



# Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:41 am BST

PDB ID : 3ABL  
Title : Bovine heart cytochrome c oxidase at the fully oxidized state (15-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 : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 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

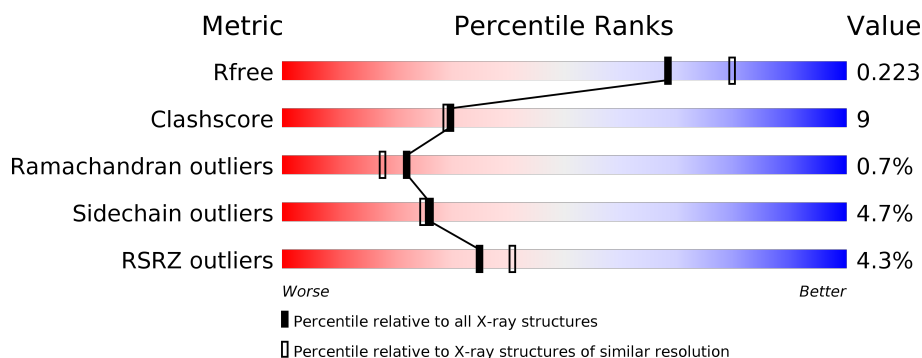
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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>76%</div> <div>21%</div> <div>.</div> </div>
1	N	514	<div> <div>78%</div> <div>20%</div> <div>.</div> </div>
2	B	227	<div> <div>75%</div> <div>21%</div> <div>..</div> </div>
2	O	227	<div> <div>2%</div> <div>71%</div> <div>23%</div> <div>5%</div> </div>
3	C	261	<div> <div>81%</div> <div>17%</div> <div>..</div> </div>
3	P	261	<div> <div>%</div> <div>80%</div> <div>17%</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	-	-	-
23	CHD	C	271	X	-	-	-
23	CHD	J	60	X	-	-	X
23	CHD	O	229	X	-	-	-
23	CHD	P	1271	X	-	-	-
23	CHD	W	1060	X	-	-	X
24	DMU	C	272	X	-	-	-
24	DMU	M	526	X	-	-	-
24	DMU	P	1272	X	-	-	-
24	DMU	Z	1526	X	-	-	-
26	CDL	G	269	-	-	X	-
26	CDL	T	1269	-	-	X	-
28	PEK	T	263	-	-	X	-



## 2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 32244 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	C	N	O	P	S	0	0	0
			675	431	129	113	1	1			
7	T	84	Total	C	N	O	P	S	0	0	0
			675	431	129	113	1	1			

- 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			

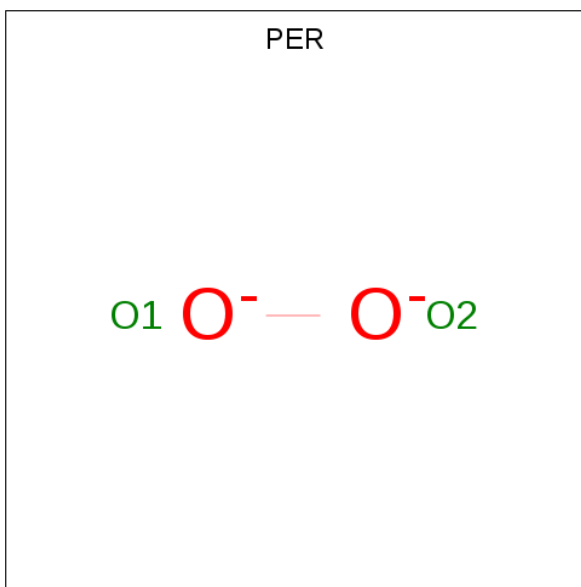
- Molecule 13 is a protein called Cytochrome c oxidase subunit 8B.

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

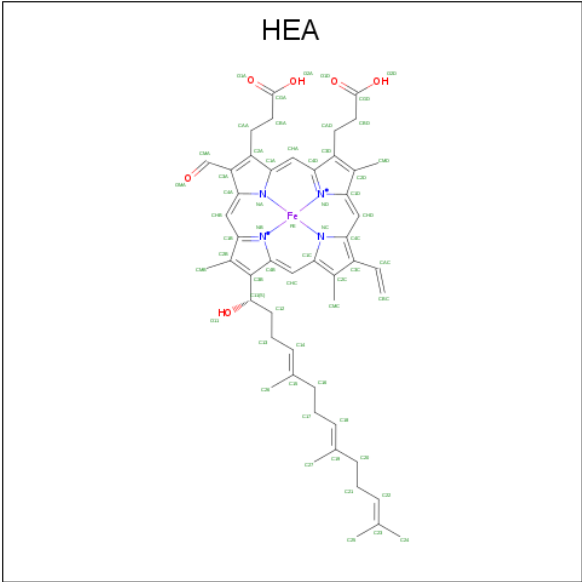
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

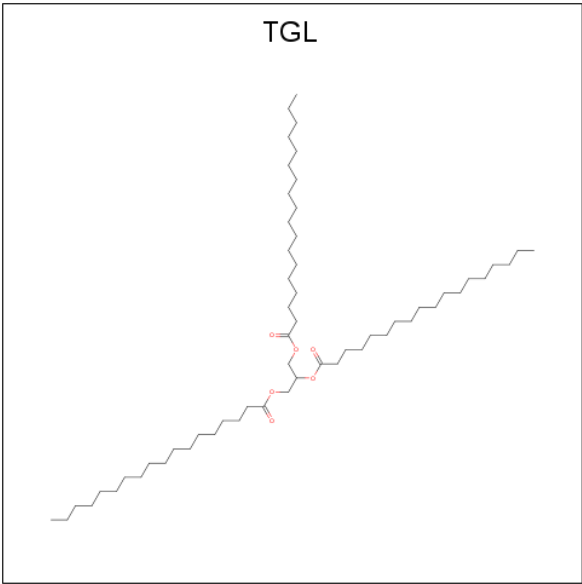
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	A	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- 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>).



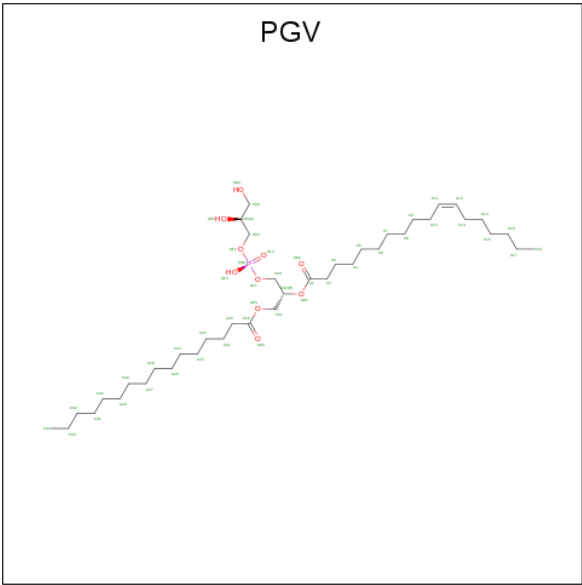
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- 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	N	1	Total	C	O	0	0
			63	57	6		
19	N	1	Total	C	O	0	0
			63	57	6		
19	Q	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).



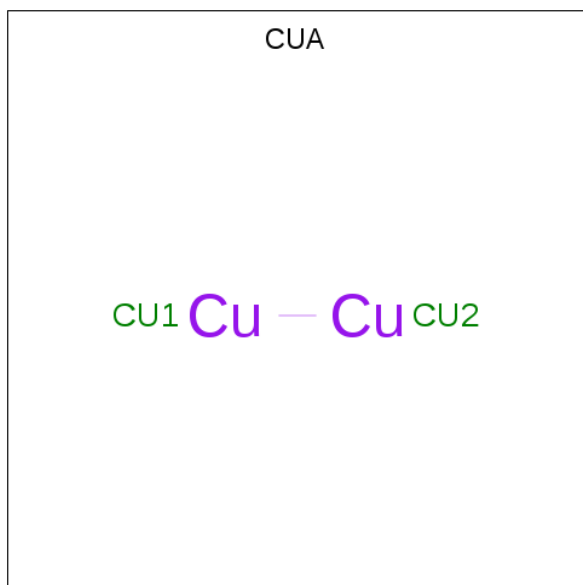
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		

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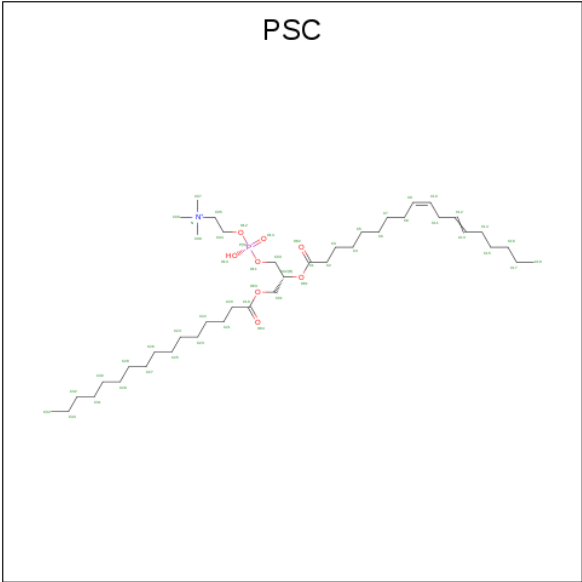
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		

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



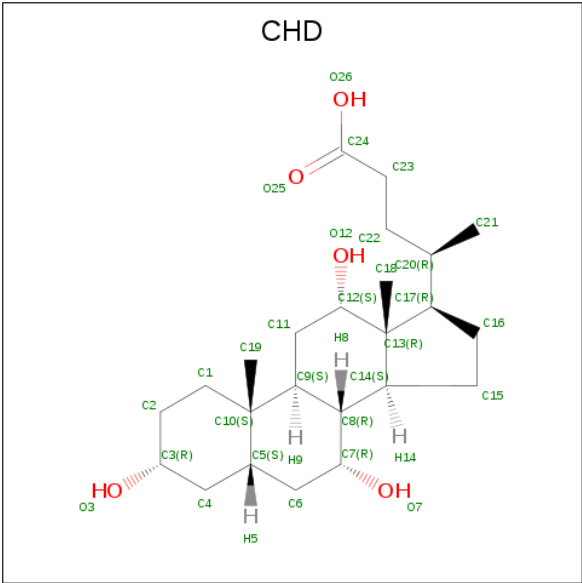
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
21	B	1	Total	Cu	0	0
			2	2		
21	O	1	Total	Cu	0	0
			2	2		

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



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

- Molecule 23 is CHOLIC ACID (three-letter code: CHD) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>5</sub>).



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

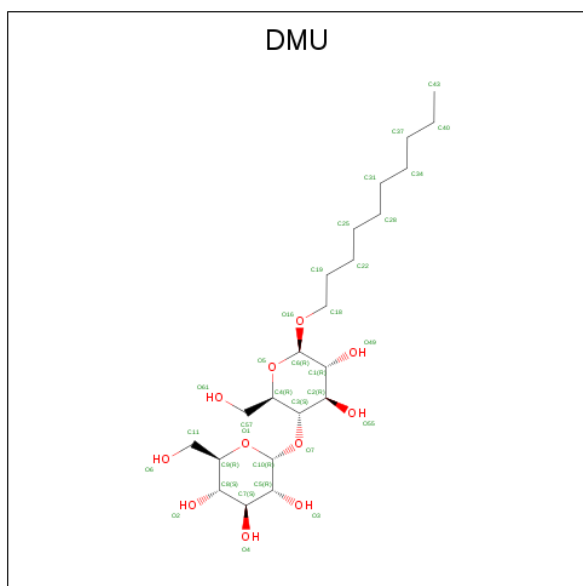
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
23	C	1	Total	C	O	0	0
			29	24	5		
23	J	1	Total	C	O	0	0
			29	24	5		
23	O	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	P	1	Total	C	O	0	0
			29	24	5		
23	W	1	Total	C	O	0	0
			29	24	5		

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

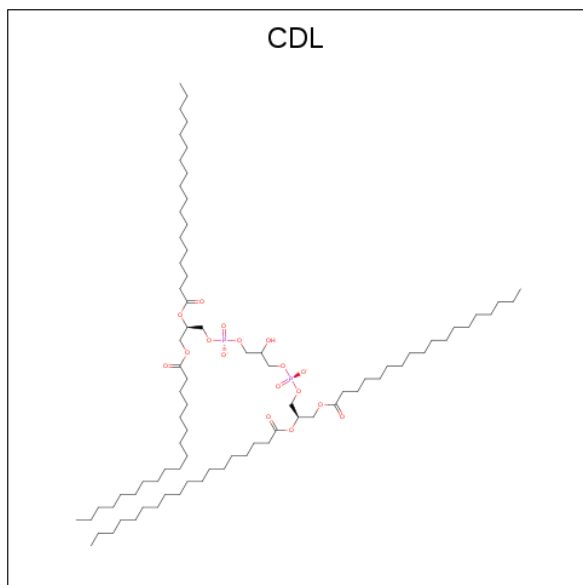


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
24	C	1	Total	C	O	0	0
			33	22	11		
24	M	1	Total	C	O	0	0
			33	22	11		
24	P	1	Total	C	O	0	0
			33	22	11		
24	Z	1	Total	C	O	0	0
			33	22	11		

- Molecule 25 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

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

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



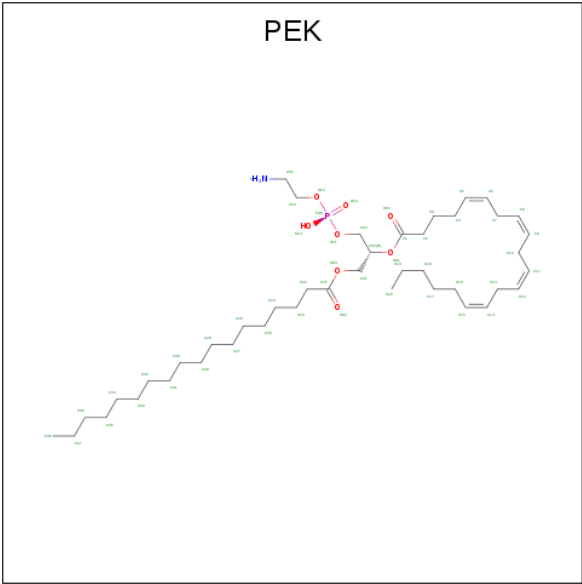
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
26	C	1	Total C O P 100 81 17 2	0	0
26	G	1	Total C O P 100 81 17 2	0	0
26	P	1	Total C O P 100 81 17 2	0	0
26	T	1	Total C O P 100 81 17 2	0	0

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

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

- Molecule 28 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
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	G	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	P	1	Total	C	N	O	P	0	0
			53	43	1	8	1		
28	T	1	Total	C	N	O	P	0	0
			53	43	1	8	1		

- Molecule 29 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	A	219	Total	O	0	0
			219	219		
29	B	139	Total	O	0	0
			139	139		
29	C	105	Total	O	0	0
			105	105		
29	D	110	Total	O	0	0
			110	110		
29	E	68	Total	O	0	0
			68	68		

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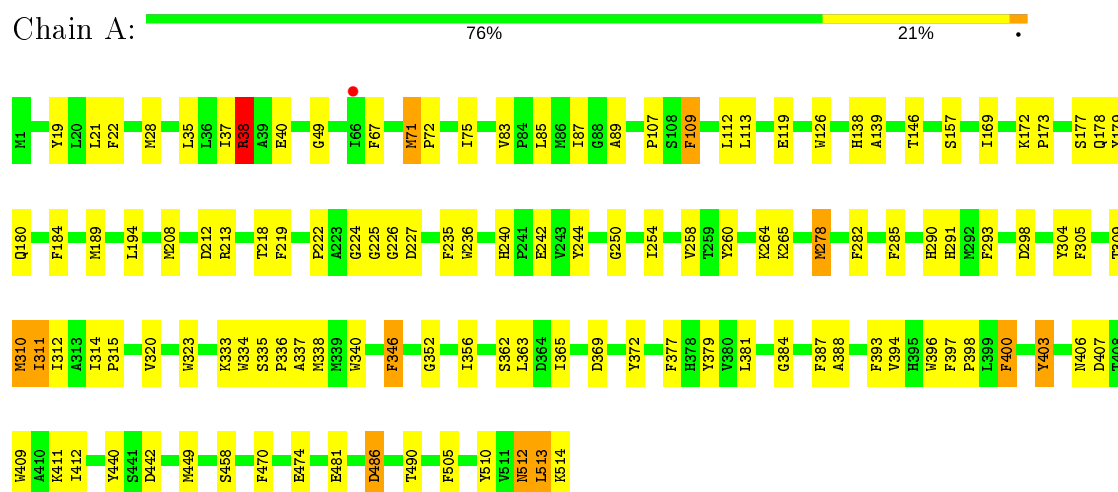
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	F	76	Total 76	O 76	0	0
29	G	45	Total 45	O 45	0	0
29	H	48	Total 48	O 48	0	0
29	I	35	Total 35	O 35	0	0
29	J	21	Total 21	O 21	0	0
29	K	22	Total 22	O 22	0	0
29	L	27	Total 27	O 27	0	0
29	M	18	Total 18	O 18	0	0
29	N	204	Total 204	O 204	0	0
29	O	109	Total 109	O 109	0	0
29	P	106	Total 106	O 106	0	0
29	Q	67	Total 67	O 67	0	0
29	R	52	Total 52	O 52	0	0
29	S	69	Total 69	O 69	0	0
29	T	48	Total 48	O 48	0	0
29	U	38	Total 38	O 38	0	0
29	V	19	Total 19	O 19	0	0
29	W	16	Total 16	O 16	0	0
29	X	16	Total 16	O 16	0	0
29	Y	17	Total 17	O 17	0	0
29	Z	14	Total 14	O 14	0	0

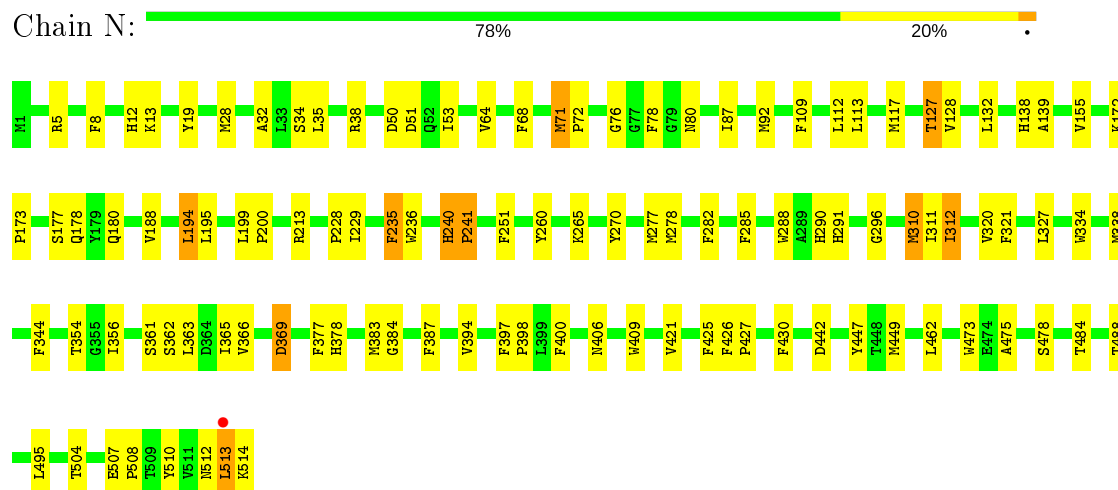
### 3 Residue-property plots

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

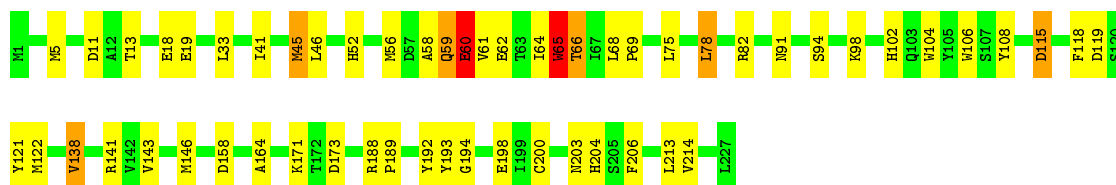


#### • Molecule 1: Cytochrome c oxidase subunit 1

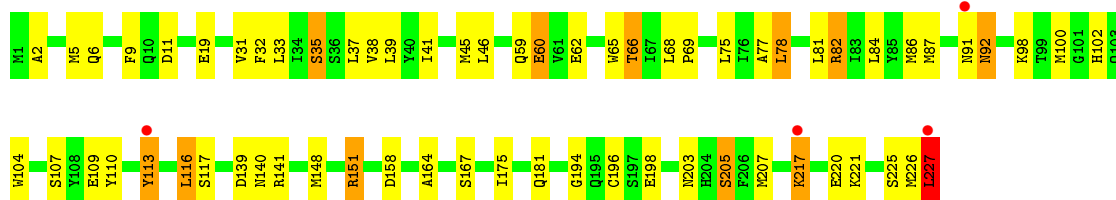


#### • Molecule 2: Cytochrome c oxidase subunit 2

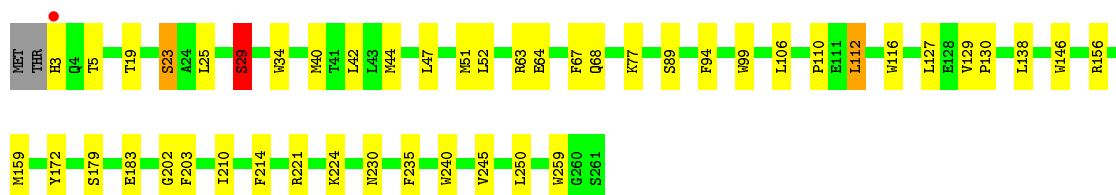
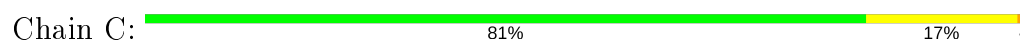




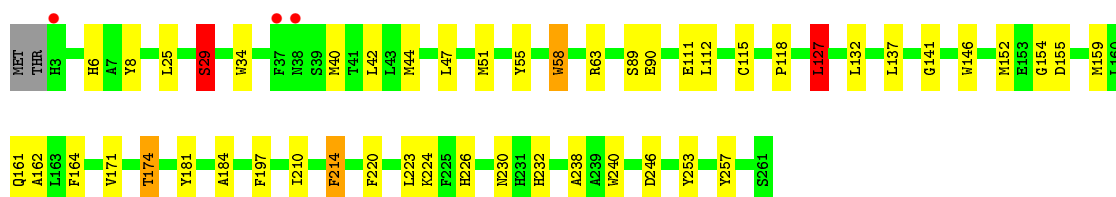
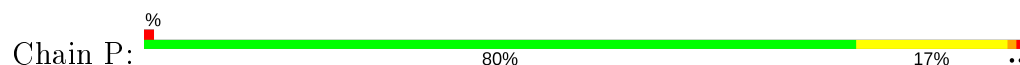
- Molecule 2: Cytochrome c oxidase subunit 2



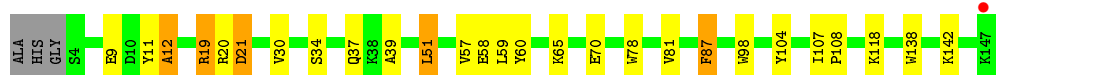
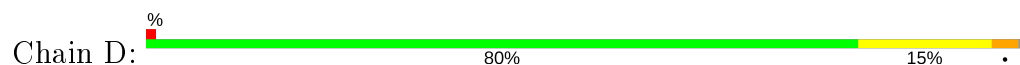
- Molecule 3: Cytochrome c oxidase subunit 3



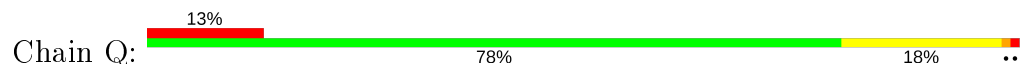
- Molecule 3: Cytochrome c oxidase subunit 3

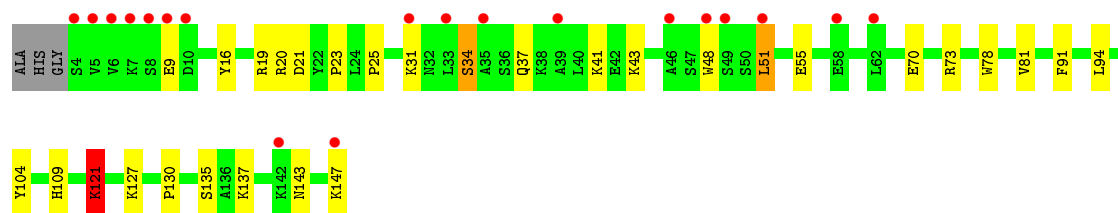


- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

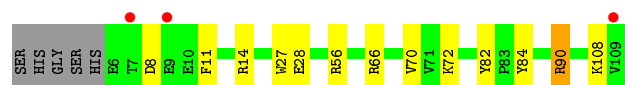
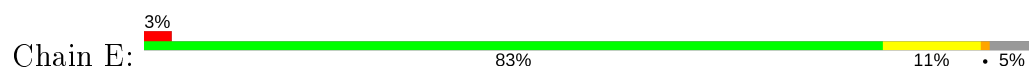


- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1

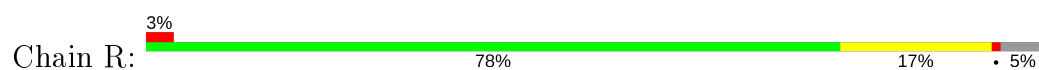




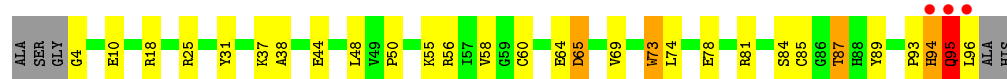
● Molecule 5: Cytochrome c oxidase subunit 5A



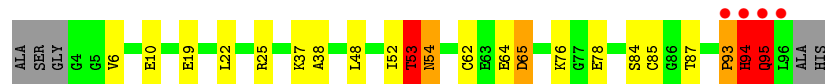
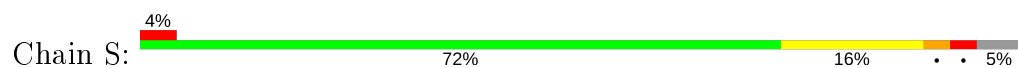
● Molecule 5: Cytochrome c oxidase subunit 5A



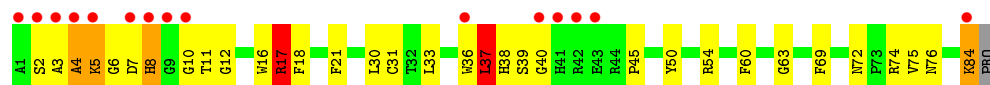
● Molecule 6: Cytochrome c oxidase subunit 5B



● Molecule 6: Cytochrome c oxidase subunit 5B

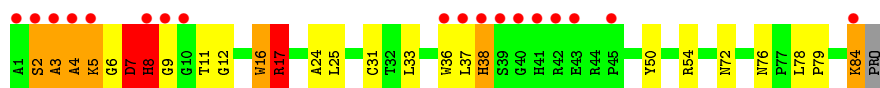


● Molecule 7: Cytochrome c oxidase subunit 6A2

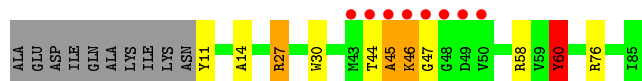
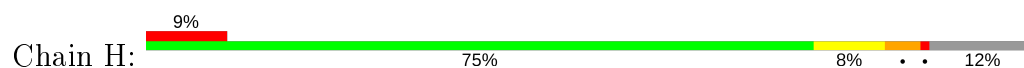


● Molecule 7: Cytochrome c oxidase subunit 6A2

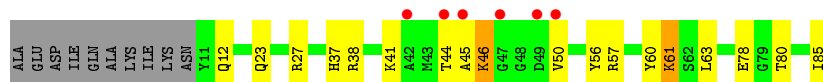




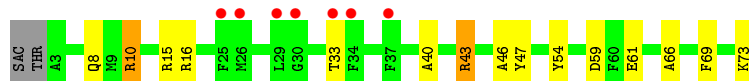
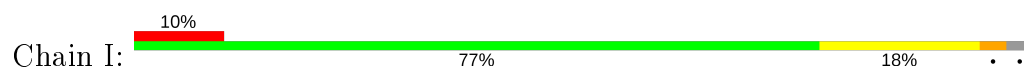
- Molecule 8: Cytochrome c oxidase subunit 6B1



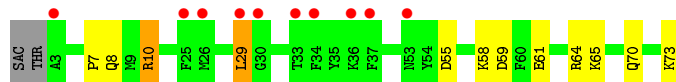
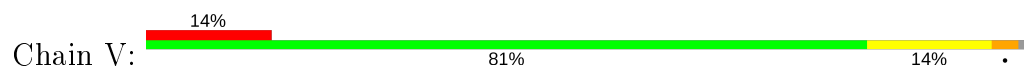
- Molecule 8: Cytochrome c oxidase subunit 6B1



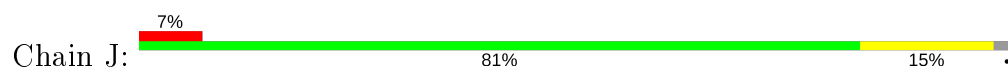
- Molecule 9: Cytochrome c oxidase subunit 6C



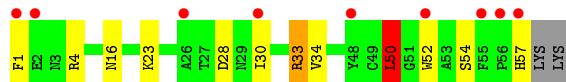
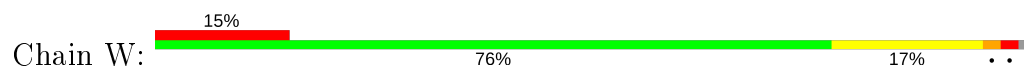
- Molecule 9: Cytochrome c oxidase subunit 6C



- Molecule 10: Cytochrome c oxidase polypeptide 7A1




- Molecule 10: Cytochrome c oxidase polypeptide 7A1




- Molecule 11: Cytochrome c oxidase subunit 7B

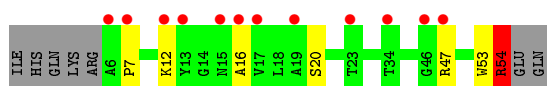


Chain K:  79% 9% 13%



- Molecule 11: Cytochrome c oxidase subunit 7B

Chain X:  21% 75% 11% 13%



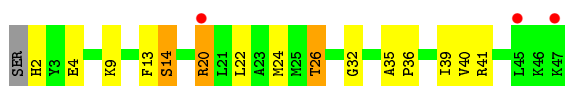
- Molecule 12: Cytochrome c oxidase subunit 7C

Chain L:  6% 68% 30%



- Molecule 12: Cytochrome c oxidase subunit 7C

Chain Y:  6% 66% 26% 6%



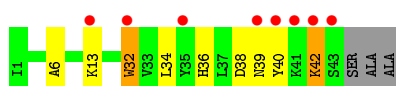
- Molecule 13: Cytochrome c oxidase subunit 8B

Chain M:  13% 67% 22% 7%



- Molecule 13: Cytochrome c oxidase subunit 8B

Chain Z:  17% 74% 15% 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	184.14Å 207.51Å 178.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 38.32 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.10) 98.6 (38.32-2.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.62 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, $R_{free}$	0.176 , 0.210 0.193 , 0.223	Depositor DCC
$R_{free}$ test set	13841 reflections (3.55%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.0	Xtriage
Anisotropy	0.482	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 62.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	32244	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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	1.72	46/4156 (1.1%)	1.25	23/5678 (0.4%)
1	N	1.55	27/4156 (0.6%)	1.16	20/5678 (0.4%)
2	B	1.61	18/1860 (1.0%)	1.29	13/2534 (0.5%)
2	O	1.36	7/1860 (0.4%)	1.11	5/2534 (0.2%)
3	C	1.52	12/2197 (0.5%)	1.04	3/3005 (0.1%)
3	P	1.53	18/2197 (0.8%)	1.07	6/3005 (0.2%)
4	D	1.67	20/1229 (1.6%)	1.24	8/1658 (0.5%)
4	Q	1.27	3/1229 (0.2%)	1.06	3/1658 (0.2%)
5	E	1.51	6/860 (0.7%)	1.17	4/1167 (0.3%)
5	R	1.27	3/860 (0.3%)	0.99	0/1167
6	F	1.57	9/733 (1.2%)	1.23	4/996 (0.4%)
6	S	1.34	2/733 (0.3%)	1.17	3/996 (0.3%)
7	G	1.44	5/690 (0.7%)	1.23	2/937 (0.2%)
7	T	1.48	5/690 (0.7%)	1.29	6/937 (0.6%)
8	H	1.51	5/648 (0.8%)	1.09	2/877 (0.2%)
8	U	1.28	2/648 (0.3%)	1.03	1/877 (0.1%)
9	I	1.53	6/598 (1.0%)	1.20	5/792 (0.6%)
9	V	1.24	0/598	1.04	2/792 (0.3%)
10	J	1.33	1/462 (0.2%)	0.99	1/625 (0.2%)
10	W	1.26	1/462 (0.2%)	1.09	3/625 (0.5%)
11	K	1.48	2/398 (0.5%)	1.06	1/546 (0.2%)
11	X	1.15	0/398	0.98	1/546 (0.2%)
12	L	1.57	4/393 (1.0%)	1.16	2/526 (0.4%)
12	Y	1.40	3/393 (0.8%)	0.98	0/526
13	M	1.54	3/345 (0.9%)	1.12	2/470 (0.4%)
13	Z	1.20	1/345 (0.3%)	0.98	0/470
All	All	1.51	209/29138 (0.7%)	1.15	120/39622 (0.3%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
6	S	0	1
All	All	0	2

All (209) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	60	CYS	CB-SG	10.42	2.00	1.82
3	P	29	SER	CB-OG	-9.66	1.29	1.42
4	D	39	ALA	CA-CB	8.57	1.70	1.52
1	N	139	ALA	CA-CB	8.38	1.70	1.52
7	G	36	TRP	CB-CG	8.16	1.65	1.50
9	I	66	ALA	CA-CB	8.16	1.69	1.52
1	A	379	TYR	CD1-CE1	7.91	1.51	1.39
3	P	58	TRP	CG-CD1	7.85	1.47	1.36
2	B	19	GLU	CB-CG	-7.77	1.37	1.52
13	M	16	ALA	CA-CB	7.66	1.68	1.52
1	N	394	VAL	CB-CG2	-7.63	1.36	1.52
8	H	60	TYR	CD2-CE2	7.63	1.50	1.39
1	A	372	TYR	CD1-CE1	7.51	1.50	1.39
3	P	161	GLN	CB-CG	-7.48	1.32	1.52
7	T	24	ALA	CA-CB	7.44	1.68	1.52
4	Q	81	VAL	CB-CG1	7.29	1.68	1.52
1	A	346	PHE	CD1-CE1	7.27	1.53	1.39
1	A	157	SER	CB-OG	7.22	1.51	1.42
6	F	4	GLY	N-CA	7.03	1.56	1.46
4	D	60	TYR	CD1-CE1	6.98	1.49	1.39
2	B	118	PHE	CE2-CZ	6.96	1.50	1.37
2	B	106	TRP	CE3-CZ3	6.96	1.50	1.38
12	L	35	ALA	CA-CB	6.95	1.67	1.52
1	N	288	TRP	CB-CG	6.95	1.62	1.50
6	S	54	ASN	CB-CG	-6.94	1.35	1.51
1	A	119	GLU	CG-CD	6.92	1.62	1.51
3	P	197	PHE	CE1-CZ	6.89	1.50	1.37
4	D	58	GLU	CD-OE2	6.85	1.33	1.25
3	P	174	THR	CB-CG2	6.84	1.75	1.52
1	A	379	TYR	CE2-CZ	6.80	1.47	1.38
4	D	19	ARG	CZ-NH2	6.77	1.41	1.33
9	I	46	ALA	CA-CB	6.77	1.66	1.52
1	N	473	TRP	CE3-CZ3	6.73	1.49	1.38
1	N	270	TYR	CD1-CE1	6.65	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	98	LYS	CE-NZ	6.62	1.65	1.49
1	N	235	PHE	CD2-CE2	6.58	1.52	1.39
1	A	83	VAL	CB-CG1	6.54	1.66	1.52
1	A	352	GLY	N-CA	6.54	1.55	1.46
3	P	240	TRP	CE3-CZ3	6.53	1.49	1.38
1	N	251	PHE	CE2-CZ	6.44	1.49	1.37
4	D	65	LYS	CE-NZ	6.42	1.65	1.49
4	D	30	VAL	CB-CG1	6.40	1.66	1.52
3	P	257	TYR	CD1-CE1	6.39	1.49	1.39
4	D	58	GLU	CG-CD	6.39	1.61	1.51
1	A	244	TYR	CD1-CE1	6.35	1.48	1.39
2	B	206	PHE	CE2-CZ	6.34	1.49	1.37
2	B	108	TYR	CG-CD1	6.33	1.47	1.39
1	N	475	ALA	CA-CB	6.33	1.65	1.52
3	P	184	ALA	CA-CB	6.32	1.65	1.52
7	T	5	LYS	CB-CG	6.30	1.69	1.52
3	P	181	TYR	CD2-CE2	6.29	1.48	1.39
1	N	320	VAL	CB-CG1	6.28	1.66	1.52
3	P	214	PHE	CD1-CE1	6.27	1.51	1.39
2	O	113	TYR	CD2-CE2	6.25	1.48	1.39
13	M	3	ALA	CA-CB	6.24	1.65	1.52
1	A	242	GLU	CG-CD	6.23	1.61	1.51
8	H	11	TYR	N-CA	6.19	1.58	1.46
1	N	188	VAL	CB-CG1	6.18	1.65	1.52
1	A	126	TRP	CZ3-CH2	6.15	1.49	1.40
5	E	14	ARG	CG-CD	6.12	1.67	1.51
1	N	507	GLU	CB-CG	6.12	1.63	1.52
1	A	440	TYR	CE1-CZ	6.12	1.46	1.38
4	D	12	ALA	CA-CB	6.11	1.65	1.52
1	A	219	PHE	CD2-CE2	6.08	1.51	1.39
4	D	70	GLU	CD-OE2	6.06	1.32	1.25
3	C	172	TYR	CD2-CE2	6.03	1.48	1.39
4	D	60	TYR	CE1-CZ	6.02	1.46	1.38
1	A	40	GLU	CB-CG	6.02	1.63	1.52
1	N	8	PHE	CD1-CE1	6.02	1.51	1.39
4	D	138	TRP	CE3-CZ3	6.01	1.48	1.38
9	I	47	TYR	CD1-CE1	6.01	1.48	1.39
2	B	18	GLU	CG-CD	6.00	1.60	1.51
1	A	244	TYR	CD2-CE2	6.00	1.48	1.39
1	A	258	VAL	CB-CG2	5.97	1.65	1.52
1	A	474	GLU	CD-OE1	5.96	1.32	1.25
2	B	115	ASP	CB-CG	5.93	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	11	TYR	CB-CG	5.92	1.60	1.51
2	O	60	GLU	CB-CG	5.92	1.63	1.52
3	C	240	TRP	CZ3-CH2	5.92	1.49	1.40
2	O	198	GLU	C-O	5.92	1.34	1.23
2	B	198	GLU	C-O	5.90	1.34	1.23
3	C	235	PHE	CE2-CZ	5.88	1.48	1.37
12	Y	32	GLY	N-CA	5.87	1.54	1.46
12	L	33	PHE	CE1-CZ	5.85	1.48	1.37
3	P	8	TYR	CD1-CE1	5.84	1.48	1.39
10	W	1	PHE	CE1-CZ	5.83	1.48	1.37
1	A	388	ALA	CA-CB	5.83	1.64	1.52
4	Q	121	LYS	CE-NZ	5.81	1.63	1.49
3	P	115	CYS	CB-SG	5.81	1.92	1.82
5	R	80	GLU	CG-CD	5.80	1.60	1.51
1	A	323	TRP	CG-CD1	5.78	1.44	1.36
5	E	27	TRP	CE3-CZ3	5.76	1.48	1.38
5	R	9	GLU	CG-CD	5.74	1.60	1.51
1	A	236	TRP	CB-CG	5.73	1.60	1.50
5	E	84	TYR	CE2-CZ	5.70	1.46	1.38
7	T	36	TRP	CB-CG	5.69	1.60	1.50
1	N	387	PHE	CE1-CZ	5.69	1.48	1.37
1	N	64	VAL	CA-CB	5.68	1.66	1.54
1	N	19	TYR	CD2-CE2	5.68	1.47	1.39
4	D	60	TYR	CD2-CE2	5.68	1.47	1.39
12	L	37	PHE	CD1-CE1	5.67	1.50	1.39
1	A	293	PHE	CE2-CZ	5.65	1.48	1.37
1	A	470	PHE	CD1-CE1	5.65	1.50	1.39
1	A	146	THR	CB-CG2	5.64	1.71	1.52
1	A	184	PHE	CE2-CZ	5.64	1.48	1.37
1	A	486	ASP	CB-CG	5.64	1.63	1.51
3	P	90	GLU	CB-CG	5.64	1.62	1.52
7	G	75	VAL	CB-CG1	5.62	1.64	1.52
1	A	474	GLU	CB-CG	5.62	1.62	1.52
12	Y	4	GLU	CG-CD	5.62	1.60	1.51
1	A	260	TYR	CD2-CE2	5.62	1.47	1.39
8	U	56	TYR	CD1-CE1	5.61	1.47	1.39
3	P	141	GLY	N-CA	5.61	1.54	1.46
1	A	403	TYR	CG-CD1	5.59	1.46	1.39
3	P	181	TYR	CD1-CE1	5.58	1.47	1.39
3	C	29	SER	CB-OG	-5.58	1.35	1.42
4	D	57	VAL	CB-CG1	5.57	1.64	1.52
1	A	387	PHE	CD2-CE2	5.56	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	5	LYS	CB-CG	5.56	1.67	1.52
3	P	253	TYR	CD1-CE1	5.55	1.47	1.39
9	I	47	TYR	CG-CD1	5.55	1.46	1.39
5	E	28	GLU	CG-CD	5.54	1.60	1.51
1	A	67	PHE	CD2-CE2	5.53	1.50	1.39
4	Q	104	TYR	CD2-CE2	5.53	1.47	1.39
2	B	192	TYR	CG-CD1	5.52	1.46	1.39
2	B	98	LYS	CD-CE	5.51	1.65	1.51
3	C	94	PHE	CG-CD2	5.51	1.47	1.38
1	A	320	VAL	CB-CG2	5.49	1.64	1.52
1	A	340	TRP	CE3-CZ3	5.47	1.47	1.38
2	B	193	TYR	CB-CG	5.47	1.59	1.51
1	A	235	PHE	N-CA	-5.46	1.35	1.46
1	A	505	PHE	CE1-CZ	5.46	1.47	1.37
2	B	138	VAL	CB-CG1	5.45	1.64	1.52
8	H	58	ARG	CZ-NH1	5.44	1.40	1.33
3	C	203	PHE	CB-CG	5.44	1.60	1.51
6	F	69	VAL	CB-CG1	5.42	1.64	1.52
3	C	116	TRP	CE3-CZ3	5.42	1.47	1.38
1	A	109	PHE	CD2-CE2	5.42	1.50	1.39
1	N	387	PHE	CB-CG	5.40	1.60	1.51
2	O	38	VAL	CB-CG2	5.40	1.64	1.52
2	O	151	ARG	CZ-NH1	5.40	1.40	1.33
1	A	224	GLY	N-CA	5.39	1.54	1.46
2	O	9	PHE	CD2-CE2	5.39	1.50	1.39
1	N	507	GLU	CG-CD	5.39	1.60	1.51
7	T	50	TYR	CD2-CE2	5.38	1.47	1.39
3	C	94	PHE	CD1-CE1	5.38	1.50	1.39
5	R	102	GLU	CG-CD	5.37	1.60	1.51
1	A	38	ARG	CD-NE	5.37	1.55	1.46
2	B	60	GLU	CB-CG	5.36	1.62	1.52
7	G	60	PHE	CE1-CZ	5.35	1.47	1.37
1	A	235	PHE	CD2-CE2	5.35	1.50	1.39
1	A	403	TYR	CE2-CZ	5.35	1.45	1.38
2	B	59	GLN	CG-CD	5.35	1.63	1.51
6	F	44	GLU	CG-CD	5.34	1.59	1.51
6	F	58	VAL	CB-CG2	5.32	1.64	1.52
7	T	16	TRP	CZ3-CH2	5.32	1.48	1.40
4	D	11	TYR	CD2-CE2	-5.32	1.31	1.39
8	H	14	ALA	CA-CB	5.32	1.63	1.52
1	N	78	PHE	CB-CG	-5.32	1.42	1.51
5	E	70	VAL	CB-CG2	5.31	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	104	TYR	CG-CD1	5.30	1.46	1.39
11	K	31	TYR	CD2-CE2	5.30	1.47	1.39
12	Y	9	LYS	CD-CE	5.30	1.64	1.51
1	A	393	PHE	CE1-CZ	5.28	1.47	1.37
2	B	108	TYR	CE1-CZ	5.27	1.45	1.38
13	M	4	LYS	CB-CG	-5.27	1.38	1.52
3	P	89	SER	CB-OG	5.27	1.49	1.42
6	F	73	TRP	CE3-CZ3	5.22	1.47	1.38
5	E	27	TRP	CB-CG	5.22	1.59	1.50
1	A	305	PHE	CD1-CE1	5.22	1.49	1.39
3	C	250	LEU	N-CA	5.22	1.56	1.46
1	A	304	TYR	CE1-CZ	5.21	1.45	1.38
2	O	19	GLU	CB-CG	-5.20	1.42	1.52
1	N	387	PHE	CD2-CE2	5.19	1.49	1.39
4	D	9	GLU	CG-CD	5.19	1.59	1.51
7	G	50	TYR	CG-CD1	5.18	1.45	1.39
3	C	89	SER	CB-OG	5.17	1.49	1.42
1	N	92	MET	CB-CG	5.17	1.67	1.51
13	Z	32	TRP	CB-CG	5.17	1.59	1.50
9	I	69	PHE	CB-CG	-5.16	1.42	1.51
12	L	4	GLU	CG-CD	5.14	1.59	1.51
1	A	458	SER	CA-CB	5.13	1.60	1.52
3	C	245	VAL	CB-CG2	5.13	1.63	1.52
1	A	400	PHE	CB-CG	5.13	1.60	1.51
1	N	473	TRP	CB-CG	5.12	1.59	1.50
1	N	128	VAL	CB-CG1	5.12	1.63	1.52
6	F	56	ARG	CG-CD	5.12	1.64	1.51
6	S	65	ASP	CB-CG	5.12	1.62	1.51
2	B	143	VAL	CB-CG2	5.11	1.63	1.52
6	F	89	TYR	CD2-CE2	5.11	1.47	1.39
8	U	56	TYR	CE1-CZ	5.11	1.45	1.38
10	J	20	VAL	CB-CG1	5.10	1.63	1.52
4	D	142	LYS	CD-CE	5.08	1.64	1.51
4	D	60	TYR	CG-CD1	5.06	1.45	1.39
4	D	81	VAL	CB-CG2	5.06	1.63	1.52
6	F	31	TYR	CE1-CZ	5.06	1.45	1.38
1	A	139	ALA	CA-CB	5.05	1.63	1.52
1	N	447	TYR	CD2-CE2	5.05	1.47	1.39
1	A	179	TYR	CE2-CZ	5.05	1.45	1.38
2	B	214	VAL	CB-CG1	5.04	1.63	1.52
1	N	354	THR	CB-CG2	5.03	1.69	1.52
3	P	238	ALA	CA-CB	5.02	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	99	TRP	CE3-CZ3	5.02	1.47	1.38
11	K	39	GLU	CB-CG	5.02	1.61	1.52
4	D	87	PHE	CD1-CE1	5.02	1.49	1.39
1	N	344	PHE	CD2-CE2	5.01	1.49	1.39
9	I	40	ALA	CA-CB	5.00	1.62	1.52
1	N	513	LEU	C-O	5.00	1.32	1.23
1	N	260	TYR	CE2-CZ	5.00	1.45	1.38

