electron density around CHD W 1060:**

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and green (positive)

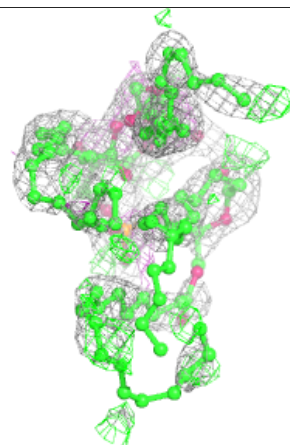
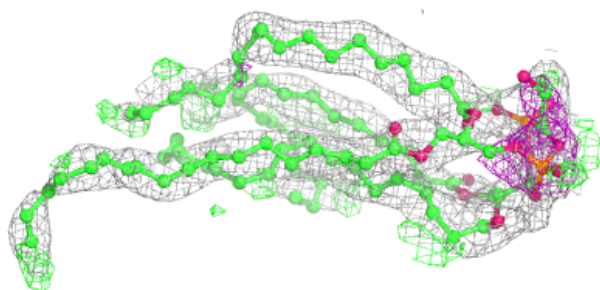
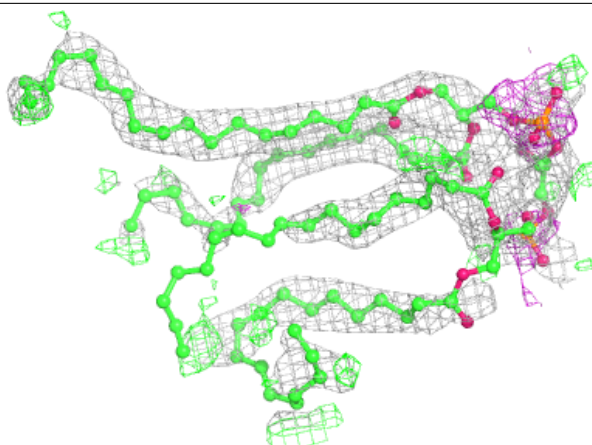
**Electron density around PGV N 1268:**

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and green (positive)

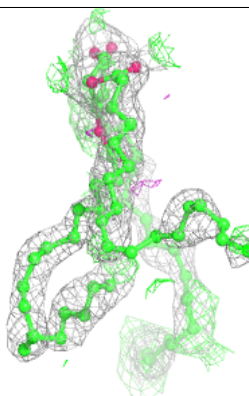
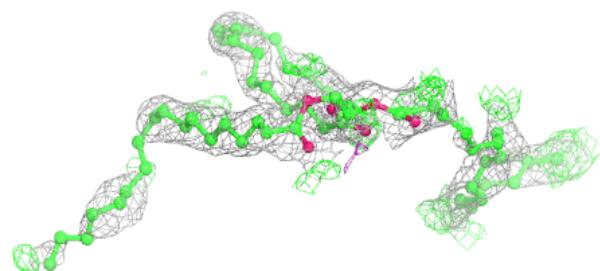
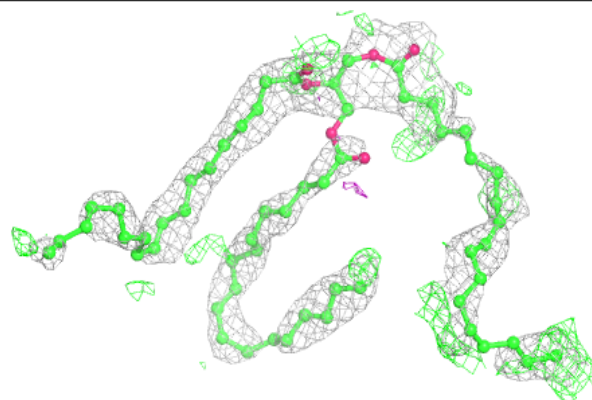


**Electron density around CDL P 1270:**

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and green (positive)

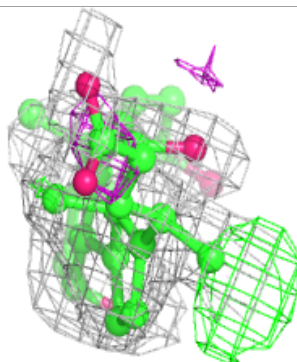
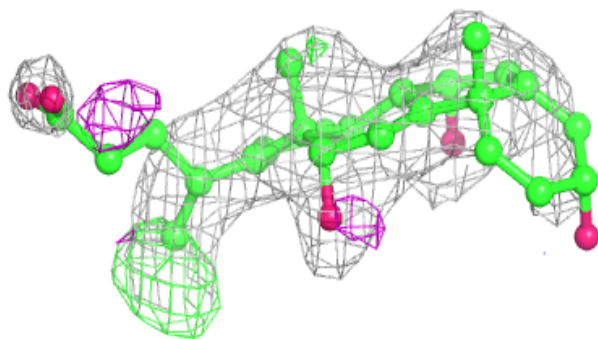
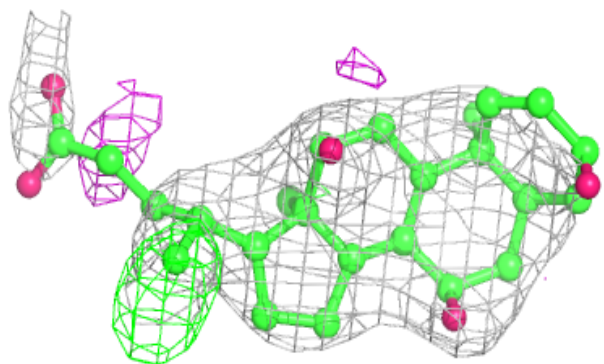
**Electron density around TGL O 1523:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