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	17	ARG	NE-CZ-NH2	-15.09	112.76	120.30
7	T	17	ARG	NE-CZ-NH2	-14.08	113.26	120.30
4	D	19	ARG	NE-CZ-NH1	-12.84	113.88	120.30
4	Q	20	ARG	NE-CZ-NH2	-12.82	113.89	120.30
5	E	90	ARG	NE-CZ-NH2	-12.63	113.99	120.30
5	E	90	ARG	NE-CZ-NH1	11.22	125.91	120.30
4	Q	20	ARG	NE-CZ-NH1	10.93	125.76	120.30
7	G	17	ARG	NE-CZ-NH1	10.44	125.52	120.30
4	D	20	ARG	NE-CZ-NH2	-10.38	115.11	120.30
4	Q	137	LYS	CD-CE-NZ	-10.32	87.96	111.70
1	A	208	MET	CG-SD-CE	9.93	116.09	100.20
2	B	188	ARG	NE-CZ-NH2	-9.47	115.56	120.30
1	A	486	ASP	CB-CG-OD1	9.38	126.75	118.30
1	N	213	ARG	NE-CZ-NH2	-9.31	115.64	120.30
7	T	17	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	N	5	ARG	NE-CZ-NH2	-8.61	116.00	120.30
4	D	21	ASP	CB-CG-OD2	8.55	125.99	118.30
1	N	369	ASP	CB-CG-OD2	8.54	125.98	118.30
1	N	312	ILE	CG1-CB-CG2	-8.34	93.05	111.40
7	T	33	LEU	CA-CB-CG	8.33	134.45	115.30
1	N	71	MET	CG-SD-CE	-8.16	87.14	100.20
2	B	158	ASP	CB-CG-OD1	8.14	125.63	118.30
2	B	82	ARG	NE-CZ-NH2	-7.71	116.44	120.30
11	X	54	ARG	NE-CZ-NH2	7.71	124.16	120.30
9	I	59	ASP	CB-CG-OD1	-7.67	111.39	118.30
2	B	188	ARG	NE-CZ-NH1	7.61	124.11	120.30
6	F	81	ARG	NE-CZ-NH1	-7.41	116.60	120.30
1	N	194	LEU	CB-CG-CD2	7.23	123.29	111.00
3	P	152	MET	CG-SD-CE	7.19	111.71	100.20
12	L	41	ARG	NE-CZ-NH1	7.19	123.89	120.30
5	E	66	ARG	NE-CZ-NH2	-7.18	116.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	141	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	310	MET	CG-SD-CE	-6.97	89.05	100.20
1	A	35	LEU	CA-CB-CG	-6.92	99.38	115.30
1	A	213	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	A	71	MET	CG-SD-CE	-6.77	89.36	100.20
1	A	298	ASP	CB-CG-OD1	-6.76	112.22	118.30
4	D	19	ARG	NE-CZ-NH2	6.71	123.66	120.30
6	S	54	ASN	CB-CA-C	-6.71	96.98	110.40
3	C	221	ARG	NE-CZ-NH1	-6.61	117.00	120.30
1	A	212	ASP	CB-CG-OD2	6.60	124.24	118.30
1	A	486	ASP	CB-CG-OD2	-6.55	112.40	118.30
3	P	137	LEU	CB-CG-CD1	-6.53	99.91	111.00
2	O	227	LEU	CA-CB-CG	-6.52	100.31	115.30
6	F	18	ARG	NE-CZ-NH2	-6.52	117.04	120.30
2	B	65	TRP	CB-CA-C	6.45	123.29	110.40
9	V	10	ARG	NE-CZ-NH2	-6.41	117.09	120.30
11	K	54	ARG	NE-CZ-NH1	-6.41	117.09	120.30
2	O	82	ARG	NE-CZ-NH2	-6.41	117.10	120.30
2	B	45	MET	CG-SD-CE	6.40	110.44	100.20
1	N	384	GLY	N-CA-C	-6.38	97.15	113.10
10	W	50	LEU	CA-CB-CG	6.36	129.92	115.30
1	N	310	MET	CG-SD-CE	-6.35	90.04	100.20
6	S	94	HIS	N-CA-C	6.20	127.73	111.00
1	N	195	LEU	CB-CG-CD1	-6.16	100.54	111.00
1	A	19	TYR	CZ-CE2-CD2	-6.05	114.36	119.80
7	T	8	HIS	N-CA-C	6.05	127.33	111.00
1	N	240	HIS	N-CA-CB	6.00	121.40	110.60
9	I	10	ARG	NE-CZ-NH1	5.99	123.30	120.30
3	P	223	LEU	CB-CG-CD1	-5.97	100.85	111.00
1	N	117	MET	CG-SD-CE	5.94	109.70	100.20
1	N	369	ASP	CB-CG-OD1	-5.91	112.98	118.30
6	S	53	THR	CA-CB-CG2	5.88	120.63	112.40
2	B	173	ASP	CB-CG-OD2	-5.85	113.04	118.30
1	N	50	ASP	CB-CG-OD2	5.77	123.49	118.30
10	J	28	ASP	CB-CG-OD1	5.76	123.48	118.30
10	W	28	ASP	CB-CG-OD1	5.74	123.47	118.30
2	O	11	ASP	CB-CG-OD2	5.72	123.45	118.30
8	H	76	ARG	NE-CZ-NH1	5.71	123.16	120.30
4	D	51	LEU	CA-CB-CG	5.71	128.43	115.30
1	N	113	LEU	CB-CG-CD1	5.68	120.67	111.00
2	B	11	ASP	CB-CG-OD2	5.67	123.40	118.30
1	N	278	MET	CA-CB-CG	-5.67	103.67	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	127	LEU	CB-CG-CD1	5.66	120.63	111.00
4	D	20	ARG	NE-CZ-NH1	5.63	123.11	120.30
4	D	59	LEU	CB-CG-CD2	-5.62	101.44	111.00
1	N	277	MET	CA-CB-CG	-5.61	103.77	113.30
5	E	56	ARG	NE-CZ-NH1	-5.59	117.50	120.30
8	H	27	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	N	366	VAL	CG1-CB-CG2	-5.58	101.97	110.90
1	A	49	GLY	N-CA-C	-5.55	99.21	113.10
1	A	512	ASN	CB-CA-C	-5.55	99.30	110.40
9	I	10	ARG	NE-CZ-NH2	-5.55	117.53	120.30
4	D	19	ARG	CB-CA-C	-5.54	99.31	110.40
1	A	312	ILE	CA-CB-CG1	-5.51	100.52	111.00
7	T	7	ASP	N-CA-C	5.50	125.86	111.00
3	C	44	MET	CG-SD-CE	5.49	108.98	100.20
1	N	442	ASP	CB-CG-OD2	5.46	123.22	118.30
2	B	122	MET	CG-SD-CE	5.45	108.92	100.20
8	U	63	LEU	CB-CG-CD2	5.44	120.25	111.00
1	A	311	ILE	CG1-CB-CG2	-5.41	99.50	111.40
2	B	102	HIS	CB-CA-C	-5.41	99.59	110.40
6	F	93	PRO	C-N-CA	5.40	135.21	121.70
7	T	17	ARG	CB-CG-CD	-5.38	97.60	111.60
9	I	43	ARG	NE-CZ-NH1	-5.34	117.63	120.30
13	M	34	LEU	CB-CG-CD1	5.34	120.08	111.00
1	A	442	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	85	LEU	CB-CG-CD1	-5.32	101.96	111.00
9	V	59	ASP	CB-CG-OD2	5.31	123.08	118.30
9	I	59	ASP	CB-CG-OD2	5.25	123.02	118.30
13	M	28	LEU	CB-CG-CD2	5.23	119.89	111.00
3	P	132	LEU	CB-CG-CD1	-5.20	102.16	111.00
10	W	33	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	244	TYR	CA-CB-CG	-5.19	103.53	113.40
3	P	214	PHE	CB-CG-CD2	-5.19	117.16	120.80
3	C	112	LEU	CB-CG-CD2	-5.16	102.22	111.00
1	A	189	MET	CA-CB-CG	-5.16	104.53	113.30
1	N	327	LEU	CB-CG-CD1	-5.14	102.26	111.00
1	A	312	ILE	CG1-CB-CG2	-5.13	100.12	111.40
1	A	113	LEU	CB-CG-CD2	5.10	119.67	111.00
1	N	132	LEU	CB-CG-CD1	5.08	119.64	111.00
1	A	384	GLY	N-CA-C	-5.08	100.40	113.10
2	O	92	ASN	N-CA-C	5.07	124.68	111.00
2	B	119	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	A	227	ASP	CB-CG-OD2	5.04	122.84	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	65	ASP	CB-CG-OD2	5.04	122.84	118.30
12	L	21	LEU	CB-CG-CD1	5.04	119.57	111.00
2	B	198	GLU	OE1-CD-OE2	-5.01	117.28	123.30
2	O	158	ASP	CB-CG-OD1	5.00	122.81	118.30
1	A	278	MET	CA-CB-CG	-5.00	104.80	113.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
6	S	93	PRO	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	61	0
1	N	4027	0	4001	54	0
2	B	1824	0	1833	27	0
2	O	1824	0	1833	41	0
3	C	2110	0	2027	29	0
3	P	2110	0	2027	28	0
4	D	1195	0	1183	17	0
4	Q	1195	0	1183	17	0
5	E	842	0	838	4	0
5	R	842	0	838	10	0
6	F	717	0	700	16	0
6	S	717	0	700	20	0
7	G	675	0	643	34	0
7	T	675	0	643	43	0
8	H	628	0	580	5	0
8	U	628	0	580	5	0
9	I	585	0	597	10	0
9	V	585	0	597	12	0
10	J	451	0	446	5	0
10	W	451	0	446	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	K	384	0	366	1	0
11	X	384	0	366	6	0
12	L	380	0	380	11	0
12	Y	380	0	380	13	0
13	M	335	0	352	2	0
13	Z	335	0	352	5	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	0	0
17	N	1	0	0	0	0
18	A	120	0	108	12	0
18	N	120	0	108	9	0
19	A	63	0	110	6	0
19	D	63	0	110	15	0
19	L	63	0	110	16	0
19	N	126	0	220	20	0
19	Q	63	0	110	5	0
20	A	102	0	152	10	0
20	C	102	0	152	6	0
20	N	102	0	152	7	0
20	P	102	0	152	8	0
21	B	2	0	0	0	0
21	O	2	0	0	0	0
22	B	52	0	80	18	0
22	O	52	0	80	12	0
23	B	29	0	37	1	0
23	C	58	0	71	5	0
23	J	29	0	36	3	0
23	O	29	0	36	2	0
23	P	58	0	71	6	0
23	W	29	0	36	4	0
24	C	33	0	37	5	0
24	M	33	0	39	1	0
24	P	33	0	40	2	0
24	Z	33	0	39	1	0
25	C	1	0	0	0	0
25	P	1	0	0	0	0
26	C	100	0	156	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	G	100	0	156	24	0
26	P	100	0	156	16	0
26	T	100	0	156	23	0
27	F	1	0	0	0	0
27	S	1	0	0	0	0
28	G	159	0	231	20	0
28	P	106	0	154	14	0
28	T	53	0	77	21	0
29	A	219	0	0	6	0
29	B	139	0	0	3	0
29	C	105	0	0	2	0
29	D	110	0	0	0	0
29	E	68	0	0	0	0
29	F	76	0	0	3	0
29	G	45	0	0	7	0
29	H	48	0	0	1	0
29	I	35	0	0	1	0
29	J	21	0	0	1	0
29	K	22	0	0	0	0
29	L	27	0	0	1	0
29	M	18	0	0	0	0
29	N	204	0	0	2	0
29	O	109	0	0	0	0
29	P	106	0	0	2	0
29	Q	67	0	0	3	0
29	R	52	0	0	0	0
29	S	69	0	0	4	0
29	T	48	0	0	4	0
29	U	38	0	0	3	0
29	V	19	0	0	0	0
29	W	16	0	0	0	0
29	X	16	0	0	0	0
29	Y	17	0	0	1	0
29	Z	14	0	0	0	0
All	All	32244	0	31064	577	0

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

All (577) 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)
1:A:75:ILE:CG1	1:A:75:ILE:CD1	1.74	1.62
3:P:174:THR:CB	3:P:174:THR:CG2	1.74	1.60
28:G:265:PEK:H383	26:G:269:CDL:C27	1.62	1.29
28:P:1265:PEK:H383	26:T:1269:CDL:C27	1.64	1.25
7:T:2:SER:OG	28:T:263:PEK:H302	1.33	1.23
28:G:265:PEK:H383	26:G:269:CDL:H272	1.18	1.15
26:G:269:CDL:HA21	26:G:269:CDL:H112	1.26	1.10
15:A:520:PER:O1	15:A:520:PER:O2	1.70	1.10
22:B:230:PSC:H072	9:I:10:ARG:HH21	1.07	1.09
7:T:84:LYS:H	7:T:84:LYS:HD2	1.13	1.07
15:N:520:PER:O2	15:N:520:PER:O1	1.70	1.07
28:P:1265:PEK:H383	26:T:1269:CDL:H271	1.22	1.06
7:G:84:LYS:HD2	7:G:84:LYS:H	1.19	1.06
22:B:230:PSC:C07	9:I:10:ARG:HH21	1.68	1.05
7:G:5:LYS:HG3	28:G:1263:PEK:H382	1.07	1.04
19:Q:1523:TGL:HC21	19:Q:1523:TGL:HG11	1.41	1.02
22:O:1230:PSC:H212	22:O:1230:PSC:O01	1.59	1.02
6:S:95:GLN:HB2	29:S:4411:HOH:O	1.60	1.01
4:D:78:TRP:HB3	19:D:523:TGL:HB22	1.40	1.00
6:F:85:CYS:SG	6:F:87:THR:HG23	2.00	1.00
12:L:20:ARG:HH22	19:L:522:TGL:HC32	1.25	0.99
9:V:65:LYS:O	11:X:54:ARG:NH1	1.94	0.98
19:N:1522:TGL:H231	19:N:1522:TGL:HA92	1.45	0.97
7:T:2:SER:OG	28:T:263:PEK:C30	2.10	0.97
28:P:1265:PEK:C38	26:T:1269:CDL:C27	2.42	0.96
7:T:5:LYS:CG	28:T:263:PEK:H383	1.94	0.96
12:L:20:ARG:NH2	19:L:522:TGL:HC32	1.81	0.95
18:N:515:HEA:HMC1	18:N:515:HEA:HBC1	1.48	0.95
1:A:486:ASP:OD2	4:D:19:ARG:HD3	1.66	0.95
7:T:5:LYS:HD2	28:T:263:PEK:H381	1.48	0.95
7:G:5:LYS:HB2	28:G:1263:PEK:H361	1.49	0.95
3:C:63:ARG:HE	26:C:270:CDL:HA22	1.31	0.93
20:C:267:PGV:H182	26:C:270:CDL:H671	1.50	0.93
7:G:5:LYS:CG	28:G:1263:PEK:H382	1.97	0.92
7:T:5:LYS:HG3	28:T:263:PEK:H383	1.51	0.91
28:G:265:PEK:C38	26:G:269:CDL:C27	2.49	0.90
7:T:31:CYS:SG	26:T:1269:CDL:H551	2.12	0.90
1:N:400:PHE:HB3	19:N:1522:TGL:H283	1.54	0.90
20:A:524:PGV:H152	20:A:524:PGV:H321	1.52	0.89
6:S:52:ILE:O	6:S:94:HIS:CE1	2.26	0.89
7:T:2:SER:HG	28:T:263:PEK:H302	1.36	0.89
26:G:269:CDL:H241	26:G:269:CDL:H541	1.54	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:84:LYS:H	7:G:84:LYS:CD	1.82	0.88
1:N:334:TRP:CH2	2:O:46:LEU:HD13	2.09	0.88
22:O:1230:PSC:C07	9:V:10:ARG:HH21	1.86	0.87
4:D:34:SER:H	4:D:37:GLN:HE21	1.20	0.87
3:C:67:PHE:HE1	26:C:270:CDL:H1	1.41	0.86
3:P:63:ARG:HE	26:P:1270:CDL:HA22	1.40	0.86
7:T:84:LYS:H	7:T:84:LYS:CD	1.89	0.86
7:G:84:LYS:N	7:G:84:LYS:HD2	1.91	0.84
7:T:72:ASN:H	7:T:76:ASN:HD22	1.25	0.83
7:G:76:ASN:HD21	28:G:264:PEK:HN2	1.23	0.81
22:B:230:PSC:H072	9:I:10:ARG:NH2	1.93	0.80
7:G:5:LYS:HG3	28:G:1263:PEK:C38	2.02	0.80
12:Y:41:ARG:HD2	13:Z:40:TYR:CZ	2.17	0.80
4:Q:109:HIS:HD2	29:Q:3152:HOH:O	1.62	0.80
3:P:25:LEU:O	3:P:29:SER:HB2	1.81	0.80
1:A:365:ILE:HD11	29:A:4260:HOH:O	1.80	0.80
1:N:321:PHE:CD2	22:O:1230:PSC:H341	2.17	0.80
18:N:516:HEA:HBC1	18:N:516:HEA:HMC1	1.65	0.79
7:T:5:LYS:HD2	28:T:263:PEK:C38	2.13	0.79
3:P:111:GLU:HG3	29:U:4543:HOH:O	1.83	0.79
2:B:41:ILE:HD13	22:B:230:PSC:C34	2.12	0.78
12:L:24:MET:HG3	29:L:4843:HOH:O	1.82	0.78
1:N:334:TRP:HH2	2:O:46:LEU:HD13	1.47	0.78
22:O:1230:PSC:H142	22:O:1230:PSC:H343	1.64	0.78
6:S:95:GLN:HE21	6:S:95:GLN:HA	1.50	0.77
20:P:1267:PGV:H182	26:P:1270:CDL:H671	1.65	0.76
19:N:1521:TGL:H142	2:O:39:LEU:CD2	2.15	0.76
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.68	0.76
22:B:230:PSC:C07	9:I:10:ARG:NH2	2.47	0.75
7:G:4:ALA:HB3	1:N:282:PHE:HA	1.65	0.75
10:W:33:ARG:HG2	23:W:1060:CHD:H152	1.68	0.75
7:G:72:ASN:H	7:G:76:ASN:HD22	1.32	0.74
19:N:1521:TGL:H142	2:O:39:LEU:HD22	1.68	0.74
7:T:11:TPO:HG22	7:T:16:TRP:HE1	1.51	0.74
22:O:1230:PSC:H072	9:V:10:ARG:HH21	1.50	0.74
28:G:265:PEK:H383	26:G:269:CDL:H273	1.66	0.74
9:I:33:THR:HG22	29:I:4648:HOH:O	1.86	0.74
3:P:55:TYR:HE1	26:P:1270:CDL:H521	1.53	0.73
20:A:524:PGV:H152	20:A:524:PGV:C32	2.17	0.73
7:T:84:LYS:N	7:T:84:LYS:HD2	1.97	0.73
4:D:78:TRP:CB	19:D:523:TGL:HB22	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:5:LYS:CD	28:T:263:PEK:C38	2.67	0.72
2:O:226:MET:O	2:O:227:LEU:C	2.25	0.72
3:C:25:LEU:O	3:C:29:SER:HB2	1.90	0.72
10:W:33:ARG:HG2	23:W:1060:CHD:C15	2.18	0.72
3:P:55:TYR:CE1	26:P:1270:CDL:H521	2.25	0.72
6:F:94:HIS:CE1	29:F:4660:HOH:O	2.42	0.71
1:N:406:ASN:HD21	20:N:1524:PGV:H21	1.55	0.71
6:S:94:HIS:CD2	6:S:95:GLN:H	2.07	0.71
2:B:41:ILE:HD13	22:B:230:PSC:H341	1.71	0.71
7:G:45:PRO:HD2	29:G:4665:HOH:O	1.90	0.71
6:S:52:ILE:O	6:S:94:HIS:HE1	1.70	0.71
7:T:31:CYS:SG	26:T:1269:CDL:H532	2.31	0.71
26:T:1269:CDL:H571	26:T:1269:CDL:H782	1.72	0.71
4:Q:78:TRP:HA	19:Q:1523:TGL:HB22	1.73	0.70
26:P:1270:CDL:OB9	26:P:1270:CDL:H522	1.92	0.70
19:N:1522:TGL:H231	19:N:1522:TGL:CA9	2.11	0.70
7:T:5:LYS:HB2	28:T:263:PEK:H362	1.74	0.70
28:G:265:PEK:C38	26:G:269:CDL:H272	2.11	0.70
28:P:1264:PEK:HN2	7:T:76:ASN:HD21	1.38	0.69
19:Q:1523:TGL:CC2	19:Q:1523:TGL:HG11	2.22	0.69
1:N:53:ILE:HD11	12:Y:40:VAL:HG13	1.75	0.69
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.57	0.69
6:S:22:LEU:O	6:S:25:ARG:HB3	1.92	0.68
2:O:82:ARG:HG2	2:O:86:MET:HE3	1.75	0.68
28:G:264:PEK:H161	28:G:264:PEK:H101	1.76	0.68
28:G:265:PEK:C38	26:G:269:CDL:H273	2.22	0.68
12:L:12:PRO:HB2	19:L:522:TGL:HG2	1.75	0.68
2:B:164:ALA:O	2:B:194:GLY:HA3	1.94	0.68
28:P:1265:PEK:C38	26:T:1269:CDL:H273	2.24	0.68
1:N:365:ILE:HD11	29:N:4837:HOH:O	1.94	0.68
4:D:34:SER:H	4:D:37:GLN:NE2	1.92	0.67
2:B:58:ALA:O	2:B:62:GLU:HG3	1.94	0.67
6:S:85:CYS:SG	6:S:87:THR:HG23	2.35	0.67
3:C:224:LYS:HE3	26:C:270:CDL:HB31	1.76	0.67
13:Z:42:LYS:HE3	13:Z:42:LYS:HA	1.76	0.67
9:V:61:GLU:HG3	9:V:64:ARG:HH21	1.60	0.66
7:T:5:LYS:CD	28:T:263:PEK:H381	2.25	0.66
6:F:94:HIS:HE1	29:F:4660:HOH:O	1.76	0.65
1:N:172:LYS:NZ	1:N:178:GLN:HE22	1.95	0.65
3:P:246:ASP:HB2	29:P:4199:HOH:O	1.96	0.65
4:D:78:TRP:HB3	19:D:523:TGL:CB2	2.23	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:72:ASN:H	7:T:76:ASN:ND2	1.94	0.65
26:G:269:CDL:C54	26:G:269:CDL:H241	2.27	0.64
7:T:5:LYS:CG	28:T:263:PEK:C38	2.75	0.64
7:G:3:ALA:O	7:G:4:ALA:HB2	1.97	0.64
26:T:1269:CDL:C11	26:T:1269:CDL:HA21	2.27	0.64
26:T:1269:CDL:H111	26:T:1269:CDL:HA21	1.78	0.64
29:B:2351:HOH:O	19:D:523:TGL:HC61	1.98	0.64
19:L:522:TGL:H231	19:L:522:TGL:CA9	2.27	0.64
2:O:141:ARG:H	9:V:70:GLN:HE22	1.46	0.64
6:F:10:GLU:OE2	6:F:25:ARG:NH2	2.30	0.64
7:T:17:ARG:HD3	29:T:3300:HOH:O	1.98	0.64
26:G:269:CDL:C11	26:G:269:CDL:HA21	2.15	0.64
3:C:29:SER:HB3	3:C:42:LEU:HD13	1.79	0.63
3:P:174:THR:CG2	3:P:174:THR:CA	2.70	0.63
4:Q:70:GLU:O	4:Q:73:ARG:HG2	1.98	0.63
6:S:64:GLU:O	6:S:65:ASP:HB2	1.97	0.63
1:A:406:ASN:HD21	20:A:524:PGV:H22	1.62	0.63
7:G:37:LEU:HD21	26:G:269:CDL:H352	1.81	0.63
26:G:269:CDL:C24	26:G:269:CDL:H541	2.29	0.62
12:L:20:ARG:HH22	19:L:522:TGL:HC62	1.64	0.62
1:N:362:SER:HA	2:O:87:MET:HE1	1.82	0.62
2:O:116:LEU:HD12	2:O:117:SER:N	2.15	0.62
20:C:267:PGV:H172	26:C:270:CDL:H652	1.81	0.62
7:G:17:ARG:HD2	29:G:2300:HOH:O	1.98	0.62
1:A:290:HIS:CD2	1:A:291:HIS:CD2	2.88	0.62
2:B:68:LEU:HG	29:B:4723:HOH:O	1.99	0.61
7:T:17:ARG:CD	29:T:3300:HOH:O	2.47	0.61
7:G:3:ALA:O	7:G:4:ALA:CB	2.48	0.61
24:C:272:DMU:O1	24:C:272:DMU:H29	2.01	0.61
3:C:5:THR:HG22	6:F:96:LEU:HD13	1.81	0.61
1:N:177:SER:H	1:N:180:GLN:NE2	1.98	0.61
3:C:3:HIS:HE1	6:F:96:LEU:CD2	2.14	0.61
20:N:1524:PGV:H011	20:N:1524:PGV:H22	1.83	0.60
2:B:62:GLU:O	2:B:66:THR:HB	2.01	0.60
1:N:229:ILE:HD11	2:O:175:ILE:HD13	1.83	0.60
19:Q:1523:TGL:HA91	19:Q:1523:TGL:H242	1.84	0.60
1:A:278:MET:SD	7:T:5:LYS:HB3	2.42	0.60
1:A:21:LEU:HD23	19:L:522:TGL:H211	1.83	0.60
18:N:515:HEA:H272	18:N:515:HEA:C16	2.32	0.60
6:S:94:HIS:CD2	6:S:95:GLN:N	2.70	0.60
20:N:1524:PGV:H011	20:N:1524:PGV:C2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:5:LYS:HB2	28:T:263:PEK:C36	2.32	0.59
1:N:177:SER:H	1:N:180:GLN:HE21	1.50	0.59
7:G:31:CYS:SG	26:G:269:CDL:H532	2.42	0.59
2:B:59:GLN:O	2:B:60:GLU:HG3	2.03	0.59
7:G:37:LEU:HD23	7:G:38:HIS:ND1	2.17	0.59
1:N:172:LYS:HZ2	1:N:178:GLN:HE22	1.50	0.59
20:A:524:PGV:H31	20:A:524:PGV:H232	1.83	0.59
6:F:95:GLN:OE1	6:F:95:GLN:HA	2.01	0.59
26:G:269:CDL:H201	1:N:311:ILE:CD1	2.32	0.59
1:A:75:ILE:CD1	1:A:75:ILE:CB	2.76	0.59
19:L:522:TGL:H231	19:L:522:TGL:HA92	1.83	0.59
9:V:55:ASP:OD2	9:V:58:LYS:HB2	2.03	0.59
2:B:41:ILE:HD13	22:B:230:PSC:H342	1.85	0.58
23:C:525:CHD:H42	3:P:127:LEU:HD21	1.84	0.58
4:Q:34:SER:H	4:Q:37:GLN:NE2	2.01	0.58
7:G:72:ASN:H	7:G:76:ASN:ND2	2.00	0.58
1:N:296:GLY:HA2	8:U:23:GLN:OE1	2.04	0.58
18:A:515:HEA:HMC1	18:A:515:HEA:HBC1	1.85	0.57
26:G:269:CDL:H473	29:G:4638:HOH:O	2.03	0.57
22:O:1230:PSC:C02	22:O:1230:PSC:H212	2.34	0.57
7:T:31:CYS:SG	26:T:1269:CDL:C55	2.90	0.57
4:D:107:ILE:HB	4:D:108:PRO:CD	2.35	0.57
7:T:38:HIS:HE2	26:T:1269:CDL:H111	1.69	0.57
2:B:59:GLN:C	2:B:60:GLU:HG3	2.26	0.57
3:P:226:HIS:HE1	26:P:1270:CDL:HB32	1.70	0.56
28:P:1265:PEK:C38	26:T:1269:CDL:H271	2.15	0.56
22:O:1230:PSC:H071	9:V:10:ARG:HH21	1.69	0.56
10:W:52:TRP:O	10:W:57:HIS:HE1	1.88	0.56
1:A:28:MET:CE	18:A:515:HEA:H271	2.36	0.56
6:S:19:GLU:HG2	29:S:4904:HOH:O	2.06	0.56
7:T:84:LYS:N	7:T:84:LYS:CD	2.64	0.56
19:D:523:TGL:H242	19:D:523:TGL:HA91	1.87	0.55
1:A:194:LEU:HD22	1:A:285:PHE:HE2	1.71	0.55
2:B:56:MET:HA	22:B:230:PSC:H202	1.87	0.55
18:N:515:HEA:H122	18:N:515:HEA:HHC	1.87	0.55
3:C:67:PHE:CE1	26:C:270:CDL:H1	2.31	0.55
4:D:78:TRP:N	19:D:523:TGL:HB21	2.21	0.55
24:C:272:DMU:H40	7:G:63:GLY:H	1.70	0.55
22:B:230:PSC:O01	22:B:230:PSC:H212	2.06	0.55
12:Y:35:ALA:O	12:Y:39:ILE:HG13	2.07	0.55
1:A:172:LYS:HZ2	1:A:178:GLN:HE22	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LYS:HE3	29:A:2385:HOH:O	2.06	0.55
8:H:45:ALA:O	8:H:47:GLY:N	2.34	0.55
3:P:58:TRP:CG	20:P:1267:PGV:H41	2.42	0.54
7:G:21:PHE:CD2	28:G:265:PEK:H222	2.42	0.54
12:L:20:ARG:HH22	19:L:522:TGL:CC6	2.20	0.54
6:F:64:GLU:O	6:F:65:ASP:HB2	2.07	0.54
4:D:118:LYS:HB3	11:K:53:TRP:HB3	1.90	0.54
19:N:1522:TGL:HC62	19:N:1522:TGL:HC22	1.89	0.54
1:N:68:PHE:HE2	1:N:112:LEU:HD13	1.73	0.54
1:N:488:THR:HB	1:N:495:LEU:HD13	1.90	0.54
19:A:521:TGL:C36	29:A:4497:HOH:O	2.56	0.54
1:A:71:MET:HB2	1:A:72:PRO:HD3	1.90	0.53
26:G:269:CDL:OA7	26:G:269:CDL:H342	2.08	0.53
1:A:172:LYS:NZ	1:A:178:GLN:HE22	2.06	0.53
4:D:78:TRP:CA	19:D:523:TGL:HB21	2.38	0.53
2:O:151:ARG:HD3	2:O:181:GLN:HE21	1.73	0.53
4:Q:78:TRP:CA	19:Q:1523:TGL:HB22	2.39	0.53
3:P:210:ILE:HG23	20:P:1267:PGV:H102	1.90	0.53
3:C:3:HIS:HB2	29:C:4631:HOH:O	2.09	0.53
20:A:522:PGV:H171	28:G:264:PEK:H352	1.89	0.53
3:P:34:TRP:HE1	24:P:1272:DMU:H29	1.74	0.53
7:T:2:SER:O	28:T:263:PEK:H332	2.09	0.53
2:O:82:ARG:HH11	2:O:86:MET:CE	2.22	0.52
1:A:407:ASP:O	1:A:411:LYS:HG3	2.10	0.52
20:P:1267:PGV:H172	26:P:1270:CDL:H662	1.91	0.52
5:R:7:THR:OG1	5:R:10:GLU:HG3	2.08	0.52
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.43	0.52
6:S:76:LYS:HE3	6:S:93:PRO:HG2	1.92	0.52
7:G:11:TPO:HG22	7:G:16:TRP:HE1	1.73	0.52
3:P:226:HIS:CE1	26:P:1270:CDL:HB32	2.45	0.52
7:T:5:LYS:HB2	28:T:263:PEK:C37	2.39	0.52
19:N:1522:TGL:HC62	19:N:1522:TGL:CC2	2.40	0.52
18:N:515:HEA:C27	18:N:515:HEA:C16	2.88	0.51
26:P:1270:CDL:H262	26:P:1270:CDL:H672	1.91	0.51
26:G:269:CDL:H201	1:N:311:ILE:HD12	1.92	0.51
12:L:14:SER:H	19:L:522:TGL:HC31	1.74	0.51
19:A:521:TGL:H361	29:A:4497:HOH:O	2.10	0.51
26:C:270:CDL:H711	26:C:270:CDL:H121	1.91	0.51
1:N:35:LEU:HD11	1:N:462:LEU:HB2	1.91	0.51
18:N:515:HEA:CB	18:N:515:HEA:HMC1	2.33	0.51
1:N:76:GLY:O	1:N:80:ASN:HB2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:LEU:HB2	2:B:69:PRO:HD3	1.92	0.51
7:T:3:ALA:O	7:T:4:ALA:HB2	2.10	0.51
1:A:290:HIS:HD2	1:A:291:HIS:CD2	2.28	0.51
1:A:449:MET:SD	2:B:5:MET:HG2	2.50	0.51
10:J:7:GLU:HG3	29:J:4578:HOH:O	2.11	0.51
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.75	0.51
2:O:82:ARG:HG2	2:O:86:MET:CE	2.39	0.51
29:B:2351:HOH:O	19:D:523:TGL:CC6	2.55	0.51
1:N:449:MET:SD	2:O:5:MET:HG2	2.50	0.51
11:X:7:PRO:O	11:X:12:LYS:HE3	2.10	0.50
19:N:1522:TGL:HA22	12:Y:13:PHE:HB3	1.93	0.50
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.93	0.50
10:W:30:ILE:O	10:W:34:VAL:HG23	2.11	0.50
22:B:230:PSC:C13	22:B:230:PSC:H343	2.41	0.50
2:O:84:LEU:HA	2:O:87:MET:HE2	1.93	0.50
19:N:1521:TGL:H142	2:O:39:LEU:HD23	1.94	0.50
8:U:78:GLU:HG2	8:U:80:THR:HG23	1.93	0.50
12:Y:2:HIS:N	29:Y:4284:HOH:O	2.45	0.50
19:N:1521:TGL:HA52	2:O:32:PHE:CE2	2.46	0.50
10:W:16:ASN:OD1	10:W:23:LYS:HE3	2.11	0.50
7:G:37:LEU:HD23	7:G:38:HIS:CE1	2.47	0.50
1:N:513:LEU:O	1:N:514:LYS:HB2	2.12	0.50
20:N:1524:PGV:O11	20:N:1524:PGV:H061	2.12	0.49
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.59	0.49
12:Y:14:SER:O	12:Y:20:ARG:NH2	2.44	0.49
2:B:41:ILE:O	2:B:45:MET:HG2	2.13	0.49
2:O:41:ILE:O	2:O:45:MET:HG2	2.12	0.49
20:A:524:PGV:H141	20:A:524:PGV:H301	1.94	0.49
19:N:1521:TGL:HC72	29:Q:4417:HOH:O	2.11	0.49
7:T:7:ASP:O	7:T:9:GLY:N	2.46	0.49
19:L:522:TGL:C23	19:L:522:TGL:HA92	2.43	0.49
22:O:1230:PSC:H222	22:O:1230:PSC:H21	1.94	0.49
11:X:54:ARG:NH2	11:X:54:ARG:HG3	2.21	0.49
10:J:37:THR:OG1	23:J:60:CHD:H7	2.12	0.49
19:N:1522:TGL:HC31	12:Y:13:PHE:HA	1.95	0.49
7:G:38:HIS:CE1	26:G:269:CDL:H111	2.48	0.49
19:D:523:TGL:H351	9:I:16:ARG:HH21	1.77	0.49
5:R:25:ASP:OD1	5:R:28:GLU:HG3	2.12	0.49
3:P:47:LEU:O	3:P:51:MET:HG2	2.13	0.49
23:O:229:CHD:H212	23:O:229:CHD:H12	1.94	0.49
4:Q:130:PRO:HA	4:Q:135:SER:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:1269:CDL:OB4	26:T:1269:CDL:H1	2.13	0.49
1:A:225:GLY:HA3	3:C:112:LEU:HD21	1.94	0.48
24:C:272:DMU:H1	7:G:69:PHE:HZ	1.78	0.48
7:G:30:LEU:HB3	26:G:269:CDL:H531	1.94	0.48
7:T:17:ARG:HD2	29:T:3300:HOH:O	2.12	0.48
12:L:24:MET:SD	19:L:522:TGL:H161	2.54	0.48
2:O:2:ALA:HA	2:O:6:GLN:OE1	2.14	0.48
10:W:33:ARG:HG2	23:W:1060:CHD:H151	1.95	0.48
1:A:107:PRO:HB3	3:C:25:LEU:HB2	1.96	0.48
26:G:269:CDL:H401	2:O:77:ALA:CB	2.44	0.48
26:C:270:CDL:H861	26:C:270:CDL:H831	1.50	0.48
23:C:271:CHD:H12A	23:C:271:CHD:H112	1.46	0.48
1:A:510:TYR:OH	1:A:512:ASN:ND2	2.45	0.48
18:A:516:HEA:HMC1	18:A:516:HEA:HBC1	1.96	0.48
2:B:104:TRP:CG	2:B:203:ASN:HB2	2.49	0.48
26:G:269:CDL:H371	2:O:81:LEU:HD12	1.96	0.48
1:A:38:ARG:HD2	18:A:515:HEA:OMA	2.13	0.48
22:B:230:PSC:H071	5:E:8:ASP:HA	1.96	0.48
18:N:515:HEA:H122	18:N:515:HEA:H262	1.94	0.48
2:O:59:GLN:O	2:O:59:GLN:HG3	2.13	0.48
1:A:311:ILE:HD12	26:T:1269:CDL:H191	1.95	0.48
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.96	0.47
1:N:514:LYS:HE2	29:S:3330:HOH:O	2.13	0.47
1:A:334:TRP:CH2	2:B:46:LEU:HD13	2.49	0.47
7:G:10:GLY:HA3	29:G:4761:HOH:O	2.14	0.47
28:G:264:PEK:C10	28:G:264:PEK:H161	2.43	0.47
6:S:53:THR:HG22	6:S:54:ASN:H	1.78	0.47
23:W:1060:CHD:H12A	23:W:1060:CHD:H112	1.63	0.47
1:A:346:PHE:HZ	19:A:521:TGL:H122	1.79	0.47
6:F:55:LYS:HA	6:F:74:LEU:O	2.14	0.47
1:N:377:PHE:CE2	1:N:378:HIS:CE1	3.02	0.47
22:B:230:PSC:H073	5:E:11:PHE:CG	2.50	0.47
1:N:310:MET:HE2	1:N:356:ILE:HG23	1.96	0.47
24:P:1272:DMU:H25	28:P:1264:PEK:H341	1.97	0.47
8:H:46:LYS:CE	29:H:4804:HOH:O	2.62	0.47
3:C:47:LEU:O	3:C:51:MET:HG2	2.15	0.47
2:O:62:GLU:O	2:O:66:THR:HB	2.15	0.47
7:T:5:LYS:CD	28:T:263:PEK:H383	2.35	0.47
19:N:1522:TGL:H251	19:N:1522:TGL:H282	1.54	0.47
2:O:100:MET:HB2	2:O:107:SER:OG	2.15	0.47
26:P:1270:CDL:H532	26:P:1270:CDL:H561	1.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:10:GLU:OE2	6:S:25:ARG:NH1	2.42	0.47
1:A:335:SER:HB2	1:A:336:PRO:HD2	1.97	0.47
1:A:37:ILE:HG21	18:A:515:HEA:CMA	2.44	0.47
20:A:524:PGV:H262	20:A:524:PGV:H71	1.97	0.47
20:C:268:PGV:H062	29:C:4909:HOH:O	2.15	0.47
4:D:12:ALA:CB	6:F:55:LYS:HE3	2.45	0.47
28:G:1263:PEK:H331	28:G:1263:PEK:H372	1.96	0.47
23:P:1271:CHD:H112	23:P:1271:CHD:H12A	1.38	0.47
26:T:1269:CDL:H761	26:T:1269:CDL:H242	1.97	0.47
3:C:3:HIS:CE1	6:F:96:LEU:CD2	2.97	0.46
20:N:1266:PGV:H181	28:P:1264:PEK:H321	1.96	0.46
2:O:164:ALA:O	2:O:194:GLY:HA3	2.14	0.46
2:O:82:ARG:NH1	2:O:86:MET:HE3	2.30	0.46
7:T:5:LYS:CB	28:T:263:PEK:H383	2.44	0.46
26:G:269:CDL:H332	2:O:78:LEU:HD12	1.97	0.46
2:O:37:LEU:O	2:O:41:ILE:HG13	2.15	0.46
5:R:80:GLU:CD	5:R:80:GLU:H	2.18	0.46
12:Y:20:ARG:NH2	12:Y:24:MET:HG3	2.29	0.46
23:B:1086:CHD:H12A	23:B:1086:CHD:H112	1.59	0.46
3:C:52:LEU:HD23	26:C:270:CDL:H362	1.97	0.46
1:A:177:SER:H	1:A:180:GLN:NE2	2.13	0.46
1:A:87:ILE:O	1:A:173:PRO:HD3	2.16	0.46
19:D:523:TGL:H122	19:D:523:TGL:HB81	1.97	0.46
26:G:269:CDL:H511	26:G:269:CDL:H181	1.97	0.46
18:N:515:HEA:CMC	18:N:515:HEA:HBC1	2.29	0.46
20:P:1268:PGV:H21	20:P:1268:PGV:H51	1.71	0.46
1:A:264:LYS:NZ	29:A:4192:HOH:O	2.48	0.46
26:C:270:CDL:H412	26:C:270:CDL:H382	1.60	0.46
4:D:78:TRP:CA	19:D:523:TGL:CB2	2.93	0.46
3:C:202:GLY:HA3	28:G:264:PEK:H21	1.98	0.46
1:A:481:GLU:HB2	13:M:4:LYS:HE2	1.96	0.46
1:N:28:MET:CE	18:N:515:HEA:H271	2.45	0.46
12:L:45:LEU:HA	12:L:45:LEU:HD23	1.77	0.46
3:P:155:ASP:OD1	3:P:155:ASP:C	2.54	0.46
2:B:68:LEU:CB	2:B:69:PRO:HD3	2.46	0.46
1:N:229:ILE:HD11	2:O:175:ILE:CD1	2.45	0.46
1:N:290:HIS:CD2	1:N:291:HIS:CD2	3.03	0.46
2:O:98:LYS:HB2	2:O:109:GLU:HB2	1.97	0.46
28:P:1264:PEK:H383	28:P:1264:PEK:H352	1.37	0.46
26:P:1270:CDL:H822	26:P:1270:CDL:H852	1.64	0.46
7:T:8:HIS:CD2	28:T:263:PEK:H232	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:MET:HE2	18:A:515:HEA:H271	1.98	0.46
28:G:264:PEK:C7	28:G:264:PEK:H32	2.46	0.46
1:N:87:ILE:O	1:N:173:PRO:HD3	2.16	0.46
6:S:94:HIS:HD2	6:S:95:GLN:H	1.58	0.46
7:G:8:HIS:ND1	28:G:1263:PEK:H312	2.30	0.46
23:J:60:CHD:H12A	23:J:60:CHD:H112	1.61	0.46
6:S:94:HIS:HA	29:S:4898:HOH:O	2.16	0.46
28:T:263:PEK:H361	28:T:263:PEK:H332	1.68	0.46
10:J:27:THR:O	10:J:27:THR:HG22	2.16	0.45
12:L:11:ILE:CG2	19:L:522:TGL:H272	2.46	0.45
1:A:218:THR:O	1:A:226:GLY:HA3	2.16	0.45
22:B:230:PSC:H073	5:E:11:PHE:CB	2.46	0.45
20:P:1268:PGV:H062	29:P:4599:HOH:O	2.15	0.45
2:B:41:ILE:CD1	22:B:230:PSC:H341	2.43	0.45
3:C:224:LYS:CD	26:C:270:CDL:HB32	2.46	0.45
4:D:98:TRP:CE2	24:M:526:DMU:H9	2.51	0.45
1:N:409:TRP:CE2	20:N:1524:PGV:H61	2.52	0.45
22:O:1230:PSC:C07	9:V:10:ARG:NH2	2.68	0.45
22:O:1230:PSC:C21	22:O:1230:PSC:O01	2.47	0.45
1:A:282:PHE:CA	7:T:4:ALA:HB3	2.44	0.45
12:Y:22:LEU:O	12:Y:26:THR:HB	2.16	0.45
8:H:44:THR:O	8:H:45:ALA:O	2.35	0.45
1:A:172:LYS:NZ	1:A:178:GLN:NE2	2.64	0.45
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.52	0.45
1:A:177:SER:H	1:A:180:GLN:HE21	1.63	0.45
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.99	0.45
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.52	0.45
6:F:94:HIS:HB3	6:F:95:GLN:NE2	2.32	0.45
19:L:522:TGL:H252	19:L:522:TGL:H283	1.62	0.45
1:N:378:HIS:CG	1:N:425:PHE:CE2	3.05	0.45
5:R:63:SER:O	5:R:67:ILE:HG13	2.17	0.45
26:P:1270:CDL:H791	26:P:1270:CDL:H231	1.99	0.45
9:V:61:GLU:CG	9:V:64:ARG:HH21	2.26	0.45
19:N:1521:TGL:HA52	2:O:32:PHE:HE2	1.82	0.45
13:Z:32:TRP:N	24:Z:1526:DMU:H1	2.32	0.45
22:B:230:PSC:H212	22:B:230:PSC:C1	2.47	0.45
3:C:34:TRP:CD1	3:C:40:MET:HG3	2.52	0.45
7:G:8:HIS:CE1	28:G:1263:PEK:H342	2.52	0.45
1:N:383:MET:HG2	1:N:421:VAL:HG21	1.97	0.45
2:O:31:VAL:O	2:O:35:SER:OG	2.34	0.45
6:S:94:HIS:CG	6:S:95:GLN:H	2.27	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:C:271:CHD:H212	23:C:271:CHD:H12	1.99	0.44
7:G:17:ARG:CD	29:G:2300:HOH:O	2.63	0.44
2:O:217:LYS:HE2	2:O:220:GLU:OE2	2.16	0.44
2:B:52:HIS:CE1	22:B:230:PSC:H211	2.52	0.44
7:G:12:GLY:HA3	29:G:2267:HOH:O	2.16	0.44
1:N:510:TYR:OH	1:N:512:ASN:ND2	2.41	0.44
1:A:334:TRP:HB2	19:D:523:TGL:HG11	2.00	0.44
20:P:1267:PGV:H12	20:P:1267:PGV:H152	1.44	0.44
8:U:37:HIS:HD2	29:U:3142:HOH:O	2.00	0.44
1:A:377:PHE:CD1	18:A:516:HEA:HAD1	2.52	0.44
20:A:522:PGV:H261	20:C:267:PGV:H292	1.98	0.44
1:A:71:MET:N	1:A:72:PRO:CD	2.81	0.44
4:D:78:TRP:HA	19:D:523:TGL:HB21	2.00	0.44
22:B:230:PSC:H071	9:I:10:ARG:NH2	2.31	0.44
10:J:52:TRP:O	10:J:57:HIS:HE1	2.01	0.44
1:N:312:ILE:HG21	1:N:312:ILE:HD13	1.61	0.44
2:O:82:ARG:HH11	2:O:86:MET:HE3	1.82	0.44
19:A:521:TGL:HA82	19:A:521:TGL:H222	2.00	0.44
13:M:17:ILE:O	13:M:21:VAL:HG23	2.16	0.44
1:N:397:PHE:HB3	1:N:398:PRO:HD3	1.98	0.44
4:Q:23:PRO:HD2	5:R:34:ASN:OD1	2.18	0.44
2:B:65:TRP:CZ3	22:B:230:PSC:H322	2.53	0.44
19:N:1522:TGL:HC62	19:N:1522:TGL:HC32	1.79	0.44
2:O:59:GLN:O	2:O:59:GLN:CG	2.65	0.44
7:T:12:GLY:HA3	29:T:3267:HOH:O	2.17	0.44
3:C:64:GLU:HA	3:C:68:GLN:HE21	1.82	0.44
19:D:523:TGL:HB42	19:D:523:TGL:HA32	2.00	0.44
1:A:87:ILE:HG13	1:A:89:ALA:HB2	1.99	0.44
3:C:179:SER:O	3:C:183:GLU:HG2	2.17	0.44
12:L:25:MET:HG2	19:L:522:TGL:HA62	2.00	0.44
19:N:1522:TGL:HC31	12:Y:14:SER:H	1.82	0.44
4:Q:109:HIS:CD2	29:Q:3152:HOH:O	2.49	0.44
4:Q:16:TYR:CE1	4:Q:25:PRO:HG2	2.52	0.44
20:A:524:PGV:H232	20:A:524:PGV:H202	1.79	0.43
26:C:270:CDL:PA1	26:C:270:CDL:HB22	2.57	0.43
2:O:102:HIS:O	2:O:104:TRP:HA	2.17	0.43
6:S:94:HIS:HD2	6:S:95:GLN:N	2.12	0.43
6:F:55:LYS:HG3	6:F:73:TRP:CZ3	2.53	0.43
9:I:73:LYS:HD2	9:I:73:LYS:HA	1.73	0.43
28:P:1264:PEK:H262	28:P:1264:PEK:H231	1.80	0.43
23:P:1525:CHD:H12	23:P:1525:CHD:H212	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:T:1269:CDL:H562	26:T:1269:CDL:H762	1.99	0.43
26:T:1269:CDL:H561	26:T:1269:CDL:H591	1.75	0.43
3:C:210:ILE:HD13	20:C:267:PGV:H301	2.00	0.43
3:C:210:ILE:HG12	20:C:267:PGV:H12	2.00	0.43
1:N:508:PRO:HG3	3:P:6:HIS:HB3	2.00	0.43
7:T:8:HIS:ND1	28:T:263:PEK:H321	2.33	0.43
12:Y:41:ARG:HH11	12:Y:41:ARG:HG2	1.82	0.43
13:Z:36:HIS:O	13:Z:39:ASN:HB2	2.18	0.43
19:A:521:TGL:HA91	19:A:521:TGL:H241	1.99	0.43
23:P:1525:CHD:H152	20:P:1268:PGV:H92	2.01	0.43
9:V:29:LEU:HD12	9:V:29:LEU:HA	1.54	0.43
24:C:272:DMU:C10	24:C:272:DMU:H29	2.49	0.43
1:N:155:VAL:CG2	28:P:1264:PEK:H381	2.48	0.43
4:Q:91:PHE:O	4:Q:94:LEU:HB2	2.18	0.43
8:U:57:ARG:O	8:U:61:LYS:HG3	2.18	0.43
8:H:60:TYR:C	8:H:60:TYR:CD1	2.91	0.43
1:N:199:LEU:N	1:N:200:PRO:CD	2.82	0.43
28:P:1265:PEK:H383	26:T:1269:CDL:H272	1.80	0.43
2:B:13:THR:HG22	2:B:13:THR:O	2.19	0.43
3:P:224:LYS:HD3	26:P:1270:CDL:HB31	2.01	0.43
2:B:200:CYS:SG	2:B:204:HIS:HA	2.59	0.43
22:O:1230:PSC:H201	22:O:1230:PSC:H231	1.70	0.43
23:P:1525:CHD:H12A	23:P:1525:CHD:H112	1.74	0.43
28:T:263:PEK:H271	28:T:263:PEK:H241	1.84	0.43
23:C:525:CHD:H112	23:C:525:CHD:H12A	1.72	0.43
19:N:1521:TGL:C28	19:N:1521:TGL:H101	2.49	0.43
26:T:1269:CDL:H252	26:T:1269:CDL:H221	1.48	0.43
26:T:1269:CDL:OA7	26:T:1269:CDL:H342	2.19	0.43
7:G:4:ALA:CB	1:N:282:PHE:HA	2.43	0.43
1:A:309:THR:HG22	18:A:516:HEA:HMB2	2.01	0.42
3:P:29:SER:HB3	3:P:42:LEU:HD13	2.01	0.42
7:T:8:HIS:HB2	28:T:263:PEK:H282	2.01	0.42
4:Q:19:ARG:HD2	4:Q:21:ASP:OD1	2.18	0.42
1:A:112:LEU:HG	29:A:4496:HOH:O	2.19	0.42
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.54	0.42
1:A:169:ILE:HG23	7:T:9:GLY:HA3	2.01	0.42
26:G:269:CDL:H661	26:G:269:CDL:H631	1.64	0.42
1:N:240:HIS:O	1:N:241:PRO:C	2.58	0.42
5:R:81:ILE:HG12	9:V:7:PRO:HG2	2.01	0.42
28:P:1265:PEK:H311	28:P:1265:PEK:H282	1.91	0.42
10:J:40:LEU:HD12	23:J:60:CHD:H183	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:N:1521:TGL:H241	19:N:1521:TGL:H211	1.78	0.42
1:N:172:LYS:NZ	1:N:178:GLN:NE2	2.63	0.42
2:B:189:PRO:HD2	9:I:54:TYR:OH	2.19	0.42
1:N:430:PHE:HE1	19:N:1521:TGL:HB21	1.83	0.42
4:Q:48:TRP:O	4:Q:51:LEU:HB2	2.19	0.42
1:A:250:GLY:O	1:A:254:ILE:HG12	2.20	0.42
1:A:486:ASP:OD2	4:D:19:ARG:CD	2.51	0.42
1:A:22:PHE:HA	19:L:522:TGL:HB71	2.02	0.42
3:C:19:THR:O	3:C:23:SER:HB3	2.20	0.42
1:N:426:PHE:HB3	1:N:427:PRO:HD3	2.02	0.42
19:A:521:TGL:H121	19:A:521:TGL:H292	1.26	0.42
4:Q:43:LYS:NZ	4:Q:55:GLU:OE1	2.42	0.42
12:Y:41:ARG:HG2	12:Y:41:ARG:NH1	2.34	0.42
1:A:381:LEU:CD2	18:A:516:HEA:HBC2	2.50	0.41
7:T:78:LEU:HB3	7:T:79:PRO:HD2	2.02	0.41
1:A:514:LYS:HG3	6:F:38:ALA:HB2	2.02	0.41
19:N:1522:TGL:H352	29:N:4536:HOH:O	2.19	0.41
5:R:82:TYR:HB3	5:R:83:PRO:HD3	2.02	0.41
10:W:50:LEU:HD22	10:W:54:SER:HG	1.84	0.41
18:A:515:HEA:H172	18:A:515:HEA:H261	1.78	0.41
1:N:236:TRP:CE3	1:N:236:TRP:HA	2.55	0.41
3:P:171:VAL:HG22	26:P:1270:CDL:H841	2.02	0.41
3:P:40:MET:O	3:P:44:MET:HG2	2.20	0.41
11:X:16:ALA:O	11:X:20:SER:HB2	2.20	0.41
2:B:64:ILE:HA	2:B:64:ILE:HD13	1.95	0.41
26:C:270:CDL:H231	26:C:270:CDL:H642	2.02	0.41
7:T:25:LEU:HD23	7:T:25:LEU:HA	1.82	0.41
23:O:229:CHD:H112	23:O:229:CHD:H12A	1.68	0.41
5:R:26:ALA:O	5:R:30:ARG:HG3	2.21	0.41
1:N:514:LYS:HA	6:S:38:ALA:HB3	2.03	0.41
4:Q:121:LYS:HG2	11:X:53:TRP:CD1	2.55	0.41
6:F:87:THR:HG21	29:F:4882:HOH:O	2.19	0.41
3:P:220:PHE:CB	26:P:1270:CDL:H712	2.51	0.41
1:A:311:ILE:CD1	26:T:1269:CDL:H191	2.51	0.41
1:A:314:ILE:HB	1:A:315:PRO:CD	2.51	0.41
1:A:396:TRP:O	1:A:397:PHE:C	2.58	0.41
1:A:513:LEU:O	1:A:513:LEU:HD13	2.21	0.41
2:B:121:TYR:O	2:B:138:VAL:HA	2.20	0.41
3:C:156:ARG:HE	23:C:271:CHD:C24	2.34	0.41
5:E:72:LYS:HB2	5:E:82:TYR:CD2	2.56	0.41
1:N:51:ASP:OD2	2:O:205:SER:OG	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:O:1230:PSC:H071	9:V:10:ARG:NH2	2.33	0.41
1:A:381:LEU:HD13	18:A:515:HEA:HAC	2.03	0.41
18:A:516:HEA:HMB1	18:A:516:HEA:H11	1.88	0.41
3:C:138:LEU:HD23	3:C:138:LEU:HA	1.84	0.41
3:C:3:HIS:HE1	6:F:96:LEU:HD21	1.85	0.41
19:D:523:TGL:HC21	19:D:523:TGL:HG12	2.03	0.41
7:G:12:GLY:CA	29:G:2267:HOH:O	2.69	0.41
1:A:334:TRP:HH2	2:B:46:LEU:HD13	1.86	0.41
1:A:400:PHE:HB3	19:L:522:TGL:H283	2.03	0.41
1:A:409:TRP:HA	1:A:412:ILE:HD12	2.03	0.41
3:C:129:VAL:N	3:C:130:PRO:CD	2.84	0.41
4:Q:34:SER:N	4:Q:37:GLN:HE21	2.19	0.41
2:B:146:MET:HA	2:B:213:LEU:HD12	2.03	0.41
1:N:365:ILE:HD11	29:U:4796:HOH:O	2.19	0.41
5:R:105:GLY:O	5:R:108:LYS:HG2	2.20	0.41
2:B:78:LEU:HA	2:B:78:LEU:HD12	1.95	0.40
2:O:139:ASP:OD2	2:O:140:ASN:N	2.53	0.40
23:P:1271:CHD:H162	23:P:1271:CHD:H232	2.03	0.40
3:P:224:LYS:CD	26:P:1270:CDL:HB31	2.51	0.40
5:R:74:LYS:HD2	5:R:74:LYS:HA	1.88	0.40
3:P:127:LEU:HG	26:T:1269:CDL:OB3	2.20	0.40
1:A:265:LYS:HB2	1:A:490:THR:HG21	2.03	0.40
4:D:19:ARG:NH1	4:D:21:ASP:OD2	2.54	0.40
24:C:272:DMU:C11	7:G:63:GLY:H	2.34	0.40
4:Q:37:GLN:O	4:Q:41:LYS:HG2	2.22	0.40
28:P:1265:PEK:C37	26:T:1269:CDL:C27	2.99	0.40
8:U:38:ARG:HG2	8:U:85:ILE:HA	2.04	0.40
1:A:398:PRO:HA	1:A:403:TYR:O	2.20	0.40
3:P:112:LEU:HD13	3:P:118:PRO:HG3	2.03	0.40
3:P:154:GLY:HA2	6:S:6:VAL:HB	2.03	0.40
6:S:62:CYS:HB3	6:S:85:CYS:HB3	2.03	0.40
3:C:106:LEU:HD21	3:C:259:TRP:CZ2	2.57	0.40
1:N:12:HIS:CE1	1:N:13:LYS:HG3	2.56	0.40
20:N:1524:PGV:H41	20:N:1524:PGV:H221	2.03	0.40
1:N:478:SER:O	13:Z:6:ALA:HB1	2.22	0.40
1:N:71:MET:HB2	1:N:72:PRO:HD3	2.03	0.40
2:O:68:LEU:CB	2:O:69:PRO:HD3	2.51	0.40
1:A:310:MET:CE	1:A:356:ILE:HG23	2.52	0.40
1:A:38:ARG:HD2	1:A:38:ARG:HH11	1.74	0.40
20:A:524:PGV:H151	4:D:87:PHE:CZ	2.57	0.40
9:I:43:ARG:HD3	9:I:43:ARG:HH11	1.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:127:THR:HG22	1:N:235:PHE:CE2	2.57	0.40
3:P:164:PHE:CD1	23:P:1271:CHD:H192	2.57	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%)	493 (96%)	19 (4%)	0	100	100
1	N	512/514 (100%)	484 (94%)	28 (6%)	0	100	100
2	B	225/227 (99%)	217 (96%)	7 (3%)	1 (0%)	34	32
2	O	225/227 (99%)	211 (94%)	13 (6%)	1 (0%)	34	32
3	C	257/261 (98%)	252 (98%)	5 (2%)	0	100	100
3	P	257/261 (98%)	252 (98%)	4 (2%)	1 (0%)	34	32
4	D	142/147 (97%)	138 (97%)	4 (3%)	0	100	100
4	Q	142/147 (97%)	133 (94%)	8 (6%)	1 (1%)	22	18
5	E	102/109 (94%)	99 (97%)	3 (3%)	0	100	100
5	R	102/109 (94%)	101 (99%)	1 (1%)	0	100	100
6	F	91/98 (93%)	88 (97%)	1 (1%)	2 (2%)	6	2
6	S	91/98 (93%)	86 (94%)	3 (3%)	2 (2%)	6	2
7	G	81/85 (95%)	66 (82%)	8 (10%)	7 (9%)	1	0
7	T	81/85 (95%)	65 (80%)	10 (12%)	6 (7%)	1	0
8	H	73/85 (86%)	69 (94%)	2 (3%)	2 (3%)	5	1
8	U	73/85 (86%)	66 (90%)	4 (6%)	3 (4%)	3	1
9	I	69/73 (94%)	68 (99%)	1 (1%)	0	100	100
9	V	69/73 (94%)	67 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	46 (98%)	1 (2%)	0	100	100
11	X	47/56 (84%)	43 (92%)	4 (8%)	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%)	40 (98%)	1 (2%)	0	100	100
13	Z	41/46 (89%)	38 (93%)	3 (7%)	0	100	100
All	All	3478/3614 (96%)	3316 (95%)	136 (4%)	26 (1%)	22	18

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	60	GLU
6	F	95	GLN
7	G	4	ALA
7	G	7	ASP
7	G	8	HIS
7	G	39	SER
7	G	40	GLY
8	H	45	ALA
8	H	46	LYS
6	S	94	HIS
7	T	4	ALA
7	T	8	HIS
8	U	50	VAL
7	G	37	LEU
7	T	7	ASP
7	G	6	GLY
8	U	45	ALA
4	Q	34	SER
6	S	95	GLN
7	T	3	ALA
7	T	37	LEU
6	F	94	HIS
2	O	92	ASN
3	P	232	HIS
7	T	6	GLY
8	U	46	LYS

### 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%)	416 (98%)	10 (2%)	50	55
1	N	426/426 (100%)	412 (97%)	14 (3%)	38	40
2	B	210/210 (100%)	199 (95%)	11 (5%)	23	21
2	O	210/210 (100%)	192 (91%)	18 (9%)	10	7
3	C	224/226 (99%)	217 (97%)	7 (3%)	40	43
3	P	224/226 (99%)	219 (98%)	5 (2%)	52	57
4	D	128/129 (99%)	127 (99%)	1 (1%)	81	86
4	Q	128/129 (99%)	121 (94%)	7 (6%)	21	19
5	E	91/95 (96%)	89 (98%)	2 (2%)	52	57
5	R	91/95 (96%)	89 (98%)	2 (2%)	52	57
6	F	79/81 (98%)	72 (91%)	7 (9%)	9	6
6	S	79/81 (98%)	72 (91%)	7 (9%)	9	6
7	G	67/68 (98%)	59 (88%)	8 (12%)	5	2
7	T	67/68 (98%)	61 (91%)	6 (9%)	9	6
8	H	67/75 (89%)	65 (97%)	2 (3%)	41	44
8	U	67/75 (89%)	60 (90%)	7 (10%)	7	4
9	I	56/57 (98%)	53 (95%)	3 (5%)	22	20
9	V	56/57 (98%)	53 (95%)	3 (5%)	22	20
10	J	48/50 (96%)	47 (98%)	1 (2%)	53	59
10	W	48/50 (96%)	46 (96%)	2 (4%)	30	30
11	K	39/46 (85%)	38 (97%)	1 (3%)	46	50
11	X	39/46 (85%)	37 (95%)	2 (5%)	24	22
12	L	39/40 (98%)	38 (97%)	1 (3%)	46	50
12	Y	39/40 (98%)	36 (92%)	3 (8%)	13	9
13	M	37/38 (97%)	30 (81%)	7 (19%)	1	0
13	Z	37/38 (97%)	33 (89%)	4 (11%)	6	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	3022/3082 (98%)	2881 (95%)	141 (5%)	26	25

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	222	PRO
1	A	333	LYS
1	A	338	MET
1	A	362	SER
1	A	363	LEU
1	A	369	ASP
1	A	513	LEU
2	B	33	LEU
2	B	60	GLU
2	B	61	VAL
2	B	65	TRP
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	94	SER
2	B	115	ASP
2	B	171	LYS
3	C	23	SER
3	C	29	SER
3	C	77	LYS
3	C	127	LEU
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
4	D	51	LEU
5	E	90	ARG
5	E	108	LYS
6	F	37	LYS
6	F	48	LEU
6	F	50	PRO
6	F	78	GLU
6	F	84	SER
6	F	87	THR

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Mol	Chain	Res	Type
6	F	95	GLN
7	G	2	SER
7	G	17	ARG
7	G	18	PHE
7	G	33	LEU
7	G	37	LEU
7	G	54	ARG
7	G	74	ARG
7	G	84	LYS
8	H	27	ARG
8	H	60	TYR
9	I	8	GLN
9	I	15	ARG
9	I	61	GLU
10	J	50	LEU
11	K	20	SER
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
13	M	43	SER
1	N	34	SER
1	N	38	ARG
1	N	109	PHE
1	N	127	THR
1	N	138	HIS
1	N	228	PRO
1	N	241	PRO
1	N	265	LYS
1	N	338	MET
1	N	361	SER
1	N	363	LEU
1	N	369	ASP
1	N	484	THR
1	N	504	THR
2	O	33	LEU
2	O	35	SER
2	O	60	GLU
2	O	65	TRP

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Mol	Chain	Res	Type
2	O	66	THR
2	O	75	LEU
2	O	78	LEU
2	O	91	ASN
2	O	110	TYR
2	O	113	TYR
2	O	116	LEU
2	O	148	MET
2	O	167	SER
2	O	205	SER
2	O	217	LYS
2	O	221	LYS
2	O	225	SER
2	O	227	LEU
3	P	29	SER
3	P	127	LEU
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	9	GLU
4	Q	31	LYS
4	Q	51	LEU
4	Q	121	LYS
4	Q	127	LYS
4	Q	143	ASN
4	Q	147	LYS
5	R	31	LYS
5	R	80	GLU
6	S	37	LYS
6	S	48	LEU
6	S	53	THR
6	S	78	GLU
6	S	84	SER
6	S	94	HIS
6	S	95	GLN
7	T	2	SER
7	T	8	HIS
7	T	17	ARG
7	T	38	HIS
7	T	54	ARG
7	T	84	LYS
8	U	12	GLN

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Mol	Chain	Res	Type
8	U	27	ARG
8	U	41	LYS
8	U	44	THR
8	U	46	LYS
8	U	60	TYR
8	U	61	LYS
9	V	8	GLN
9	V	29	LEU
9	V	73	LYS
10	W	4	ARG
10	W	50	LEU
11	X	47	ARG
11	X	54	ARG
12	Y	14	SER
12	Y	20	ARG
12	Y	26	THR
13	Z	13	LYS
13	Z	34	LEU
13	Z	38	ASP
13	Z	42	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	178	GLN
1	A	180	GLN
1	A	360	ASN
1	A	503	HIS
1	A	512	ASN
2	B	10	GLN
2	B	195	GLN
3	C	3	HIS
3	C	68	GLN
3	C	149	HIS
4	D	29	HIS
4	D	37	GLN
4	D	109	HIS
5	E	94	ASN
7	G	76	ASN
10	J	29	ASN
10	J	57	HIS

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Mol	Chain	Res	Type
1	N	99	ASN
1	N	178	GLN
1	N	180	GLN
1	N	512	ASN
2	O	10	GLN
2	O	22	HIS
2	O	181	GLN
2	O	195	GLN
3	P	68	GLN
4	Q	37	GLN
4	Q	101	HIS
4	Q	109	HIS
4	Q	143	ASN
5	R	94	ASN
6	S	80	GLN
6	S	94	HIS
6	S	95	GLN
7	T	76	ASN
8	U	31	GLN
9	V	8	GLN
9	V	70	GLN
10	W	29	ASN
10	W	57	HIS
11	X	35	GLN

### 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
7	TPO	G	11	7	8,10,11	2.15	4 (50%)	10,14,16	2.14	3 (30%)
2	FME	O	1	2	8,9,10	1.26	1 (12%)	7,9,11	6.50	5 (71%)
1	FME	N	1	1	8,9,10	0.84	0	7,9,11	4.95	3 (42%)
2	FME	B	1	2	8,9,10	2.25	4 (50%)	7,9,11	6.43	5 (71%)
1	FME	A	1	1	8,9,10	1.43	2 (25%)	7,9,11	5.22	3 (42%)
7	TPO	T	11	7	8,10,11	2.25	4 (50%)	10,14,16	1.46	3 (30%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

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

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	O1-CN	-4.06	1.10	1.22
7	G	11	TPO	P-O1P	3.70	1.62	1.50
7	T	11	TPO	P-O1P	3.42	1.61	1.50
2	B	1	FME	CA-N	3.42	1.51	1.46
7	T	11	TPO	P-OG1	3.29	1.65	1.59
2	O	1	FME	O1-CN	-2.59	1.15	1.22
7	G	11	TPO	O-C	2.54	1.30	1.19
7	T	11	TPO	P-O3P	2.54	1.64	1.54
1	A	1	FME	CB-CA	-2.54	1.48	1.53
1	A	1	FME	O1-CN	-2.53	1.15	1.22
7	T	11	TPO	O-C	2.43	1.29	1.19
7	G	11	TPO	P-OG1	2.39	1.63	1.59
7	G	11	TPO	P-O2P	2.22	1.63	1.54
2	B	1	FME	O-C	2.22	1.28	1.19
2	B	1	FME	CB-CG	2.06	1.59	1.51

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	1	FME	CA-N-CN	-15.94	98.31	122.82
2	B	1	FME	CA-N-CN	-14.83	100.01	122.82
1	A	1	FME	CA-N-CN	-13.10	102.67	122.82
1	N	1	FME	CA-N-CN	-12.51	103.58	122.82
2	B	1	FME	C-CA-N	5.54	119.73	109.73
2	B	1	FME	CG-CB-CA	-5.27	98.30	112.95
7	G	11	TPO	CG2-CB-CA	4.89	122.81	113.16
2	O	1	FME	C-CA-N	3.68	116.37	109.73
2	O	1	FME	CE-SD-CG	3.57	112.66	100.40
7	G	11	TPO	O2P-P-OG1	3.31	120.81	105.99
7	T	11	TPO	CG2-CB-CA	3.01	119.11	113.16
2	O	1	FME	CG-CB-CA	-2.93	104.82	112.95
1	N	1	FME	CE-SD-CG	2.72	109.75	100.40
2	B	1	FME	O1-CN-N	2.63	132.20	125.27
1	A	1	FME	CG-CB-CA	-2.47	106.09	112.95
1	A	1	FME	CE-SD-CG	2.38	108.58	100.40
7	G	11	TPO	OG1-P-O1P	-2.33	100.39	109.39
2	O	1	FME	O1-CN-N	-2.25	119.34	125.27
7	T	11	TPO	O-C-CA	-2.11	119.24	124.78
7	T	11	TPO	O3P-P-OG1	2.09	115.36	105.99
2	B	1	FME	O-C-CA	-2.08	119.32	124.78
1	N	1	FME	O1-CN-N	2.05	130.66	125.27

There are no chirality outliers.

All (17) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
7	G	11	TPO	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 56 ligands modelled in this entry, 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
15	PER	N	520	18,14	0,1,1	0.00	-	-		
26	CDL	G	269	-	99,99,99	1.41	12 (12%)	105,111,111	1.30	13 (12%)
23	CHD	W	1060	-	29,32,32	0.85	1 (3%)	48,51,51	5.06	36 (75%)
20	PGV	A	524	-	50,50,50	1.20	3 (6%)	53,56,56	1.44	8 (15%)
15	PER	A	520	18,14	0,1,1	0.00	-	-		
28	PEK	P	1264	-	52,52,52	1.05	4 (7%)	55,57,57	1.65	8 (14%)
22	PSC	O	1230	-	51,51,51	1.25	3 (5%)	57,59,59	1.27	6 (10%)
18	HEA	A	515	1	44,67,67	1.37	6 (13%)	37,103,103	2.60	14 (37%)
24	DMU	Z	1526	-	34,34,34	1.02	2 (5%)	45,45,45	3.22	25 (55%)
20	PGV	N	1524	-	50,50,50	1.18	2 (4%)	53,56,56	1.25	7 (13%)
20	PGV	P	1268	-	50,50,50	1.22	2 (4%)	53,56,56	1.42	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
24	DMU	M	526	-	34,34,34	0.90	1 (2%)	45,45,45	3.18	24 (53%)
19	TGL	A	521	-	62,62,62	1.44	7 (11%)	65,65,65	2.32	14 (21%)
20	PGV	C	268	-	50,50,50	1.25	2 (4%)	53,56,56	1.41	4 (7%)
21	CUA	B	228	2	0,1,1	0.00	-	-		
28	PEK	T	263	-	52,52,52	1.32	3 (5%)	55,57,57	1.30	6 (10%)
28	PEK	G	1263	-	52,52,52	1.18	2 (3%)	55,57,57	1.29	6 (10%)
28	PEK	G	265	-	52,52,52	1.18	3 (5%)	55,57,57	1.09	4 (7%)
18	HEA	N	515	1	44,67,67	1.21	4 (9%)	37,103,103	2.74	16 (43%)
23	CHD	C	525	-	29,32,32	1.69	7 (24%)	48,51,51	5.31	38 (79%)
18	HEA	N	516	1,15	44,67,67	1.26	5 (11%)	37,103,103	2.01	11 (29%)
28	PEK	G	264	-	52,52,52	0.92	2 (3%)	55,57,57	2.27	12 (21%)
19	TGL	N	1522	-	62,62,62	1.50	7 (11%)	65,65,65	1.54	10 (15%)
24	DMU	C	272	-	34,34,34	1.22	1 (2%)	45,45,45	3.32	22 (48%)
28	PEK	P	1265	-	52,52,52	1.22	2 (3%)	55,57,57	1.31	6 (10%)
19	TGL	Q	1523	-	62,62,62	1.41	6 (9%)	65,65,65	1.37	10 (15%)
26	CDL	T	1269	-	99,99,99	1.35	12 (12%)	105,111,111	1.50	15 (14%)
23	CHD	B	1086	-	29,32,32	1.86	7 (24%)	48,51,51	5.37	36 (75%)
20	PGV	P	1267	-	50,50,50	0.89	3 (6%)	53,56,56	1.50	11 (20%)
20	PGV	N	1266	-	50,50,50	0.88	1 (2%)	53,56,56	1.63	11 (20%)
21	CUA	O	228	2	0,1,1	0.00	-	-		
23	CHD	O	229	-	29,32,32	1.66	7 (24%)	48,51,51	5.98	32 (66%)
23	CHD	C	271	-	29,32,32	0.80	1 (3%)	48,51,51	5.16	33 (68%)
18	HEA	A	516	1,15	44,67,67	1.39	7 (15%)	37,103,103	2.57	11 (29%)
20	PGV	C	267	-	50,50,50	0.96	3 (6%)	53,56,56	1.48	11 (20%)
19	TGL	L	522	-	62,62,62	1.48	7 (11%)	65,65,65	1.85	12 (18%)
26	CDL	P	1270	-	99,99,99	1.37	13 (13%)	105,111,111	1.43	16 (15%)
19	TGL	N	1521	-	62,62,62	1.34	6 (9%)	65,65,65	1.59	12 (18%)
23	CHD	J	60	-	29,32,32	0.71	0	48,51,51	4.99	37 (77%)
23	CHD	P	1525	-	29,32,32	1.34	5 (17%)	48,51,51	5.65	38 (79%)
24	DMU	P	1272	-	34,34,34	1.25	3 (8%)	45,45,45	3.09	23 (51%)
20	PGV	A	522	-	50,50,50	1.12	2 (4%)	53,56,56	1.40	8 (15%)
22	PSC	B	230	-	51,51,51	1.39	3 (5%)	57,59,59	1.24	4 (7%)
23	CHD	P	1271	-	29,32,32	0.85	1 (3%)	48,51,51	5.33	36 (75%)
26	CDL	C	270	-	99,99,99	1.43	13 (13%)	105,111,111	1.61	17 (16%)
19	TGL	D	523	-	62,62,62	1.61	7 (11%)	65,65,65	1.71	12 (18%)



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
26	CDL	G	269	-	-	57/110/110/110	-
23	CHD	W	1060	-	2/2/12/12	5/7/74/74	0/4/4/4
20	PGV	A	524	-	-	31/55/55/55	-
28	PEK	P	1264	-	-	25/56/56/56	-
22	PSC	O	1230	-	-	31/55/55/55	-
18	HEA	A	515	1	3/3/7/16	3/24/76/76	-
24	DMU	Z	1526	-	5/5/10/10	11/19/59/59	0/2/2/2
20	PGV	N	1524	-	-	30/55/55/55	-
20	PGV	P	1268	-	-	32/55/55/55	-
19	TGL	Q	1523	-	-	35/65/65/65	-
19	TGL	A	521	-	-	36/65/65/65	-
20	PGV	C	268	-	-	34/55/55/55	-
28	PEK	T	263	-	-	33/56/56/56	-
28	PEK	G	1263	-	-	32/56/56/56	-
28	PEK	G	265	-	-	25/56/56/56	-
18	HEA	N	515	1	2/2/7/16	5/24/76/76	-
23	CHD	C	525	-	-	0/7/74/74	0/4/4/4
18	HEA	N	516	1,15	3/3/7/16	0/24/76/76	-
28	PEK	G	264	-	-	23/56/56/56	-
19	TGL	N	1522	-	-	36/65/65/65	-
24	DMU	C	272	-	6/6/10/10	10/19/59/59	0/2/2/2
28	PEK	P	1265	-	-	25/56/56/56	-
24	DMU	M	526	-	5/5/10/10	9/19/59/59	0/2/2/2
26	CDL	T	1269	-	-	61/110/110/110	-
23	CHD	B	1086	-	-	0/7/74/74	0/4/4/4
20	PGV	P	1267	-	-	13/55/55/55	-
20	PGV	N	1266	-	-	14/55/55/55	-
23	CHD	O	229	-	1/1/12/12	0/7/74/74	0/4/4/4
23	CHD	C	271	-	1/1/12/12	5/7/74/74	0/4/4/4
18	HEA	A	516	1,15	3/3/7/16	0/24/76/76	-
20	PGV	C	267	-	-	12/55/55/55	-
19	TGL	L	522	-	-	40/65/65/65	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CDL	P	1270	-	-	66/110/110/110	-
19	TGL	N	1521	-	-	31/65/65/65	-
23	CHD	J	60	-	2/2/12/12	4/7/74/74	0/4/4/4
23	CHD	P	1525	-	-	0/7/74/74	0/4/4/4
24	DMU	P	1272	-	5/5/10/10	11/19/59/59	0/2/2/2
20	PGV	A	522	-	-	21/55/55/55	-
22	PSC	B	230	-	-	30/55/55/55	-
23	CHD	P	1271	-	1/1/12/12	5/7/74/74	0/4/4/4
26	CDL	C	270	-	-	66/110/110/110	-
19	TGL	D	523	-	-	33/65/65/65	-

All (188) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	T	263	PEK	O03-C21	6.10	1.51	1.33
19	N	1522	TGL	OG2-CB1	6.00	1.51	1.34
19	L	522	TGL	OG2-CB1	5.99	1.51	1.34
19	D	523	TGL	OG1-CA1	5.74	1.50	1.33
19	N	1521	TGL	OG2-CB1	5.55	1.50	1.34
20	A	522	PGV	O03-C19	5.52	1.49	1.33
20	C	268	PGV	O01-C1	5.51	1.49	1.34
28	T	263	PEK	O01-C1	5.48	1.49	1.34
19	A	521	TGL	OG1-CA1	5.48	1.49	1.33
22	B	230	PSC	O03-C19	5.45	1.49	1.33
20	N	1524	PGV	O03-C19	5.40	1.49	1.33
19	A	521	TGL	OG2-CB1	5.38	1.49	1.34
20	P	1268	PGV	O01-C1	5.37	1.49	1.34
19	D	523	TGL	OG2-CB1	5.37	1.49	1.34
19	Q	1523	TGL	OG3-CC1	5.31	1.48	1.33
19	Q	1523	TGL	OG2-CB1	5.30	1.49	1.34
26	C	270	CDL	OA8-CA7	5.28	1.48	1.33
20	A	524	PGV	O03-C19	5.24	1.48	1.33
22	B	230	PSC	O01-C1	5.21	1.49	1.34
19	L	522	TGL	OG1-CA1	5.19	1.48	1.33
28	G	1263	PEK	O03-C21	5.17	1.48	1.33
28	P	1265	PEK	O03-C21	5.15	1.48	1.33
28	G	265	PEK	O01-C1	5.11	1.48	1.34
28	P	1265	PEK	O01-C1	5.09	1.48	1.34
19	D	523	TGL	OG3-CC1	5.08	1.48	1.33
19	N	1522	TGL	OG1-CA1	5.00	1.47	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	270	CDL	OA6-CA5	4.97	1.48	1.34
26	P	1270	CDL	OA8-CA7	4.97	1.47	1.33
19	N	1522	TGL	OG3-CC1	4.97	1.47	1.33
22	O	1230	PSC	O01-C1	4.92	1.48	1.34
19	N	1521	TGL	OG1-CA1	4.84	1.47	1.33
26	G	269	CDL	OA8-CA7	4.77	1.47	1.33
26	G	269	CDL	OA6-CA5	4.76	1.47	1.34
26	C	270	CDL	OB8-CB7	4.70	1.47	1.33
26	G	269	CDL	OB6-CB5	4.69	1.47	1.34
26	G	269	CDL	OB8-CB7	4.69	1.47	1.33
24	P	1272	DMU	O16-C6	4.68	1.48	1.40
28	G	1263	PEK	O01-C1	4.67	1.47	1.34
26	P	1270	CDL	OA6-CA5	4.67	1.47	1.34
28	G	265	PEK	O03-C21	4.64	1.46	1.33
19	D	523	TGL	OB1-CB1	4.64	1.36	1.22
20	C	268	PGV	O03-C19	4.62	1.46	1.33
26	T	1269	CDL	OA6-CA5	4.58	1.47	1.34
19	Q	1523	TGL	OG1-CA1	4.57	1.46	1.33
26	C	270	CDL	OB6-CB5	4.54	1.47	1.34
26	P	1270	CDL	OB8-CB7	4.54	1.46	1.33
26	T	1269	CDL	OB8-CB7	4.51	1.46	1.33
24	C	272	DMU	O16-C6	4.50	1.47	1.40
20	N	1524	PGV	O01-C1	4.48	1.46	1.34
26	T	1269	CDL	OB6-CB5	4.47	1.46	1.34
23	O	229	CHD	C4-C5	4.43	1.61	1.53
20	P	1268	PGV	O03-C19	4.24	1.45	1.33
26	P	1270	CDL	OB6-CB5	4.21	1.46	1.34
19	N	1521	TGL	OG3-CC1	4.19	1.45	1.33
26	T	1269	CDL	OA8-CA7	4.13	1.45	1.33
20	A	524	PGV	O01-C1	4.11	1.45	1.34
22	B	230	PSC	C13-C12	4.07	1.55	1.31
23	C	525	CHD	O12-C12	4.02	1.50	1.43
22	O	1230	PSC	O03-C19	3.99	1.45	1.33
23	B	1086	CHD	C8-C7	-3.97	1.46	1.53
22	O	1230	PSC	C13-C12	3.92	1.54	1.31
23	B	1086	CHD	C4-C3	3.91	1.59	1.51
19	L	522	TGL	OG3-CC1	3.84	1.44	1.33
18	A	516	HEA	C16-C15	3.81	1.59	1.51
23	C	525	CHD	C11-C9	3.81	1.60	1.53
19	A	521	TGL	OG3-CC1	3.74	1.44	1.33
18	A	515	HEA	C3B-C11	-3.73	1.50	1.52
23	C	525	CHD	C13-C12	-3.64	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	269	CDL	C59-C58	-3.52	1.31	1.51
28	P	1264	PEK	O03-C01	-3.50	1.37	1.45
19	A	521	TGL	C10-CB9	-3.48	1.32	1.51
23	B	1086	CHD	C13-C12	-3.47	1.49	1.54
19	N	1521	TGL	C10-CB9	-3.45	1.32	1.51
19	L	522	TGL	C20-CA9	-3.44	1.32	1.51
19	L	522	TGL	C10-CB9	-3.43	1.32	1.51
28	G	264	PEK	O01-C1	3.43	1.44	1.34
20	N	1266	PGV	O03-C19	3.41	1.43	1.33
28	P	1264	PEK	O01-C1	3.38	1.43	1.34
26	C	270	CDL	C79-C78	-3.37	1.32	1.51
23	B	1086	CHD	C18-C13	3.37	1.59	1.54
26	P	1270	CDL	C59-C58	-3.35	1.32	1.51
26	T	1269	CDL	C59-C58	-3.33	1.32	1.51
19	N	1522	TGL	C20-CA9	-3.31	1.33	1.51
18	N	516	HEA	C3C-C2C	-3.28	1.35	1.40
26	T	1269	CDL	C42-C41	-3.27	1.33	1.51
18	N	515	HEA	C3B-C11	-3.24	1.50	1.52
24	Z	1526	DMU	C3-C4	-3.22	1.44	1.52
26	C	270	CDL	C59-C58	-3.22	1.33	1.51
26	G	269	CDL	C39-C38	-3.21	1.33	1.51
19	N	1522	TGL	C10-CB9	-3.18	1.33	1.51
26	G	269	CDL	C62-C61	-3.14	1.33	1.51
26	T	1269	CDL	C62-C61	-3.11	1.34	1.51
24	M	526	DMU	C3-C4	-3.10	1.44	1.52
20	C	267	PGV	O03-C19	3.08	1.42	1.33
26	G	269	CDL	C42-C41	-3.07	1.34	1.51
18	A	515	HEA	O11-C11	3.06	1.49	1.42
23	B	1086	CHD	C10-C5	-3.04	1.50	1.55
26	P	1270	CDL	C22-C21	-3.03	1.34	1.51
18	A	515	HEA	C3C-CAC	3.03	1.54	1.47
26	T	1269	CDL	C19-C18	-3.02	1.34	1.51
26	P	1270	CDL	C79-C78	-3.01	1.34	1.51
20	P	1267	PGV	C03-C02	3.00	1.59	1.50
26	C	270	CDL	C39-C38	-2.96	1.35	1.51
19	D	523	TGL	C15-CC9	-2.96	1.35	1.51
26	P	1270	CDL	C19-C18	-2.95	1.35	1.51
26	C	270	CDL	C62-C61	-2.94	1.35	1.51
18	N	515	HEA	C1C-CHC	2.94	1.49	1.41
26	C	270	CDL	C22-C21	-2.94	1.35	1.51
23	O	229	CHD	C11-C9	2.93	1.58	1.53
26	G	269	CDL	C19-C18	-2.92	1.35	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	P	1270	CDL	C39-C38	-2.90	1.35	1.51
26	C	270	CDL	C82-C81	-2.88	1.35	1.51
19	N	1522	TGL	C15-CC9	-2.88	1.35	1.51
26	G	269	CDL	C22-C21	-2.86	1.35	1.51
19	Q	1523	TGL	C10-CB9	-2.86	1.35	1.51
26	C	270	CDL	C19-C18	-2.86	1.35	1.51
26	P	1270	CDL	C62-C61	-2.85	1.35	1.51
18	A	516	HEA	C18-C19	2.85	1.39	1.33
19	Q	1523	TGL	C15-CC9	-2.84	1.35	1.51
28	G	264	PEK	C2-C1	2.81	1.58	1.50
23	B	1086	CHD	C13-C14	-2.80	1.50	1.55
19	A	521	TGL	C20-CA9	-2.79	1.35	1.51
19	N	1521	TGL	C15-CC9	-2.76	1.36	1.51
19	A	521	TGL	OC1-CC1	-2.76	1.14	1.22
26	T	1269	CDL	C39-C38	-2.76	1.36	1.51
20	P	1267	PGV	O03-C19	2.75	1.41	1.33
26	P	1270	CDL	C82-C81	-2.75	1.36	1.51
18	A	516	HEA	C13-C14	2.75	1.59	1.50
26	P	1270	CDL	C42-C41	-2.75	1.36	1.51
26	T	1269	CDL	C79-C78	-2.74	1.36	1.51
26	C	270	CDL	C42-C41	-2.73	1.36	1.51
28	P	1264	PEK	C2-C1	2.71	1.58	1.50
26	T	1269	CDL	C22-C21	-2.71	1.36	1.51
23	B	1086	CHD	C15-C14	-2.70	1.48	1.54
18	N	515	HEA	CMB-C2B	2.69	1.57	1.51
26	T	1269	CDL	C82-C81	-2.68	1.36	1.51
23	C	271	CHD	C20-C17	2.67	1.59	1.54
23	O	229	CHD	C15-C14	-2.67	1.48	1.54
19	L	522	TGL	C15-CC9	-2.66	1.36	1.51
23	P	1525	CHD	C13-C12	-2.65	1.50	1.54
19	Q	1523	TGL	C20-CA9	-2.65	1.36	1.51
26	G	269	CDL	C79-C78	-2.63	1.36	1.51
26	G	269	CDL	C82-C81	-2.61	1.36	1.51
18	A	515	HEA	C3C-C2C	2.61	1.44	1.40
19	D	523	TGL	C10-CB9	-2.57	1.37	1.51
19	A	521	TGL	C15-CC9	-2.53	1.37	1.51
19	D	523	TGL	C20-CA9	-2.52	1.37	1.51
23	C	525	CHD	C18-C13	2.51	1.58	1.54
18	A	515	HEA	C16-C15	2.49	1.56	1.51
23	P	1271	CHD	C20-C17	2.48	1.58	1.54
20	C	267	PGV	C03-C02	2.46	1.58	1.50
20	P	1267	PGV	O02-C1	2.44	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	1060	CHD	C11-C9	2.43	1.57	1.53
23	C	525	CHD	C11-C12	2.41	1.57	1.53
23	O	229	CHD	C18-C13	2.40	1.58	1.54
23	P	1525	CHD	C16-C17	2.40	1.59	1.54
24	P	1272	DMU	O1-C10	2.37	1.47	1.41
18	N	515	HEA	C4C-NC	2.36	1.41	1.36
24	Z	1526	DMU	O1-C10	2.36	1.47	1.41
18	N	516	HEA	C27-C19	-2.34	1.44	1.50
19	N	1521	TGL	C20-CA9	-2.33	1.38	1.51
23	O	229	CHD	C10-C5	-2.33	1.51	1.55
26	P	1270	CDL	PB2-OB2	2.32	1.68	1.59
20	C	267	PGV	O01-C1	2.32	1.40	1.34
19	L	522	TGL	CG1-CG2	2.29	1.57	1.50
23	O	229	CHD	C4-C3	2.27	1.56	1.51
23	P	1525	CHD	C1-C10	-2.27	1.50	1.54
18	A	515	HEA	CMB-C2B	2.26	1.56	1.51
28	P	1264	PEK	C3-C2	2.23	1.60	1.52
28	T	263	PEK	C01-C02	2.20	1.57	1.50
23	P	1525	CHD	C13-C14	-2.18	1.51	1.55
23	P	1525	CHD	C16-C15	2.15	1.59	1.54
28	G	265	PEK	P-O12	2.14	1.67	1.59
18	N	516	HEA	C16-C15	2.11	1.55	1.51
18	A	516	HEA	C3C-CAC	2.10	1.52	1.47
23	C	525	CHD	C4-C3	2.09	1.55	1.51
26	C	270	CDL	CB2-C1	2.07	1.58	1.51
19	N	1522	TGL	CG3-CG2	2.07	1.57	1.50
18	N	516	HEA	CAD-C3D	2.07	1.55	1.52
18	A	516	HEA	C26-C15	2.06	1.56	1.50
18	N	516	HEA	O11-C11	2.05	1.47	1.42
18	A	516	HEA	C21-C22	2.05	1.57	1.50
23	C	525	CHD	C6-C7	-2.04	1.49	1.52
24	P	1272	DMU	C3-C4	-2.04	1.47	1.52
20	A	524	PGV	O02-C1	2.02	1.28	1.22
20	A	522	PGV	C3-C2	2.02	1.59	1.52
23	O	229	CHD	C13-C12	-2.02	1.51	1.54
18	A	516	HEA	O11-C11	2.01	1.47	1.42