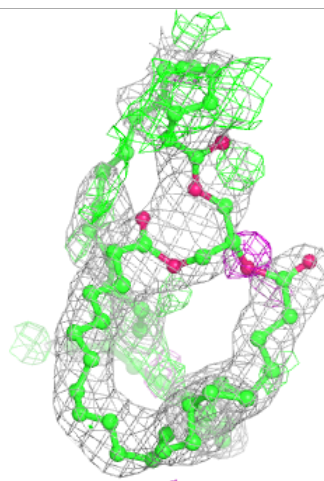
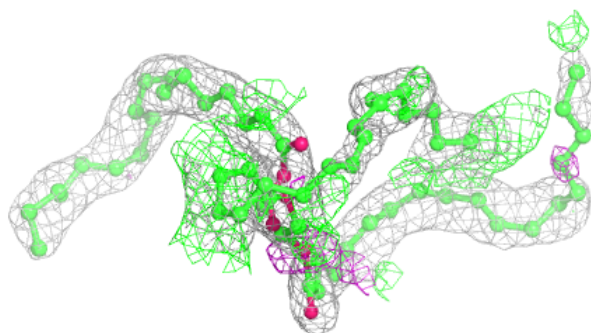
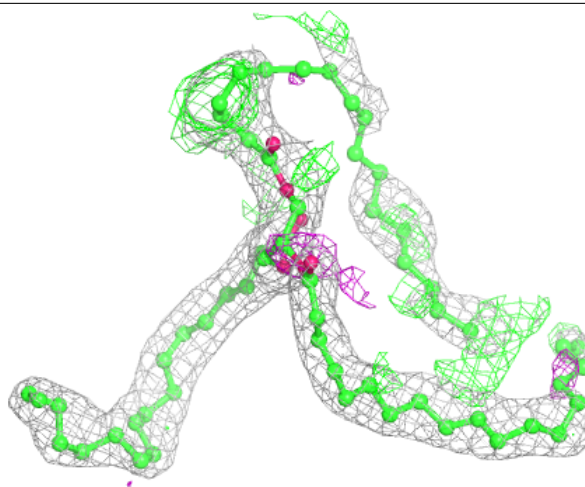
**Electron density around CHD J 60:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



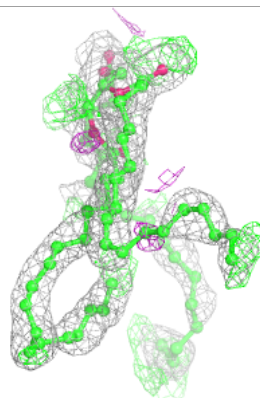
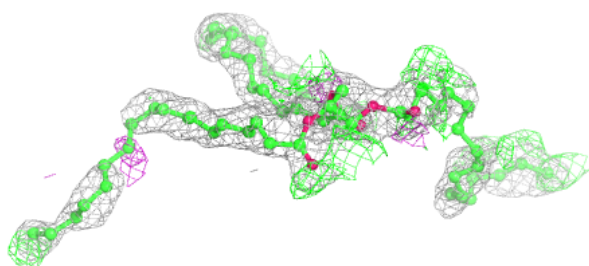
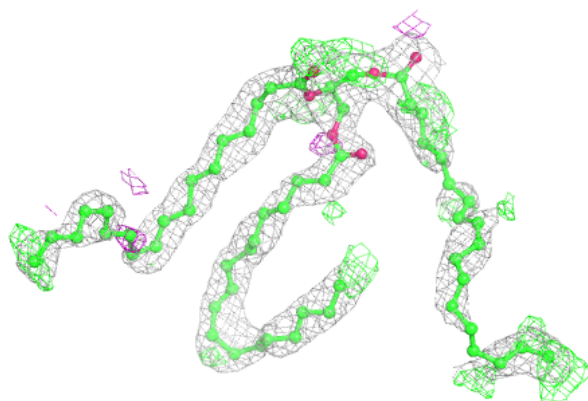
**Electron density around TGL L 522:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

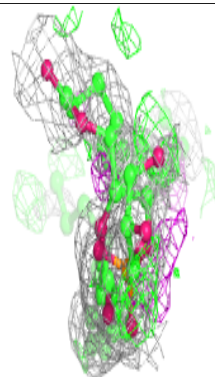
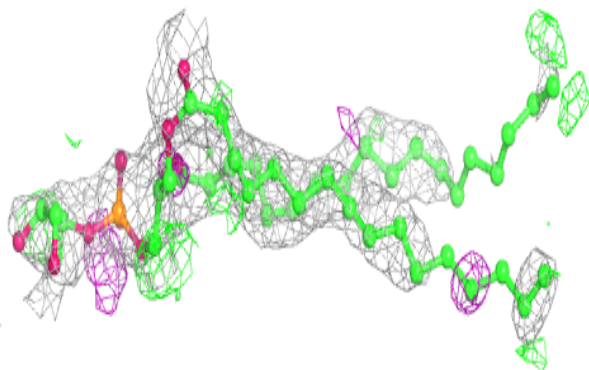
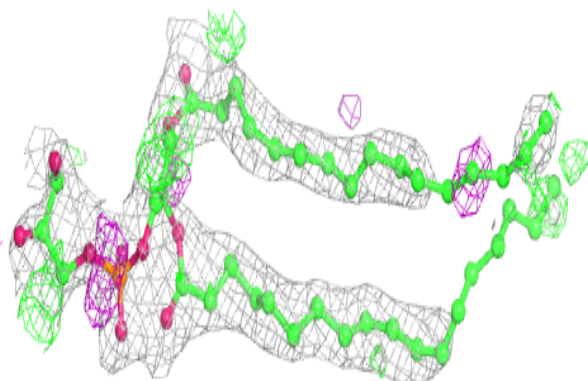


**Electron density around TGL D 523:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around PGV A 524:**

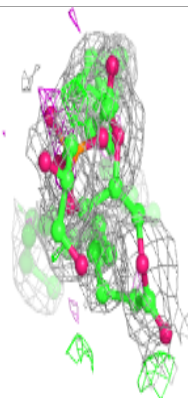
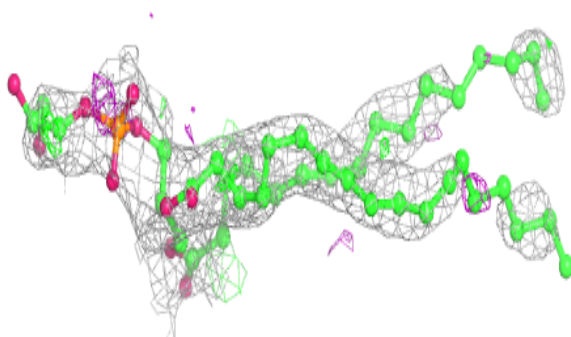
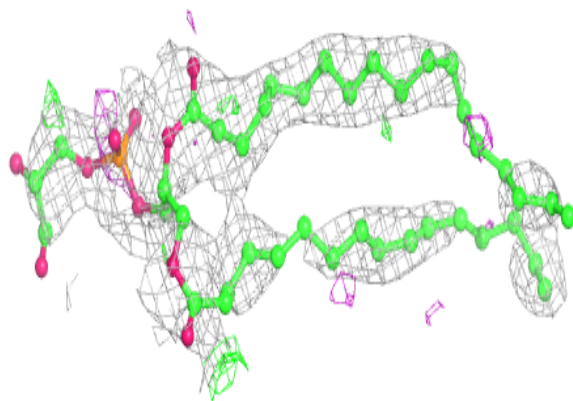
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