All (681) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	O	229	CHD	C6-C5-C10	16.20	129.86	112.66
23	P	1271	CHD	C10-C9-C8	15.44	128.40	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	271	CHD	C10-C9-C8	14.65	127.55	111.82
23	B	1086	CHD	C1-C10-C5	14.22	128.80	107.77
23	P	1525	CHD	C6-C5-C10	13.10	126.57	112.66
23	C	525	CHD	C19-C10-C9	-12.73	93.64	111.18
23	W	1060	CHD	C10-C9-C8	12.37	125.10	111.82
23	J	60	CHD	C10-C9-C8	11.90	124.59	111.82
23	O	229	CHD	C19-C10-C9	-11.81	94.91	111.18
23	P	1525	CHD	C1-C10-C5	11.74	125.13	107.77
23	B	1086	CHD	C14-C13-C12	11.62	118.22	107.40
23	O	229	CHD	C1-C10-C5	11.41	124.65	107.77
28	G	264	PEK	C2-C3-C4	11.29	133.35	113.23
23	O	229	CHD	C17-C13-C12	10.89	127.61	117.67
23	B	1086	CHD	C6-C5-C10	10.78	124.11	112.66
23	B	1086	CHD	C18-C13-C12	-10.64	98.23	109.07
23	C	525	CHD	C6-C5-C10	10.51	123.81	112.66
23	O	229	CHD	C18-C13-C12	-10.43	98.45	109.07
23	P	1525	CHD	C19-C10-C9	-10.40	96.85	111.18
23	C	525	CHD	C1-C10-C5	10.37	123.11	107.77
23	C	525	CHD	C10-C9-C8	9.92	122.47	111.82
23	O	229	CHD	C9-C8-C7	9.85	123.66	111.88
23	O	229	CHD	C6-C5-C4	-9.59	100.15	111.19
23	P	1271	CHD	C18-C13-C12	-9.44	99.46	109.07
23	P	1525	CHD	C4-C3-C2	9.38	121.75	110.55
23	P	1525	CHD	C17-C13-C12	9.31	126.16	117.67
23	B	1086	CHD	C10-C9-C8	9.10	121.59	111.82
23	P	1525	CHD	C18-C13-C17	-9.02	97.09	111.21
23	C	271	CHD	C16-C17-C20	9.02	126.10	112.15
23	O	229	CHD	C14-C13-C12	8.82	115.61	107.40
23	P	1525	CHD	C11-C9-C10	8.77	122.77	113.73
23	C	525	CHD	C4-C3-C2	8.68	120.92	110.55
23	P	1525	CHD	C17-C13-C14	8.66	108.83	100.09
18	A	516	HEA	C13-C12-C11	-8.58	101.47	114.35
23	C	271	CHD	C6-C5-C10	8.57	121.75	112.66
23	O	229	CHD	C10-C9-C8	8.56	121.01	111.82
23	C	271	CHD	C18-C13-C12	-8.41	100.51	109.07
19	A	521	TGL	CG2-OG2-CB1	8.37	138.39	117.79
23	B	1086	CHD	C4-C3-C2	8.23	120.38	110.55
23	P	1271	CHD	C6-C5-C10	8.22	121.39	112.66
23	C	525	CHD	C17-C13-C12	8.22	125.17	117.67
19	A	521	TGL	OG2-CB1-CB2	8.05	128.85	111.50
23	C	271	CHD	C15-C14-C8	8.03	129.56	118.33
23	W	1060	CHD	C1-C10-C5	7.91	119.47	107.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1271	CHD	C15-C14-C8	7.90	129.38	118.33
23	C	271	CHD	C6-C7-C8	7.87	119.88	111.48
23	C	271	CHD	C1-C2-C3	7.85	120.54	110.47
24	M	526	DMU	O5-C6-C1	7.82	126.91	110.35
23	P	1271	CHD	C6-C7-C8	7.82	119.82	111.48
23	W	1060	CHD	C14-C8-C7	7.78	122.12	111.81
23	O	229	CHD	C5-C4-C3	7.77	124.17	112.76
23	W	1060	CHD	C5-C6-C7	7.72	122.98	114.46
23	W	1060	CHD	C13-C17-C20	7.72	128.71	119.50
23	P	1271	CHD	C5-C4-C3	7.67	124.02	112.76
23	P	1525	CHD	C9-C8-C7	7.65	121.03	111.88
23	W	1060	CHD	C16-C17-C13	7.59	111.00	103.55
23	W	1060	CHD	C4-C3-C2	7.59	119.61	110.55
23	P	1271	CHD	C11-C9-C8	7.55	121.92	110.88
23	J	60	CHD	C6-C7-C8	7.53	119.52	111.48
23	P	1271	CHD	C1-C10-C5	7.43	118.76	107.77
24	M	526	DMU	O1-C9-C8	7.40	123.14	109.69
23	B	1086	CHD	C17-C13-C14	7.37	107.52	100.09
23	B	1086	CHD	C6-C7-C8	7.36	119.34	111.48
23	C	525	CHD	C14-C13-C12	7.34	114.23	107.40
23	J	60	CHD	C1-C10-C5	7.33	118.61	107.77
23	J	60	CHD	C13-C17-C20	7.32	128.23	119.50
23	O	229	CHD	C17-C13-C14	7.32	107.47	100.09
23	J	60	CHD	C14-C13-C12	7.31	114.21	107.40
23	W	1060	CHD	C6-C5-C10	7.19	120.30	112.66
23	J	60	CHD	C1-C2-C3	7.16	119.66	110.47
24	Z	1526	DMU	O1-C9-C8	7.14	122.67	109.69
23	P	1271	CHD	C14-C13-C12	7.11	114.03	107.40
23	J	60	CHD	C6-C5-C10	7.11	120.21	112.66
24	C	272	DMU	O1-C9-C8	7.10	122.59	109.69
23	P	1271	CHD	C16-C17-C20	7.02	123.02	112.15
23	C	525	CHD	C5-C4-C3	6.94	122.94	112.76
24	Z	1526	DMU	O5-C6-C1	6.91	124.97	110.35
23	C	271	CHD	C14-C13-C12	6.91	113.83	107.40
23	W	1060	CHD	C6-C7-C8	6.91	118.85	111.48
23	B	1086	CHD	C19-C10-C5	-6.91	98.65	110.36
23	C	271	CHD	C1-C10-C5	6.90	117.97	107.77
23	O	229	CHD	C11-C9-C8	6.85	120.90	110.88
24	C	272	DMU	O16-C6-C1	6.80	118.92	108.30
23	C	271	CHD	C5-C4-C3	6.80	122.74	112.76
19	L	522	TGL	OG3-CC1-OC1	-6.78	106.47	123.59
24	P	1272	DMU	O16-C6-C1	6.76	118.86	108.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	525	CHD	O12-C12-C13	-6.73	99.65	111.03
23	B	1086	CHD	C9-C11-C12	6.71	123.17	114.30
24	P	1272	DMU	O1-C9-C8	6.71	121.88	109.69
23	J	60	CHD	C5-C4-C3	6.70	122.60	112.76
26	T	1269	CDL	OB6-CB5-C51	6.67	125.87	111.50
23	P	1525	CHD	C10-C9-C8	6.66	118.97	111.82
23	J	60	CHD	C5-C6-C7	6.65	121.80	114.46
23	P	1271	CHD	C19-C10-C9	-6.63	102.04	111.18
23	J	60	CHD	C4-C3-C2	6.62	118.46	110.55
23	W	1060	CHD	C5-C4-C3	6.62	122.47	112.76
23	P	1271	CHD	C4-C3-C2	6.58	118.41	110.55
23	P	1271	CHD	C5-C6-C7	6.57	121.71	114.46
23	O	229	CHD	C18-C13-C17	-6.50	101.04	111.21
23	W	1060	CHD	C17-C13-C12	6.47	123.58	117.67
23	W	1060	CHD	C9-C11-C12	6.47	122.84	114.30
24	Z	1526	DMU	O16-C6-C1	6.40	118.30	108.30
24	M	526	DMU	O1-C10-C5	6.39	123.87	110.35
23	J	60	CHD	C17-C13-C12	6.39	123.50	117.67
23	O	229	CHD	C18-C13-C14	-6.38	101.23	111.21
23	C	271	CHD	C5-C6-C7	6.37	121.49	114.46
23	B	1086	CHD	C1-C2-C3	6.34	118.61	110.47
23	P	1525	CHD	O12-C12-C13	-6.31	100.36	111.03
24	C	272	DMU	O1-C10-C5	6.29	123.66	110.35
23	P	1271	CHD	C1-C2-C3	6.26	118.50	110.47
23	W	1060	CHD	C15-C14-C8	6.23	127.05	118.33
23	O	229	CHD	O12-C12-C13	-6.23	100.50	111.03
23	C	525	CHD	C18-C13-C12	-6.23	102.73	109.07
18	N	515	HEA	C1B-C2B-C3B	-6.21	102.68	107.00
23	J	60	CHD	C14-C8-C7	6.19	120.02	111.81
23	W	1060	CHD	C1-C2-C3	6.18	118.40	110.47
24	Z	1526	DMU	O1-C10-C5	6.18	123.43	110.35
23	P	1525	CHD	C16-C17-C20	6.15	121.66	112.15
24	C	272	DMU	C18-O16-C6	6.14	124.02	113.84
23	C	525	CHD	C23-C22-C20	-6.12	106.48	114.72
23	J	60	CHD	C16-C17-C13	6.11	109.55	103.55
23	P	1525	CHD	C11-C12-C13	6.08	117.49	111.24
23	J	60	CHD	C15-C14-C13	6.05	109.48	103.55
23	O	229	CHD	C11-C12-C13	6.04	117.45	111.24
23	W	1060	CHD	C14-C13-C12	6.04	113.03	107.40
23	P	1525	CHD	C18-C13-C14	-6.03	101.77	111.21
24	P	1272	DMU	O1-C10-C5	6.02	123.10	110.35
20	P	1268	PGV	O03-C19-C20	6.01	130.77	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	271	CHD	C17-C13-C12	5.94	123.09	117.67
26	T	1269	CDL	OA6-CA5-C11	5.94	124.30	111.50
23	C	525	CHD	C13-C17-C20	5.93	126.58	119.50
28	G	264	PEK	O01-C1-O02	-5.92	109.38	123.70
23	J	60	CHD	C18-C13-C12	-5.91	103.05	109.07
18	A	515	HEA	C26-C15-C16	5.90	125.20	115.27
23	O	229	CHD	C1-C2-C3	5.89	118.03	110.47
23	C	271	CHD	C11-C9-C8	5.82	119.40	110.88
23	C	525	CHD	C18-C13-C14	-5.81	102.12	111.21
23	C	271	CHD	C15-C14-C13	5.79	109.23	103.55
23	P	1271	CHD	C17-C13-C14	5.77	105.91	100.09
24	P	1272	DMU	O5-C4-C3	5.76	121.89	109.75
23	W	1060	CHD	C2-C1-C10	5.75	122.65	112.78
19	A	521	TGL	OG3-CC1-OC1	-5.75	109.09	123.59
26	G	269	CDL	OB6-CB5-C51	5.71	123.82	111.50
23	P	1271	CHD	C2-C1-C10	5.70	122.56	112.78
18	A	515	HEA	C3C-C4C-NC	5.70	116.58	109.21
24	P	1272	DMU	O1-C9-C11	5.69	120.59	106.44
19	N	1521	TGL	CG2-OG2-CB1	5.64	131.67	117.79
23	C	271	CHD	C2-C1-C10	5.62	122.42	112.78
23	O	229	CHD	C16-C17-C20	5.62	120.84	112.15
24	M	526	DMU	C2-C3-C4	5.61	123.78	110.93
26	C	270	CDL	CB4-OB6-CB5	-5.60	103.99	117.79
18	N	515	HEA	C27-C19-C20	5.60	124.69	115.27
23	B	1086	CHD	C19-C10-C9	-5.60	103.47	111.18
24	P	1272	DMU	C8-C7-C5	5.60	120.60	110.82
23	C	525	CHD	C17-C13-C14	5.59	105.73	100.09
23	J	60	CHD	C2-C1-C10	5.59	122.36	112.78
23	J	60	CHD	C15-C14-C8	5.58	126.14	118.33
18	N	515	HEA	C27-C19-C18	-5.58	109.37	123.68
23	P	1525	CHD	C5-C4-C3	5.54	120.89	112.76
18	A	515	HEA	C1B-C2B-C3B	-5.53	103.15	107.00
23	J	60	CHD	C11-C12-C13	5.51	116.91	111.24
18	A	516	HEA	C27-C19-C20	5.50	124.52	115.27
23	C	525	CHD	C2-C1-C10	5.50	122.21	112.78
24	C	272	DMU	O5-C4-C57	5.49	120.08	106.44
24	Z	1526	DMU	C8-C7-C5	5.47	120.37	110.82
19	N	1522	TGL	OG2-CB1-CB2	5.46	123.27	111.50
23	J	60	CHD	C16-C17-C20	5.45	120.58	112.15
23	P	1271	CHD	C16-C17-C13	5.44	108.89	103.55
23	B	1086	CHD	C11-C9-C10	5.43	119.32	113.73
28	P	1264	PEK	O01-C1-O02	-5.42	110.60	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	P	1271	CHD	C23-C22-C20	-5.40	107.44	114.72
24	C	272	DMU	C8-C7-C5	5.40	120.25	110.82
23	C	525	CHD	C11-C12-C13	5.38	116.77	111.24
18	A	515	HEA	C20-C21-C22	-5.37	94.24	111.88
23	C	271	CHD	C17-C13-C14	5.36	105.50	100.09
23	C	271	CHD	C4-C5-C10	5.35	118.34	112.66
23	P	1525	CHD	O3-C3-C4	5.32	120.44	109.85
23	P	1525	CHD	C14-C13-C12	5.31	112.35	107.40
23	P	1271	CHD	C14-C8-C7	5.31	118.85	111.81
23	J	60	CHD	C4-C5-C10	5.31	118.29	112.66
24	M	526	DMU	C8-C7-C5	5.30	120.08	110.82
23	C	271	CHD	C4-C3-C2	5.29	116.88	110.55
23	C	271	CHD	C16-C17-C13	5.28	108.73	103.55
19	A	521	TGL	OG3-CC1-CC2	5.28	128.48	111.91
24	C	272	DMU	O5-C6-C1	5.28	121.52	110.35
23	W	1060	CHD	C11-C12-C13	5.27	116.66	111.24
23	C	525	CHD	O12-C12-C11	-5.26	98.40	109.12
23	O	229	CHD	C13-C14-C8	5.25	121.44	114.74
24	Z	1526	DMU	O5-C4-C57	5.24	119.47	106.44
20	C	268	PGV	O01-C1-C2	5.24	122.80	111.50
24	C	272	DMU	O5-C4-C3	5.23	120.79	109.75
20	C	268	PGV	O03-C19-C20	5.23	128.33	111.91
23	J	60	CHD	C11-C9-C8	5.23	118.53	110.88
23	J	60	CHD	C9-C11-C12	5.22	121.20	114.30
23	C	525	CHD	C9-C8-C7	5.21	118.10	111.88
24	Z	1526	DMU	O5-C4-C3	5.20	120.71	109.75
23	P	1271	CHD	O7-C7-C6	-5.15	97.17	109.94
23	O	229	CHD	C4-C3-C2	5.15	116.70	110.55
23	W	1060	CHD	C1-C10-C9	-5.13	103.30	111.35
23	C	525	CHD	C5-C6-C7	5.11	120.10	114.46
23	P	1525	CHD	C6-C5-C4	-5.09	105.33	111.19
23	B	1086	CHD	C15-C14-C8	5.09	125.44	118.33
23	J	60	CHD	C6-C5-C4	-5.04	105.38	111.19
23	W	1060	CHD	C19-C10-C5	-5.04	101.82	110.36
24	Z	1526	DMU	O1-C9-C11	5.04	118.96	106.44
23	P	1525	CHD	C1-C10-C9	-5.03	103.44	111.35
19	A	521	TGL	CG3-OG3-CC1	5.03	135.76	117.12
23	C	525	CHD	C22-C23-C24	-5.02	102.81	113.59
19	D	523	TGL	OG2-CB1-CB2	-5.01	100.69	111.50
23	B	1086	CHD	C1-C10-C9	-5.01	103.48	111.35
23	C	525	CHD	C11-C9-C10	5.00	118.88	113.73
24	C	272	DMU	C2-C3-C4	4.99	122.36	110.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	270	CDL	OA6-CA5-C11	4.98	122.23	111.50
23	C	525	CHD	C9-C11-C12	4.95	120.84	114.30
23	C	271	CHD	C18-C13-C17	-4.93	103.49	111.21
23	P	1525	CHD	C15-C14-C13	4.93	108.39	103.55
28	P	1264	PEK	O03-C01-C02	-4.93	94.08	108.43
24	M	526	DMU	O5-C4-C3	4.93	120.14	109.75
23	B	1086	CHD	C18-C13-C14	-4.92	103.51	111.21
23	J	60	CHD	C1-C10-C9	-4.91	103.63	111.35
23	C	271	CHD	C11-C12-C13	4.91	116.28	111.24
23	W	1060	CHD	C6-C5-C4	-4.91	105.54	111.19
28	G	1263	PEK	O01-C1-C2	4.91	122.07	111.50
23	J	60	CHD	C22-C20-C17	4.90	120.40	110.28
20	N	1266	PGV	O03-C19-O04	-4.87	111.31	123.59
23	P	1525	CHD	C9-C11-C12	4.86	120.71	114.30
28	P	1265	PEK	O03-C21-C22	4.85	127.14	111.91
20	C	267	PGV	C27-C26-C25	-4.85	89.79	114.42
18	N	516	HEA	C4B-C3B-C2B	-4.85	103.48	106.87
18	N	515	HEA	C26-C15-C16	4.84	123.41	115.27
20	N	1266	PGV	O03-C19-C20	4.83	127.06	111.91
23	P	1271	CHD	C18-C13-C17	-4.82	103.66	111.21
19	L	522	TGL	OG3-CC1-CC2	4.81	127.01	111.91
23	P	1271	CHD	C9-C11-C12	4.81	120.65	114.30
23	P	1525	CHD	O12-C12-C11	-4.81	99.33	109.12
23	P	1525	CHD	C6-C7-C8	4.76	116.56	111.48
18	A	516	HEA	C20-C19-C18	-4.76	111.49	121.12
28	T	263	PEK	O01-C1-C2	4.73	121.70	111.50
23	C	271	CHD	C9-C11-C12	4.72	120.53	114.30
23	C	271	CHD	C6-C5-C4	-4.72	105.76	111.19
23	W	1060	CHD	C15-C14-C13	4.71	108.18	103.55
23	B	1086	CHD	C5-C4-C3	4.71	119.68	112.76
26	P	1270	CDL	OA6-CA5-C11	4.70	121.64	111.50
23	P	1525	CHD	C19-C10-C5	-4.70	102.39	110.36
23	C	525	CHD	C18-C13-C17	-4.70	103.86	111.21
23	P	1525	CHD	C19-C10-C1	4.69	115.81	108.26
24	Z	1526	DMU	C2-C3-C4	4.67	121.63	110.93
18	A	515	HEA	C13-C12-C11	4.66	121.34	114.35
18	N	516	HEA	C13-C12-C11	-4.64	107.38	114.35
28	P	1264	PEK	C2-C3-C4	4.64	121.49	113.23
20	A	524	PGV	C02-O01-C1	4.63	129.18	117.79
23	B	1086	CHD	C17-C13-C12	4.62	121.88	117.67
23	J	60	CHD	C9-C10-C5	4.62	115.06	108.58
23	P	1525	CHD	C22-C20-C17	-4.61	100.76	110.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	515	HEA	C3C-C4C-NC	4.61	115.17	109.21
23	O	229	CHD	C15-C14-C13	4.58	108.05	103.55
23	C	271	CHD	C23-C22-C20	-4.57	108.56	114.72
24	P	1272	DMU	O5-C6-C1	4.57	120.02	110.35
19	D	523	TGL	OG2-CB1-OB1	4.56	134.72	123.70
18	A	515	HEA	C16-C17-C18	4.55	126.85	111.88
26	G	269	CDL	OA6-CA5-C11	4.55	121.30	111.50
20	P	1268	PGV	O01-C1-C2	4.54	121.29	111.50
23	B	1086	CHD	O12-C12-C11	-4.53	99.90	109.12
23	W	1060	CHD	C11-C9-C8	4.52	117.50	110.88
23	C	271	CHD	C19-C10-C9	-4.51	104.96	111.18
23	B	1086	CHD	C18-C13-C17	-4.51	104.15	111.21
23	C	271	CHD	O7-C7-C6	-4.50	98.77	109.94
19	A	521	TGL	OG3-CG3-CG2	4.48	121.46	108.43
23	C	525	CHD	C15-C14-C13	4.45	107.92	103.55
24	P	1272	DMU	O5-C4-C57	4.45	117.51	106.44
19	N	1521	TGL	OG2-CB1-CB2	4.45	121.10	111.50
18	N	515	HEA	C12-C11-C3B	4.44	124.21	112.56
19	L	522	TGL	CC3-CC2-CC1	4.42	129.70	113.62
23	O	229	CHD	O12-C12-C11	-4.42	100.12	109.12
23	W	1060	CHD	C18-C13-C12	-4.41	104.57	109.07
23	B	1086	CHD	C9-C8-C7	4.41	117.15	111.88
23	W	1060	CHD	C4-C5-C10	4.41	117.34	112.66
23	C	525	CHD	C6-C5-C4	-4.38	106.15	111.19
23	P	1271	CHD	C11-C12-C13	4.38	115.74	111.24
23	P	1271	CHD	C15-C14-C13	4.37	107.84	103.55
23	P	1525	CHD	C4-C5-C10	-4.36	108.03	112.66
24	M	526	DMU	C18-O16-C6	4.36	121.06	113.84
19	D	523	TGL	CG1-OG1-CA1	4.34	133.20	117.12
23	P	1271	CHD	C4-C5-C10	4.34	117.26	112.66
19	Q	1523	TGL	OG3-CC1-CC2	4.32	125.45	111.91
23	B	1086	CHD	C14-C8-C9	4.31	115.62	109.71
23	W	1060	CHD	C16-C17-C20	4.30	118.81	112.15
26	C	270	CDL	OB8-CB7-C71	4.29	125.37	111.91
24	M	526	DMU	O5-C4-C57	4.28	117.09	106.44
20	A	524	PGV	C8-C9-C10	-4.27	95.19	113.79
19	A	521	TGL	OG1-CA1-CA2	4.27	125.30	111.91
24	C	272	DMU	C6-C1-C2	4.25	118.85	110.00
22	B	230	PSC	O01-C1-C2	4.25	120.66	111.50
19	N	1521	TGL	CG3-OG3-CC1	4.24	132.83	117.12
23	B	1086	CHD	C15-C14-C13	4.22	107.69	103.55
23	W	1060	CHD	C9-C10-C5	4.22	114.51	108.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	515	HEA	C16-C17-C18	4.22	125.75	111.88
26	C	270	CDL	OA8-CA7-C31	4.21	125.13	111.91
19	L	522	TGL	OG1-CG1-CG2	4.21	120.68	108.43
24	P	1272	DMU	C7-C8-C9	4.16	117.66	110.24
23	B	1086	CHD	C11-C9-C8	4.16	116.96	110.88
26	P	1270	CDL	OB8-CB7-C71	4.16	124.96	111.91
19	A	521	TGL	OB1-CB1-CB2	-4.16	107.52	123.73
23	P	1271	CHD	C11-C9-C10	-4.15	109.45	113.73
24	Z	1526	DMU	O7-C10-C5	-4.14	97.37	108.10
23	C	525	CHD	C6-C7-C8	4.14	115.90	111.48
23	W	1060	CHD	O7-C7-C6	-4.14	99.67	109.94
18	N	516	HEA	C17-C18-C19	4.13	137.60	127.66
23	O	229	CHD	C1-C10-C9	-4.13	104.86	111.35
18	N	515	HEA	C16-C15-C14	-4.12	112.78	121.12
23	B	1086	CHD	C22-C23-C24	-4.09	104.79	113.59
23	P	1525	CHD	C13-C17-C20	4.09	124.38	119.50
24	P	1272	DMU	C1-C2-C3	4.09	119.02	109.68
23	P	1271	CHD	C17-C13-C12	4.09	121.40	117.67
19	L	522	TGL	OG1-CA1-CA2	4.07	124.69	111.91
18	A	515	HEA	C12-C11-C3B	4.06	123.21	112.56
20	N	1524	PGV	O01-C1-C2	4.05	120.24	111.50
19	L	522	TGL	CG2-OG2-CB1	4.05	127.77	117.79
23	B	1086	CHD	O12-C12-C13	-4.05	104.19	111.03
22	O	1230	PSC	O01-C1-C2	4.02	120.16	111.50
28	G	265	PEK	O03-C21-C22	4.01	124.51	111.91
23	P	1525	CHD	C23-C22-C20	-4.00	109.33	114.72
24	Z	1526	DMU	C7-C8-C9	3.99	117.36	110.24
24	P	1272	DMU	C6-C1-C2	3.99	118.31	110.00
23	J	60	CHD	C19-C10-C5	-3.99	103.60	110.36
18	A	516	HEA	CAD-CBD-CGD	-3.99	105.98	112.67
18	A	516	HEA	C4B-C3B-C2B	-3.98	104.09	106.87
18	N	515	HEA	CAA-CBA-CGA	-3.95	106.04	112.67
23	O	229	CHD	C4-C5-C10	-3.95	108.46	112.66
24	C	272	DMU	C7-C8-C9	3.91	117.22	110.24
24	P	1272	DMU	C6-O5-C4	3.91	121.36	113.69
23	J	60	CHD	C18-C13-C14	-3.90	105.11	111.21
23	P	1525	CHD	C2-C1-C10	3.88	119.43	112.78
24	C	272	DMU	O1-C9-C11	3.87	116.06	106.44
24	C	272	DMU	O7-C3-C4	3.85	119.99	109.45
24	C	272	DMU	O7-C3-C2	3.82	117.45	107.28
23	O	229	CHD	C14-C8-C9	3.81	114.94	109.71
20	P	1267	PGV	C8-C9-C10	-3.80	97.23	113.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	D	523	TGL	CG2-OG2-CB1	3.78	127.09	117.79
23	P	1271	CHD	O12-C12-C13	-3.76	104.67	111.03
20	N	1266	PGV	O01-C1-O02	-3.75	114.63	123.70
28	T	263	PEK	O03-C01-C02	3.74	119.32	108.43
19	D	523	TGL	OG1-CA1-CA2	3.72	123.58	111.91
20	A	522	PGV	O03-C19-C20	3.72	123.58	111.91
24	M	526	DMU	C11-C9-C8	3.72	121.71	113.00
28	G	264	PEK	C24-C23-C22	-3.69	99.91	113.19
23	P	1271	CHD	O12-C12-C11	-3.69	101.61	109.12
23	W	1060	CHD	C22-C20-C17	3.69	117.90	110.28
23	P	1525	CHD	O7-C7-C6	-3.69	100.80	109.94
24	P	1272	DMU	C2-C3-C4	3.68	119.35	110.93
28	G	264	PEK	C25-C24-C23	-3.66	95.83	114.42
23	P	1525	CHD	C13-C14-C8	3.66	119.41	114.74
18	N	515	HEA	C4B-C3B-C2B	3.65	109.42	106.87
23	C	271	CHD	O12-C12-C11	-3.63	101.72	109.12
23	B	1086	CHD	C14-C8-C7	3.63	116.62	111.81
24	Z	1526	DMU	O7-C3-C2	3.62	116.92	107.28
23	O	229	CHD	C2-C1-C10	3.62	118.98	112.78
23	P	1525	CHD	C11-C9-C8	3.60	116.15	110.88
23	W	1060	CHD	O12-C12-C11	-3.60	101.79	109.12
28	P	1265	PEK	O01-C1-C2	3.58	119.23	111.50
18	A	515	HEA	CAA-CBA-CGA	-3.57	106.68	112.67
18	A	516	HEA	CAA-CBA-CGA	-3.56	106.70	112.67
24	C	272	DMU	C11-C9-C8	3.56	121.34	113.00
26	C	270	CDL	C52-C51-CB5	-3.53	100.77	113.62
28	G	265	PEK	O03-C21-O04	-3.53	114.69	123.59
26	C	270	CDL	OB8-CB7-OB9	-3.52	114.70	123.59
23	W	1060	CHD	C18-C13-C17	-3.51	105.71	111.21
24	P	1272	DMU	C10-O1-C9	3.51	120.58	113.69
23	C	525	CHD	C11-C9-C8	3.51	116.01	110.88
23	P	1525	CHD	C14-C8-C9	3.48	114.49	109.71
28	P	1265	PEK	O03-C21-O04	-3.47	114.83	123.59
20	A	524	PGV	O03-C19-C20	3.47	122.79	111.91
23	O	229	CHD	C15-C14-C8	3.47	123.18	118.33
26	C	270	CDL	OA8-CA6-CA4	3.46	118.50	108.43
23	W	1060	CHD	C18-C13-C14	-3.44	105.82	111.21
23	P	1271	CHD	C21-C20-C17	3.43	118.18	112.92
24	C	272	DMU	C10-O1-C9	3.43	120.42	113.69
24	M	526	DMU	O5-C6-O16	3.42	118.06	109.97
26	T	1269	CDL	OA6-CA5-OA7	-3.41	115.45	123.70
23	W	1060	CHD	C13-C14-C8	3.41	119.09	114.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	M	526	DMU	O16-C6-C1	3.41	113.62	108.30
23	J	60	CHD	O12-C12-C11	-3.40	102.21	109.12
24	C	272	DMU	O7-C10-C5	3.37	116.82	108.10
20	N	1524	PGV	C02-O01-C1	3.36	126.05	117.79
26	P	1270	CDL	OA8-CA7-C31	3.34	122.38	111.91
24	C	272	DMU	C6-O5-C4	3.33	120.23	113.69
19	Q	1523	TGL	CG3-OG3-CC1	3.33	129.45	117.12
23	O	229	CHD	O3-C3-C4	3.32	116.45	109.85
23	B	1086	CHD	C6-C5-C4	-3.31	107.38	111.19
22	O	1230	PSC	O03-C19-C20	3.31	122.29	111.91
23	C	525	CHD	C14-C8-C9	3.31	114.25	109.71
24	M	526	DMU	O1-C9-C11	3.29	114.61	106.44
23	J	60	CHD	C18-C13-C17	-3.27	106.09	111.21
19	N	1522	TGL	OG3-CG3-CG2	3.27	117.94	108.43
23	O	229	CHD	C9-C11-C12	3.25	118.59	114.30
24	M	526	DMU	C57-C4-C3	3.25	122.77	113.33
24	Z	1526	DMU	C6-O5-C4	3.24	120.05	113.69
23	C	525	CHD	C15-C14-C8	3.23	122.84	118.33
23	J	60	CHD	C17-C13-C14	3.22	103.34	100.09
28	G	265	PEK	O01-C1-C2	3.21	118.42	111.50
26	P	1270	CDL	O1-C1-CA2	-3.21	98.30	109.56
26	T	1269	CDL	OB6-CB5-OB7	-3.20	115.97	123.70
18	N	516	HEA	C1B-C2B-C3B	3.20	109.22	107.00
19	Q	1523	TGL	OG2-CB1-CB2	3.19	118.38	111.50
20	A	522	PGV	C8-C9-C10	-3.19	99.90	113.79
19	Q	1523	TGL	OG1-CA1-OA1	-3.19	115.54	123.59
24	M	526	DMU	C1-C2-C3	3.17	116.93	109.68
19	N	1521	TGL	OG1-CA1-CA2	3.17	121.86	111.91
18	N	516	HEA	OMA-CMA-C3A	-3.17	118.01	124.91
18	A	516	HEA	CMC-C2C-C1C	-3.16	123.60	128.46
19	N	1522	TGL	OG1-CA1-CA2	3.14	121.77	111.91
20	P	1267	PGV	C27-C26-C25	-3.14	98.48	114.42
23	C	525	CHD	C13-C14-C8	3.14	118.75	114.74
23	B	1086	CHD	O3-C3-C4	3.13	116.08	109.85
24	M	526	DMU	C10-C5-C7	3.13	116.51	110.00
28	G	1263	PEK	O03-C21-C22	3.13	121.72	111.91
24	Z	1526	DMU	C1-C2-C3	3.11	116.79	109.68
20	C	267	PGV	C8-C9-C10	-3.11	100.23	113.79
24	Z	1526	DMU	C10-O1-C9	3.11	119.79	113.69
18	N	516	HEA	CBD-CAD-C3D	3.10	118.20	112.49
19	N	1521	TGL	OG3-CC1-CC2	3.10	121.63	111.91
19	D	523	TGL	C21-C20-CA9	3.10	130.14	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	P	1268	PGV	O04-C19-C20	-3.09	111.66	123.73
19	N	1522	TGL	OG1-CG1-CG2	3.09	117.43	108.43
28	P	1264	PEK	C03-C02-C01	-3.08	104.50	111.79
28	G	1263	PEK	O03-C01-C02	3.08	117.41	108.43
24	M	526	DMU	O7-C10-C5	-3.08	100.12	108.10
19	A	521	TGL	OG2-CG2-CG1	3.08	119.53	108.40
20	P	1267	PGV	O03-C01-C02	3.07	117.37	108.43
20	A	522	PGV	O03-C01-C02	3.06	117.35	108.43
19	D	523	TGL	CB3-CB2-CB1	3.06	124.76	113.62
23	B	1086	CHD	O7-C7-C6	-3.05	102.37	109.94
23	C	271	CHD	C19-C10-C1	-3.03	103.38	108.26
24	M	526	DMU	O7-C10-O1	-3.02	102.23	110.67
24	M	526	DMU	C7-C8-C9	3.02	115.62	110.24
20	N	1524	PGV	O03-C19-C20	3.02	121.38	111.91
19	N	1522	TGL	CC3-CC2-CC1	3.02	124.59	113.62
23	P	1271	CHD	O3-C3-C4	-3.01	103.86	109.85
23	J	60	CHD	O7-C7-C6	-3.01	102.48	109.94
26	P	1270	CDL	OB8-CB7-OB9	-3.00	116.01	123.59
23	B	1086	CHD	C13-C17-C20	2.98	123.05	119.50
24	P	1272	DMU	O5-C6-O16	2.97	117.00	109.97
26	G	269	CDL	OB6-CB5-OB7	-2.96	116.54	123.70
18	A	516	HEA	CMB-C2B-C1B	2.96	133.01	128.46
23	C	525	CHD	O3-C3-C4	2.96	115.74	109.85
23	B	1086	CHD	O7-C7-C8	-2.94	102.84	109.43
24	P	1272	DMU	C10-C5-C7	2.94	116.12	110.00
20	A	524	PGV	O01-C02-C01	2.94	119.04	108.40
19	D	523	TGL	OG3-CC1-CC2	2.92	121.07	111.91
18	A	516	HEA	CMC-C2C-C3C	2.91	130.13	124.68
24	C	272	DMU	O4-C7-C5	2.91	117.07	110.35
23	W	1060	CHD	C9-C8-C7	2.89	115.33	111.88
23	C	525	CHD	C16-C17-C20	2.87	116.60	112.15
24	Z	1526	DMU	C10-C5-C7	2.87	115.97	110.00
24	M	526	DMU	C10-O1-C9	2.86	119.31	113.69
18	N	516	HEA	O11-C11-C3B	-2.86	103.75	112.00
23	C	525	CHD	C1-C10-C9	-2.85	106.87	111.35
26	T	1269	CDL	OA8-CA7-C31	2.84	120.83	111.91
26	P	1270	CDL	OA8-CA7-OA9	-2.84	116.42	123.59
28	T	263	PEK	O03-C21-C22	2.84	120.82	111.91
24	C	272	DMU	C1-C2-C3	2.84	116.16	109.68
23	P	1525	CHD	C1-C2-C3	2.83	114.10	110.47
23	O	229	CHD	C11-C9-C10	2.83	116.65	113.73
20	P	1267	PGV	C3-C2-C1	-2.83	103.33	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G	269	CDL	OA8-CA7-C31	2.82	120.77	111.91
24	Z	1526	DMU	O49-C1-C6	-2.82	103.20	110.05
19	D	523	TGL	C10-CB9-CB8	2.81	128.68	114.42
19	Q	1523	TGL	OG1-CA1-CA2	2.80	120.69	111.91
20	C	268	PGV	O04-C19-C20	-2.80	112.82	123.73
19	D	523	TGL	CG3-OG3-CC1	2.79	127.45	117.12
26	G	269	CDL	OA6-CA5-OA7	-2.79	116.97	123.70
20	C	267	PGV	C4-C3-C2	-2.78	103.20	113.19
19	L	522	TGL	OG2-CG2-CG1	2.77	118.43	108.40
20	P	1268	PGV	C03-C02-C01	-2.77	105.24	111.79
26	C	270	CDL	O1-C1-CB2	2.77	119.27	109.56
20	C	267	PGV	C3-C2-C1	-2.77	103.55	113.62
28	T	263	PEK	C01-O03-C21	2.77	127.36	117.12
24	P	1272	DMU	O7-C10-O1	2.76	118.37	110.67
19	Q	1523	TGL	OG3-CC1-OC1	-2.75	116.64	123.59
23	C	525	CHD	C4-C5-C10	-2.74	109.74	112.66
24	C	272	DMU	O5-C6-O16	2.74	116.47	109.97
22	B	230	PSC	C29-C28-C27	-2.74	100.52	114.42
20	N	1266	PGV	C01-O03-C19	-2.73	107.00	117.12
23	J	60	CHD	C9-C8-C7	2.73	115.14	111.88
24	M	526	DMU	O4-C7-C8	2.73	116.66	110.35
24	P	1272	DMU	O7-C10-C5	2.72	115.16	108.10
23	O	229	CHD	C22-C23-C24	-2.72	107.74	113.59
19	D	523	TGL	C11-C10-CB9	2.72	128.24	114.42
28	P	1264	PEK	C24-C23-C22	-2.72	103.43	113.19
23	C	525	CHD	O7-C7-C6	-2.70	103.25	109.94
24	Z	1526	DMU	C6-C1-C2	2.70	115.62	110.00
19	N	1522	TGL	CG2-OG2-CB1	2.69	124.42	117.79
26	P	1270	CDL	CB4-OB6-CB5	-2.68	111.19	117.79
20	A	524	PGV	C4-C3-C2	-2.68	103.55	113.19
23	W	1060	CHD	C17-C13-C14	2.68	102.80	100.09
24	Z	1526	DMU	O3-C5-C7	2.68	116.54	110.35
18	A	515	HEA	CAD-C3D-C2D	2.67	134.93	127.25
24	C	272	DMU	C10-C5-C7	2.67	115.56	110.00
19	N	1521	TGL	OG3-CG3-CG2	2.67	116.20	108.43
26	C	270	CDL	OB6-CB5-C51	2.66	117.23	111.50
19	N	1522	TGL	OG3-CC1-OC1	-2.65	116.91	123.59
22	O	1230	PSC	C31-C30-C29	-2.64	101.02	114.42
26	C	270	CDL	C42-C41-C40	2.64	127.83	114.42
24	Z	1526	DMU	O5-C6-O16	2.64	116.22	109.97
23	C	525	CHD	C19-C10-C1	2.63	112.51	108.26
28	G	264	PEK	C26-C25-C24	-2.63	101.06	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	P	1267	PGV	C03-C02-C01	-2.62	105.58	111.79
26	P	1270	CDL	OB6-CB4-CB6	2.62	117.90	108.40
23	W	1060	CHD	C11-C9-C10	2.61	116.42	113.73
23	B	1086	CHD	C4-C5-C10	-2.61	109.89	112.66
20	N	1524	PGV	O01-C02-C01	2.60	117.83	108.40
23	C	271	CHD	C14-C8-C7	2.60	115.25	111.81
18	N	515	HEA	C17-C18-C19	-2.59	121.41	127.66
28	G	264	PEK	C31-C30-C29	-2.59	101.30	114.42
28	G	264	PEK	O01-C1-C2	2.58	117.07	111.50
20	C	267	PGV	O01-C02-C03	-2.58	99.05	108.40
26	G	269	CDL	CA6-OA8-CA7	2.58	126.66	117.12
26	T	1269	CDL	OB8-CB7-OB9	-2.58	117.09	123.59
24	M	526	DMU	O3-C5-C7	2.57	116.28	110.35
23	P	1525	CHD	O7-C7-C8	-2.56	103.70	109.43
26	G	269	CDL	OB8-CB7-OB9	-2.56	117.13	123.59
20	P	1267	PGV	O14-P-O13	2.56	124.89	112.24
26	T	1269	CDL	C83-C82-C81	2.56	127.40	114.42
19	N	1521	TGL	CG1-OG1-CA1	2.54	126.51	117.12
26	P	1270	CDL	C39-C38-C37	2.53	127.29	114.42
26	G	269	CDL	C82-C81-C80	2.53	127.28	114.42
26	T	1269	CDL	C80-C79-C78	2.52	127.24	114.42
28	T	263	PEK	C02-O01-C1	2.52	124.00	117.79
24	M	526	DMU	C6-O5-C4	2.51	118.61	113.69
20	N	1266	PGV	C02-O01-C1	2.51	123.97	117.79
26	P	1270	CDL	C42-C41-C40	2.51	127.15	114.42
20	A	522	PGV	O03-C19-O04	-2.50	117.28	123.59
24	P	1272	DMU	C57-C4-C3	2.50	120.60	113.33
26	C	270	CDL	OA8-CA7-OA9	-2.50	117.29	123.59
20	C	267	PGV	O12-P-O13	-2.48	99.36	109.07
23	J	60	CHD	C19-C10-C9	-2.48	107.77	111.18
19	A	521	TGL	C15-CC9-CC8	2.47	126.96	114.42
22	B	230	PSC	O03-C19-C20	2.47	119.64	111.91
28	P	1265	PEK	O03-C01-C02	2.46	115.61	108.43
26	T	1269	CDL	CB6-OB8-CB7	2.46	126.24	117.12
20	N	1266	PGV	O01-C1-C2	2.46	116.80	111.50
18	N	516	HEA	CAD-CBD-CGD	-2.46	108.55	112.67
20	N	1524	PGV	C01-O03-C19	2.46	126.21	117.12
20	P	1267	PGV	O01-C1-O02	-2.45	117.77	123.70
19	Q	1523	TGL	OG2-CG2-CG3	2.45	117.29	108.40
28	P	1264	PEK	O04-C21-C22	2.45	133.31	123.73
28	G	264	PEK	O02-C1-C2	2.45	133.30	123.73
23	C	525	CHD	O7-C7-C8	-2.45	103.95	109.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	271	CHD	O12-C12-C13	-2.44	106.90	111.03
18	N	516	HEA	CMC-C2C-C1C	-2.44	124.72	128.46
20	C	267	PGV	O01-C1-O02	-2.44	117.81	123.70
19	N	1521	TGL	OG3-CC1-OC1	-2.42	117.48	123.59
26	C	270	CDL	C63-C62-C61	2.42	126.71	114.42
19	N	1522	TGL	CB3-CB2-CB1	2.41	122.38	113.62
20	P	1268	PGV	O03-C19-O04	-2.40	117.53	123.59
22	O	1230	PSC	O03-C19-O04	-2.40	117.53	123.59
20	A	522	PGV	C24-C23-C22	2.40	126.61	114.42
18	N	515	HEA	C20-C21-C22	-2.40	103.99	111.88
24	P	1272	DMU	O7-C3-C4	2.40	116.02	109.45
19	A	521	TGL	CB7-CB6-CB5	-2.40	102.26	114.42
18	N	516	HEA	CAA-CBA-CGA	-2.40	108.65	112.67
20	N	1266	PGV	O14-P-O11	2.39	118.85	107.75
19	L	522	TGL	CA5-CA4-CA3	-2.38	102.33	114.42
26	T	1269	CDL	OB8-CB6-CB4	2.38	115.37	108.43
26	G	269	CDL	C83-C82-C81	2.38	126.51	114.42
23	P	1525	CHD	C18-C13-C12	-2.38	106.64	109.07
22	B	230	PSC	C02-O01-C1	2.38	123.64	117.79
19	L	522	TGL	OG2-CB1-CB2	2.37	116.61	111.50
28	P	1264	PEK	O01-C1-C2	2.37	116.60	111.50
18	N	515	HEA	CAD-C3D-C2D	2.37	134.04	127.25
20	C	268	PGV	O03-C01-C02	2.36	115.32	108.43
26	C	270	CDL	OB8-CB6-CB4	-2.36	101.56	108.43
26	T	1269	CDL	OB8-CB7-C71	2.36	119.32	111.91
23	J	60	CHD	C13-C14-C8	2.36	117.75	114.74
20	N	1266	PGV	C8-C7-C6	-2.36	102.47	114.42
24	P	1272	DMU	C18-O16-C6	2.35	117.74	113.84
18	A	516	HEA	CAA-C2A-C3A	-2.35	121.07	126.86
20	N	1266	PGV	O03-C01-C02	2.35	115.27	108.43
24	Z	1526	DMU	O2-C8-C7	-2.35	104.92	110.35
26	G	269	CDL	C80-C79-C78	2.35	126.33	114.42
20	P	1267	PGV	O06-C06-C05	-2.35	98.95	110.20
19	N	1522	TGL	OG3-CC1-CC2	2.34	119.25	111.91
26	P	1270	CDL	CA6-CA4-CA3	-2.34	106.26	111.79
23	C	525	CHD	C15-C16-C17	2.34	109.76	105.13
24	M	526	DMU	O49-C1-C2	2.33	115.73	110.35
20	P	1267	PGV	O12-P-O13	-2.33	99.98	109.07
26	C	270	CDL	C39-C38-C37	2.33	126.23	114.42
18	A	515	HEA	C16-C15-C14	-2.32	116.41	121.12
28	G	264	PEK	O03-C01-C02	-2.32	101.68	108.43
19	D	523	TGL	OG3-CC1-OC1	-2.31	117.76	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	P	1272	DMU	O7-C3-C2	2.31	113.42	107.28
23	P	1271	CHD	C19-C10-C5	-2.30	106.46	110.36
19	L	522	TGL	CA9-CA8-CA7	-2.30	102.76	114.42
18	N	515	HEA	C20-C19-C18	2.30	125.76	121.12
26	P	1270	CDL	CB6-CB4-CB3	-2.29	106.36	111.79
20	N	1266	PGV	C03-C02-C01	-2.29	106.37	111.79
20	C	267	PGV	C22-C21-C20	-2.29	104.97	113.19
24	Z	1526	DMU	C11-C9-C8	2.28	118.36	113.00
23	C	271	CHD	C21-C20-C17	2.28	116.41	112.92
23	P	1271	CHD	C22-C23-C24	-2.28	108.69	113.59
19	A	521	TGL	OG1-CA1-OA1	-2.28	117.85	123.59
19	N	1522	TGL	CG3-OG3-CC1	2.27	125.54	117.12
23	P	1525	CHD	C21-C20-C22	-2.27	106.81	110.36
23	B	1086	CHD	C13-C14-C8	2.27	117.64	114.74
20	A	524	PGV	C3-C2-C1	2.27	121.86	113.62
20	A	522	PGV	C28-C27-C26	2.26	125.92	114.42
20	A	524	PGV	C01-O03-C19	2.26	125.50	117.12
19	L	522	TGL	CB9-CB8-CB7	-2.26	102.94	114.42
23	B	1086	CHD	C21-C20-C22	-2.26	106.82	110.36
28	G	264	PEK	C32-C31-C30	-2.26	102.97	114.42
24	Z	1526	DMU	C31-C28-C25	-2.25	102.99	114.42
19	N	1521	TGL	CB3-CB2-CB1	2.25	121.78	113.62
23	P	1271	CHD	C6-C5-C4	-2.24	108.61	111.19
26	T	1269	CDL	C23-C22-C21	2.24	125.80	114.42
24	P	1272	DMU	O16-C18-C19	2.23	117.36	109.56
28	G	1263	PEK	O01-C1-O02	-2.22	118.33	123.70
23	J	60	CHD	C11-C9-C10	2.22	116.02	113.73
26	T	1269	CDL	OA8-CA7-OA9	-2.21	118.00	123.59
24	Z	1526	DMU	C57-C4-C3	2.21	119.75	113.33
22	O	1230	PSC	O01-C1-O02	-2.21	118.37	123.70
26	C	270	CDL	CA6-CA4-CA3	-2.20	106.58	111.79
26	P	1270	CDL	OB6-CB4-CB3	-2.20	100.42	108.40
18	A	515	HEA	CMB-C2B-C3B	2.20	129.00	124.69
28	T	263	PEK	O04-C21-C22	-2.20	115.15	123.73
24	M	526	DMU	C34-C31-C28	-2.20	103.26	114.42
18	N	515	HEA	CMB-C2B-C3B	2.20	128.99	124.69
23	P	1271	CHD	C13-C14-C8	2.19	117.53	114.74
20	P	1267	PGV	C9-C8-C7	-2.18	103.35	114.42
26	P	1270	CDL	OA6-CA5-OA7	-2.18	118.44	123.70
20	C	267	PGV	O03-C19-O04	-2.18	118.09	123.59
19	Q	1523	TGL	C21-C20-CA9	2.18	125.48	114.42
26	T	1269	CDL	OB5-PB2-OB3	-2.18	100.57	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	C	271	CHD	C22-C23-C24	-2.17	108.92	113.59
28	P	1264	PEK	O02-C1-C2	2.17	132.20	123.73
18	A	515	HEA	CMD-C2D-C3D	2.17	129.03	124.94
18	N	515	HEA	CMD-C2D-C3D	2.17	129.03	124.94
28	G	1263	PEK	C18-C17-C16	-2.16	104.36	113.79
23	B	1086	CHD	C16-C17-C20	2.16	115.48	112.15
19	Q	1523	TGL	C16-C15-CC9	2.14	125.30	114.42
28	G	264	PEK	O12-P-O14	2.13	117.39	109.07
20	N	1524	PGV	O01-C1-O02	-2.13	118.56	123.70
26	G	269	CDL	CA6-CA4-CA3	2.12	116.80	111.79
26	C	270	CDL	C53-C52-C51	-2.11	105.61	113.19
19	N	1521	TGL	C15-CC9-CC8	2.11	125.12	114.42
20	P	1268	PGV	C21-C20-C19	-2.11	105.96	113.62
18	A	515	HEA	C26-C15-C14	-2.11	118.28	123.68
26	C	270	CDL	C57-C56-C55	-2.10	103.74	114.42
26	G	269	CDL	OB8-CB7-C71	2.09	118.46	111.91
20	A	522	PGV	C3-C2-C1	-2.09	106.03	113.62
18	A	515	HEA	C12-C13-C14	-2.09	106.72	112.23
28	P	1265	PEK	P-O11-C03	2.08	133.90	121.68
23	O	229	CHD	C19-C10-C5	2.08	113.89	110.36
28	P	1265	PEK	C33-C32-C31	-2.08	103.87	114.42
19	L	522	TGL	C24-C23-C22	-2.08	103.87	114.42
24	Z	1526	DMU	C28-C25-C22	-2.07	103.90	114.42
19	N	1521	TGL	OG1-CA1-OA1	-2.07	118.36	123.59
20	A	522	PGV	C03-C02-C01	-2.07	106.89	111.79
19	N	1521	TGL	OG2-CG2-CG3	2.07	115.89	108.40
23	P	1271	CHD	C16-C15-C14	2.07	109.23	105.13
19	A	521	TGL	C20-CA9-CA8	2.07	124.92	114.42
28	G	264	PEK	C3-C2-C1	-2.06	106.12	113.62
20	N	1524	PGV	O03-C19-O04	-2.06	118.41	123.59
22	O	1230	PSC	C27-C26-C25	-2.05	104.01	114.42
20	C	267	PGV	O06-C06-C05	-2.05	100.38	110.20
20	C	267	PGV	O14-P-O13	2.04	122.35	112.24
18	A	516	HEA	C3A-C4A-NA	-2.04	107.08	110.94
20	P	1267	PGV	C10-C11-C12	-2.04	109.04	124.73
26	P	1270	CDL	C20-C19-C18	2.03	124.72	114.42
23	C	271	CHD	C14-C8-C9	2.03	112.49	109.71
28	G	1263	PEK	C02-O01-C1	2.02	122.77	117.79
20	A	524	PGV	O03-C19-O04	-2.02	118.49	123.59
19	Q	1523	TGL	OG3-CG3-CG2	2.02	114.32	108.43
19	A	521	TGL	C21-C20-CA9	2.02	124.67	114.42
26	T	1269	CDL	CA4-OA6-CA5	-2.02	112.83	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	G	265	PEK	C01-O03-C21	2.02	124.58	117.12
23	J	60	CHD	C21-C20-C17	-2.02	109.83	112.92
20	N	1266	PGV	O14-P-O12	-2.02	98.39	107.75
23	W	1060	CHD	C16-C15-C14	2.01	109.12	105.13
26	P	1270	CDL	O1-C1-CB2	2.01	116.61	109.56
18	N	516	HEA	C26-C15-C16	2.01	118.65	115.27
26	G	269	CDL	C20-C19-C18	2.01	124.61	114.42

All (39) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
23	W	1060	CHD	C17
23	W	1060	CHD	C9
18	A	515	HEA	ND
18	A	515	HEA	NA
18	A	515	HEA	NB
24	Z	1526	DMU	C2
24	Z	1526	DMU	C4
24	Z	1526	DMU	C6
24	Z	1526	DMU	C9
24	Z	1526	DMU	C5
24	M	526	DMU	C2
24	M	526	DMU	C4
24	M	526	DMU	C6
24	M	526	DMU	C9
24	M	526	DMU	C5
18	N	515	HEA	ND
18	N	515	HEA	NB
23	C	271	CHD	C9
18	N	516	HEA	ND
18	N	516	HEA	NA
18	N	516	HEA	NB
24	C	272	DMU	C5
24	C	272	DMU	C6
24	C	272	DMU	C9
24	C	272	DMU	C4
24	C	272	DMU	C2
24	C	272	DMU	C3
23	O	229	CHD	C9
18	A	516	HEA	ND
18	A	516	HEA	NA
18	A	516	HEA	NB

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Mol	Chain	Res	Type	Atom
23	J	60	CHD	C17
23	J	60	CHD	C9
24	P	1272	DMU	C2
24	P	1272	DMU	C4
24	P	1272	DMU	C9
24	P	1272	DMU	C6
24	P	1272	DMU	C5
23	P	1271	CHD	C9

All (940) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	G	269	CDL	CA2-OA2-PA1-OA3
26	G	269	CDL	CA3-OA5-PA1-OA2
26	G	269	CDL	CA3-OA5-PA1-OA4
26	G	269	CDL	C11-CA5-OA6-CA4
26	G	269	CDL	C1-CB2-OB2-PB2
23	W	1060	CHD	C13-C17-C20-C22
23	W	1060	CHD	C16-C17-C20-C21
23	W	1060	CHD	C16-C17-C20-C22
23	W	1060	CHD	C20-C22-C23-C24
20	A	524	PGV	C03-O11-P-O12
20	A	524	PGV	C03-O11-P-O14
20	A	524	PGV	C03-C02-O01-C1
20	A	524	PGV	C02-C03-O11-P
20	A	524	PGV	O02-C1-O01-C02
20	A	524	PGV	C2-C1-O01-C02
20	A	524	PGV	O04-C19-O03-C01
20	A	524	PGV	C20-C19-O03-C01
22	O	1230	PSC	C03-O11-P-O12
22	O	1230	PSC	C03-O11-P-O14
18	A	515	HEA	C14-C15-C16-C17
18	A	515	HEA	C26-C15-C16-C17
18	A	515	HEA	C16-C17-C18-C19
24	Z	1526	DMU	O5-C6-O16-C18
20	N	1524	PGV	C03-O11-P-O14
20	N	1524	PGV	C04-O12-P-O14
20	N	1524	PGV	C02-C03-O11-P
20	N	1524	PGV	O02-C1-O01-C02
20	N	1524	PGV	C2-C1-O01-C02
20	N	1524	PGV	C10-C11-C12-C13
20	P	1268	PGV	O03-C01-C02-O01

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Mol	Chain	Res	Type	Atoms
20	P	1268	PGV	C04-C05-C06-O06
24	M	526	DMU	O5-C6-O16-C18
24	M	526	DMU	C19-C18-O16-C6
19	A	521	TGL	CB2-CB1-OG2-CG2
19	A	521	TGL	CG2-CG3-OG3-CC1
20	C	268	PGV	O01-C02-C03-O11
20	C	268	PGV	C04-C05-C06-O06
28	T	263	PEK	C03-O11-P-O13
28	T	263	PEK	O12-C04-C05-N
28	T	263	PEK	C5-C6-C7-C8
28	T	263	PEK	C11-C12-C13-C14
28	T	263	PEK	C13-C14-C15-C16
28	G	1263	PEK	C03-O11-P-O12
28	G	1263	PEK	C03-O11-P-O13
28	G	1263	PEK	C03-O11-P-O14
28	G	1263	PEK	C04-O12-P-O13
28	G	1263	PEK	C04-O12-P-O14
28	G	1263	PEK	O03-C01-C02-O01
28	G	1263	PEK	C7-C8-C9-C10
28	G	1263	PEK	C13-C14-C15-C16
28	G	265	PEK	O12-C04-C05-N
28	G	265	PEK	C4-C5-C6-C7
28	G	264	PEK	C6-C7-C8-C9
19	N	1522	TGL	CB2-CB1-OG2-CG2
28	P	1264	PEK	C6-C7-C8-C9
28	P	1265	PEK	C04-O12-P-O11
28	P	1265	PEK	C04-O12-P-O14
28	P	1265	PEK	C4-C5-C6-C7
28	P	1265	PEK	C6-C7-C8-C9
26	T	1269	CDL	C1-CB2-OB2-PB2
26	T	1269	CDL	CB3-OB5-PB2-OB3
19	L	522	TGL	CB2-CB1-OG2-CG2
26	P	1270	CDL	CA2-OA2-PA1-OA3
26	P	1270	CDL	C11-CA5-OA6-CA4
26	P	1270	CDL	CB3-OB5-PB2-OB3
26	P	1270	CDL	C51-CB5-OB6-CB4
23	J	60	CHD	C16-C17-C20-C22
24	P	1272	DMU	C1-C6-O16-C18
22	B	230	PSC	C04-O12-P-O13
26	C	270	CDL	CA2-OA2-PA1-OA3
26	C	270	CDL	CA3-OA5-PA1-OA2
26	C	270	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
26	C	270	CDL	CA4-CA3-OA5-PA1
26	C	270	CDL	C11-CA5-OA6-CA4
26	C	270	CDL	CB2-OB2-PB2-OB3
26	C	270	CDL	OB7-CB5-OB6-CB4
26	C	270	CDL	C51-CB5-OB6-CB4
19	D	523	TGL	CC2-CC1-OG3-CG3
19	D	523	TGL	OC1-CC1-OG3-CG3
20	N	1524	PGV	O04-C19-O03-C01
19	Q	1523	TGL	OC1-CC1-OG3-CG3
19	N	1521	TGL	CG2-CG3-OG3-CC1
20	N	1524	PGV	C20-C19-O03-C01
19	A	521	TGL	OC1-CC1-OG3-CG3
19	N	1521	TGL	OC1-CC1-OG3-CG3
24	M	526	DMU	O5-C4-C57-O61
24	C	272	DMU	O6-C11-C9-O1
26	G	269	CDL	OA7-CA5-OA6-CA4
19	A	521	TGL	OB1-CB1-OG2-CG2
19	N	1522	TGL	OB1-CB1-OG2-CG2
26	P	1270	CDL	OA7-CA5-OA6-CA4
26	P	1270	CDL	OB7-CB5-OB6-CB4
26	C	270	CDL	OA7-CA5-OA6-CA4
19	A	521	TGL	CC2-CC1-OG3-CG3
19	Q	1523	TGL	CC2-CC1-OG3-CG3
19	L	522	TGL	CC3-CC4-CC5-CC6
22	O	1230	PSC	C20-C19-O03-C01
19	N	1522	TGL	CA2-CA1-OG1-CG1
19	L	522	TGL	CA2-CA1-OG1-CG1
19	N	1521	TGL	CC2-CC1-OG3-CG3
22	O	1230	PSC	C11-C10-C9-C8
28	G	1263	PEK	C4-C5-C6-C7
28	G	265	PEK	C7-C8-C9-C10
28	G	265	PEK	C10-C11-C12-C13
28	G	264	PEK	C10-C11-C12-C13
28	G	264	PEK	C13-C14-C15-C16
28	P	1265	PEK	C10-C11-C12-C13
20	P	1267	PGV	C10-C11-C12-C13
19	N	1522	TGL	CC3-CC4-CC5-CC6
19	L	522	TGL	OB1-CB1-OG2-CG2
22	O	1230	PSC	O04-C19-O03-C01
19	N	1521	TGL	CB3-CB4-CB5-CB6
26	C	270	CDL	C83-C84-C85-C86
23	J	60	CHD	C16-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
24	Z	1526	DMU	O5-C4-C57-O61
26	T	1269	CDL	O1-C1-CA2-OA2
26	P	1270	CDL	O1-C1-CB2-OB2
22	B	230	PSC	C20-C19-O03-C01
26	P	1270	CDL	C82-C83-C84-C85
24	P	1272	DMU	O6-C11-C9-O1
19	N	1522	TGL	CC1-CC2-CC3-CC4
19	L	522	TGL	CC1-CC2-CC3-CC4
26	G	269	CDL	C59-C60-C61-C62
26	T	1269	CDL	C56-C57-C58-C59
26	T	1269	CDL	C79-C80-C81-C82
19	N	1521	TGL	C21-C20-CA9-CA8
22	B	230	PSC	C20-C21-C22-C23
26	C	270	CDL	C38-C39-C40-C41
19	N	1522	TGL	OA1-CA1-OG1-CG1
19	A	521	TGL	C12-C13-C14-C29
19	Q	1523	TGL	C17-C18-C19-C33
26	T	1269	CDL	C73-C74-C75-C76
22	O	1230	PSC	C20-C21-C22-C23
24	Z	1526	DMU	O6-C11-C9-O1
24	C	272	DMU	O5-C4-C57-O61
28	P	1265	PEK	C28-C29-C30-C31
26	P	1270	CDL	C61-C62-C63-C64
19	D	523	TGL	CB9-C10-C11-C12
19	L	522	TGL	OA1-CA1-OG1-CG1
19	Q	1523	TGL	C21-C22-C23-C24
19	D	523	TGL	C21-C22-C23-C24
23	P	1271	CHD	C21-C20-C22-C23
24	C	272	DMU	O5-C6-O16-C18
18	N	515	HEA	C15-C16-C17-C18
26	C	270	CDL	C78-C79-C80-C81
19	Q	1523	TGL	CA2-CA1-OG1-CG1
26	T	1269	CDL	C71-CB7-OB8-CB6
28	P	1264	PEK	C7-C8-C9-C10
22	B	230	PSC	O04-C19-O03-C01
26	C	270	CDL	CB2-C1-CA2-OA2
23	C	271	CHD	C21-C20-C22-C23
19	Q	1523	TGL	OA1-CA1-OG1-CG1
19	A	521	TGL	C21-C20-CA9-CA8
28	G	265	PEK	C34-C35-C36-C37
26	C	270	CDL	C71-CB7-OB8-CB6
26	G	269	CDL	C79-C80-C81-C82

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Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	C22-C23-C24-C25
26	C	270	CDL	OB5-CB3-CB4-OB6
28	T	263	PEK	C33-C34-C35-C36
26	C	270	CDL	O1-C1-CA2-OA2
26	G	269	CDL	CA7-C31-C32-C33
20	A	524	PGV	C19-C20-C21-C22
24	C	272	DMU	C1-C6-O16-C18
19	N	1522	TGL	C20-C21-C22-C23
28	G	265	PEK	C28-C29-C30-C31
23	J	60	CHD	C13-C17-C20-C21
26	G	269	CDL	CB5-C51-C52-C53
23	P	1271	CHD	C17-C20-C22-C23
26	G	269	CDL	CA5-C11-C12-C13
20	A	524	PGV	C1-C2-C3-C4
28	G	1263	PEK	C21-C22-C23-C24
19	L	522	TGL	CB1-CB2-CB3-CB4
26	P	1270	CDL	CB7-C71-C72-C73
22	B	230	PSC	C19-C20-C21-C22
20	C	267	PGV	C10-C11-C12-C13
24	M	526	DMU	O6-C11-C9-C8
26	G	269	CDL	C63-C64-C65-C66
22	O	1230	PSC	C1-C2-C3-C4
20	N	1524	PGV	C19-C20-C21-C22
19	N	1522	TGL	CB1-CB2-CB3-CB4
28	P	1264	PEK	C1-C2-C3-C4
26	T	1269	CDL	CB7-C71-C72-C73
28	G	1263	PEK	C33-C34-C35-C36
22	O	1230	PSC	C04-C05-N-C06
22	O	1230	PSC	C04-C05-N-C08
28	G	265	PEK	C1-C2-C3-C4
20	P	1267	PGV	C1-C2-C3-C4
19	D	523	TGL	CB1-CB2-CB3-CB4
23	P	1271	CHD	C20-C22-C23-C24
26	C	270	CDL	OB9-CB7-OB8-CB6
24	Z	1526	DMU	O16-C18-C19-C22
24	P	1272	DMU	O16-C18-C19-C22
26	T	1269	CDL	O1-C1-CB2-OB2
28	G	265	PEK	C22-C21-O03-C01
26	T	1269	CDL	OB9-CB7-OB8-CB6
23	J	60	CHD	C13-C17-C20-C22
22	O	1230	PSC	C11-C12-C13-C14
28	T	263	PEK	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
28	G	264	PEK	C7-C8-C9-C10
28	P	1264	PEK	C10-C11-C12-C13
18	N	515	HEA	C16-C17-C18-C19
26	G	269	CDL	CA2-OA2-PA1-OA5
20	N	1524	PGV	C03-O11-P-O12
28	T	263	PEK	C03-O11-P-O12
28	G	1263	PEK	C04-O12-P-O11
26	T	1269	CDL	CB3-OB5-PB2-OB2
26	P	1270	CDL	CA3-OA5-PA1-OA2
26	P	1270	CDL	CB2-OB2-PB2-OB5
22	B	230	PSC	C04-O12-P-O11
26	C	270	CDL	CA2-OA2-PA1-OA5
26	C	270	CDL	CB2-OB2-PB2-OB5
26	G	269	CDL	C40-C41-C42-C43
26	G	269	CDL	CA2-C1-CB2-OB2
26	T	1269	CDL	CA2-C1-CB2-OB2
22	B	230	PSC	C04-C05-N-C08
23	C	271	CHD	C20-C22-C23-C24
23	W	1060	CHD	C13-C17-C20-C21
24	P	1272	DMU	C3-C4-C57-O61
28	G	264	PEK	C25-C26-C27-C28
19	L	522	TGL	C18-C19-C33-C34
26	P	1270	CDL	C12-C13-C14-C15
26	P	1270	CDL	C17-C18-C19-C20
19	N	1521	TGL	CB4-CB5-CB6-CB7
19	N	1521	TGL	C16-C17-C18-C19
20	C	268	PGV	C2-C1-O01-C02
23	C	271	CHD	C17-C20-C22-C23
26	G	269	CDL	C36-C37-C38-C39
26	G	269	CDL	C37-C38-C39-C40
26	G	269	CDL	C75-C76-C77-C78
20	N	1524	PGV	C14-C15-C16-C17
20	P	1268	PGV	C13-C14-C15-C16
20	P	1268	PGV	C14-C15-C16-C17
19	A	521	TGL	CA5-CA6-CA7-CA8
19	A	521	TGL	CC4-CC5-CC6-CC7
19	N	1522	TGL	CB5-CB6-CB7-CB8
19	N	1522	TGL	C12-C13-C14-C29
26	T	1269	CDL	C36-C37-C38-C39
20	C	267	PGV	C7-C8-C9-C10
26	P	1270	CDL	C15-C16-C17-C18
26	P	1270	CDL	C77-C78-C79-C80

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Mol	Chain	Res	Type	Atoms
26	C	270	CDL	C57-C58-C59-C60
26	C	270	CDL	C58-C59-C60-C61
26	G	269	CDL	C34-C35-C36-C37
24	Z	1526	DMU	C28-C31-C34-C37
20	N	1524	PGV	C2-C3-C4-C5
20	C	268	PGV	C30-C31-C32-C33
24	C	272	DMU	C28-C31-C34-C37
26	T	1269	CDL	C61-C62-C63-C64
26	P	1270	CDL	C14-C15-C16-C17
20	A	522	PGV	C27-C28-C29-C30
19	D	523	TGL	CG3-CG2-OG2-CB1
20	C	268	PGV	O02-C1-O01-C02
20	A	524	PGV	C20-C21-C22-C23
28	T	263	PEK	C16-C17-C18-C19
26	T	1269	CDL	C63-C64-C65-C66
26	P	1270	CDL	C16-C17-C18-C19
26	P	1270	CDL	C72-C73-C74-C75
26	P	1270	CDL	C73-C74-C75-C76
19	N	1521	TGL	CA4-CA5-CA6-CA7
26	C	270	CDL	C16-C17-C18-C19
20	P	1268	PGV	C02-C03-O11-P
28	G	264	PEK	C4-C5-C6-C7
26	G	269	CDL	C77-C78-C79-C80
22	O	1230	PSC	C2-C3-C4-C5
19	N	1522	TGL	CC6-CC7-CC8-CC9
19	N	1522	TGL	C21-C22-C23-C24
28	P	1264	PEK	C25-C26-C27-C28
28	P	1265	PEK	C33-C34-C35-C36
19	Q	1523	TGL	CC2-CC3-CC4-CC5
19	L	522	TGL	C17-C18-C19-C33
26	P	1270	CDL	C37-C38-C39-C40
26	C	270	CDL	C39-C40-C41-C42
26	G	269	CDL	O1-C1-CB2-OB2
22	O	1230	PSC	C27-C28-C29-C30
28	P	1264	PEK	C32-C33-C34-C35
19	Q	1523	TGL	CC5-CC6-CC7-CC8
26	T	1269	CDL	C34-C35-C36-C37
26	T	1269	CDL	C54-C55-C56-C57
26	P	1270	CDL	C62-C63-C64-C65
26	P	1270	CDL	C63-C64-C65-C66
22	B	230	PSC	C24-C25-C26-C27
20	C	267	PGV	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
20	N	1524	PGV	C22-C23-C24-C25
19	A	521	TGL	CB4-CB5-CB6-CB7
19	N	1522	TGL	CA2-CA3-CA4-CA5
19	N	1522	TGL	C23-C24-C25-C26
26	T	1269	CDL	C19-C20-C21-C22
19	L	522	TGL	C10-C11-C12-C13
26	G	269	CDL	C35-C36-C37-C38
20	A	524	PGV	C24-C25-C26-C27
28	T	263	PEK	C26-C27-C28-C29
19	N	1522	TGL	C16-C17-C18-C19
26	T	1269	CDL	C11-C12-C13-C14
19	L	522	TGL	C22-C23-C24-C25
19	N	1521	TGL	C11-C12-C13-C14
26	C	270	CDL	C19-C20-C21-C22
19	N	1521	TGL	CA1-CA2-CA3-CA4
26	G	269	CDL	C62-C63-C64-C65
26	G	269	CDL	C71-C72-C73-C74
26	G	269	CDL	C73-C74-C75-C76
24	Z	1526	DMU	C22-C25-C28-C31
20	C	268	PGV	C23-C24-C25-C26
19	N	1522	TGL	CA3-CA4-CA5-CA6
19	N	1522	TGL	C22-C23-C24-C25
19	Q	1523	TGL	CB6-CB7-CB8-CB9
20	P	1267	PGV	C13-C14-C15-C16
26	P	1270	CDL	C59-C60-C61-C62
22	B	230	PSC	C30-C31-C32-C33
26	G	269	CDL	C58-C59-C60-C61
19	A	521	TGL	C11-C12-C13-C14
19	A	521	TGL	CC7-CC8-CC9-C15
19	A	521	TGL	C14-C29-C30-C31
20	C	268	PGV	C6-C7-C8-C9
19	N	1522	TGL	C16-C15-CC9-CC8
19	Q	1523	TGL	CC6-CC7-CC8-CC9
26	T	1269	CDL	C51-CB5-OB6-CB4
22	O	1230	PSC	C24-C25-C26-C27
20	P	1268	PGV	C2-C3-C4-C5
19	N	1522	TGL	C11-C12-C13-C14
28	P	1264	PEK	C33-C34-C35-C36
20	P	1267	PGV	C7-C8-C9-C10
20	N	1266	PGV	C6-C7-C8-C9
26	P	1270	CDL	C58-C59-C60-C61
26	C	270	CDL	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
20	C	268	PGV	C12-C13-C14-C15
28	P	1264	PEK	C15-C16-C17-C18
20	P	1267	PGV	C12-C13-C14-C15
28	G	264	PEK	C1-C2-C3-C4
22	B	230	PSC	C1-C2-C3-C4
26	G	269	CDL	C54-C55-C56-C57
26	G	269	CDL	C56-C57-C58-C59
22	O	1230	PSC	C26-C27-C28-C29
24	Z	1526	DMU	C25-C28-C31-C34
28	G	265	PEK	C29-C30-C31-C32
19	N	1522	TGL	CB4-CB5-CB6-CB7
20	P	1267	PGV	C24-C25-C26-C27
19	L	522	TGL	CC6-CC7-CC8-CC9
26	P	1270	CDL	C81-C82-C83-C84
19	N	1521	TGL	CC7-CC8-CC9-C15
26	C	270	CDL	C14-C15-C16-C17
19	D	523	TGL	CB2-CB3-CB4-CB5
22	B	230	PSC	C02-C01-O03-C19
19	A	521	TGL	CA6-CA7-CA8-CA9
19	A	521	TGL	C11-C10-CB9-CB8
19	A	521	TGL	CC5-CC6-CC7-CC8
19	A	521	TGL	C22-C23-C24-C25
20	C	268	PGV	C26-C27-C28-C29
28	T	263	PEK	C25-C26-C27-C28
28	T	263	PEK	C29-C30-C31-C32
28	G	265	PEK	C33-C34-C35-C36
19	N	1522	TGL	CC4-CC5-CC6-CC7
26	T	1269	CDL	C59-C60-C61-C62
26	P	1270	CDL	C74-C75-C76-C77
19	N	1521	TGL	CB9-C10-C11-C12
19	N	1521	TGL	C15-C16-C17-C18
19	D	523	TGL	C19-C33-C34-C35
28	P	1265	PEK	O12-C04-C05-N
19	L	522	TGL	C21-C20-CA9-CA8
26	C	270	CDL	C12-C13-C14-C15
20	A	522	PGV	C19-C20-C21-C22
28	G	265	PEK	O04-C21-O03-C01
22	O	1230	PSC	C28-C29-C30-C31
26	T	1269	CDL	C75-C76-C77-C78
19	D	523	TGL	CC5-CC6-CC7-CC8
26	T	1269	CDL	C17-C18-C19-C20
19	N	1521	TGL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
20	A	524	PGV	C28-C29-C30-C31
19	Q	1523	TGL	C16-C15-CC9-CC8
20	N	1266	PGV	C23-C24-C25-C26
20	C	267	PGV	C28-C29-C30-C31
26	C	270	CDL	C35-C36-C37-C38
19	D	523	TGL	C15-C16-C17-C18
28	G	1263	PEK	C22-C23-C24-C25
19	N	1522	TGL	C17-C18-C19-C33
20	A	524	PGV	O03-C01-C02-C03
26	T	1269	CDL	OB7-CB5-OB6-CB4
20	A	524	PGV	C10-C11-C12-C13
19	A	521	TGL	CA9-C20-C21-C22
19	Q	1523	TGL	C12-C13-C14-C29
26	T	1269	CDL	C31-C32-C33-C34
19	D	523	TGL	C17-C18-C19-C33
28	T	263	PEK	C21-C22-C23-C24
28	G	264	PEK	C28-C29-C30-C31
19	N	1521	TGL	C14-C29-C30-C31
20	N	1524	PGV	C4-C5-C6-C7
26	T	1269	CDL	C51-C52-C53-C54
20	A	522	PGV	C14-C15-C16-C17
20	A	522	PGV	C24-C25-C26-C27
20	P	1268	PGV	O05-C05-C06-O06
20	C	268	PGV	O05-C05-C06-O06
28	P	1264	PEK	C30-C31-C32-C33
19	Q	1523	TGL	CB2-CB3-CB4-CB5
19	N	1521	TGL	CC4-CC5-CC6-CC7
24	P	1272	DMU	C19-C22-C25-C28
22	B	230	PSC	C29-C30-C31-C32
20	C	268	PGV	C11-C10-C9-C8
28	G	264	PEK	C2-C3-C4-C5
19	A	521	TGL	C13-C14-C29-C30
26	P	1270	CDL	C22-C23-C24-C25
20	P	1268	PGV	C3-C4-C5-C6
26	P	1270	CDL	C71-C72-C73-C74
19	D	523	TGL	C16-C17-C18-C19
19	N	1521	TGL	OB1-CB1-OG2-CG2
26	G	269	CDL	C60-C61-C62-C63
28	P	1265	PEK	C29-C30-C31-C32
19	N	1521	TGL	CA5-CA6-CA7-CA8
19	A	521	TGL	CB6-CB7-CB8-CB9
20	C	268	PGV	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
28	P	1264	PEK	C35-C36-C37-C38
26	C	270	CDL	C43-C44-C45-C46
22	O	1230	PSC	C04-C05-N-C07
26	G	269	CDL	C14-C15-C16-C17
26	G	269	CDL	C31-C32-C33-C34
20	P	1268	PGV	C22-C23-C24-C25
24	M	526	DMU	C28-C31-C34-C37
19	L	522	TGL	CA5-CA6-CA7-CA8
19	Q	1523	TGL	CB5-CB6-CB7-CB8
24	P	1272	DMU	O5-C4-C57-O61
19	N	1522	TGL	C25-C26-C27-C28
26	T	1269	CDL	C55-C56-C57-C58
26	P	1270	CDL	C64-C65-C66-C67
18	N	515	HEA	C26-C15-C16-C17
19	N	1521	TGL	CC5-CC6-CC7-CC8
20	N	1266	PGV	C11-C10-C9-C8
26	T	1269	CDL	OA7-CA5-OA6-CA4
26	G	269	CDL	CB7-C71-C72-C73
20	C	268	PGV	C29-C30-C31-C32
19	L	522	TGL	C25-C26-C27-C28
22	B	230	PSC	C4-C5-C6-C7
28	G	1263	PEK	C25-C26-C27-C28
28	P	1264	PEK	C26-C27-C28-C29
26	C	270	CDL	C71-C72-C73-C74
19	Q	1523	TGL	CA6-CA7-CA8-CA9
26	P	1270	CDL	C38-C39-C40-C41
22	B	230	PSC	C28-C29-C30-C31
26	C	270	CDL	C51-C52-C53-C54
26	C	270	CDL	C72-C73-C74-C75
19	L	522	TGL	CC4-CC5-CC6-CC7
19	L	522	TGL	C19-C33-C34-C35
26	C	270	CDL	C32-C33-C34-C35
20	P	1268	PGV	C2-C1-O01-C02
26	T	1269	CDL	C11-CA5-OA6-CA4
19	N	1521	TGL	CB2-CB1-OG2-CG2
19	A	521	TGL	C16-C17-C18-C19
28	P	1265	PEK	C25-C26-C27-C28
20	P	1268	PGV	O12-C04-C05-O05
20	P	1268	PGV	C6-C7-C8-C9
26	T	1269	CDL	C35-C36-C37-C38
26	G	269	CDL	OB6-CB4-CB6-OB8
20	C	268	PGV	O03-C01-C02-O01

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Mol	Chain	Res	Type	Atoms
19	D	523	TGL	OG1-CG1-CG2-OG2
28	G	265	PEK	C24-C25-C26-C27
22	O	1230	PSC	C4-C5-C6-C7
19	Q	1523	TGL	CA4-CA5-CA6-CA7
20	C	267	PGV	C29-C30-C31-C32
28	T	263	PEK	C2-C3-C4-C5
19	A	521	TGL	CB1-CB2-CB3-CB4
18	N	515	HEA	C14-C15-C16-C17
26	G	269	CDL	C18-C19-C20-C21
22	B	230	PSC	C2-C3-C4-C5
20	C	268	PGV	C10-C11-C12-C13
28	P	1264	PEK	C13-C14-C15-C16
20	C	268	PGV	C4-C5-C6-C7
19	N	1522	TGL	C10-C11-C12-C13
26	P	1270	CDL	C35-C36-C37-C38
19	D	523	TGL	CA6-CA7-CA8-CA9
28	G	1263	PEK	C27-C28-C29-C30
28	P	1265	PEK	C30-C31-C32-C33
26	C	270	CDL	C74-C75-C76-C77
19	D	523	TGL	CC6-CC7-CC8-CC9
26	P	1270	CDL	CA2-OA2-PA1-OA5
19	L	522	TGL	C13-C14-C29-C30
19	D	523	TGL	C13-C14-C29-C30
26	G	269	CDL	C74-C75-C76-C77
26	T	1269	CDL	C71-C72-C73-C74
20	A	524	PGV	C01-C02-C03-O11
20	C	268	PGV	C01-C02-C03-O11
26	P	1270	CDL	OA5-CA3-CA4-CA6
26	C	270	CDL	OA5-CA3-CA4-CA6
26	C	270	CDL	OB5-CB3-CB4-CB6
26	C	270	CDL	C41-C42-C43-C44
28	G	264	PEK	C23-C24-C25-C26
26	P	1270	CDL	C13-C14-C15-C16
28	G	265	PEK	C25-C26-C27-C28
19	L	522	TGL	CB4-CB5-CB6-CB7
26	C	270	CDL	C15-C16-C17-C18
26	C	270	CDL	C82-C83-C84-C85
28	G	265	PEK	C15-C16-C17-C18
20	C	268	PGV	C14-C15-C16-C17
26	T	1269	CDL	C32-C33-C34-C35
26	G	269	CDL	C31-CA7-OA8-CA6
28	G	265	PEK	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
28	P	1264	PEK	C16-C17-C18-C19
20	A	522	PGV	C26-C27-C28-C29
19	L	522	TGL	CB5-CB6-CB7-CB8
19	N	1521	TGL	C13-C14-C29-C30
20	P	1268	PGV	C26-C27-C28-C29
28	G	265	PEK	C26-C27-C28-C29
20	N	1524	PGV	O03-C01-C02-C03
20	P	1268	PGV	O03-C01-C02-C03
24	M	526	DMU	C25-C28-C31-C34
20	C	268	PGV	O03-C01-C02-C03
26	P	1270	CDL	CA3-CA4-CA6-OA8
26	P	1270	CDL	CB3-CB4-CB6-OB8
26	C	270	CDL	C37-C38-C39-C40
28	P	1264	PEK	C4-C5-C6-C7
20	N	1266	PGV	C10-C11-C12-C13
20	C	268	PGV	C31-C32-C33-C34
19	L	522	TGL	C33-C34-C35-C36
26	G	269	CDL	C76-C77-C78-C79
20	P	1268	PGV	C31-C32-C33-C34
20	C	267	PGV	C31-C32-C33-C34
20	A	522	PGV	C15-C16-C17-C18
20	A	522	PGV	C30-C31-C32-C33
20	P	1268	PGV	O02-C1-O01-C02
19	A	521	TGL	C25-C26-C27-C28
19	A	521	TGL	C29-C30-C31-C32
19	D	523	TGL	CC2-CC3-CC4-CC5
19	D	523	TGL	C16-C15-CC9-CC8
20	N	1266	PGV	C7-C8-C9-C10
20	N	1524	PGV	C11-C12-C13-C14
20	N	1266	PGV	C5-C6-C7-C8
26	C	270	CDL	C79-C80-C81-C82
20	P	1268	PGV	C12-C13-C14-C15
28	P	1265	PEK	C15-C16-C17-C18
20	P	1267	PGV	C11-C10-C9-C8
20	N	1266	PGV	C12-C13-C14-C15
26	T	1269	CDL	CA7-C31-C32-C33
22	O	1230	PSC	C31-C32-C33-C34
20	N	1266	PGV	C31-C32-C33-C34
20	A	522	PGV	C7-C8-C9-C10
19	D	523	TGL	C33-C34-C35-C36
19	D	523	TGL	CA1-CA2-CA3-CA4
28	P	1265	PEK	C22-C21-O03-C01

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Mol	Chain	Res	Type	Atoms
26	P	1270	CDL	C44-C45-C46-C47
22	O	1230	PSC	O03-C19-C20-C21
26	P	1270	CDL	C42-C43-C44-C45
20	A	524	PGV	C25-C26-C27-C28
26	T	1269	CDL	C16-C17-C18-C19
19	L	522	TGL	CA9-C20-C21-C22
19	A	521	TGL	CA7-CA8-CA9-C20
28	T	263	PEK	O01-C02-C03-O11
22	B	230	PSC	C04-C05-N-C07
19	L	522	TGL	CB2-CB3-CB4-CB5
19	Q	1523	TGL	CA5-CA6-CA7-CA8
28	P	1265	PEK	O04-C21-O03-C01
19	N	1521	TGL	CA7-CA8-CA9-C20
19	Q	1523	TGL	CB1-CB2-CB3-CB4
19	A	521	TGL	OG2-CG2-CG3-OG3
28	T	263	PEK	O03-C01-C02-O01
26	G	269	CDL	C12-C13-C14-C15
20	N	1524	PGV	C24-C25-C26-C27
28	G	264	PEK	C27-C28-C29-C30
20	C	268	PGV	C15-C16-C17-C18
26	T	1269	CDL	C52-C53-C54-C55
26	G	269	CDL	OA9-CA7-OA8-CA6
24	C	272	DMU	C4-C3-O7-C10
24	P	1272	DMU	C34-C37-C40-C43
20	P	1268	PGV	O12-C04-C05-C06
22	O	1230	PSC	O02-C1-O01-C02
22	O	1230	PSC	C2-C1-O01-C02
20	N	1524	PGV	C6-C7-C8-C9
20	A	524	PGV	C31-C32-C33-C34
20	P	1267	PGV	C15-C16-C17-C18
20	C	268	PGV	C9-C10-C11-C12
22	O	1230	PSC	C22-C23-C24-C25
26	T	1269	CDL	C81-C82-C83-C84
20	N	1524	PGV	C01-C02-C03-O11
28	P	1264	PEK	C31-C32-C33-C34
26	P	1270	CDL	C19-C20-C21-C22
19	L	522	TGL	CC2-CC3-CC4-CC5
28	G	264	PEK	C24-C25-C26-C27
19	Q	1523	TGL	CB3-CB4-CB5-CB6
19	L	522	TGL	OG1-CA1-CA2-CA3
20	C	268	PGV	C19-C20-C21-C22
28	G	1263	PEK	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
19	N	1521	TGL	C21-C22-C23-C24
28	P	1264	PEK	C3-C4-C5-C6
26	G	269	CDL	C13-C14-C15-C16
20	C	268	PGV	C21-C22-C23-C24
26	T	1269	CDL	C20-C21-C22-C23
26	P	1270	CDL	C41-C42-C43-C44
20	A	524	PGV	C12-C13-C14-C15
28	G	1263	PEK	C22-C21-O03-C01
19	N	1522	TGL	CA9-C20-C21-C22
26	G	269	CDL	CB3-CB4-CB6-OB8
28	T	263	PEK	O03-C01-C02-C03
28	G	1263	PEK	O03-C01-C02-C03
19	Q	1523	TGL	OG1-CG1-CG2-CG3
19	D	523	TGL	OG1-CG1-CG2-CG3
28	P	1265	PEK	C26-C27-C28-C29
28	T	263	PEK	C7-C8-C9-C10
28	P	1265	PEK	C13-C14-C15-C16
28	G	1263	PEK	C26-C27-C28-C29
19	N	1522	TGL	C29-C30-C31-C32
24	P	1272	DMU	C28-C31-C34-C37
19	D	523	TGL	CB4-CB5-CB6-CB7
28	T	263	PEK	C27-C28-C29-C30
19	Q	1523	TGL	CC3-CC4-CC5-CC6
26	P	1270	CDL	C84-C85-C86-C87
26	P	1270	CDL	C36-C37-C38-C39
20	P	1268	PGV	C23-C24-C25-C26
28	G	265	PEK	C30-C31-C32-C33
22	O	1230	PSC	C9-C10-C11-C12
28	G	1263	PEK	C11-C10-C9-C8
28	G	1263	PEK	C9-C10-C11-C12
28	G	1263	PEK	C11-C12-C13-C14
28	G	265	PEK	C5-C6-C7-C8
28	G	265	PEK	C6-C7-C8-C9
28	G	264	PEK	C9-C10-C11-C12
28	P	1264	PEK	C9-C10-C11-C12
28	P	1265	PEK	C5-C6-C7-C8
28	P	1265	PEK	C11-C10-C9-C8
26	P	1270	CDL	CB3-OB5-PB2-OB2
22	B	230	PSC	C9-C10-C11-C12
22	B	230	PSC	C10-C11-C12-C13
19	L	522	TGL	C15-C16-C17-C18
26	P	1270	CDL	C40-C41-C42-C43

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Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	C21-C22-C23-C24
19	L	522	TGL	C11-C10-CB9-CB8
26	C	270	CDL	C73-C74-C75-C76
19	L	522	TGL	C16-C15-CC9-CC8
22	B	230	PSC	C22-C23-C24-C25
19	D	523	TGL	CA9-C20-C21-C22
19	A	521	TGL	OG1-CG1-CG2-OG2
19	N	1521	TGL	OG1-CG1-CG2-OG2
19	D	523	TGL	OG2-CB1-CB2-CB3
19	A	521	TGL	C16-C15-CC9-CC8
20	P	1268	PGV	C5-C6-C7-C8
22	B	230	PSC	C11-C10-C9-C8
19	A	521	TGL	CB9-C10-C11-C12
22	B	230	PSC	C31-C32-C33-C34
24	P	1272	DMU	C25-C28-C31-C34
26	T	1269	CDL	C37-C38-C39-C40
19	L	522	TGL	CC5-CC6-CC7-CC8
20	A	524	PGV	C05-C04-O12-P
26	T	1269	CDL	CB4-CB3-OB5-PB2
20	C	267	PGV	C02-C03-O11-P
26	P	1270	CDL	CA4-CA3-OA5-PA1
26	C	270	CDL	C1-CA2-OA2-PA1
26	C	270	CDL	C84-C85-C86-C87
19	D	523	TGL	CA4-CA5-CA6-CA7
19	A	521	TGL	C15-C16-C17-C18
26	T	1269	CDL	C62-C63-C64-C65
24	M	526	DMU	C34-C37-C40-C43
26	P	1270	CDL	C21-C22-C23-C24
26	P	1270	CDL	C24-C25-C26-C27
26	T	1269	CDL	OB5-CB3-CB4-CB6
26	T	1269	CDL	C13-C14-C15-C16
22	O	1230	PSC	C23-C24-C25-C26
26	G	269	CDL	C33-C34-C35-C36
26	P	1270	CDL	C57-C58-C59-C60
20	C	268	PGV	C24-C25-C26-C27
26	G	269	CDL	C44-C45-C46-C47
20	C	268	PGV	C13-C14-C15-C16
26	C	270	CDL	C36-C37-C38-C39
20	N	1524	PGV	C01-C02-O01-C1
28	G	264	PEK	C16-C17-C18-C19
20	P	1267	PGV	C02-C03-O11-P
28	P	1264	PEK	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
28	G	1263	PEK	O04-C21-O03-C01
20	N	1524	PGV	O03-C01-C02-O01
26	P	1270	CDL	OA6-CA4-CA6-OA8
26	P	1270	CDL	OB6-CB4-CB6-OB8
20	P	1268	PGV	C15-C16-C17-C18
22	B	230	PSC	C5-C6-C7-C8
20	C	267	PGV	C22-C23-C24-C25
26	P	1270	CDL	C51-C52-C53-C54
28	G	265	PEK	C13-C14-C15-C16
20	A	522	PGV	C10-C11-C12-C13
20	P	1268	PGV	O01-C1-C2-C3
26	G	269	CDL	C61-C62-C63-C64
20	P	1268	PGV	C29-C30-C31-C32
20	N	1524	PGV	C7-C8-C9-C10
26	T	1269	CDL	C44-C45-C46-C47
20	A	522	PGV	C5-C6-C7-C8
20	A	524	PGV	C11-C10-C9-C8
20	C	268	PGV	C04-O12-P-O11
26	T	1269	CDL	CB2-OB2-PB2-OB5
20	N	1524	PGV	C05-C04-O12-P
20	P	1268	PGV	C05-C04-O12-P
20	C	268	PGV	C05-C04-O12-P
26	C	270	CDL	C42-C43-C44-C45
26	G	269	CDL	CA3-OA5-PA1-OA3
20	N	1524	PGV	C04-O12-P-O13
20	C	268	PGV	C04-O12-P-O14
26	T	1269	CDL	CB3-OB5-PB2-OB4
26	P	1270	CDL	CA2-OA2-PA1-OA4
26	P	1270	CDL	CA3-OA5-PA1-OA3
26	P	1270	CDL	CB2-OB2-PB2-OB3
26	P	1270	CDL	CB2-OB2-PB2-OB4
26	P	1270	CDL	CB3-OB5-PB2-OB4
22	B	230	PSC	C04-C05-N-C06
26	C	270	CDL	CA2-OA2-PA1-OA4
26	C	270	CDL	CB2-OB2-PB2-OB4
26	P	1270	CDL	C78-C79-C80-C81
26	P	1270	CDL	C83-C84-C85-C86
28	T	263	PEK	C01-C02-C03-O11
28	G	1263	PEK	C01-C02-C03-O11
20	C	267	PGV	C30-C31-C32-C33
20	A	522	PGV	C23-C24-C25-C26
28	P	1265	PEK	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
20	C	268	PGV	C7-C8-C9-C10
28	P	1264	PEK	C2-C1-O01-C02
19	D	523	TGL	C12-C13-C14-C29
20	A	522	PGV	C12-C13-C14-C15
26	G	269	CDL	C16-C17-C18-C19
26	C	270	CDL	C59-C60-C61-C62
19	N	1522	TGL	C21-C20-CA9-CA8
19	N	1521	TGL	CB5-CB6-CB7-CB8
20	A	524	PGV	O01-C02-C03-O11
20	P	1268	PGV	O01-C02-C03-O11
28	G	1263	PEK	O01-C02-C03-O11
26	C	270	CDL	OA5-CA3-CA4-OA6
26	G	269	CDL	C78-C79-C80-C81
20	A	524	PGV	C11-C12-C13-C14
19	A	521	TGL	C18-C19-C33-C34
23	P	1271	CHD	C16-C17-C20-C22
20	P	1268	PGV	C1-C2-C3-C4
28	T	263	PEK	C1-C2-C3-C4
19	Q	1523	TGL	CB4-CB5-CB6-CB7
19	L	522	TGL	CA7-CA8-CA9-C20
19	D	523	TGL	C11-C10-CB9-CB8
20	A	522	PGV	C25-C26-C27-C28
26	G	269	CDL	C32-C33-C34-C35
19	N	1522	TGL	CG1-CG2-CG3-OG3
19	Q	1523	TGL	CB7-CB8-CB9-C10
19	N	1522	TGL	OG2-CG2-CG3-OG3
28	T	263	PEK	C28-C29-C30-C31
26	C	270	CDL	C77-C78-C79-C80
20	P	1268	PGV	C10-C11-C12-C13
19	Q	1523	TGL	CB9-C10-C11-C12
20	N	1524	PGV	C9-C10-C11-C12
26	G	269	CDL	C20-C21-C22-C23
19	N	1521	TGL	C18-C19-C33-C34
28	G	1263	PEK	C32-C33-C34-C35
20	A	524	PGV	C15-C16-C17-C18
19	A	521	TGL	C17-C18-C19-C33
19	N	1522	TGL	CB7-CB8-CB9-C10
28	P	1265	PEK	C22-C23-C24-C25
26	G	269	CDL	C52-C51-CB5-OB6
19	D	523	TGL	OG1-CA1-CA2-CA3
19	A	521	TGL	C20-C21-C22-C23
20	N	1524	PGV	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
19	A	521	TGL	CG1-CG2-OG2-CB1
19	Q	1523	TGL	CG3-CG2-OG2-CB1
22	B	230	PSC	C01-C02-O01-C1
26	C	270	CDL	CA2-C1-CB2-OB2
24	Z	1526	DMU	C19-C22-C25-C28
20	P	1268	PGV	C4-C5-C6-C7
26	P	1270	CDL	CA5-C11-C12-C13
28	P	1264	PEK	C34-C35-C36-C37
19	D	523	TGL	C18-C19-C33-C34
26	P	1270	CDL	OA5-CA3-CA4-OA6
20	A	524	PGV	C7-C8-C9-C10
20	P	1268	PGV	C24-C25-C26-C27
20	N	1266	PGV	C29-C30-C31-C32
19	Q	1523	TGL	C10-C11-C12-C13
19	N	1521	TGL	C23-C24-C25-C26
26	G	269	CDL	CB2-OB2-PB2-OB5
20	A	524	PGV	C04-O12-P-O11
20	P	1268	PGV	C04-O12-P-O11
28	G	265	PEK	C04-O12-P-O11
26	C	270	CDL	CB3-OB5-PB2-OB2
28	T	263	PEK	C34-C35-C36-C37
24	C	272	DMU	C31-C34-C37-C40
20	N	1266	PGV	C13-C14-C15-C16
19	N	1522	TGL	C11-C10-CB9-CB8
19	A	521	TGL	CB3-CB4-CB5-CB6
26	P	1270	CDL	CA7-C31-C32-C33
24	M	526	DMU	C31-C34-C37-C40
23	C	271	CHD	C16-C17-C20-C22
28	T	263	PEK	C35-C36-C37-C38
20	C	268	PGV	C02-C03-O11-P
28	G	1263	PEK	C02-C03-O11-P
26	C	270	CDL	C1-CB2-OB2-PB2
28	P	1264	PEK	C17-C18-C19-C20
19	L	522	TGL	C29-C30-C31-C32
28	G	1263	PEK	C10-C11-C12-C13
24	Z	1526	DMU	C34-C37-C40-C43
22	O	1230	PSC	O04-C19-C20-C21
19	Q	1523	TGL	C21-C20-CA9-CA8
20	N	1266	PGV	C25-C26-C27-C28
18	N	515	HEA	C12-C13-C14-C15
24	P	1272	DMU	C18-C19-C22-C25
20	A	522	PGV	C02-C01-O03-C19