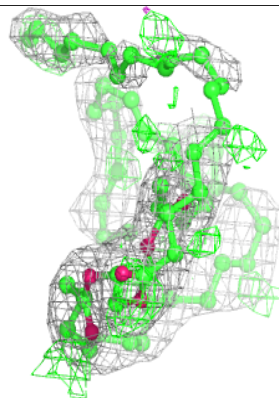
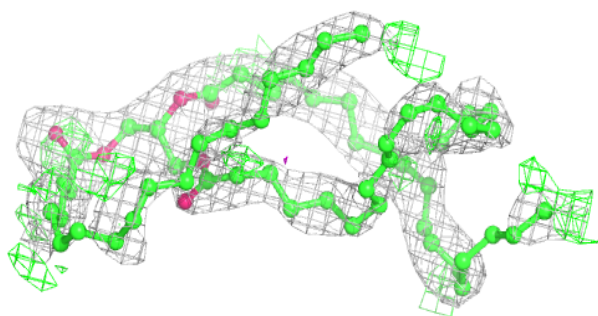
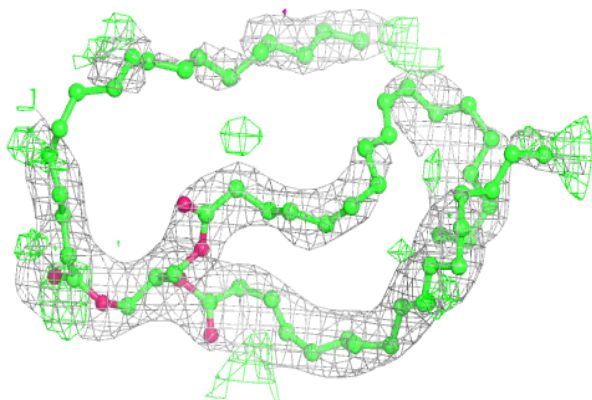


**Electron density around PGV N 1524:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

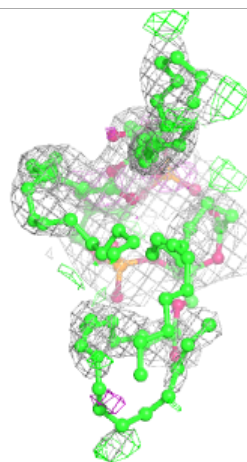
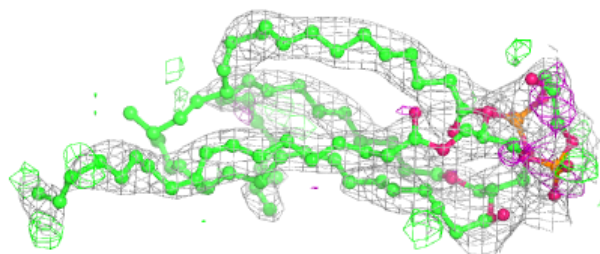
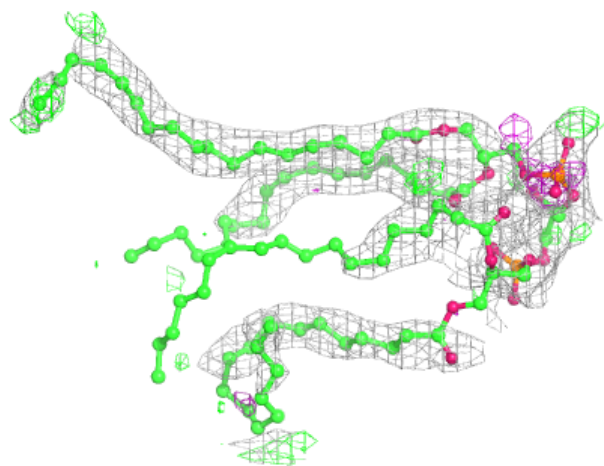
**Electron density around TGL O 1521:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



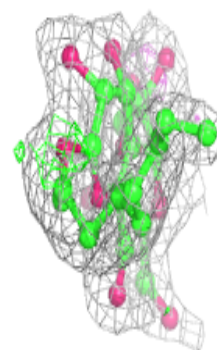
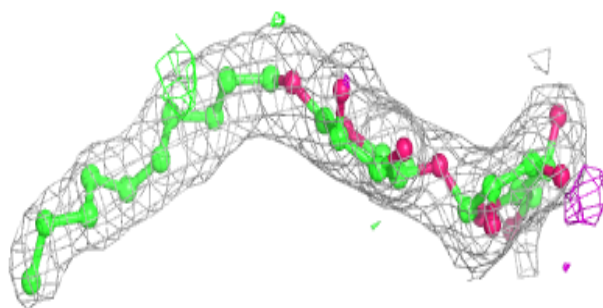
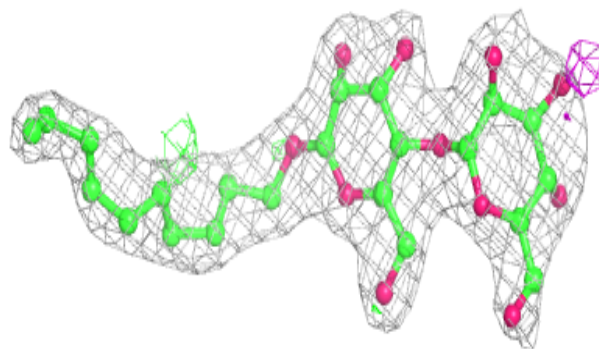
**Electron density around CDL C 270:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

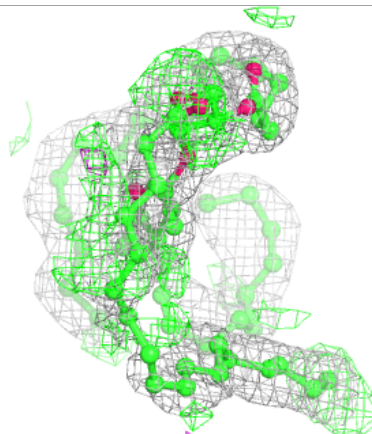
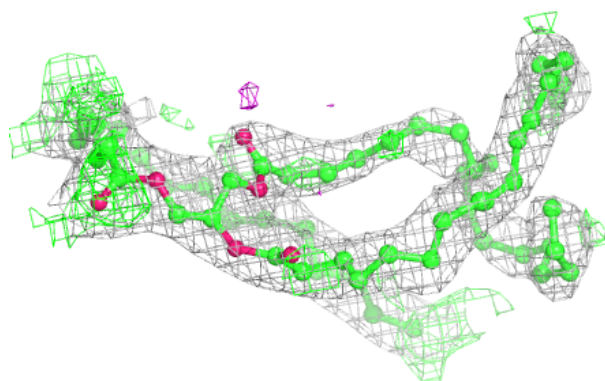
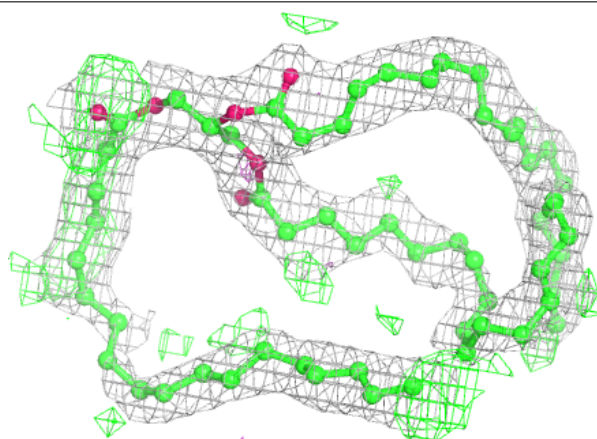


**Electron density around DMU Z 1526:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around TGL A 521:**

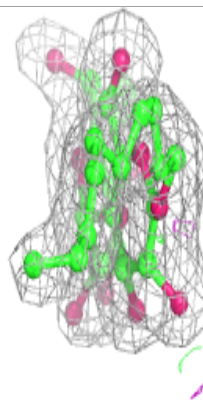
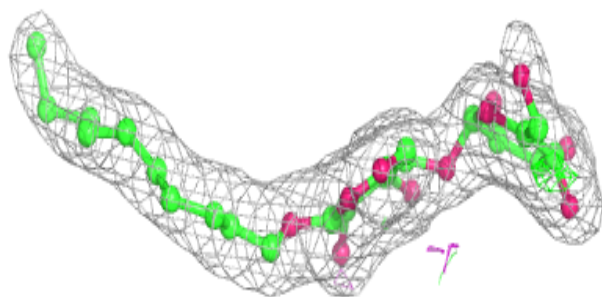
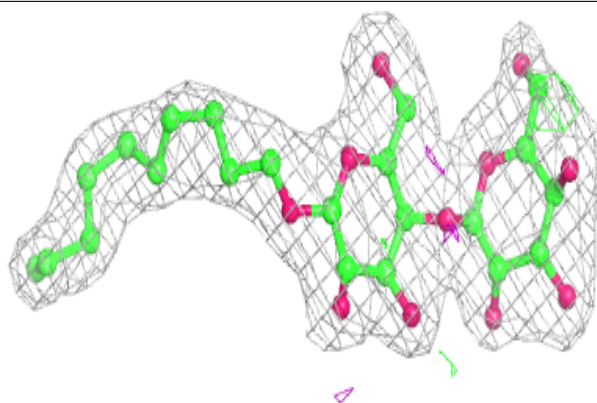
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



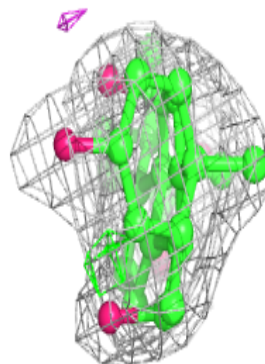
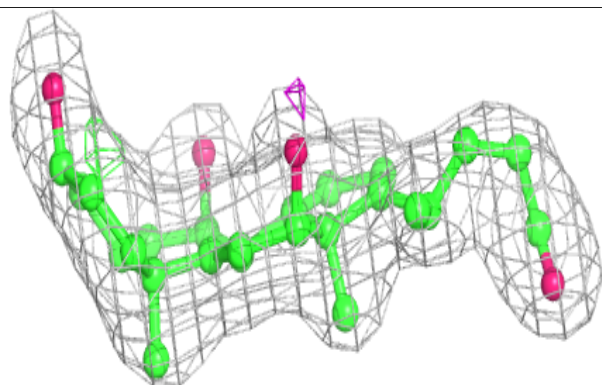
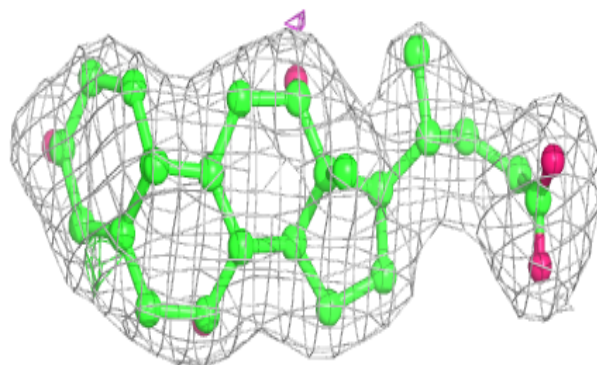