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Mol	Chain	Res	Type	Atoms
26	C	270	CDL	C20-C21-C22-C23
28	G	264	PEK	C32-C33-C34-C35
26	T	1269	CDL	C15-C16-C17-C18
26	T	1269	CDL	CA3-CA4-CA6-OA8
28	G	265	PEK	O02-C1-O01-C02
20	A	524	PGV	C23-C24-C25-C26
20	N	1524	PGV	C5-C6-C7-C8
24	M	526	DMU	O16-C18-C19-C22
28	G	264	PEK	C22-C23-C24-C25
20	C	267	PGV	C12-C13-C14-C15
26	P	1270	CDL	C20-C21-C22-C23
22	O	1230	PSC	C03-C02-O01-C1
22	B	230	PSC	C03-C02-O01-C1
28	T	263	PEK	C3-C4-C5-C6
20	P	1267	PGV	C3-C4-C5-C6
19	D	523	TGL	CC3-CC4-CC5-CC6
22	O	1230	PSC	C10-C11-C12-C13
20	N	1524	PGV	C04-O12-P-O11
28	T	263	PEK	C6-C7-C8-C9
28	T	263	PEK	C9-C10-C11-C12
28	G	1263	PEK	C12-C13-C14-C15
28	G	265	PEK	C11-C10-C9-C8
28	G	265	PEK	C9-C10-C11-C12
22	B	230	PSC	C14-C15-C16-C17
26	T	1269	CDL	C64-C65-C66-C67
28	G	1263	PEK	C34-C35-C36-C37
26	G	269	CDL	C17-C18-C19-C20
20	C	267	PGV	C15-C16-C17-C18
26	C	270	CDL	C31-C32-C33-C34
19	N	1521	TGL	CA9-C20-C21-C22
26	G	269	CDL	OA6-CA4-CA6-OA8
28	P	1265	PEK	O03-C01-C02-O01
28	G	264	PEK	C35-C36-C37-C38
19	A	521	TGL	C10-C11-C12-C13
28	T	263	PEK	C4-C5-C6-C7
26	T	1269	CDL	CB2-C1-CA2-OA2
26	P	1270	CDL	CA2-C1-CB2-OB2
26	T	1269	CDL	C72-C73-C74-C75
19	Q	1523	TGL	CA3-CA4-CA5-CA6
19	N	1522	TGL	OG2-CB1-CB2-CB3
22	B	230	PSC	C26-C27-C28-C29
19	Q	1523	TGL	C19-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
26	T	1269	CDL	C38-C39-C40-C41
19	N	1521	TGL	CB7-CB8-CB9-C10
26	T	1269	CDL	C52-C51-CB5-OB6
20	A	522	PGV	O03-C19-C20-C21
22	B	230	PSC	O01-C1-C2-C3
19	N	1522	TGL	CA1-CA2-CA3-CA4
26	T	1269	CDL	C60-C61-C62-C63
20	P	1267	PGV	C14-C15-C16-C17
24	C	272	DMU	C5-C10-O7-C3
24	C	272	DMU	C19-C22-C25-C28
26	T	1269	CDL	OA9-CA7-OA8-CA6
19	N	1522	TGL	C13-C14-C29-C30
22	O	1230	PSC	O01-C02-C03-O11
19	Q	1523	TGL	C33-C34-C35-C36
20	A	522	PGV	C29-C30-C31-C32
26	T	1269	CDL	C24-C25-C26-C27
20	P	1267	PGV	C05-C04-O12-P
19	L	522	TGL	OA1-CA1-CA2-CA3
20	N	1524	PGV	O03-C19-C20-C21
28	G	1263	PEK	C2-C1-O01-C02
26	T	1269	CDL	C31-CA7-OA8-CA6
19	N	1521	TGL	C22-C23-C24-C25
26	C	270	CDL	C24-C25-C26-C27
26	C	270	CDL	C64-C65-C66-C67
20	A	524	PGV	C14-C15-C16-C17
28	T	263	PEK	C24-C25-C26-C27
19	N	1522	TGL	CA6-CA7-CA8-CA9
19	N	1522	TGL	OG1-CA1-CA2-CA3
20	N	1266	PGV	O03-C19-C20-C21
20	N	1266	PGV	C9-C10-C11-C12
20	N	1266	PGV	C20-C21-C22-C23
28	G	1263	PEK	C16-C17-C18-C19
23	P	1271	CHD	C16-C17-C20-C21
28	T	263	PEK	O02-C1-O01-C02
19	L	522	TGL	CC7-CC8-CC9-C15
20	P	1268	PGV	C19-C20-C21-C22
26	C	270	CDL	C62-C63-C64-C65
23	C	271	CHD	C16-C17-C20-C21
28	G	264	PEK	O01-C1-C2-C3
19	L	522	TGL	OG3-CC1-CC2-CC3
20	A	524	PGV	C9-C10-C11-C12
22	O	1230	PSC	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
28	G	264	PEK	C14-C15-C16-C17
28	P	1264	PEK	C2-C3-C4-C5
26	G	269	CDL	C53-C54-C55-C56
28	P	1264	PEK	O01-C1-C2-C3
19	D	523	TGL	OB1-CB1-CB2-CB3
20	P	1268	PGV	C9-C10-C11-C12
28	P	1265	PEK	C3-C4-C5-C6
20	A	522	PGV	C9-C10-C11-C12
19	Q	1523	TGL	C29-C30-C31-C32
26	T	1269	CDL	C82-C83-C84-C85
28	T	263	PEK	O01-C1-C2-C3
28	P	1265	PEK	O01-C1-C2-C3
28	G	264	PEK	C26-C27-C28-C29
26	C	270	CDL	OB6-CB4-CB6-OB8
26	C	270	CDL	CA7-C31-C32-C33
19	D	523	TGL	CA5-CA6-CA7-CA8
19	Q	1523	TGL	OG3-CC1-CC2-CC3
26	C	270	CDL	C52-C51-CB5-OB6
24	P	1272	DMU	C5-C10-O7-C3
20	A	522	PGV	C31-C32-C33-C34
22	B	230	PSC	C3-C4-C5-C6
28	G	265	PEK	C2-C1-O01-C02
26	P	1270	CDL	C12-C11-CA5-OA6
20	C	268	PGV	C25-C26-C27-C28
19	L	522	TGL	C21-C22-C23-C24
28	T	263	PEK	C2-C1-O01-C02
24	C	272	DMU	C18-C19-C22-C25
20	P	1267	PGV	C4-C5-C6-C7
20	N	1524	PGV	C04-C05-C06-O06
28	G	264	PEK	C34-C35-C36-C37
19	N	1521	TGL	C17-C18-C19-C33
26	C	270	CDL	C40-C41-C42-C43
19	Q	1523	TGL	OC1-CC1-CC2-CC3
26	C	270	CDL	CB3-CB4-CB6-OB8
20	C	268	PGV	O12-C04-C05-O05
19	L	522	TGL	OC1-CC1-CC2-CC3
26	G	269	CDL	CB2-OB2-PB2-OB3
26	G	269	CDL	CB3-OB5-PB2-OB4
20	A	524	PGV	C04-O12-P-O13
28	P	1265	PEK	C03-O11-P-O14
20	A	522	PGV	C04-O12-P-O13
22	B	230	PSC	C03-O11-P-O14

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Mol	Chain	Res	Type	Atoms
19	L	522	TGL	CA3-CA4-CA5-CA6
19	L	522	TGL	C11-C12-C13-C14
19	D	523	TGL	C29-C30-C31-C32
28	G	264	PEK	O02-C1-C2-C3
22	O	1230	PSC	C01-C02-C03-O11
26	T	1269	CDL	C83-C84-C85-C86
28	P	1264	PEK	O12-C04-C05-N
28	P	1265	PEK	O02-C1-C2-C3
19	L	522	TGL	C23-C24-C25-C26
19	Q	1523	TGL	OG2-CB1-CB2-CB3
28	P	1264	PEK	O02-C1-C2-C3
26	G	269	CDL	C64-C65-C66-C67
22	O	1230	PSC	C05-C04-O12-P
28	G	264	PEK	C05-C04-O12-P
26	T	1269	CDL	C33-C34-C35-C36
20	C	267	PGV	C13-C14-C15-C16
28	T	263	PEK	O02-C1-C2-C3
26	C	270	CDL	C52-C51-CB5-OB7
24	Z	1526	DMU	O6-C11-C9-C8
24	Z	1526	DMU	C19-C18-O16-C6
19	Q	1523	TGL	OG1-CA1-CA2-CA3
26	P	1270	CDL	C12-C11-CA5-OA7
26	C	270	CDL	O1-C1-CB2-OB2
20	A	524	PGV	O03-C19-C20-C21
20	C	268	PGV	O01-C1-C2-C3
20	A	522	PGV	C4-C5-C6-C7
20	A	522	PGV	C11-C12-C13-C14
19	L	522	TGL	OG2-CB1-CB2-CB3

There are no ring outliers.

44 monomers are involved in 285 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	N	520	PER	1	0
26	G	269	CDL	24	0
23	W	1060	CHD	4	0
20	A	524	PGV	8	0
15	A	520	PER	1	0
28	P	1264	PEK	6	0
22	O	1230	PSC	12	0
18	A	515	HEA	7	0
24	Z	1526	DMU	1	0

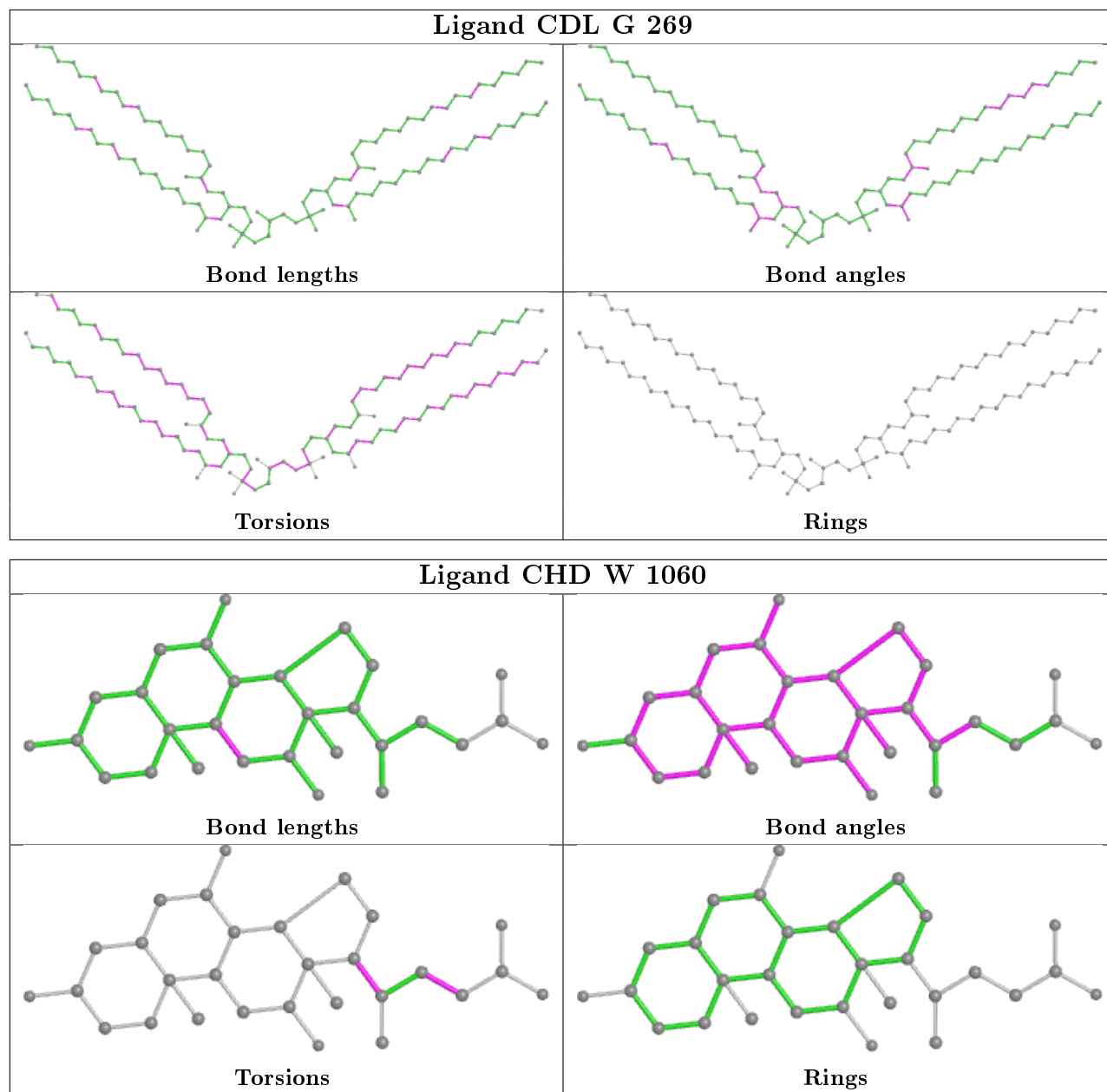
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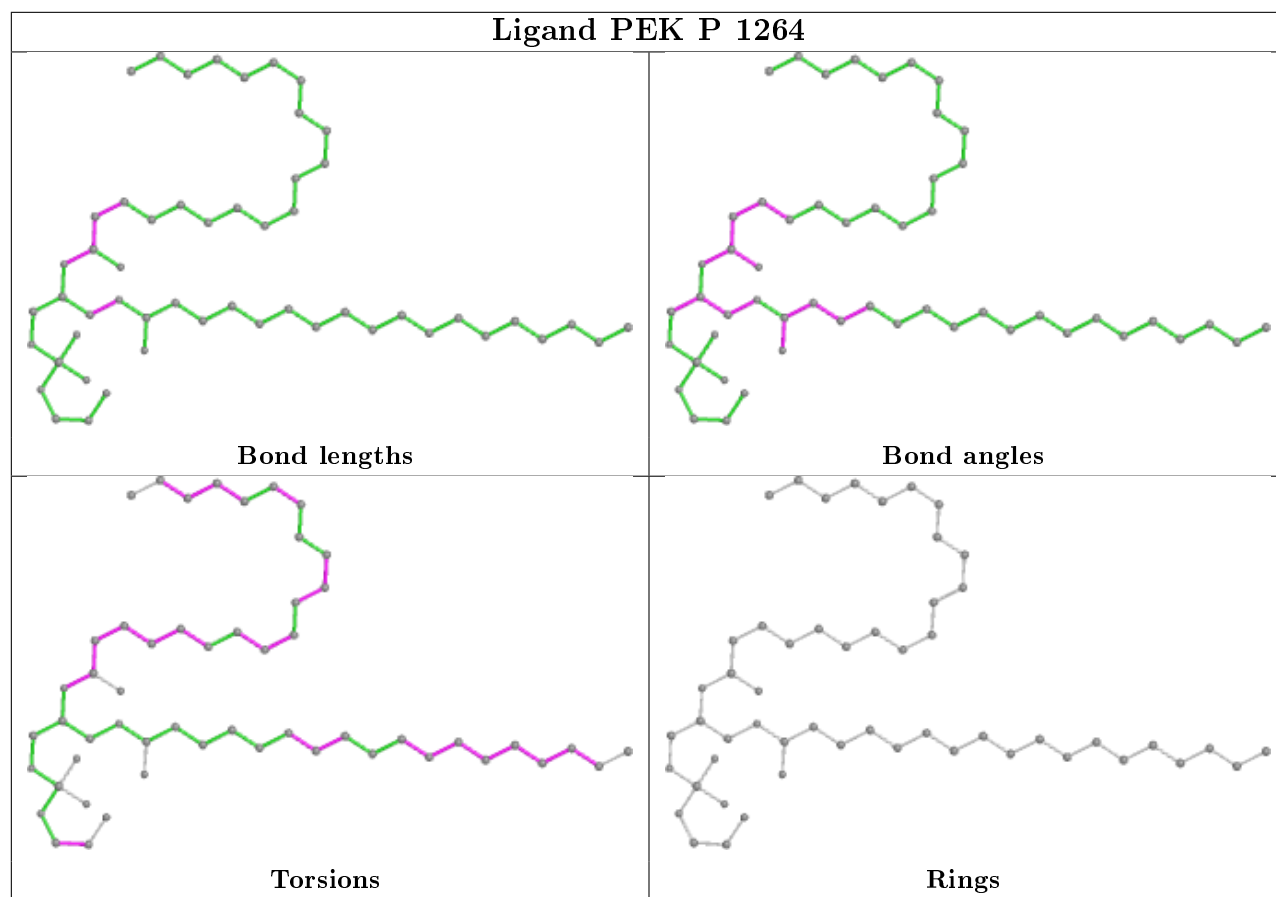
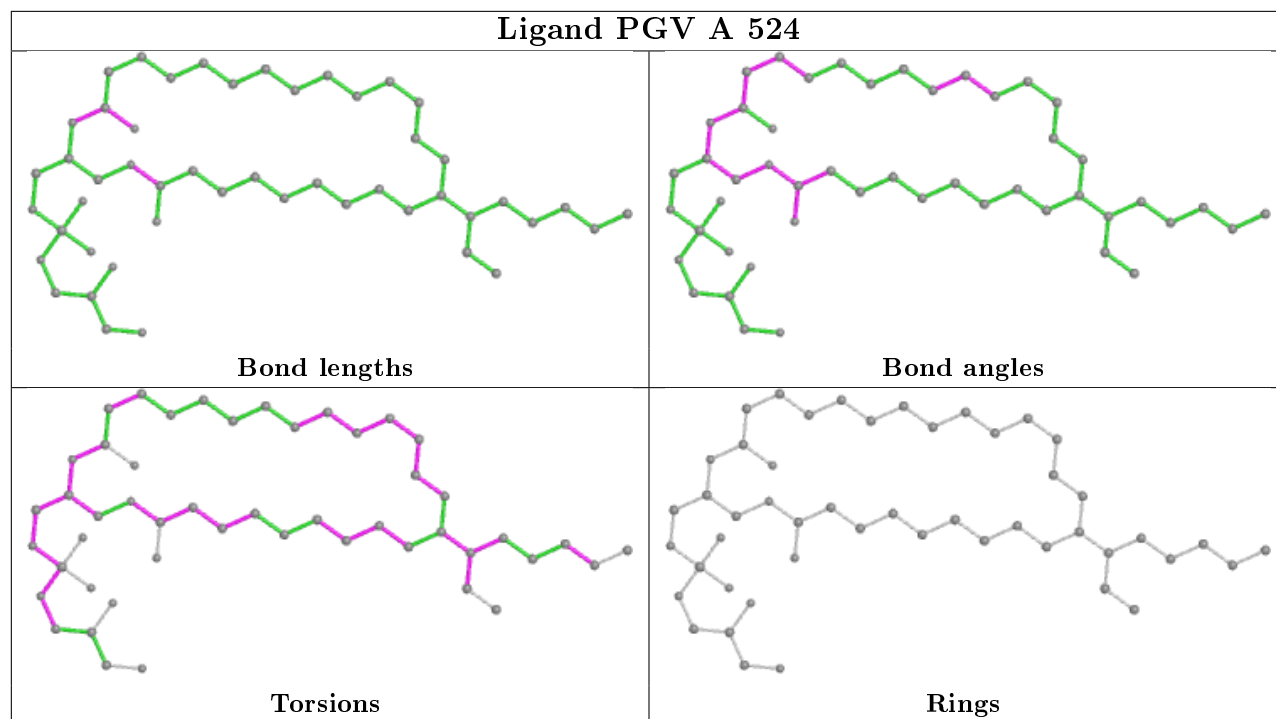
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	N	1524	PGV	6	0
20	P	1268	PGV	3	0
24	M	526	DMU	1	0
19	A	521	TGL	6	0
20	C	268	PGV	1	0
28	T	263	PEK	21	0
28	G	1263	PEK	7	0
28	G	265	PEK	7	0
18	N	515	HEA	8	0
23	C	525	CHD	2	0
18	N	516	HEA	1	0
28	G	264	PEK	6	0
19	N	1522	TGL	11	0
24	C	272	DMU	5	0
28	P	1265	PEK	8	0
19	Q	1523	TGL	5	0
26	T	1269	CDL	23	0
23	B	1086	CHD	1	0
20	P	1267	PGV	5	0
20	N	1266	PGV	1	0
23	O	229	CHD	2	0
23	C	271	CHD	3	0
18	A	516	HEA	5	0
20	C	267	PGV	5	0
19	L	522	TGL	16	0
26	P	1270	CDL	16	0
19	N	1521	TGL	9	0
23	J	60	CHD	3	0
23	P	1525	CHD	3	0
24	P	1272	DMU	2	0
20	A	522	PGV	2	0
22	B	230	PSC	18	0
23	P	1271	CHD	3	0
26	C	270	CDL	13	0
19	D	523	TGL	15	0

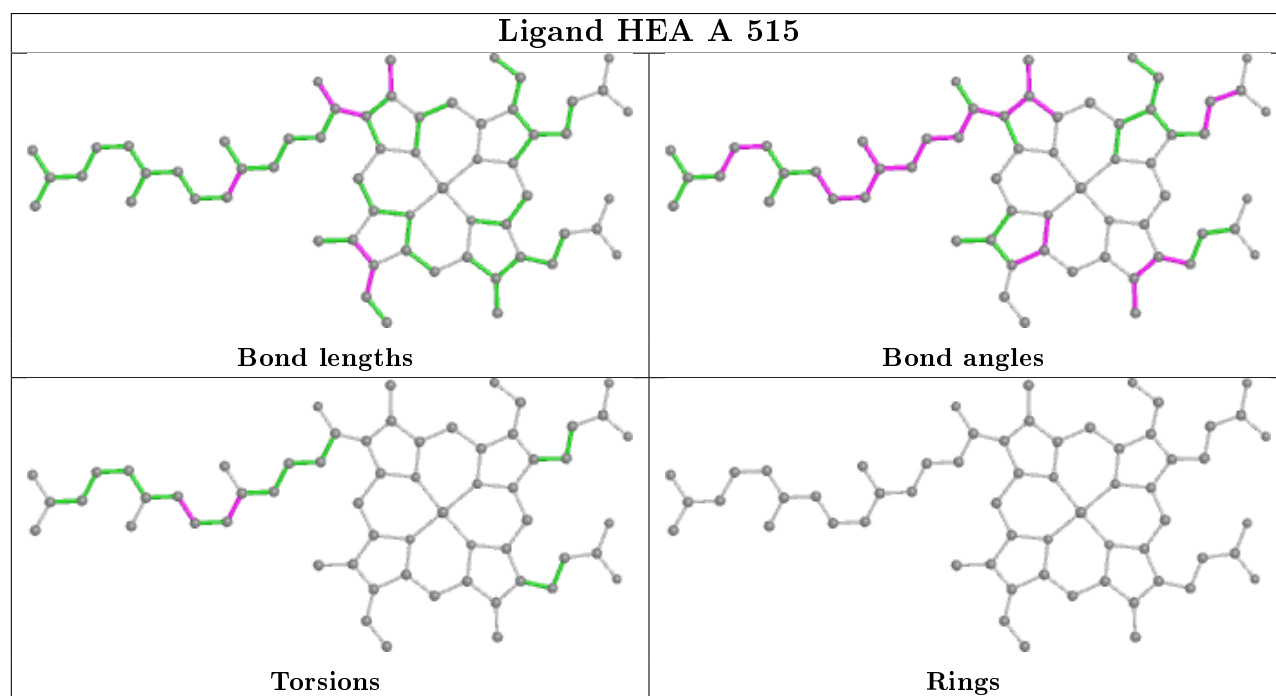
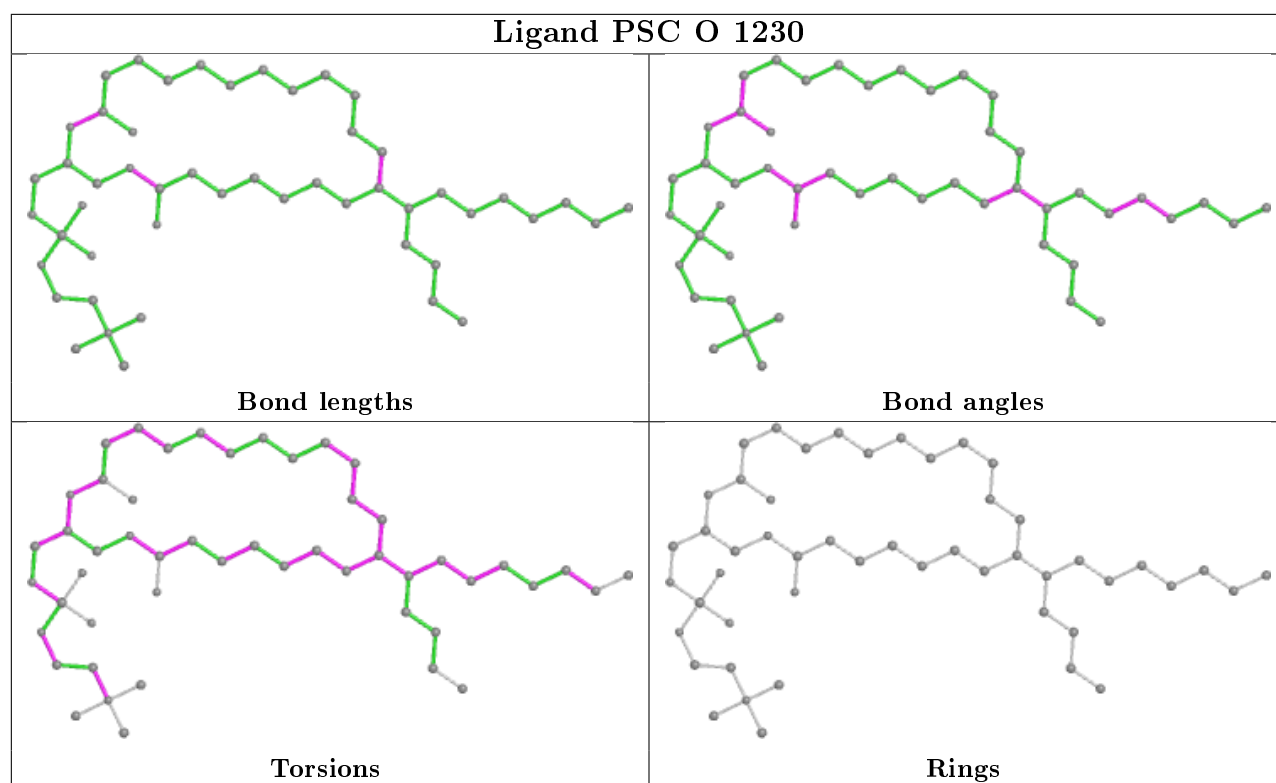
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

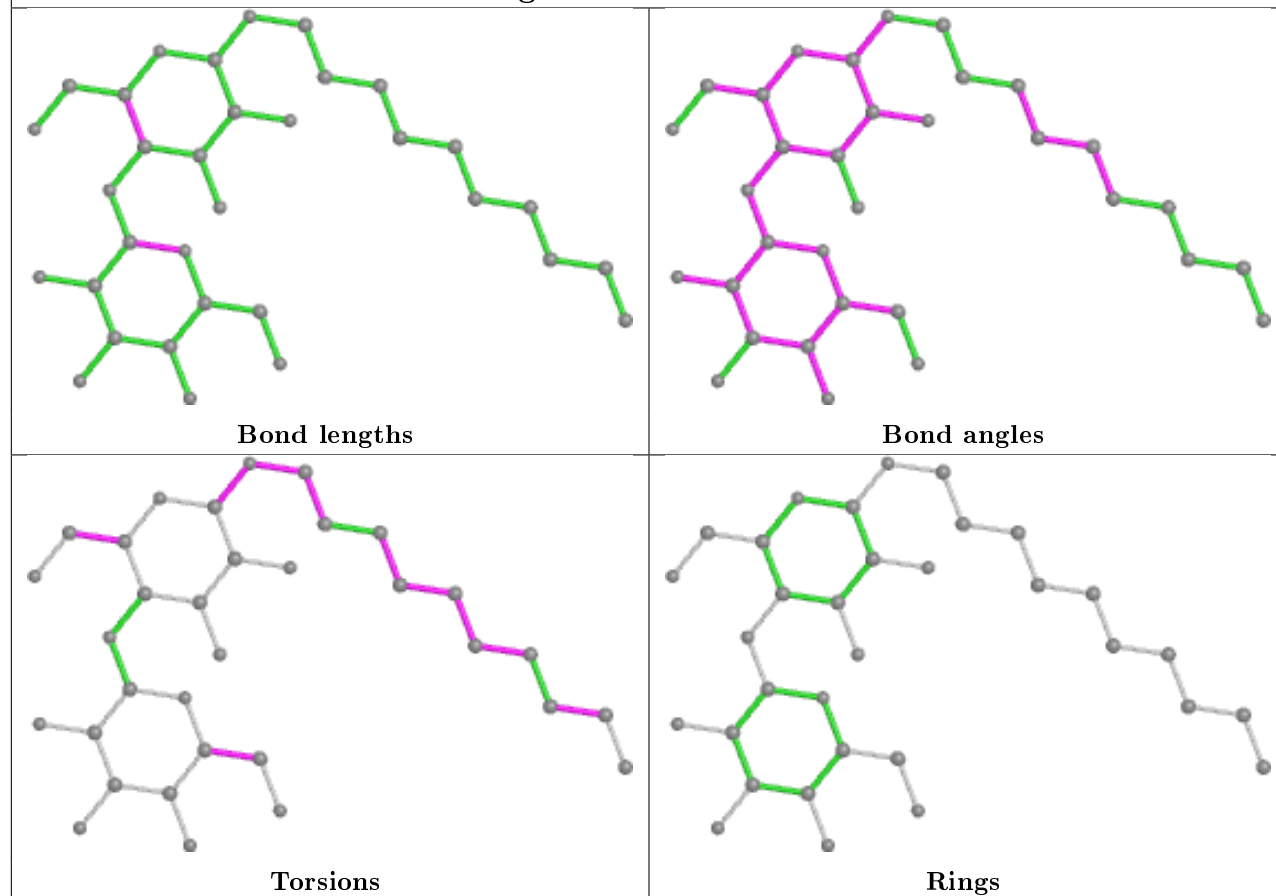




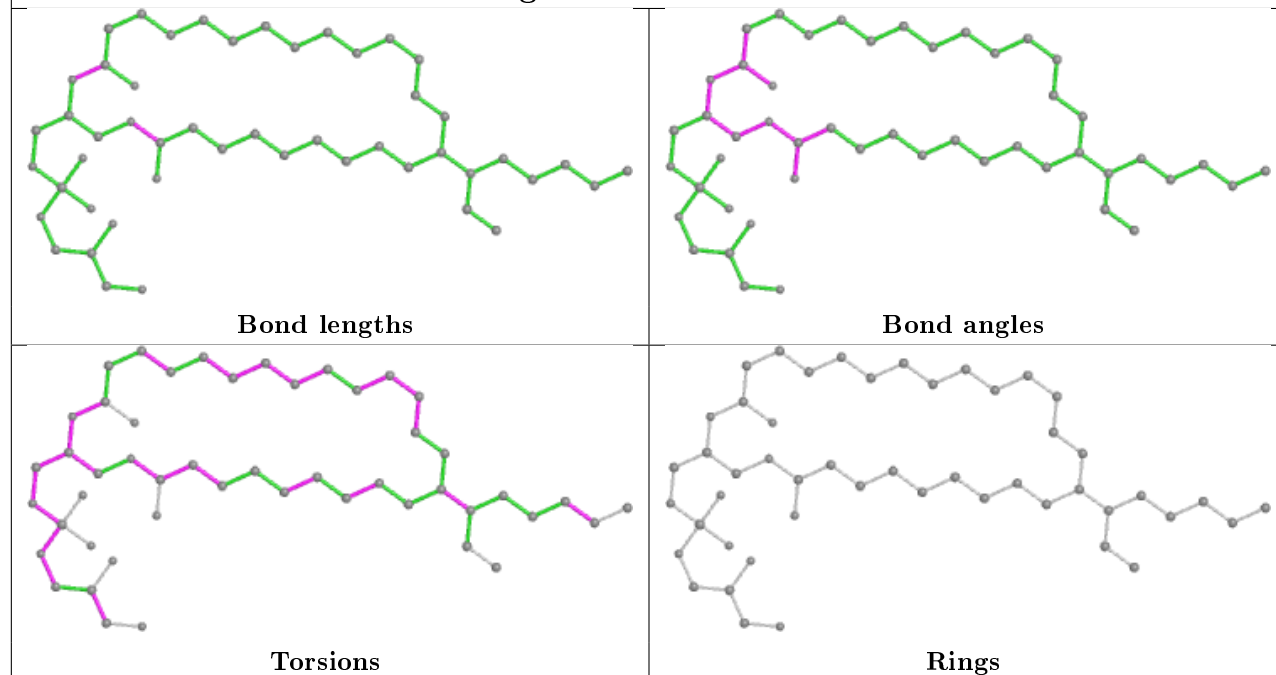




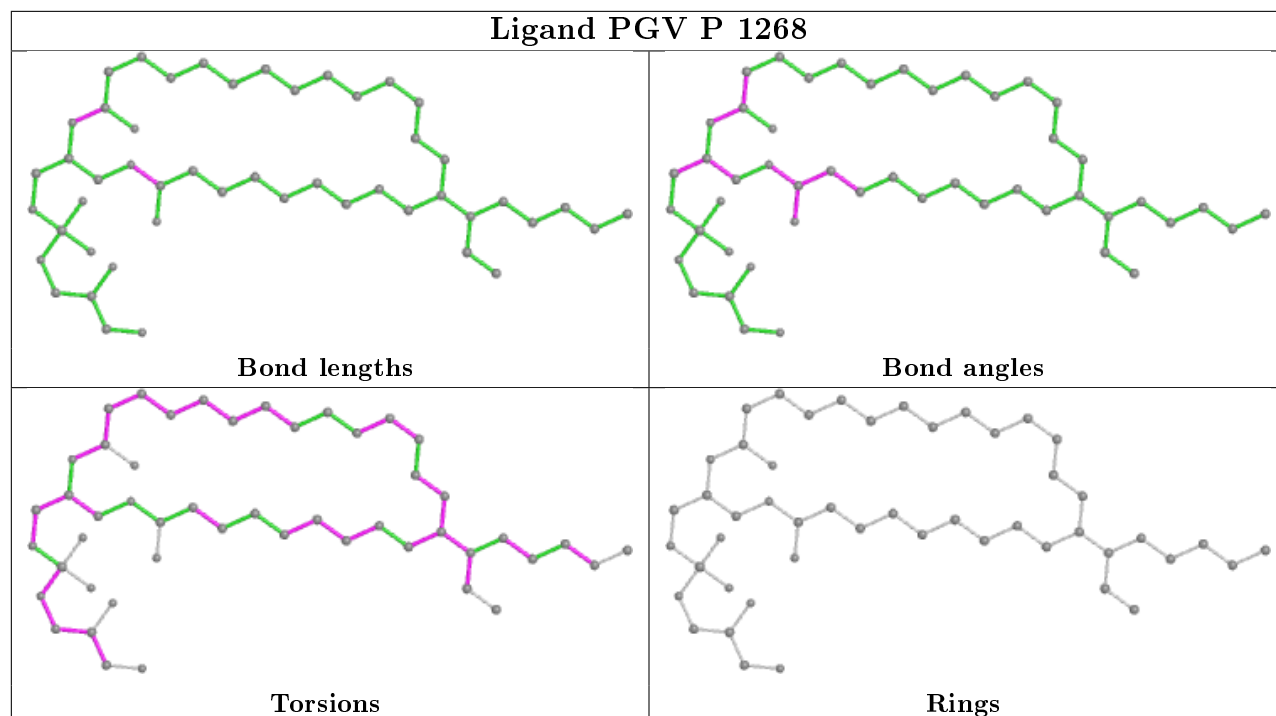
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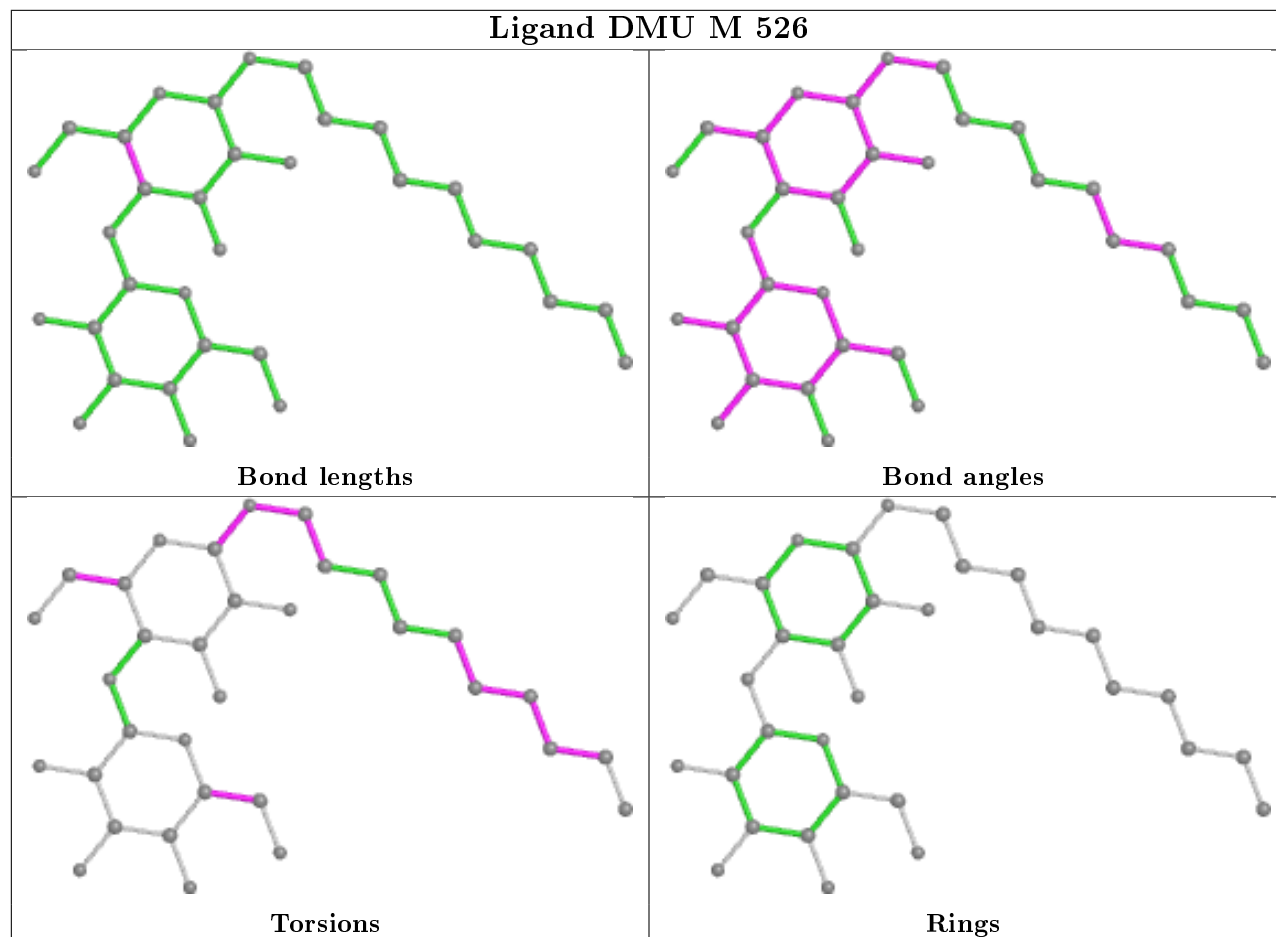
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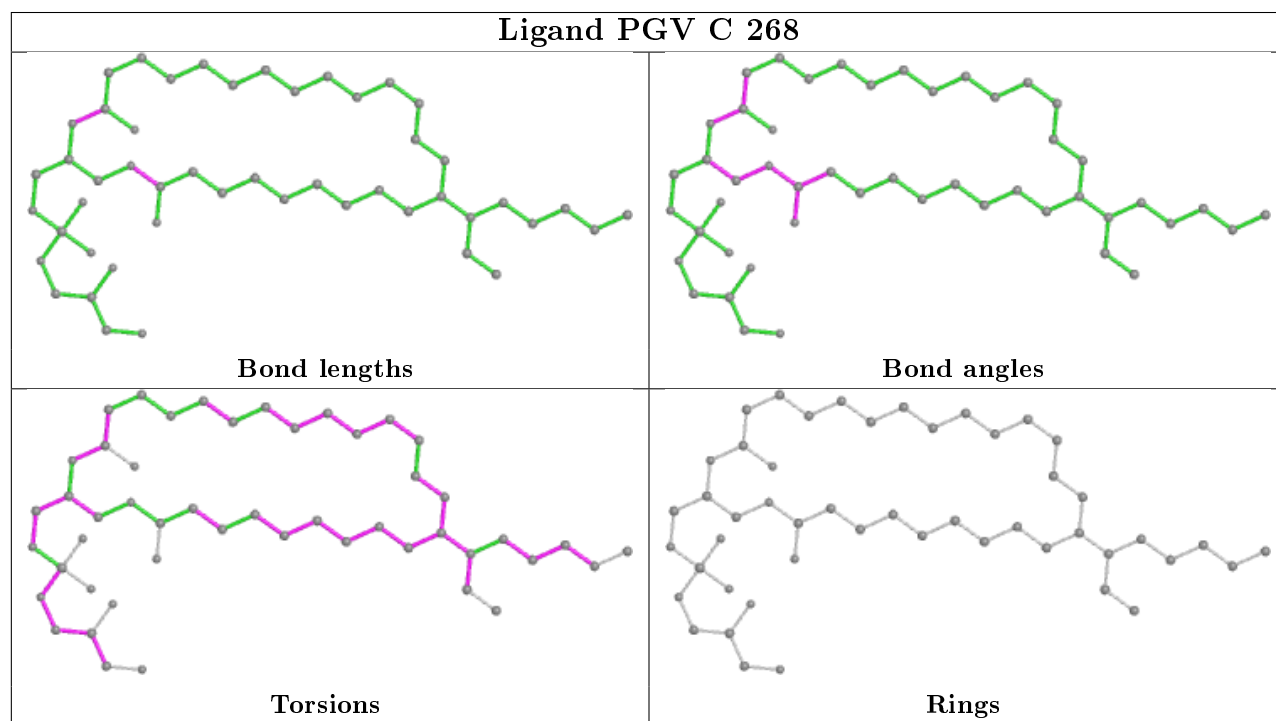
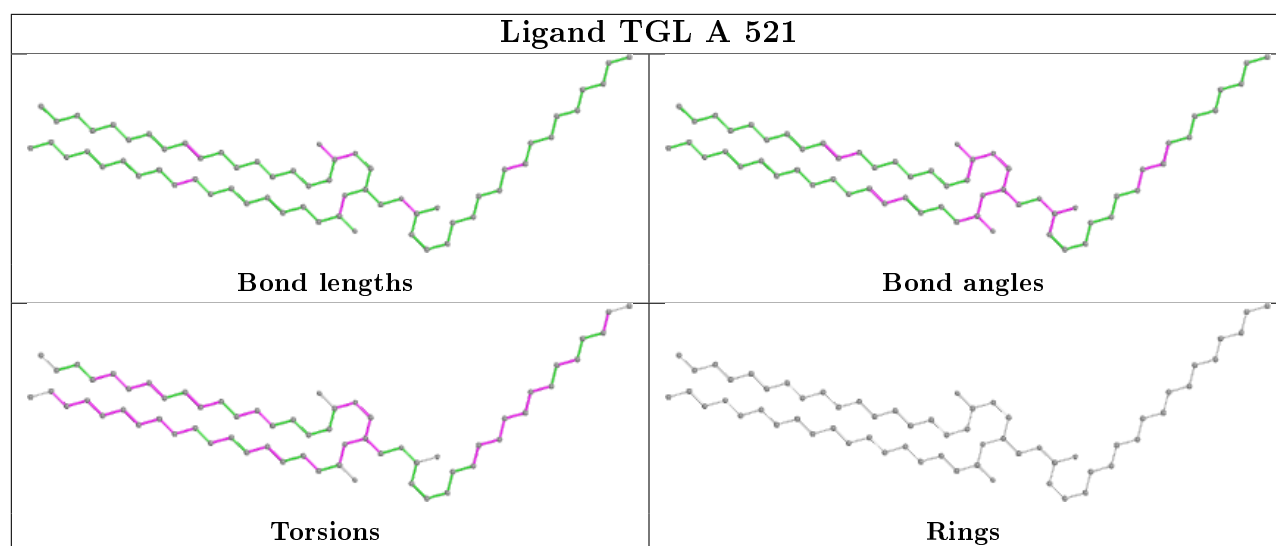


## Ligand PGV P 1268

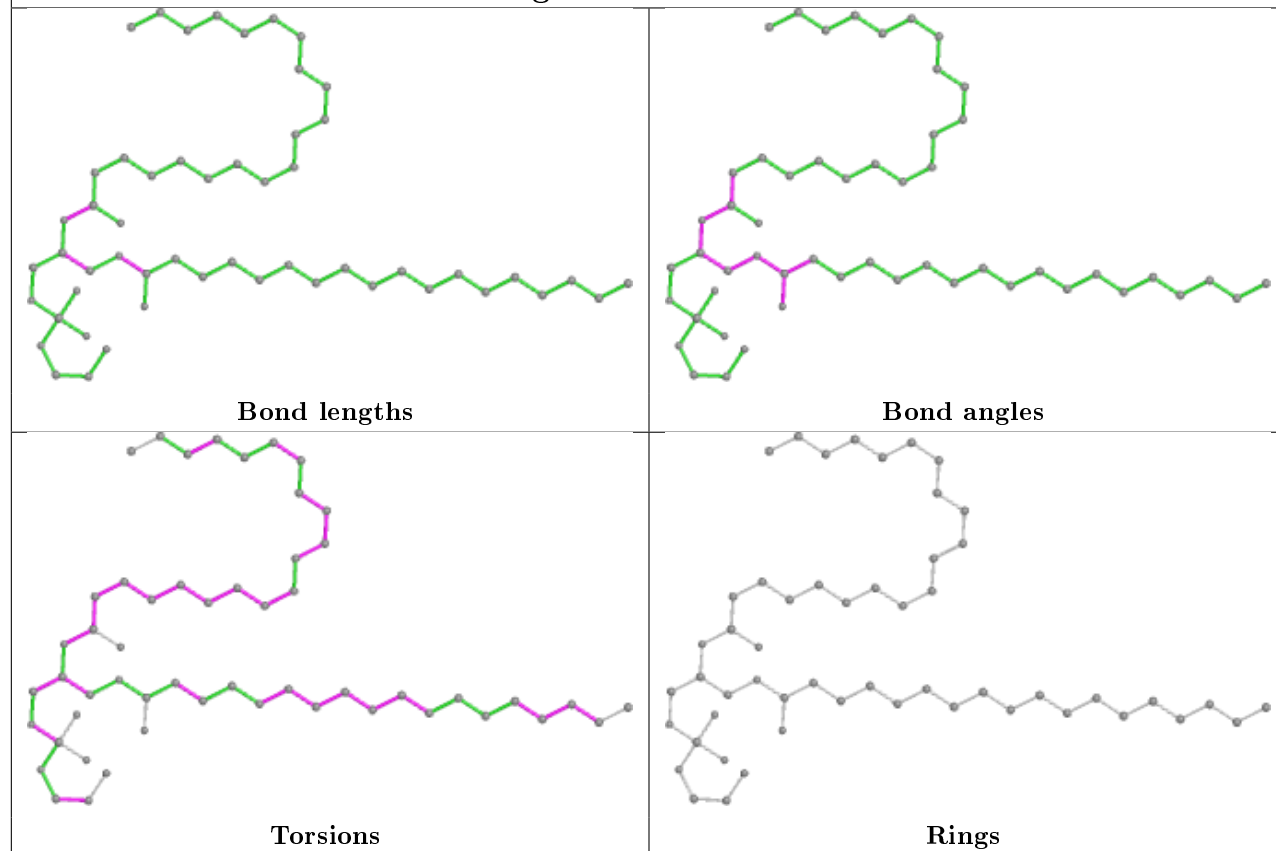


## Ligand DMU M 526

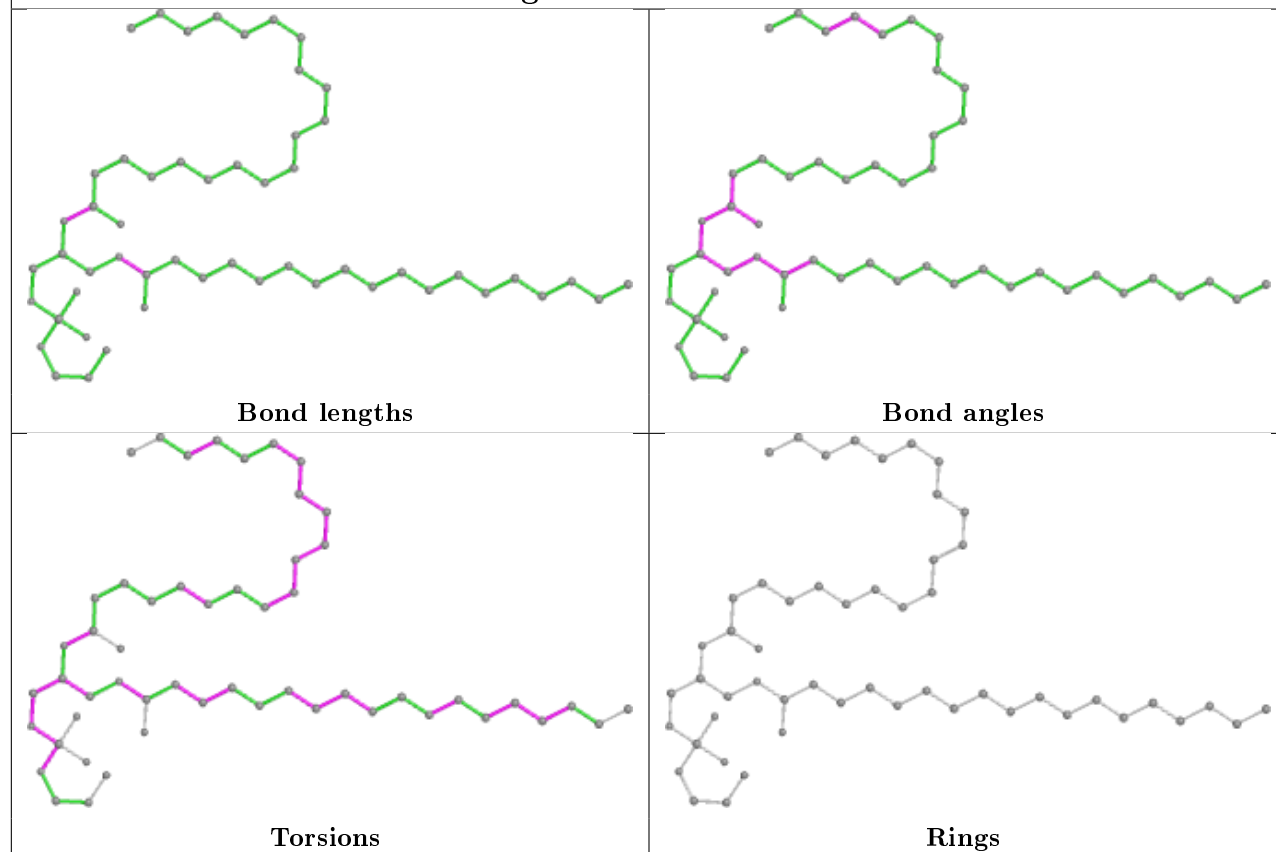




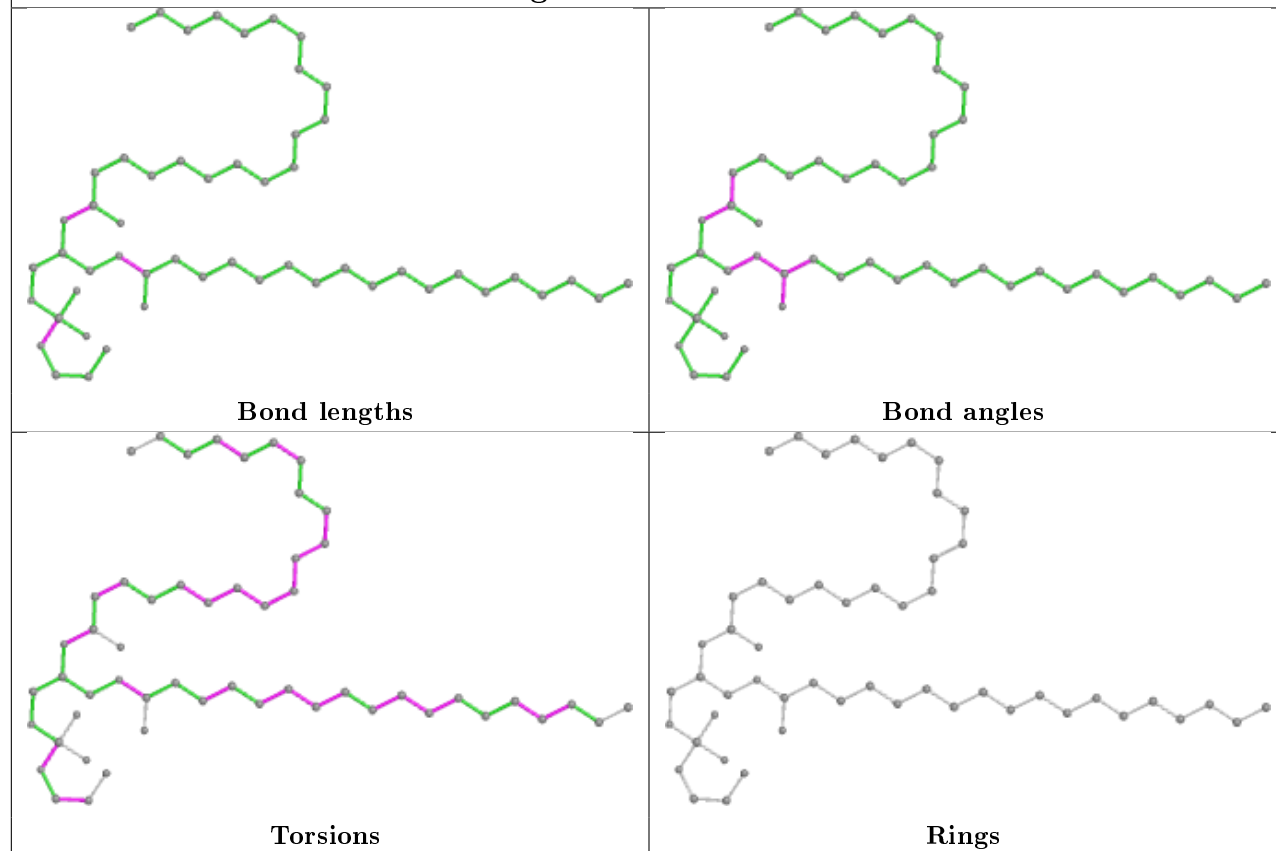
## Ligand PEK T 263



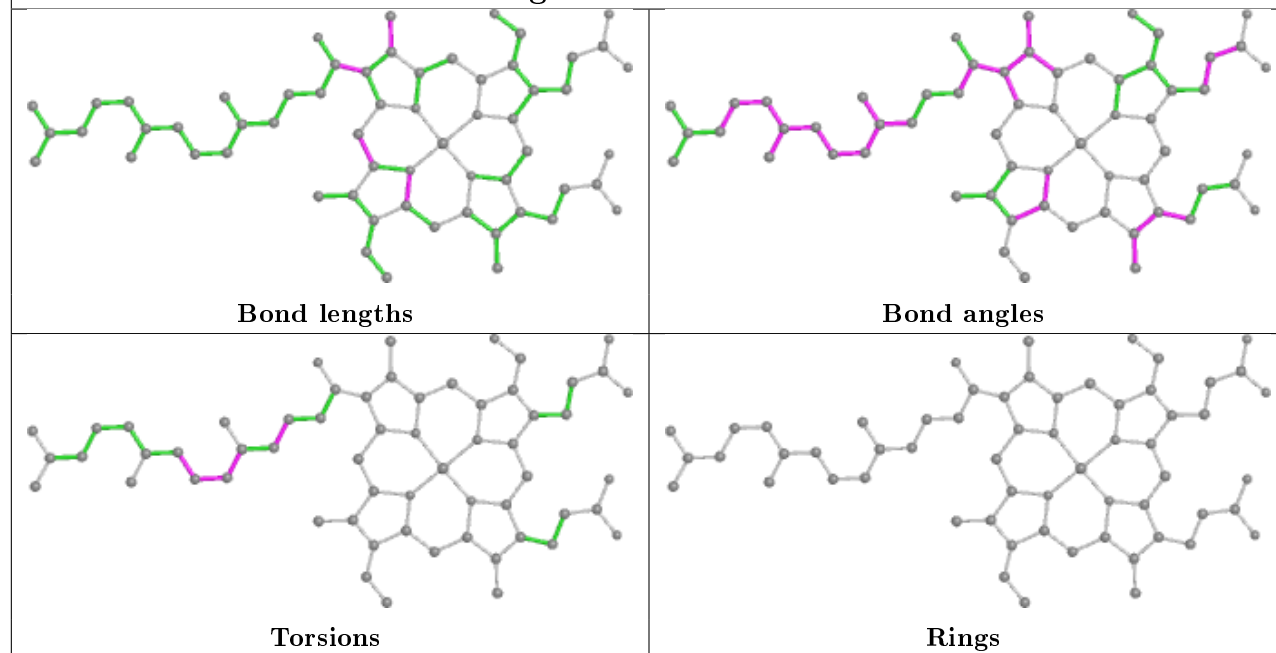
## Ligand PEK G 1263

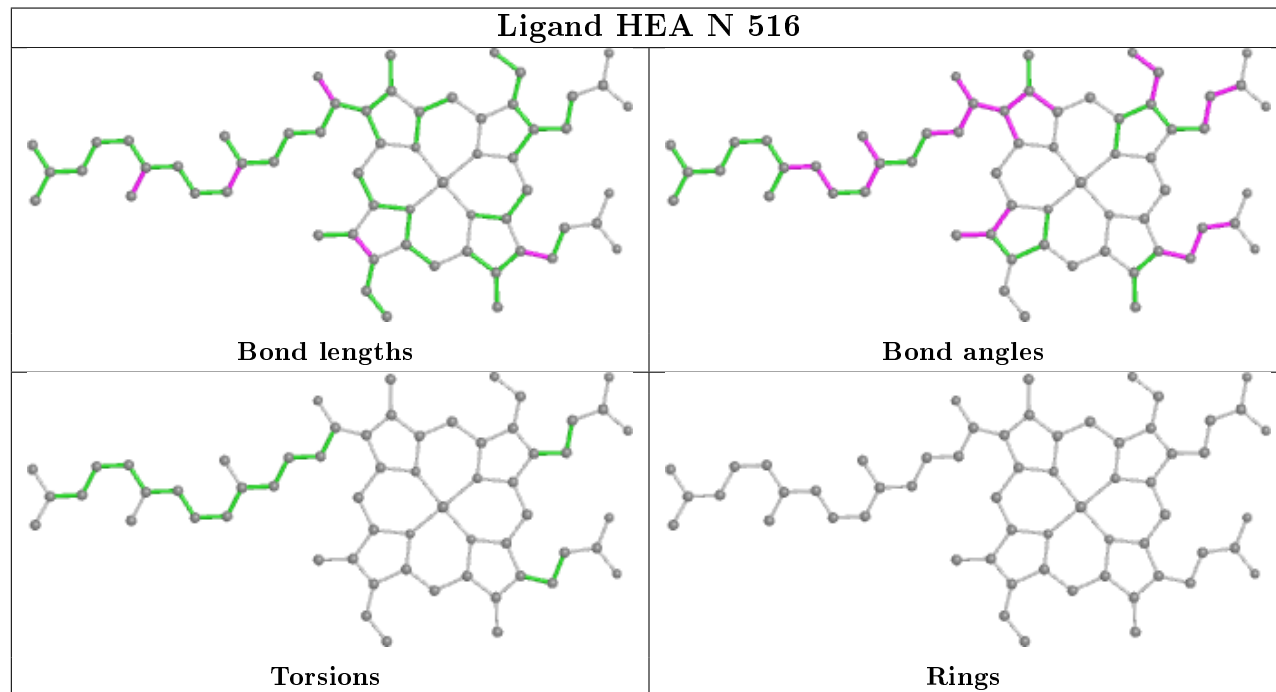
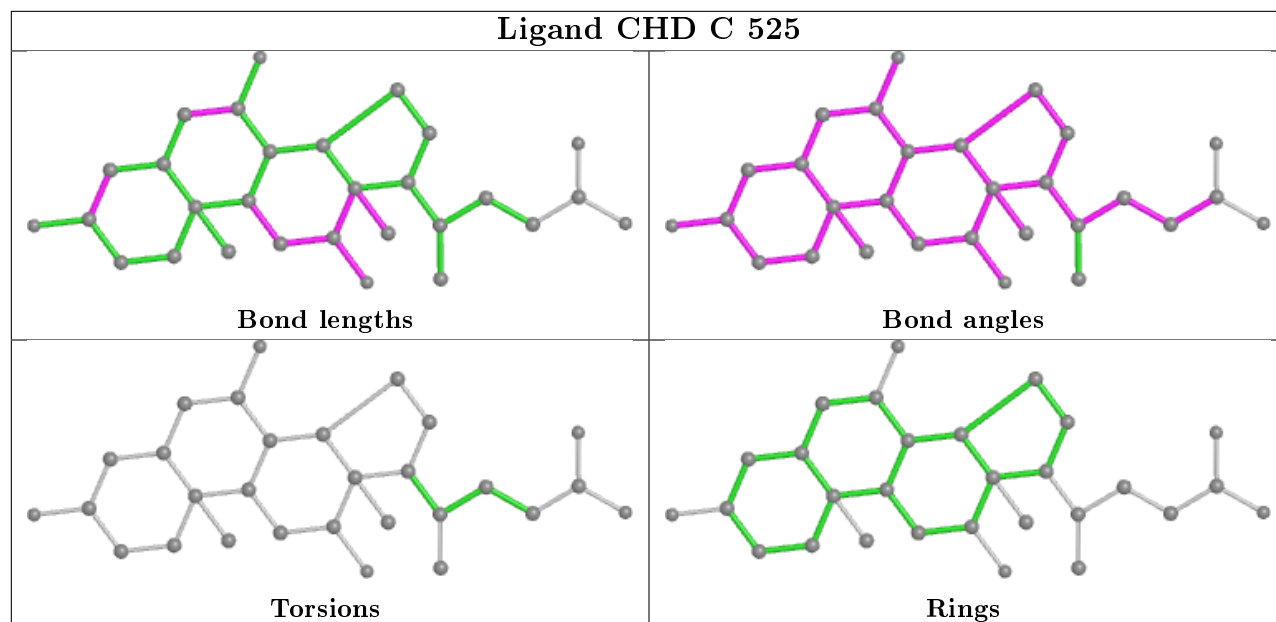


## Ligand PEK G 265

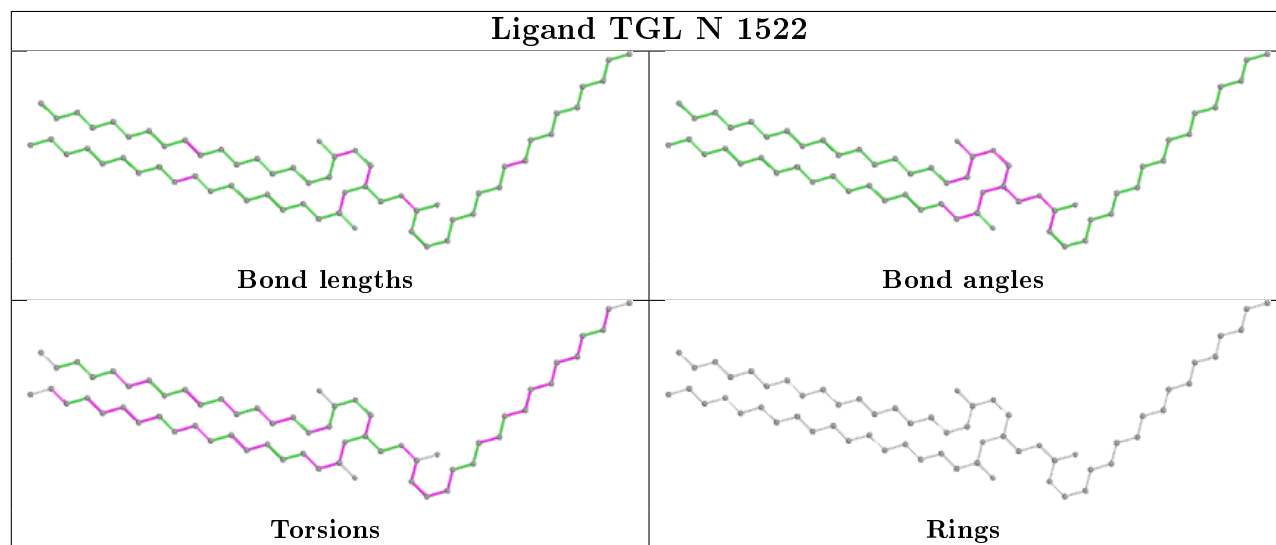
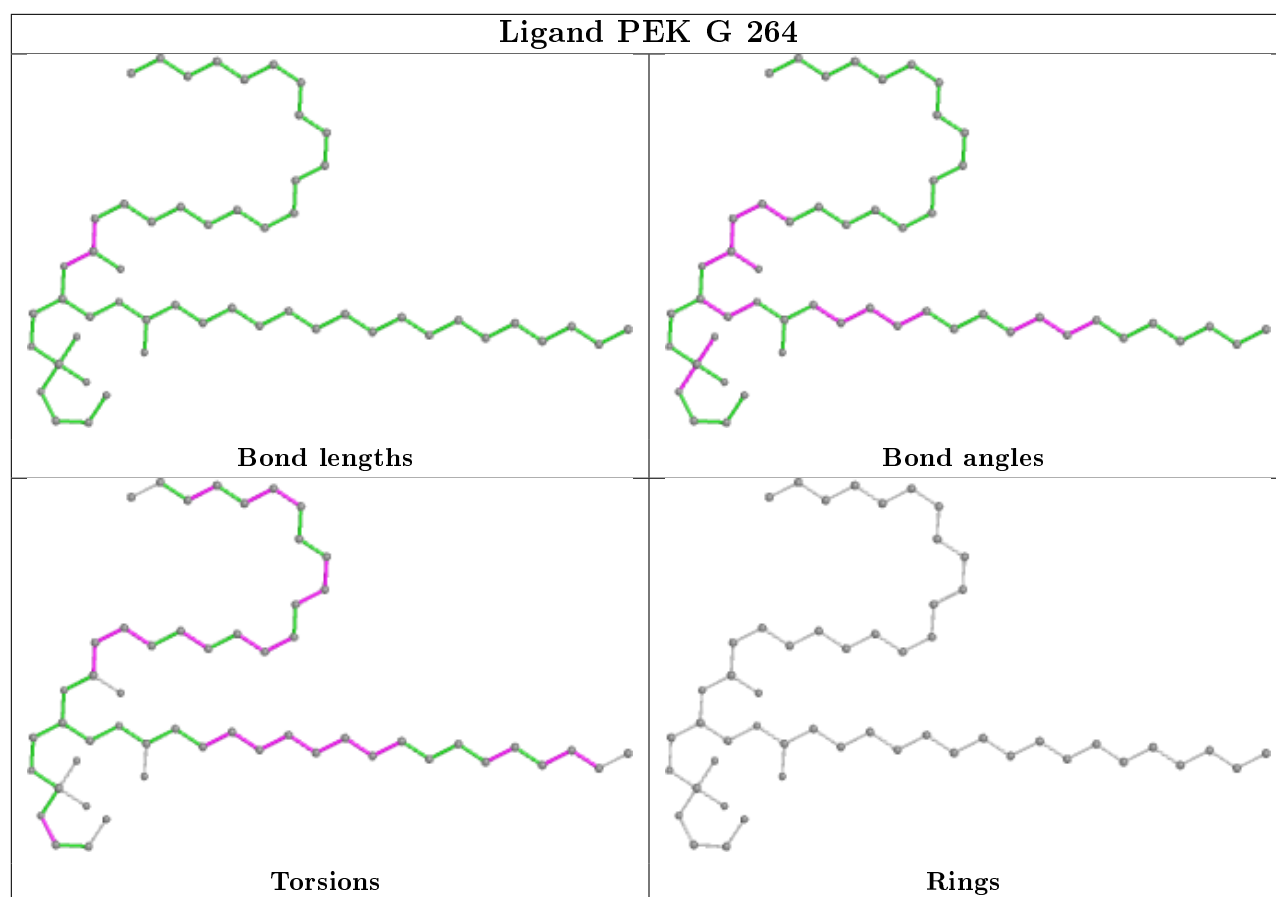


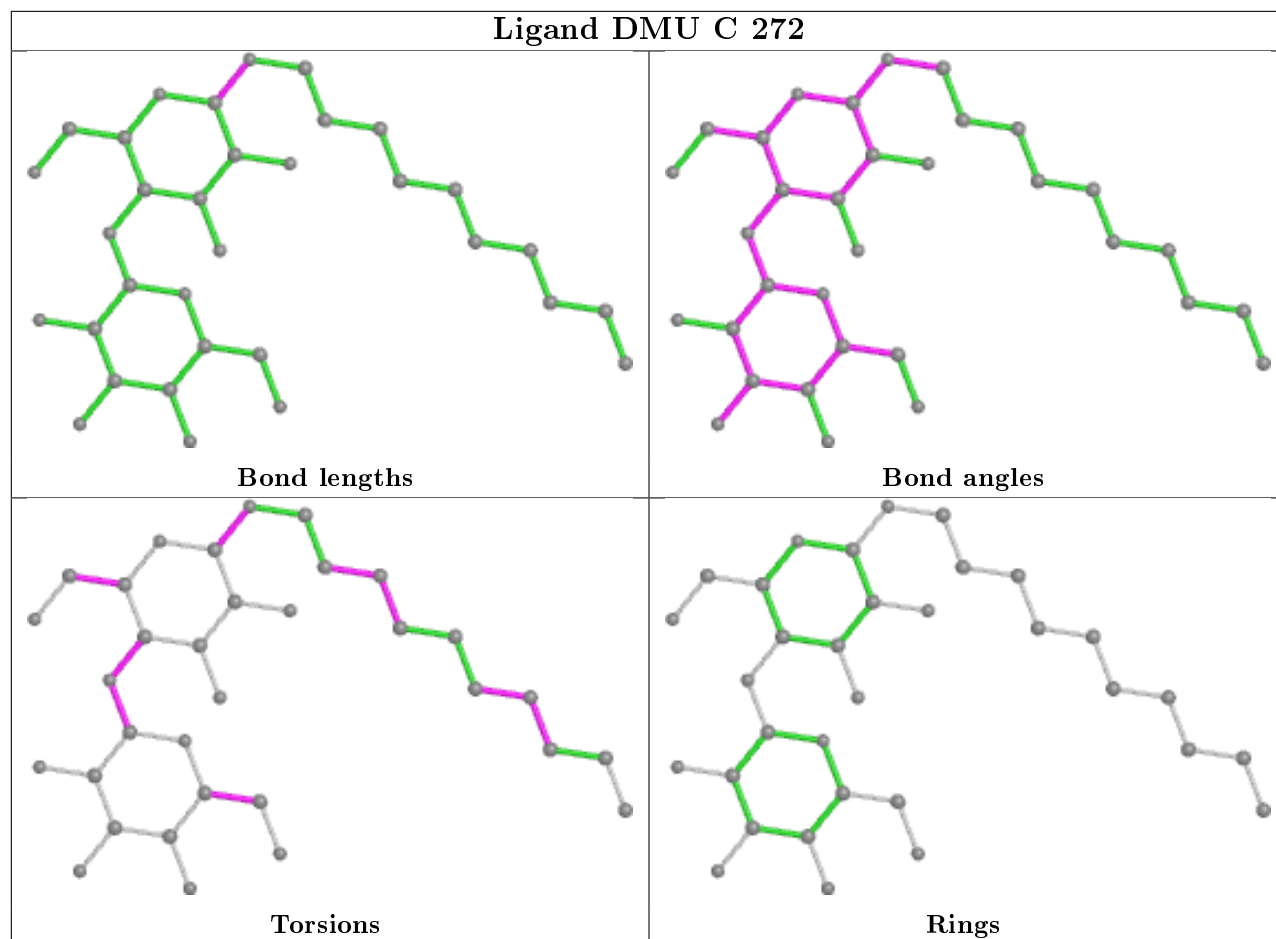
## Ligand HEA N 515

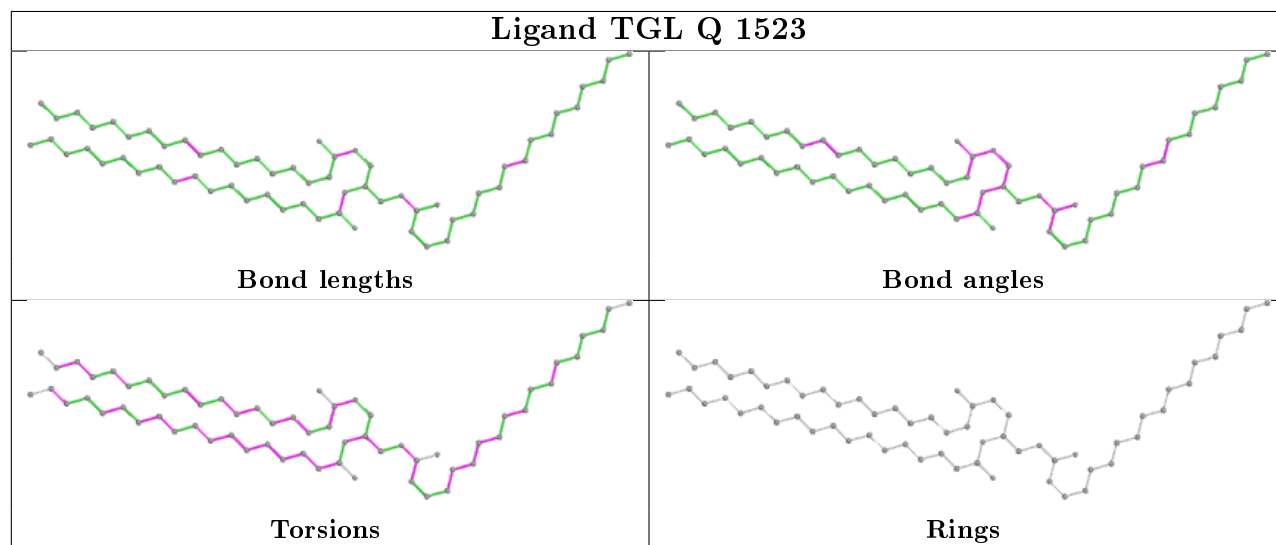
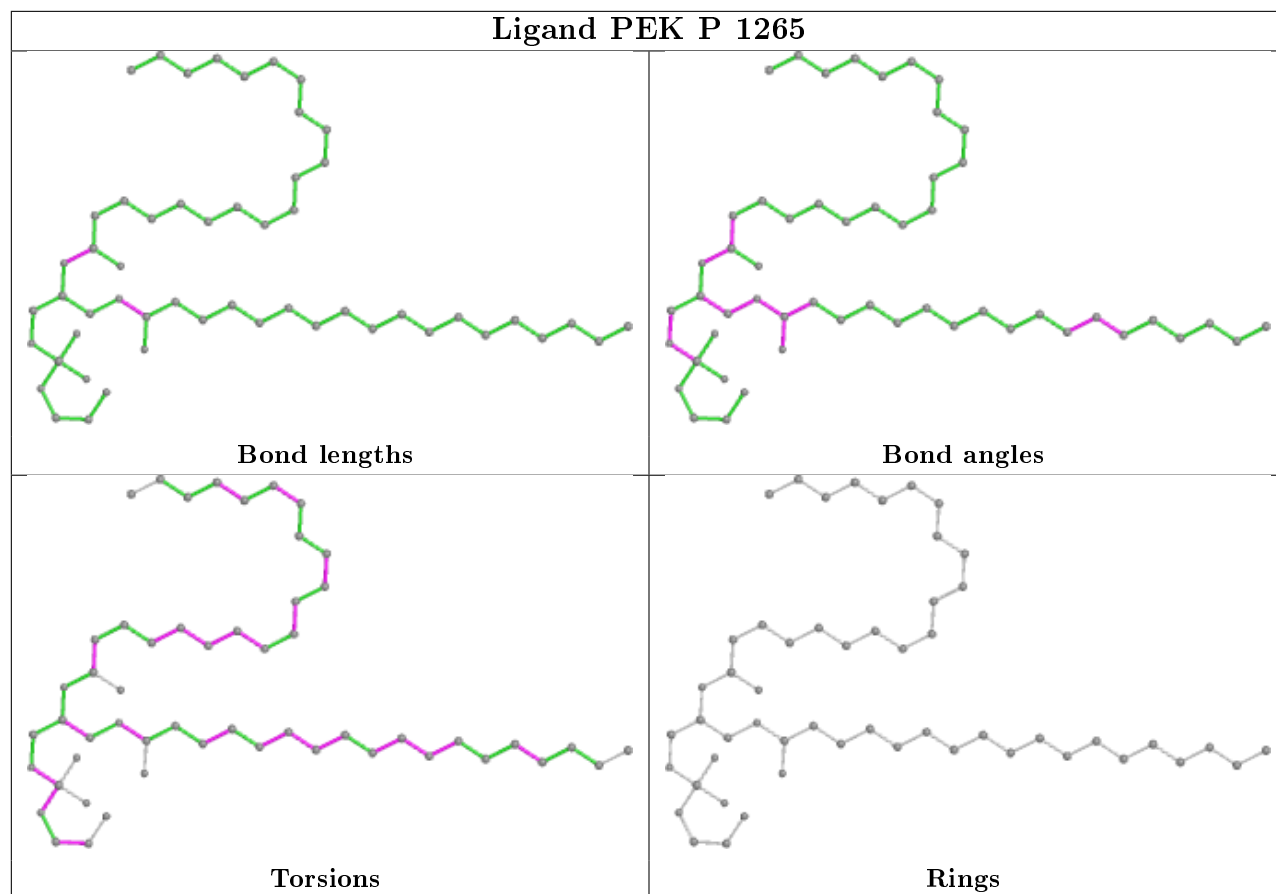


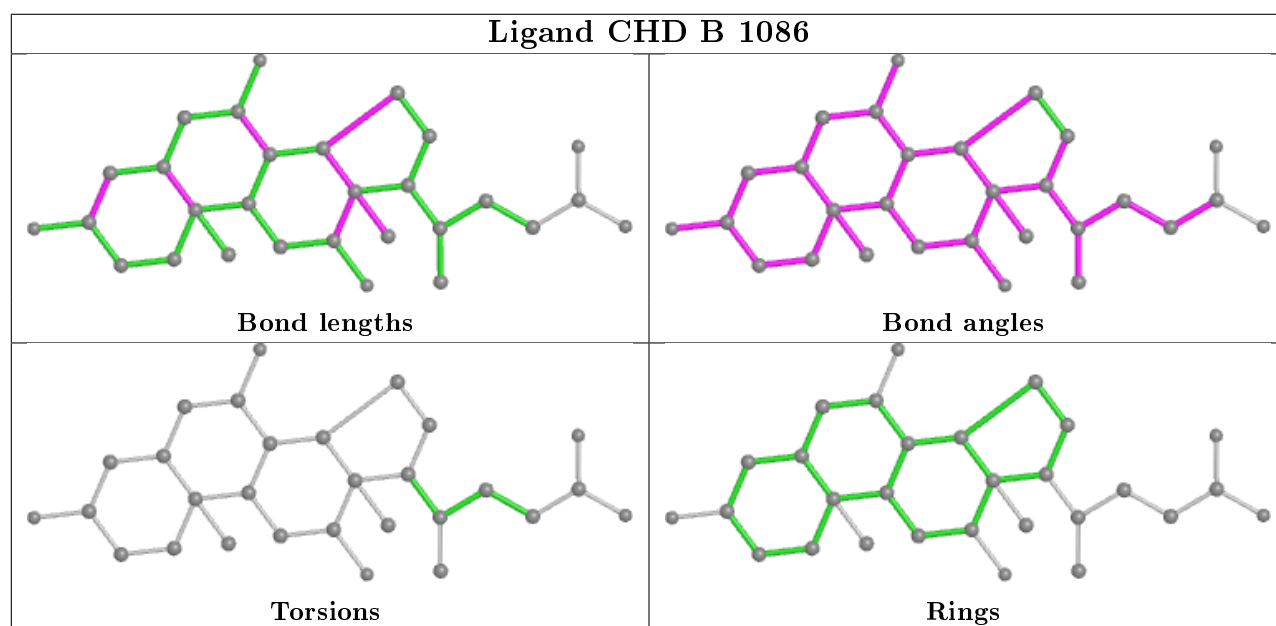
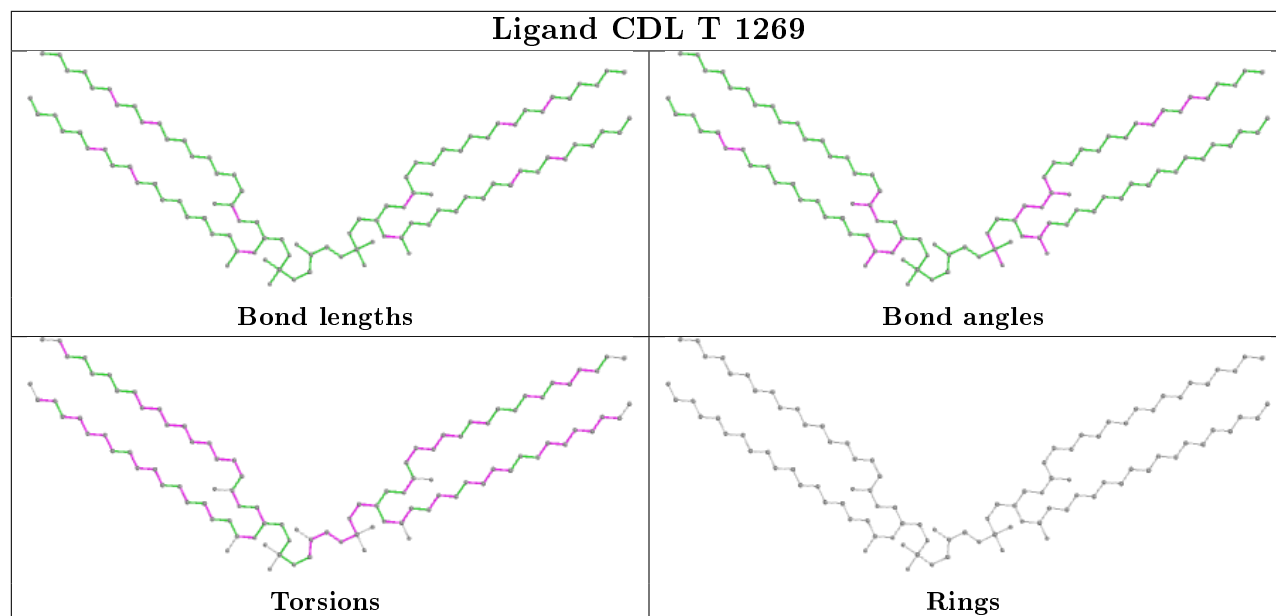


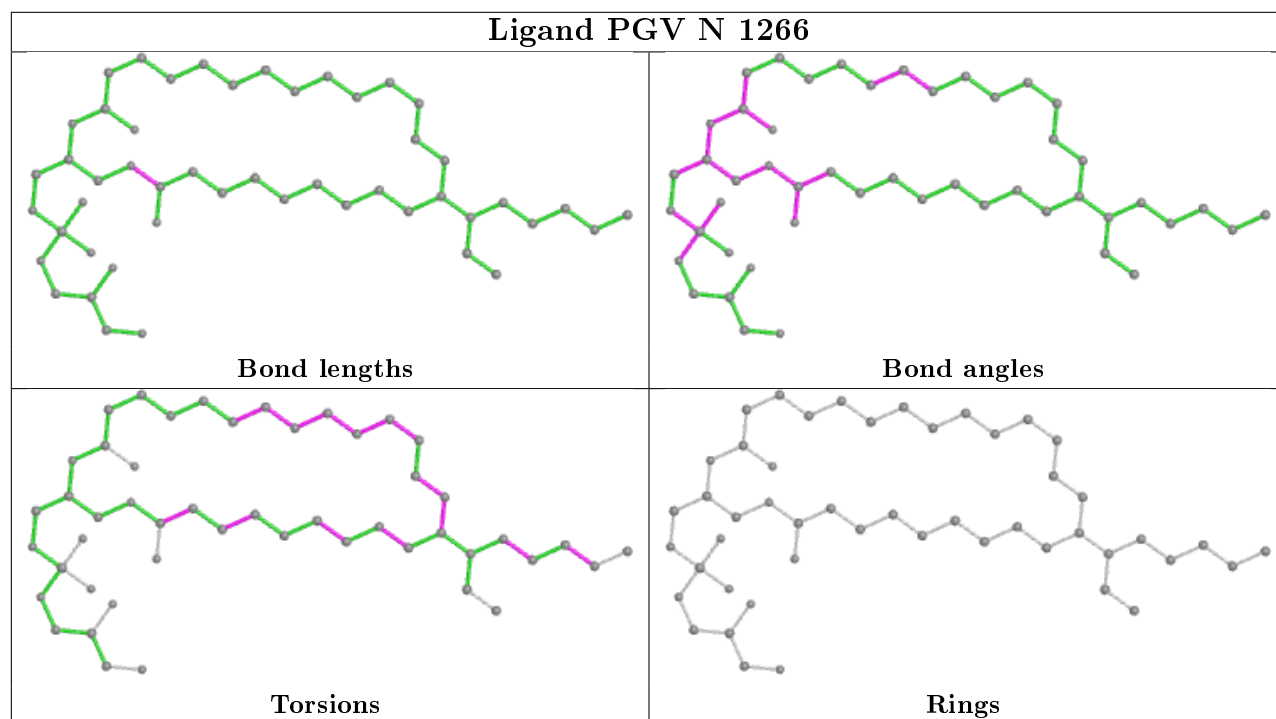
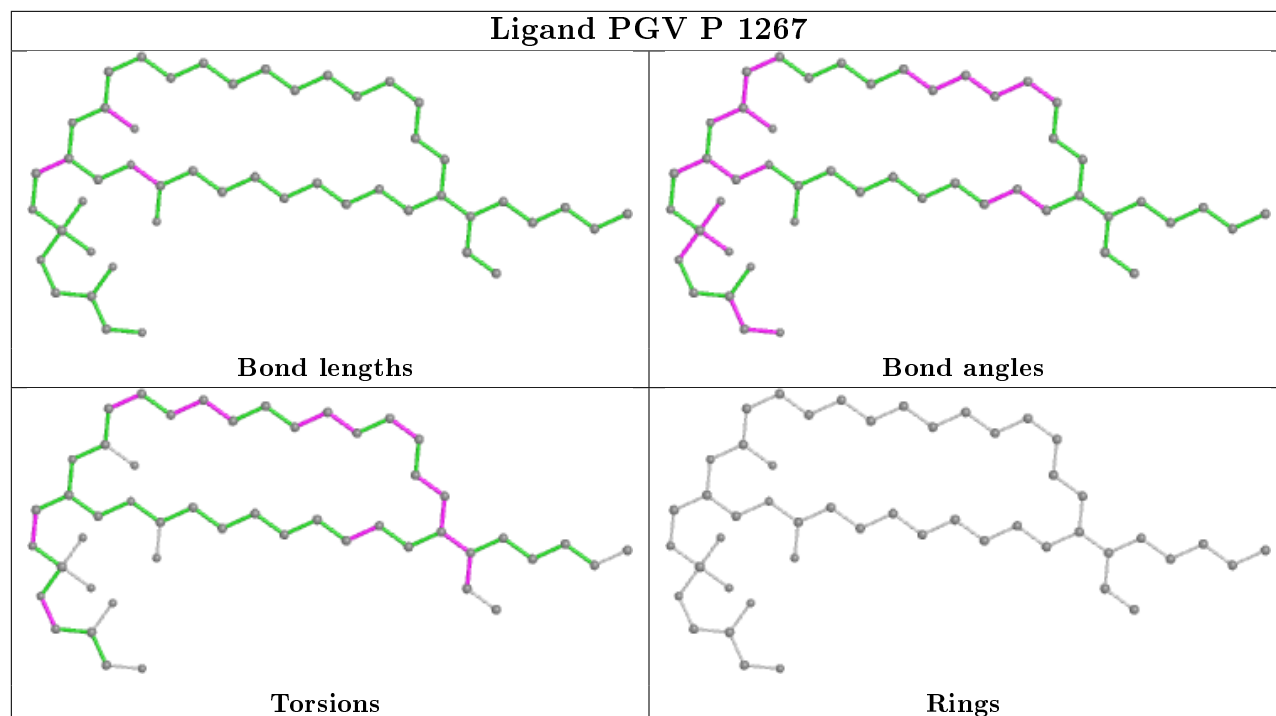


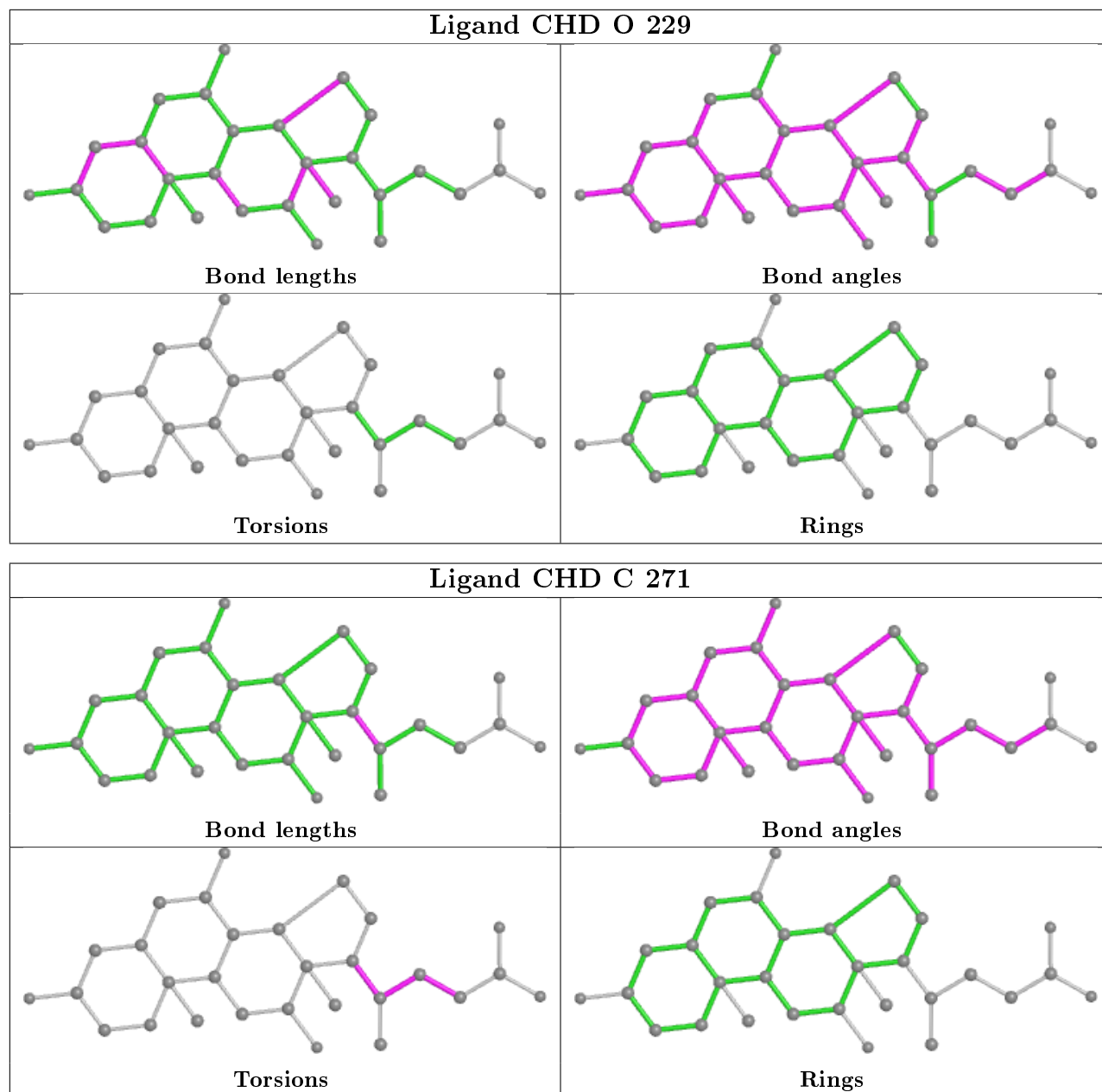


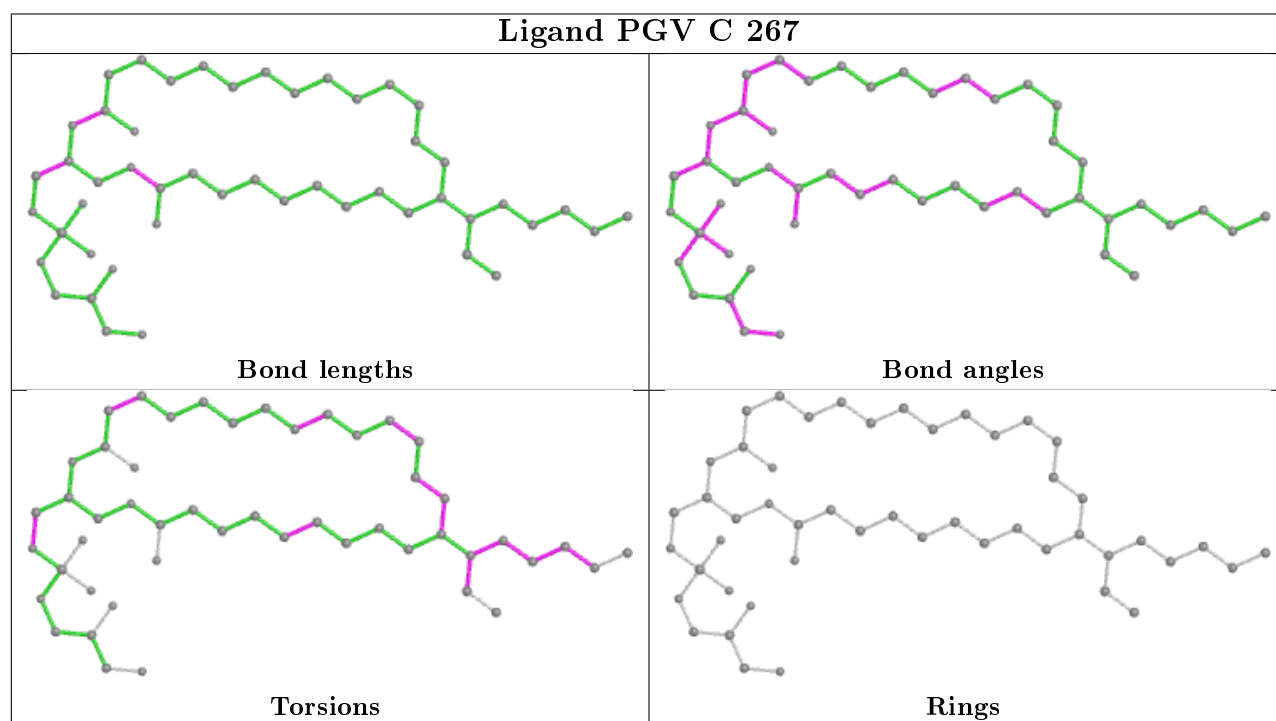
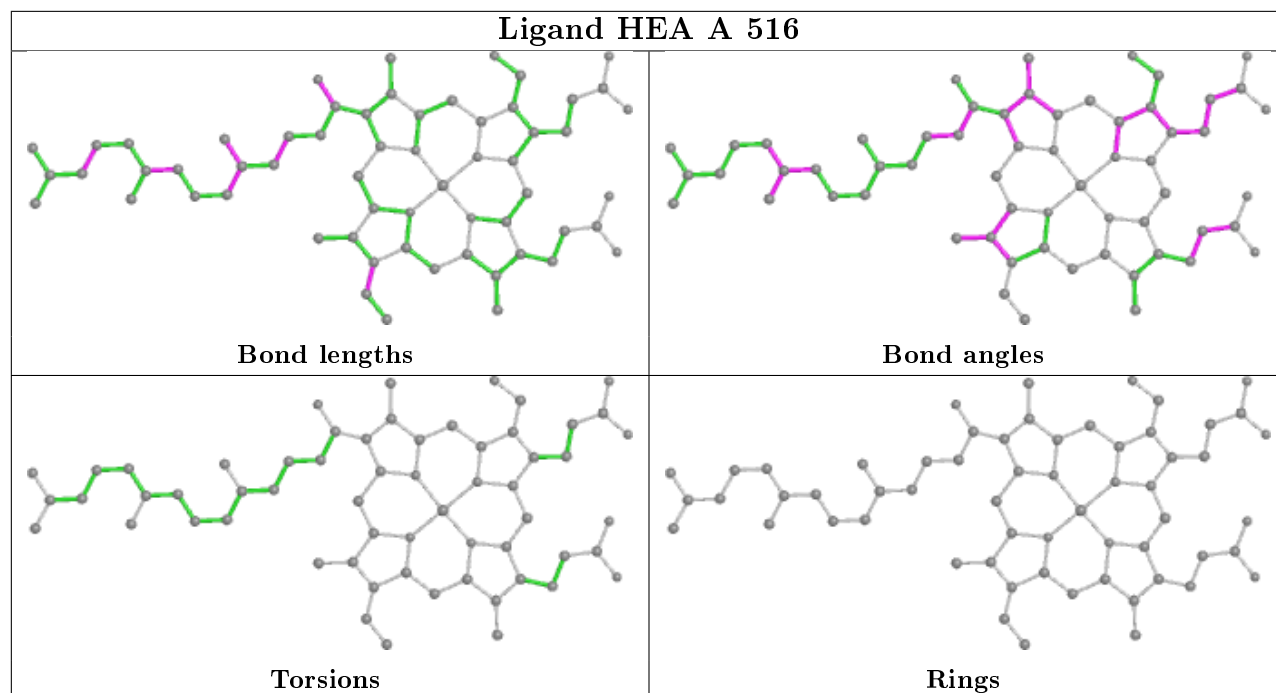