**Electron density around DMU M 526:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

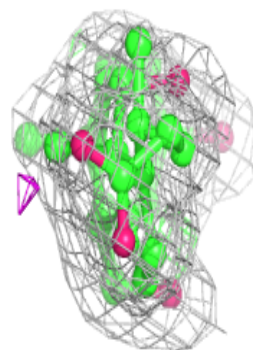
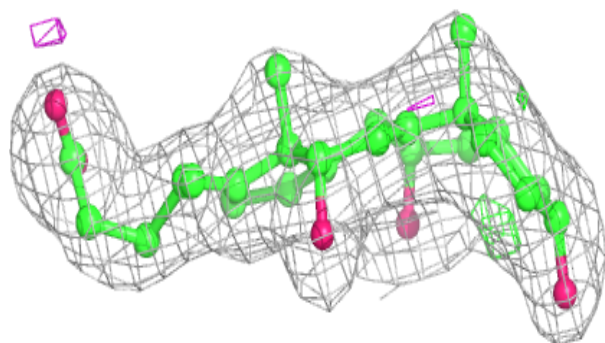
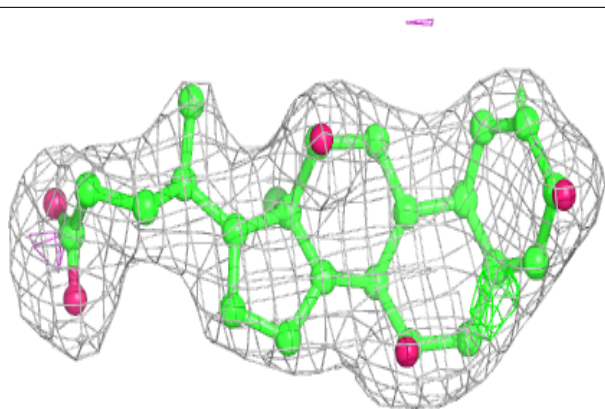
**Electron density around CHD C 271:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

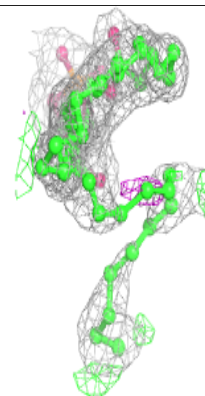
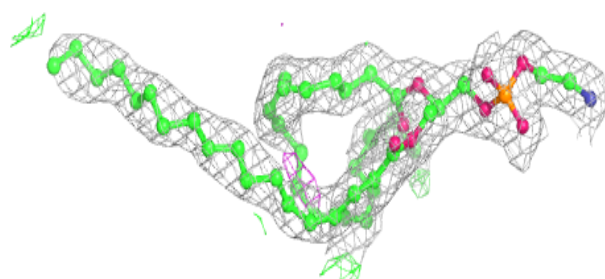
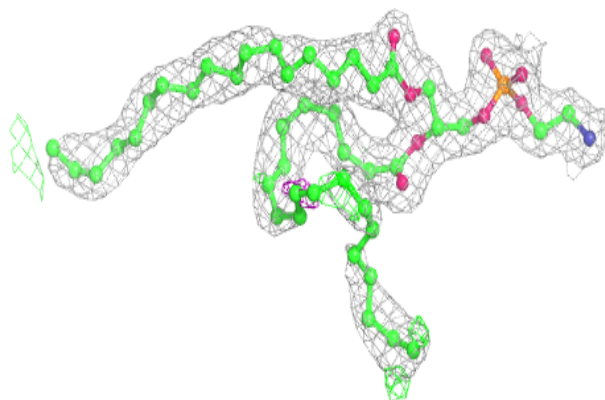


**Electron density around CHD P 1271:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

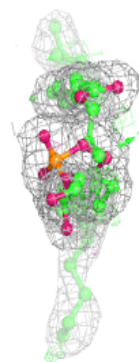
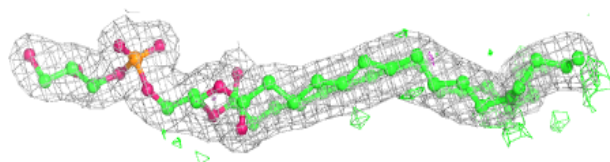
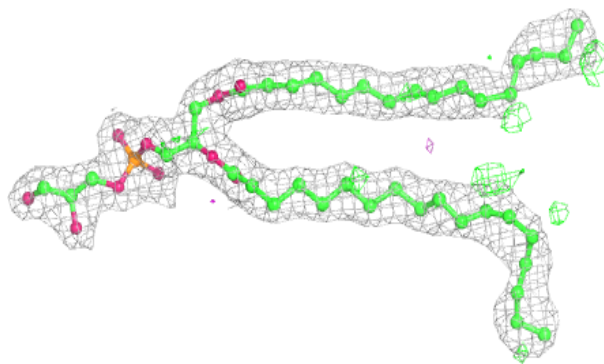
**Electron density around PEK P 1264:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

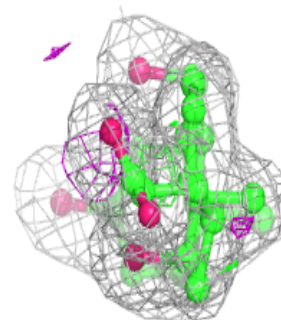
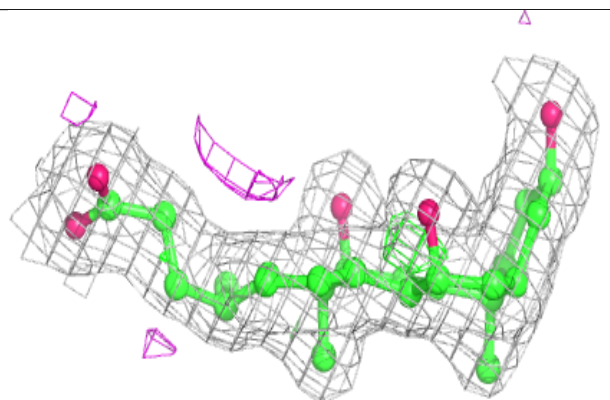
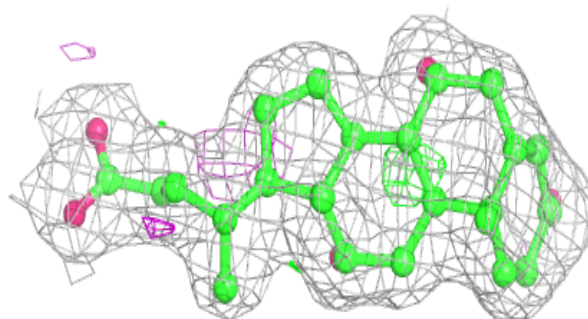


**Electron density around PGV C 267:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

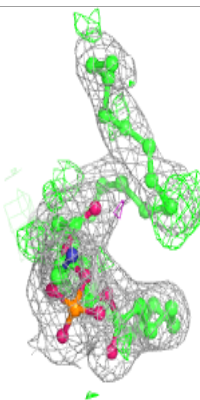
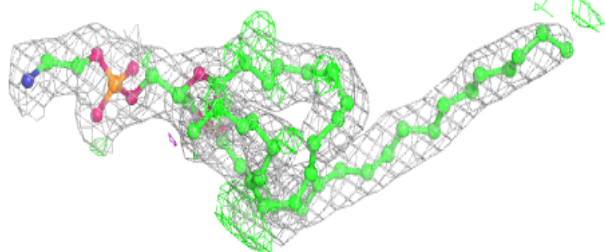
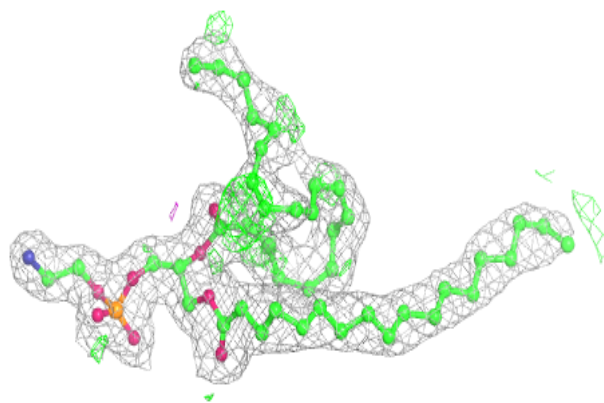
**Electron density around CHD O 229:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

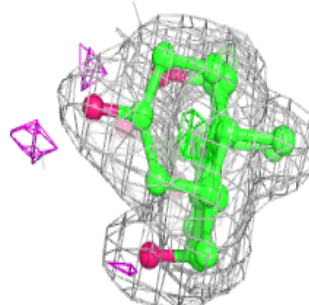
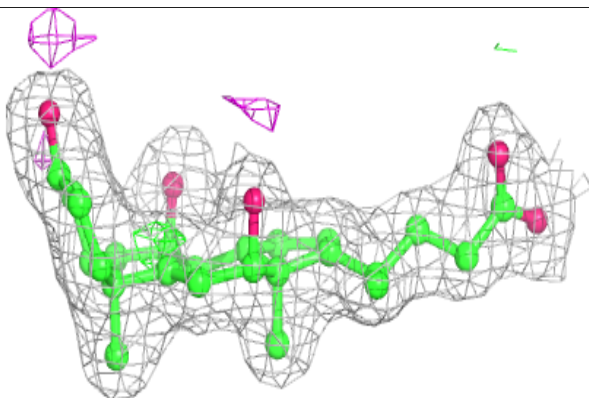


**Electron density around PEK C 264:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CHD C 525:**

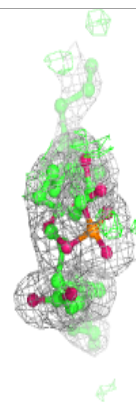
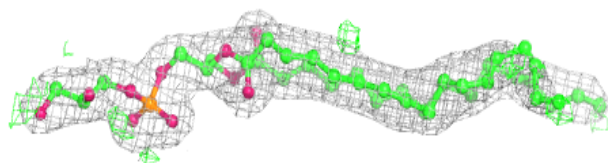
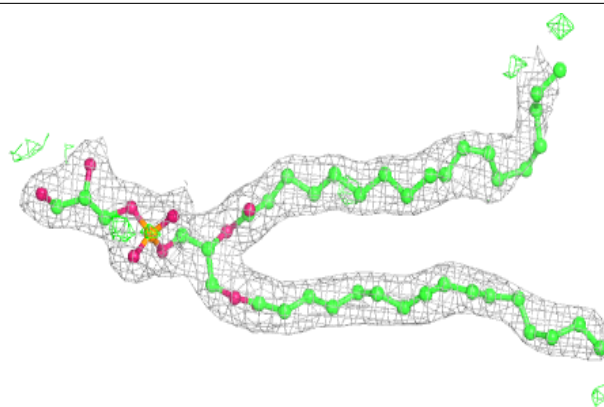
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



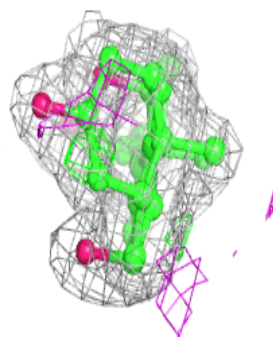
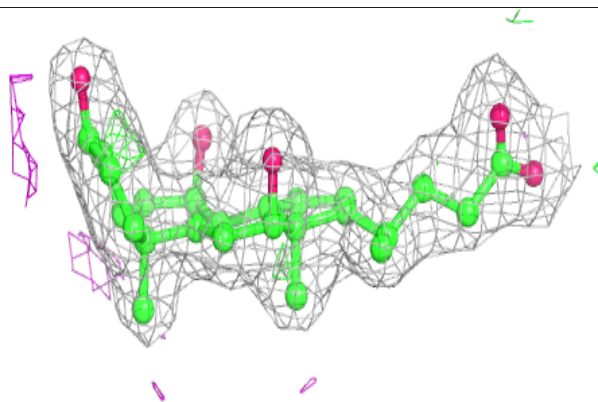
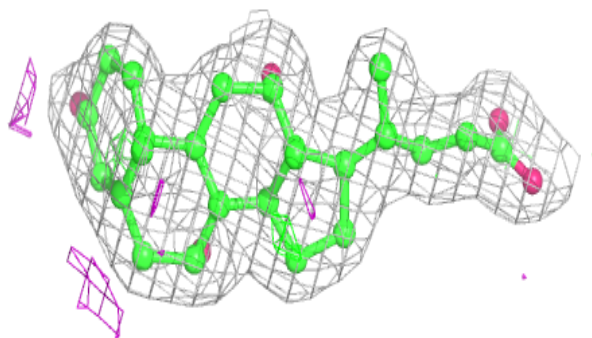


**Electron density around PGV P 1267:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

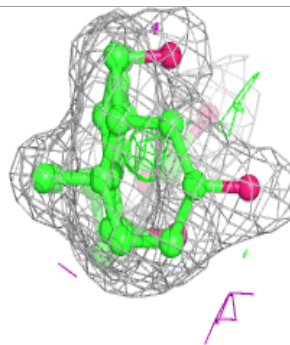
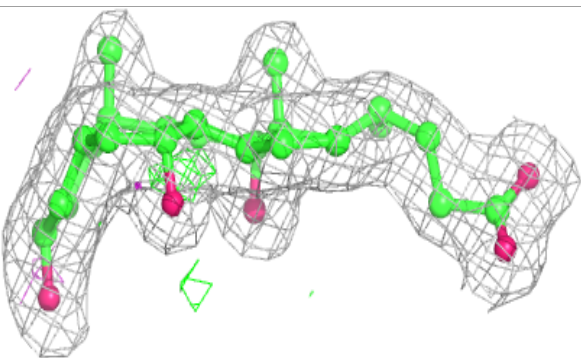
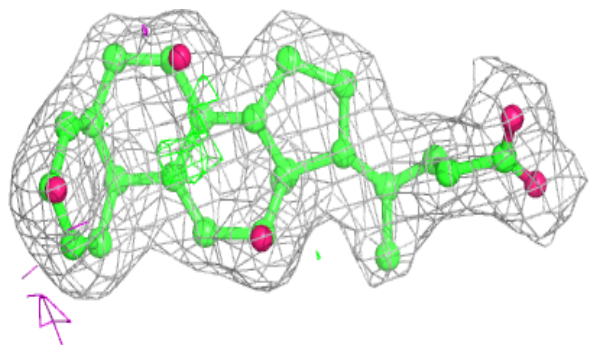
**Electron density around CHD P 1525:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

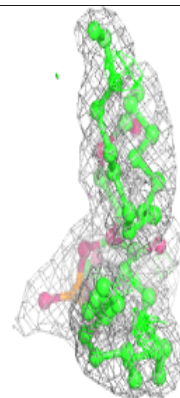
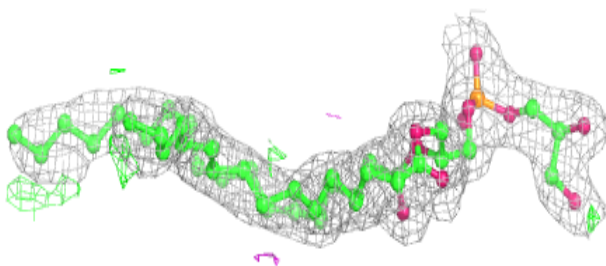
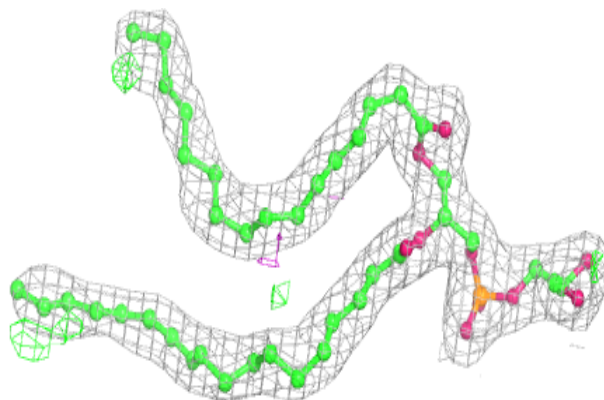


**Electron density around CHD B 1086:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

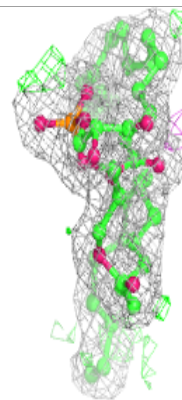
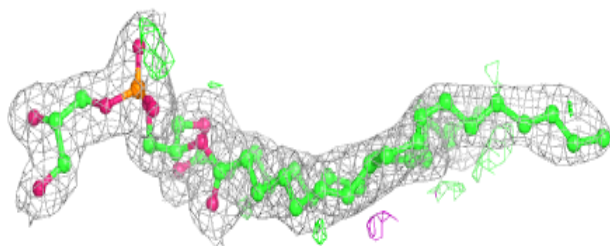
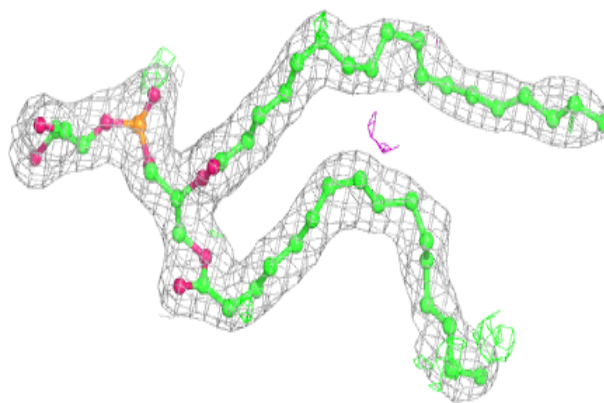
**Electron density around PGV N 1266:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

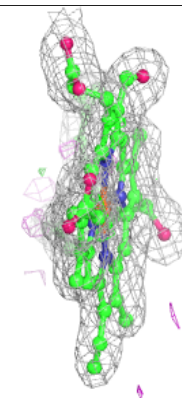
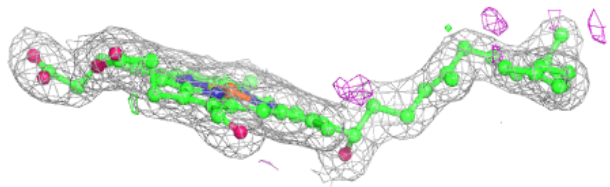
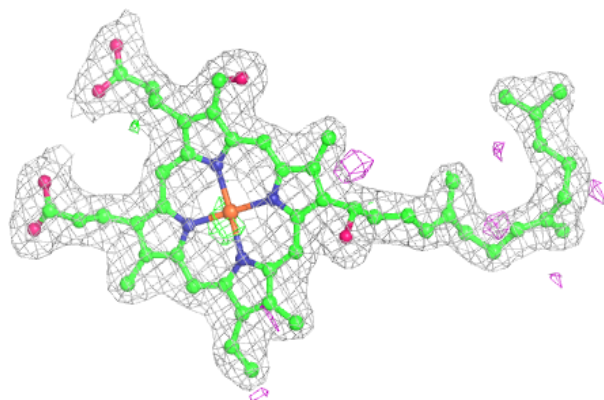


**Electron density around PGV A 522:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

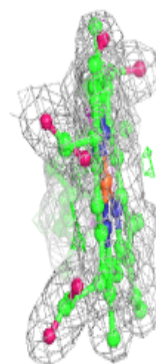
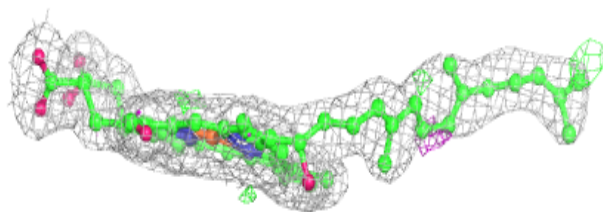
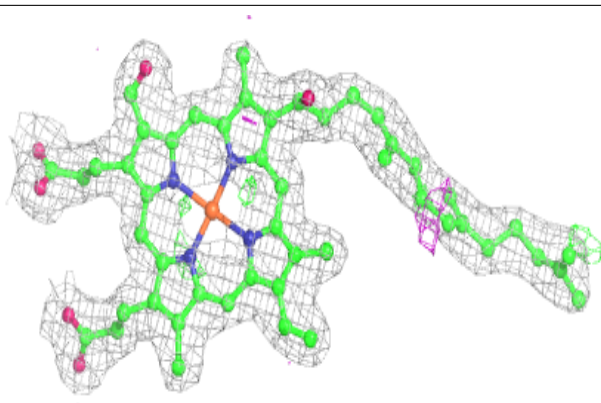
**Electron density around HEA N 516:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

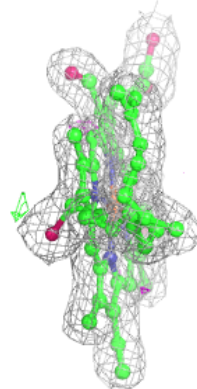
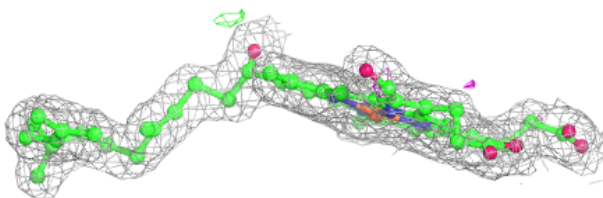
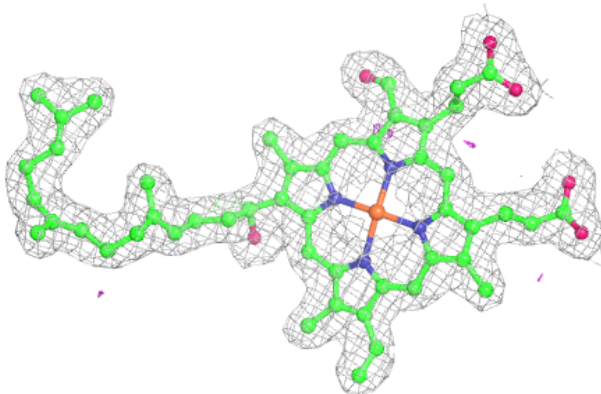


**Electron density around HEA N 515:**

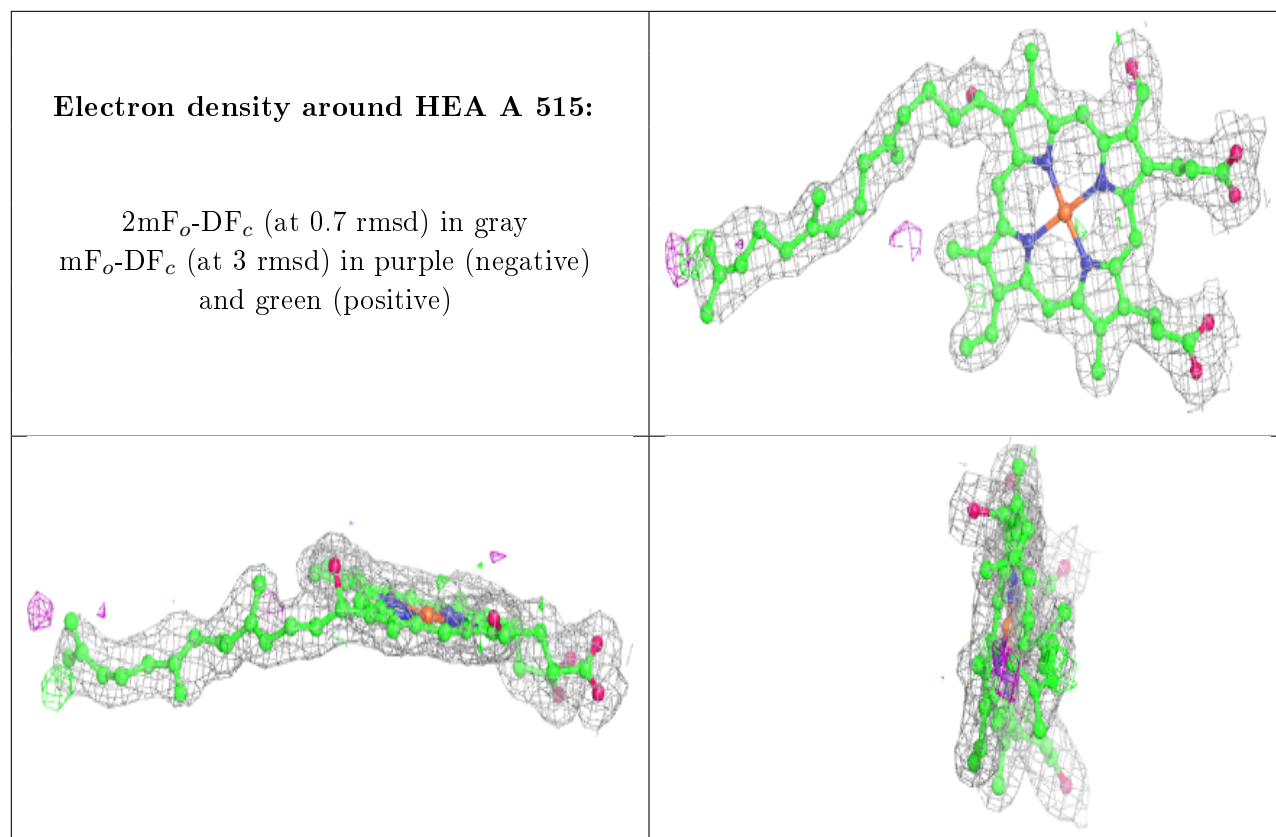
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around HEA A 516:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)







## 6.5 Other polymers [i](#)

There are no such residues in this entry.