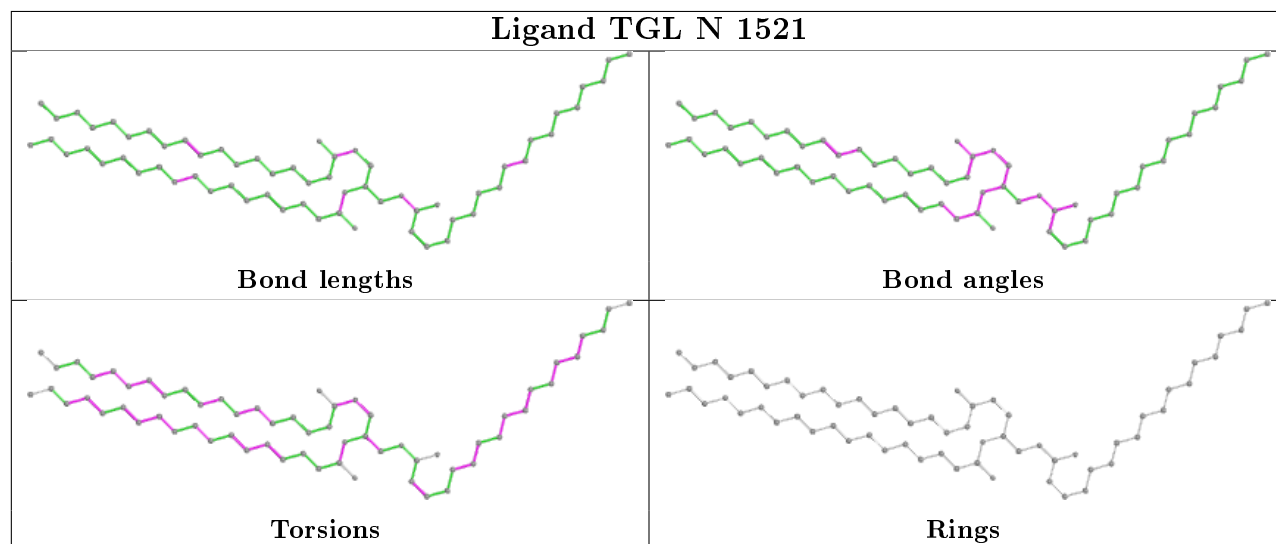
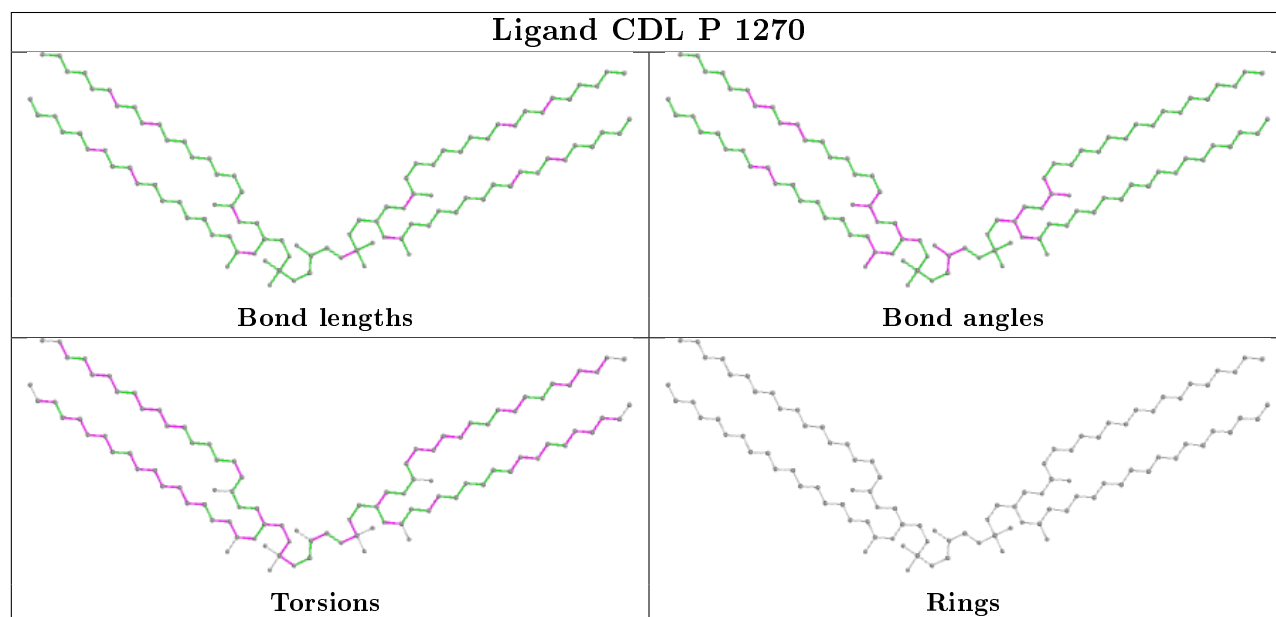
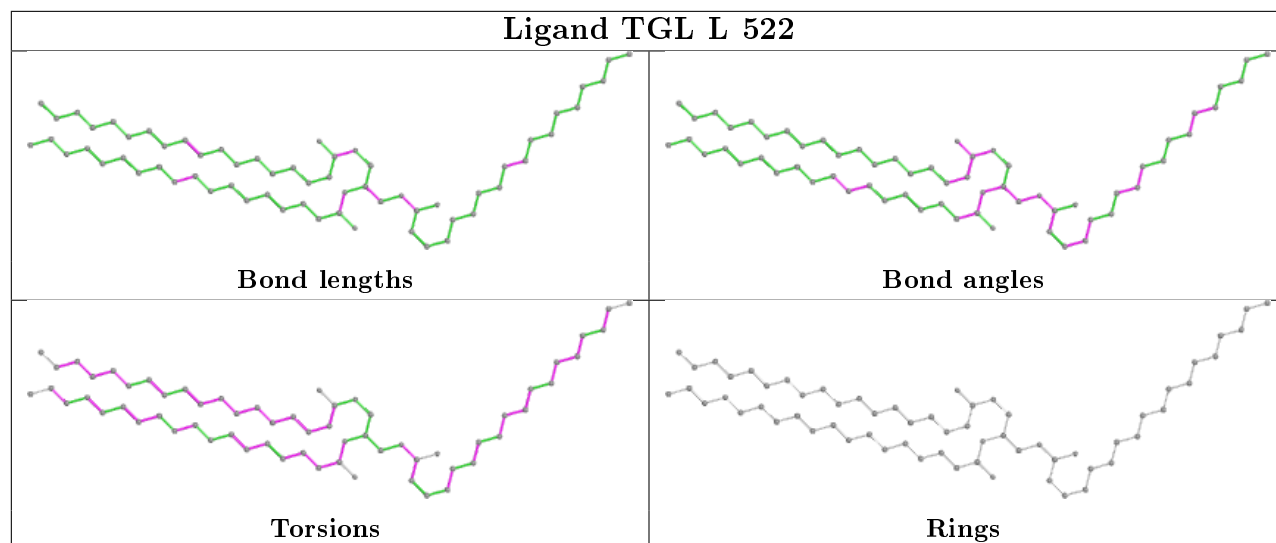






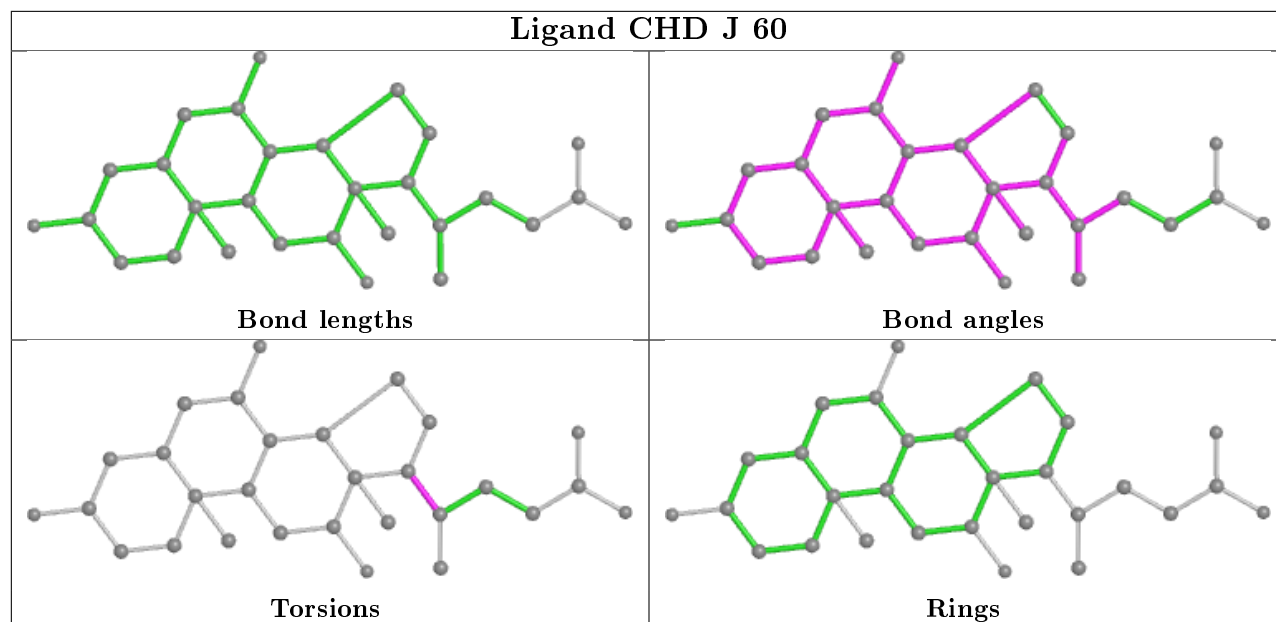




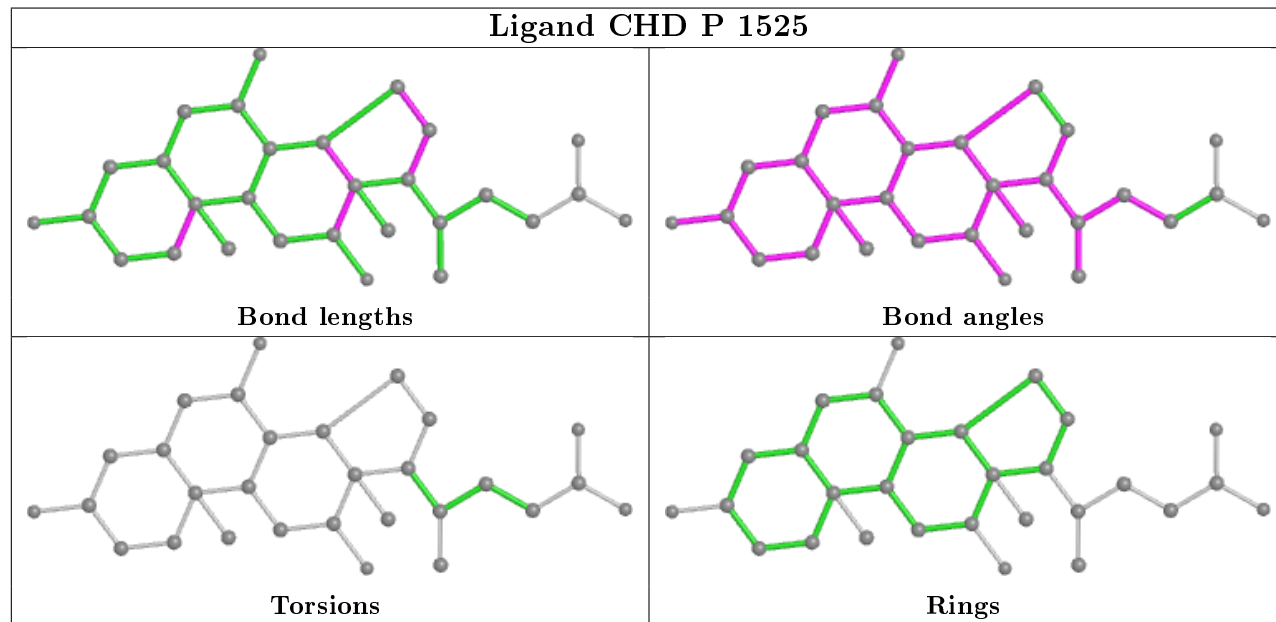




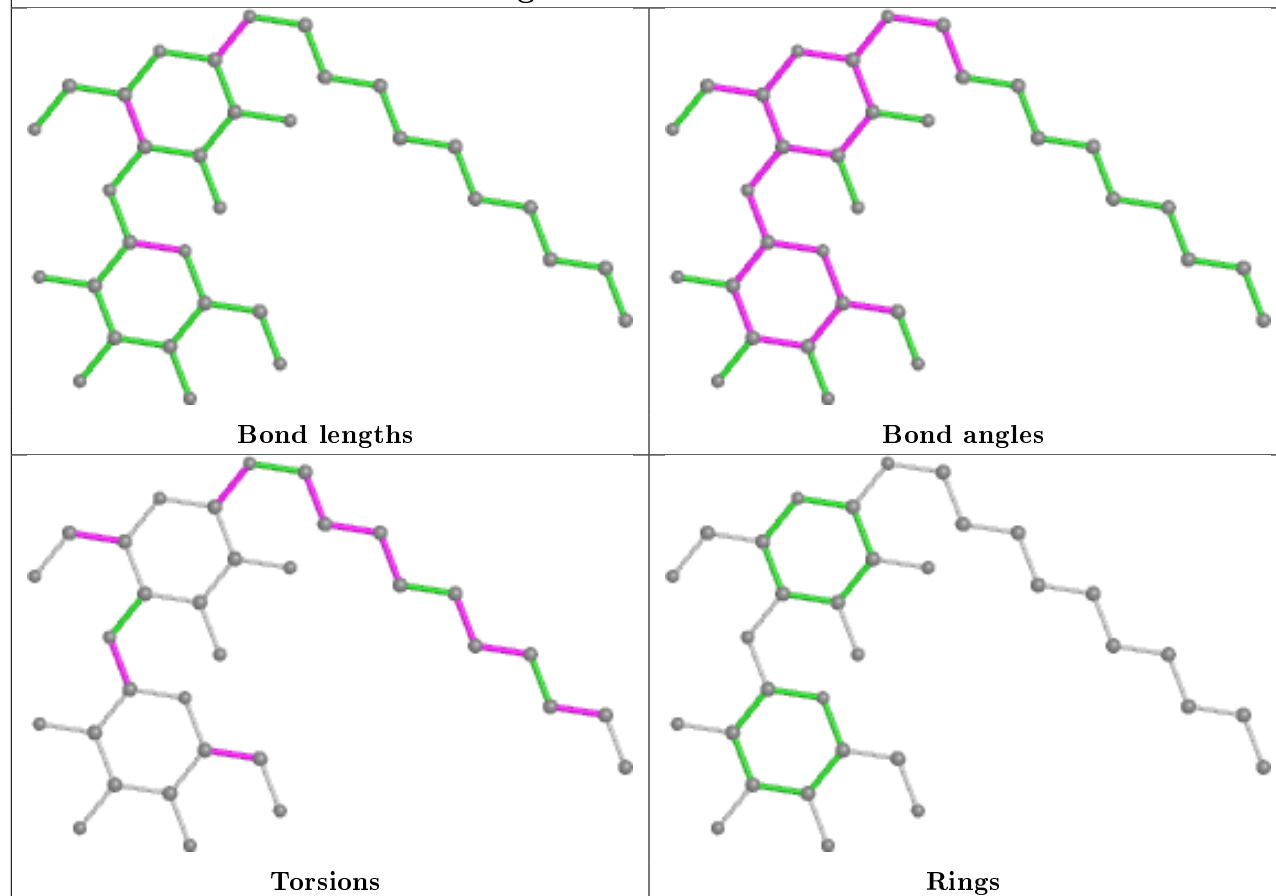
## Ligand CHD J 60



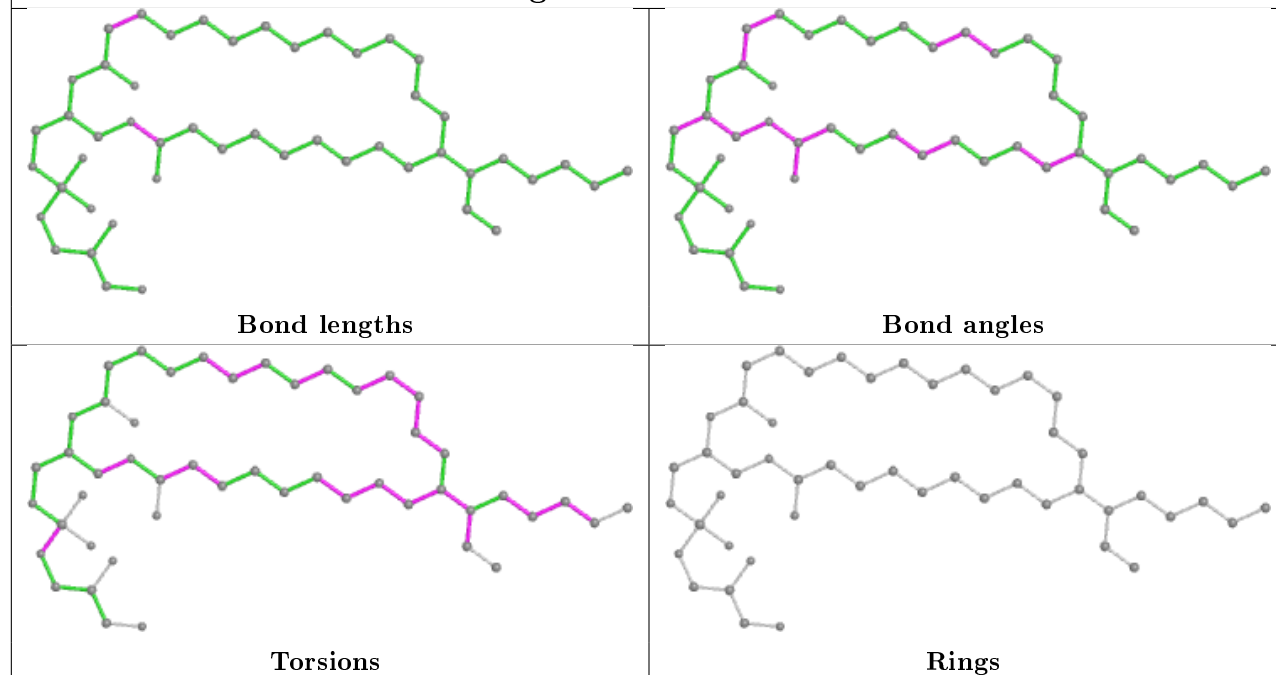
## Ligand CHD P 1525



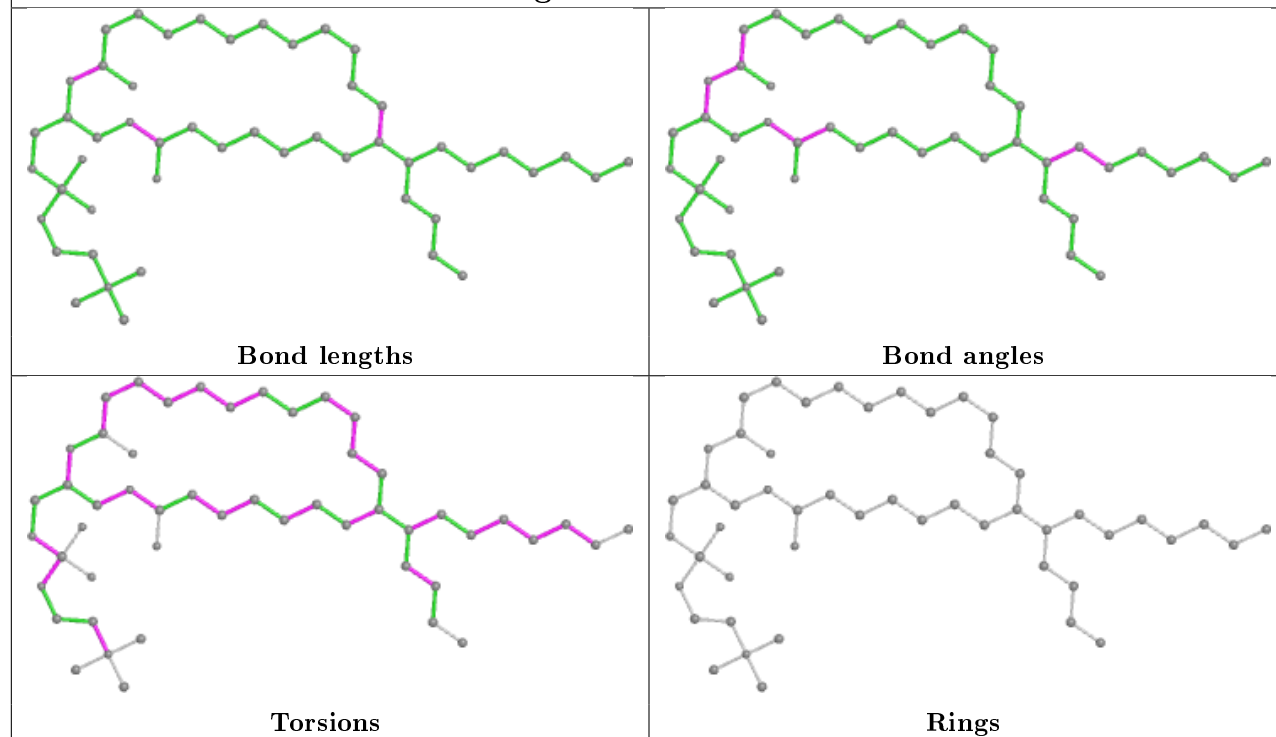
## Ligand DMU P 1272



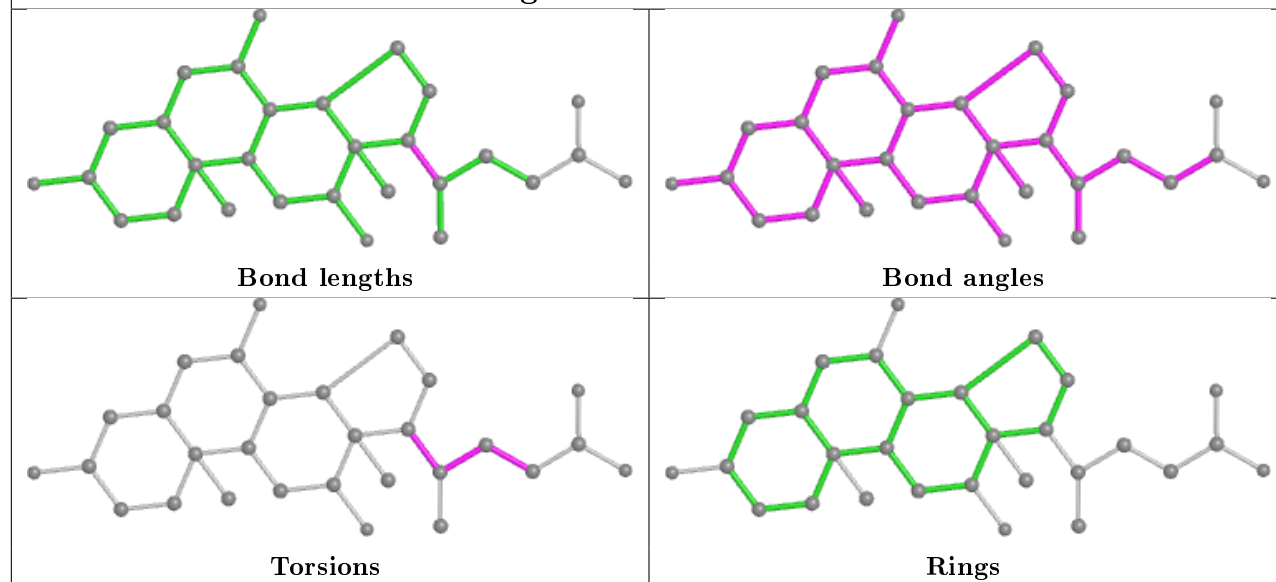
## Ligand PGV A 522

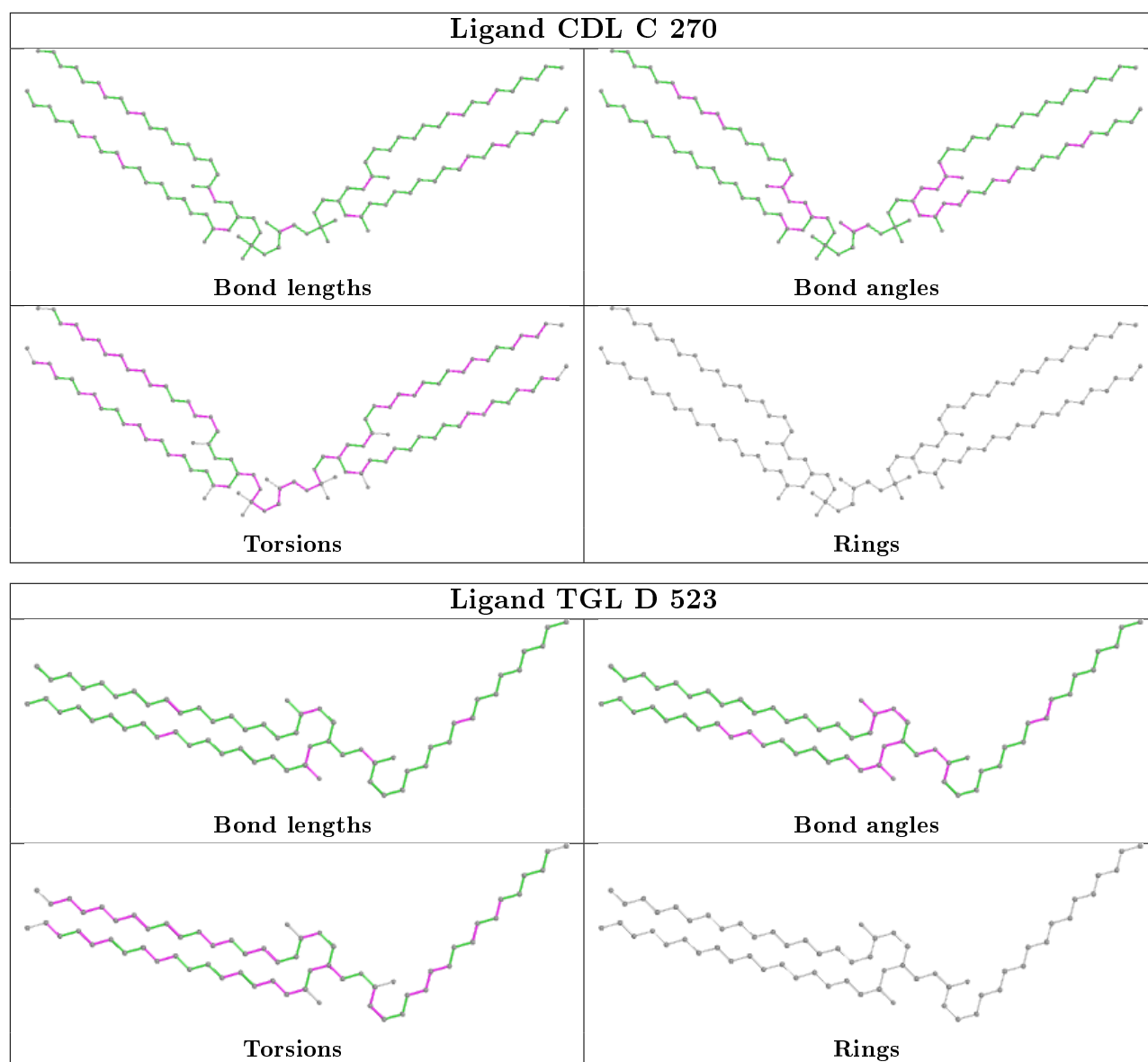


## Ligand PSC B 230



## Ligand CHD P 1271





## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.14	1 (0%) 95 95	20, 25, 32, 63	0
1	N	513/514 (99%)	-0.22	1 (0%) 95 95	24, 31, 38, 63	0
2	B	226/227 (99%)	-0.54	0 100 100	21, 29, 49, 77	0
2	O	226/227 (99%)	-0.26	4 (1%) 68 72	28, 37, 56, 77	0
3	C	259/261 (99%)	-0.66	1 (0%) 92 93	22, 28, 40, 63	0
3	P	259/261 (99%)	-0.53	3 (1%) 79 82	25, 32, 43, 63	0
4	D	144/147 (97%)	-0.55	1 (0%) 87 89	25, 31, 48, 64	0
4	Q	144/147 (97%)	0.72	19 (13%) 3 4	33, 44, 67, 108	0
5	E	104/109 (95%)	-0.57	3 (2%) 51 57	26, 31, 51, 65	0
5	R	104/109 (95%)	-0.14	3 (2%) 51 57	31, 38, 58, 74	0
6	F	93/98 (94%)	-0.18	3 (3%) 47 54	23, 34, 52, 94	0
6	S	93/98 (94%)	0.19	4 (4%) 35 41	29, 38, 59, 91	0
7	G	83/85 (97%)	0.33	15 (18%) 1 1	25, 35, 94, 102	0
7	T	83/85 (97%)	0.53	18 (21%) 0 0	27, 38, 93, 100	0
8	H	75/85 (88%)	-0.13	8 (10%) 6 7	28, 36, 69, 75	0
8	U	75/85 (88%)	0.14	6 (8%) 12 16	32, 41, 72, 76	0
9	I	71/73 (97%)	0.18	7 (9%) 7 9	28, 38, 65, 70	0
9	V	71/73 (97%)	0.61	10 (14%) 2 3	30, 48, 65, 75	0
10	J	57/59 (96%)	-0.17	4 (7%) 16 20	28, 37, 57, 70	0
10	W	57/59 (96%)	0.52	9 (15%) 2 2	33, 42, 62, 79	0
11	K	49/56 (87%)	-0.26	0 100 100	28, 35, 47, 55	0
11	X	49/56 (87%)	1.39	12 (24%) 0 0	38, 45, 60, 71	0
12	L	46/47 (97%)	-0.42	3 (6%) 18 23	26, 31, 51, 75	0
12	Y	46/47 (97%)	0.06	3 (6%) 18 23	33, 39, 60, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/46 (93%)	-0.09	6 (13%) 2 3	27, 30, 65, 89	0
13	Z	43/46 (93%)	0.57	8 (18%) 1 1	35, 39, 77, 95	0
All	All	3526/3614 (97%)	-0.15	152 (4%) 35 41	20, 33, 58, 108	0

All (152) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	6	VAL	17.1
4	Q	5	VAL	11.8
4	Q	4	SER	10.4
6	F	96	LEU	9.0
4	Q	8	SER	8.9
13	Z	43	SER	8.6
6	S	96	LEU	7.7
7	G	8	HIS	7.0
10	W	57	HIS	6.7
6	S	94	HIS	6.4
11	X	6	ALA	6.4
13	M	43	SER	6.2
10	W	52	TRP	6.2
6	F	95	GLN	5.9
12	Y	47	LYS	5.8
7	T	36	TRP	5.5
7	T	42	ARG	5.4
7	T	8	HIS	5.3
7	G	40	GLY	5.3
6	S	95	GLN	5.1
7	G	3	ALA	5.0
8	H	45	ALA	5.0
10	W	56	PRO	4.9
11	X	13	TYR	4.9
13	Z	42	LYS	4.8
11	X	7	PRO	4.8
9	V	37	PHE	4.6
4	Q	7	LYS	4.6
10	W	55	PHE	4.6
7	T	3	ALA	4.6
9	I	29	LEU	4.5
2	O	113	TYR	4.4
7	T	40	GLY	4.4
7	G	2	SER	4.4

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Mol	Chain	Res	Type	RSRZ
6	F	94	HIS	4.4
13	Z	39	ASN	4.3
9	I	37	PHE	4.3
6	S	93	PRO	4.3
7	G	42	ARG	4.3
7	T	39	SER	4.2
13	M	42	LYS	4.1
7	T	84	LYS	4.1
7	G	5	LYS	4.0
7	T	41	HIS	3.9
13	Z	40	TYR	3.9
2	O	227	LEU	3.9
4	Q	147	LYS	3.9
9	I	34	PHE	3.9
8	H	47	GLY	3.8
7	T	2	SER	3.8
2	O	91	ASN	3.7
7	G	10	GLY	3.7
3	P	3	HIS	3.6
11	X	19	ALA	3.6
7	T	4	ALA	3.6
9	V	30	GLY	3.5
7	T	1	ALA	3.5
7	T	10	GLY	3.5
7	G	1	ALA	3.4
9	I	25	PHE	3.4
9	V	34	PHE	3.4
5	R	109	VAL	3.4
11	X	23	THR	3.4
7	G	36	TRP	3.4
10	W	48	TYR	3.3
12	L	2	HIS	3.3
11	X	12	LYS	3.2
8	U	45	ALA	3.2
4	Q	51	LEU	3.2
9	I	33	THR	3.2
10	J	57	HIS	3.2
7	T	5	LYS	3.2
9	I	26	MET	3.1
10	J	52	TRP	3.1
7	T	37	LEU	3.1
4	Q	9	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
7	G	84	LYS	3.0
4	Q	33	LEU	3.0
10	J	56	PRO	3.0
11	X	47	ARG	3.0
8	U	50	VAL	2.9
7	G	41	HIS	2.9
10	W	1	PHE	2.9
3	P	38	ASN	2.9
9	V	29	LEU	2.9
5	E	109	VAL	2.8
12	L	45	LEU	2.8
5	R	108	LYS	2.8
8	U	44	THR	2.8
9	V	26	MET	2.8
13	M	40	TYR	2.8
4	Q	48	TRP	2.8
8	U	49	ASP	2.8
4	Q	46	ALA	2.7
10	W	26	ALA	2.7
10	J	1	PHE	2.7
4	Q	58	GLU	2.7
7	T	43	GLU	2.7
9	V	53	ASN	2.7
5	R	96	LEU	2.7
2	O	217	LYS	2.7
4	Q	39	ALA	2.7
7	G	7	ASP	2.7
7	G	4	ALA	2.7
1	N	513	LEU	2.7
8	U	47	GLY	2.6
8	H	49	ASP	2.6
13	M	39	ASN	2.6
9	V	33	THR	2.5
13	Z	35	TYR	2.5
13	Z	41	LYS	2.5
13	Z	32	TRP	2.5
5	E	7	THR	2.5
8	U	42	ALA	2.5
4	Q	10	ASP	2.4
9	V	36	LYS	2.4
11	X	17	VAL	2.4
4	Q	35	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
11	X	34	THR	2.4
11	X	46	GLY	2.4
4	Q	142	LYS	2.3
12	L	47	LYS	2.3
7	G	9	GLY	2.3
7	G	43	GLU	2.3
9	V	3	ALA	2.3
3	P	37	PHE	2.3
9	V	25	PHE	2.3
10	W	30	ILE	2.3
10	W	2	GLU	2.3
4	D	147	LYS	2.2
4	Q	62	LEU	2.2
13	Z	13	LYS	2.2
13	M	38	ASP	2.2
11	X	16	ALA	2.2
8	H	48	GLY	2.2
8	H	46	LYS	2.2
8	H	44	THR	2.2
4	Q	49	SER	2.1
5	E	9	GLU	2.1
12	Y	45	LEU	2.1
4	Q	31	LYS	2.1
8	H	43	MET	2.1
13	M	41	LYS	2.1
1	A	66	ILE	2.1
11	X	15	ASN	2.1
3	C	3	HIS	2.1
9	I	30	GLY	2.1
7	T	45	PRO	2.0
7	T	9	GLY	2.0
7	T	38	HIS	2.0
12	Y	20	ARG	2.0
8	H	50	VAL	2.0

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

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( $\text{\AA}^2$ )	Q<0.9
7	TPO	T	11	11/12	0.38	0.36	70,77,97,98	0
7	TPO	G	11	11/12	0.53	0.34	68,74,91,92	0
1	FME	A	1	10/11	0.91	0.16	42,48,68,76	0
1	FME	N	1	10/11	0.91	0.21	48,54,69,70	0
2	FME	O	1	10/11	0.96	0.11	36,37,46,55	0
2	FME	B	1	10/11	0.97	0.14	27,29,39,57	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( $\text{\AA}^2$ )	Q<0.9
24	DMU	C	272	33/33	0.30	0.36	70,99,105,105	0
24	DMU	P	1272	33/33	0.47	0.40	89,103,109,111	0
28	PEK	G	265	53/53	0.49	0.27	45,91,106,111	0
23	CHD	W	1060	29/29	0.52	0.46	107,109,111,111	0
28	PEK	T	263	53/53	0.54	0.30	48,93,126,127	0
28	PEK	G	1263	53/53	0.58	0.32	50,107,128,129	0
28	PEK	P	1265	53/53	0.59	0.30	42,86,105,108	0
19	TGL	N	1522	63/63	0.59	0.31	45,73,89,92	0
22	PSC	O	1230	52/52	0.66	0.30	41,93,121,122	0
26	CDL	G	269	100/100	0.66	0.26	62,86,114,116	0
23	CHD	J	60	29/29	0.67	0.41	99,100,106,106	0
19	TGL	Q	1523	63/63	0.67	0.20	53,78,92,94	0
25	UNX	C	262	1/1	0.68	0.27	39,39,39,39	0
22	PSC	B	230	52/52	0.68	0.28	39,96,121,123	0
26	CDL	T	1269	100/100	0.69	0.22	52,85,111,116	0
19	TGL	L	522	63/63	0.71	0.26	36,66,84,86	0
26	CDL	P	1270	100/100	0.72	0.27	43,87,117,123	0
20	PGV	C	268	51/51	0.72	0.19	59,88,104,105	0
20	PGV	P	1268	51/51	0.73	0.23	64,97,112,113	0
19	TGL	N	1521	63/63	0.74	0.23	53,75,92,94	0
20	PGV	N	1524	51/51	0.75	0.22	43,72,104,106	0
25	UNX	P	1262	1/1	0.76	0.33	40,40,40,40	0
19	TGL	D	523	63/63	0.76	0.19	41,69,96,98	0

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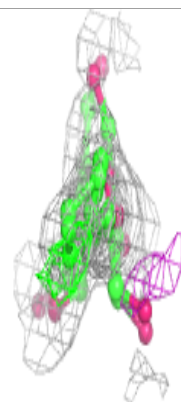
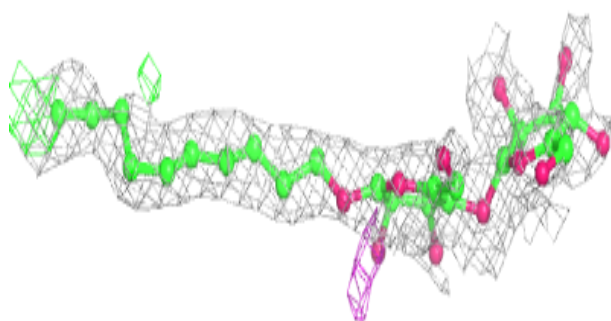
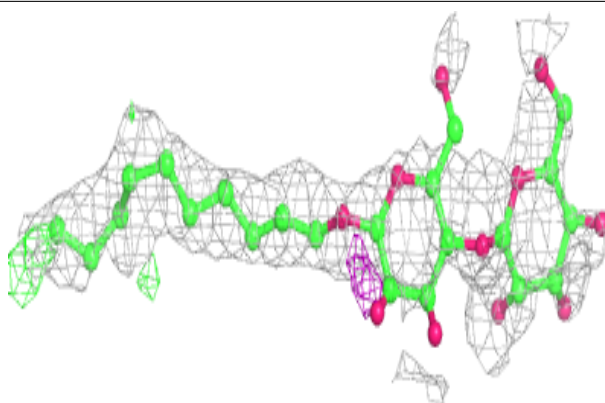
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
20	PGV	A	524	51/51	0.77	0.23	33,71,98,101	0
26	CDL	C	270	100/100	0.77	0.25	43,84,127,129	0
24	DMU	Z	1526	33/33	0.77	0.20	42,51,63,65	0
19	TGL	A	521	63/63	0.81	0.21	47,71,92,98	0
24	DMU	M	526	33/33	0.85	0.14	35,44,55,60	0
23	CHD	C	271	29/29	0.85	0.24	59,69,71,72	0
23	CHD	P	1271	29/29	0.88	0.21	68,74,77,78	0
16	MG	N	1518	1/1	0.91	0.09	29,29,29,29	0
23	CHD	P	1525	29/29	0.94	0.09	25,33,39,39	0
17	NA	N	1519	1/1	0.95	0.06	30,30,30,30	0
23	CHD	C	525	29/29	0.95	0.08	24,32,36,43	0
28	PEK	P	1264	53/53	0.95	0.17	26,47,80,82	0
23	CHD	O	229	29/29	0.96	0.07	21,25,34,39	0
20	PGV	C	267	51/51	0.96	0.17	20,31,74,77	0
23	CHD	B	1086	29/29	0.96	0.08	23,28,35,44	0
20	PGV	P	1267	51/51	0.96	0.17	21,37,76,85	0
20	PGV	N	1266	51/51	0.96	0.21	28,41,63,64	0
28	PEK	G	264	53/53	0.96	0.18	23,43,71,73	0
21	CUA	O	228	2/2	0.97	0.07	31,31,31,32	0
18	HEA	N	515	60/60	0.97	0.15	22,28,54,56	0
15	PER	N	520	2/2	0.97	0.13	20,20,20,27	0
20	PGV	A	522	51/51	0.97	0.18	25,37,63,68	0
18	HEA	A	515	60/60	0.98	0.15	16,23,46,47	0
18	HEA	N	516	60/60	0.98	0.12	23,28,35,38	0
16	MG	A	518	1/1	0.98	0.12	21,21,21,21	0
17	NA	A	519	1/1	0.98	0.07	25,25,25,25	0
15	PER	A	520	2/2	0.99	0.21	16,16,16,19	0
18	HEA	A	516	60/60	0.99	0.11	13,22,29,32	0
14	CU	A	517	1/1	0.99	0.11	24,24,24,24	0
27	ZN	S	99	1/1	0.99	0.06	34,34,34,34	0
27	ZN	F	99	1/1	1.00	0.07	30,30,30,30	0
21	CUA	B	228	2/2	1.00	0.10	23,23,23,26	0
14	CU	N	517	1/1	1.00	0.13	30,30,30,30	0

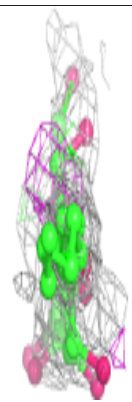
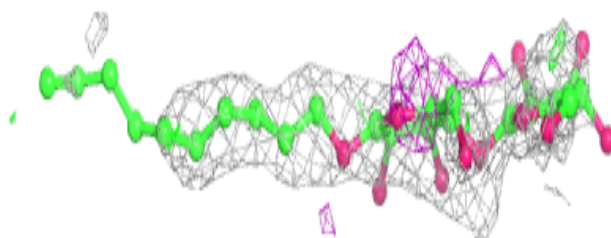
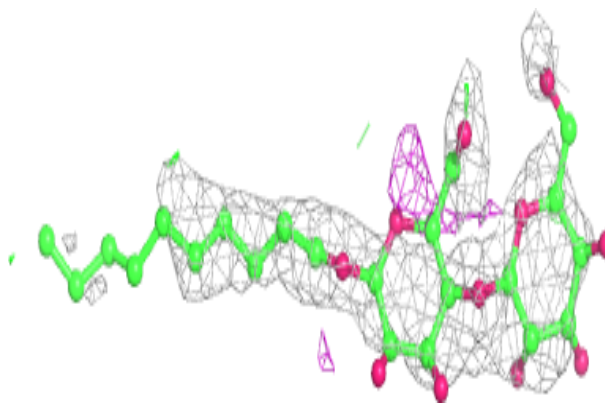
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around DMU C 272:**

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

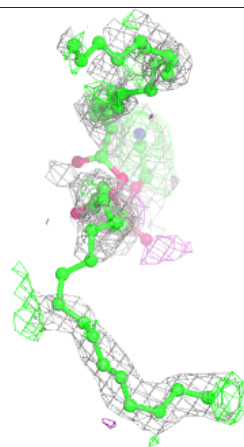
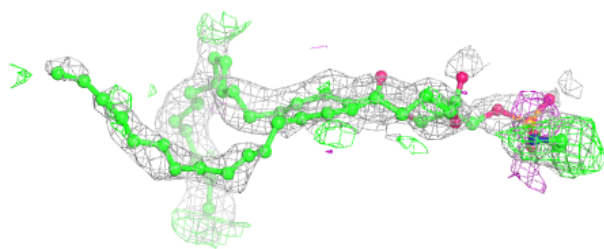
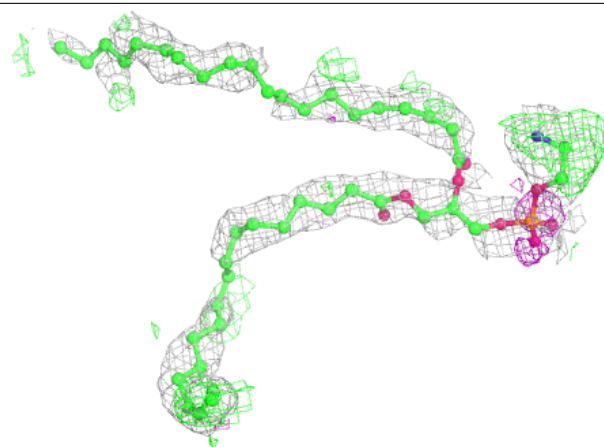
**Electron density around DMU P 1272:**

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

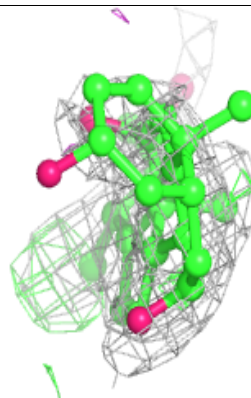
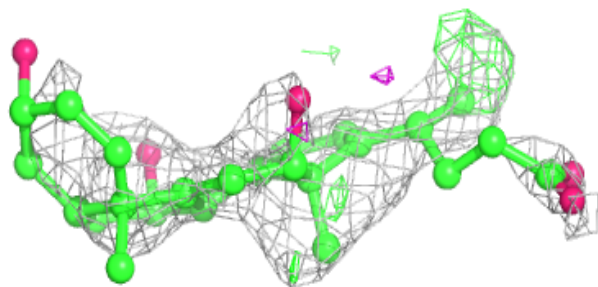
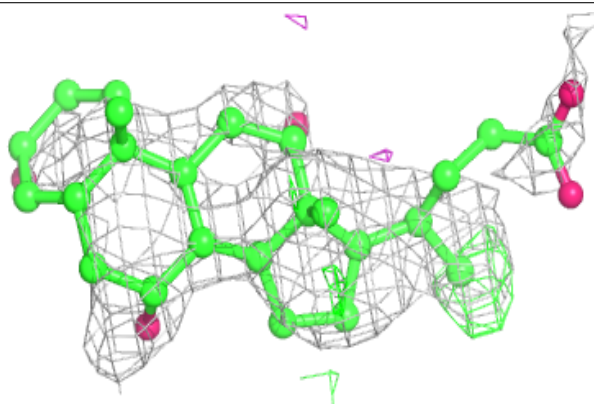


**Electron density around PEK G 265:**

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

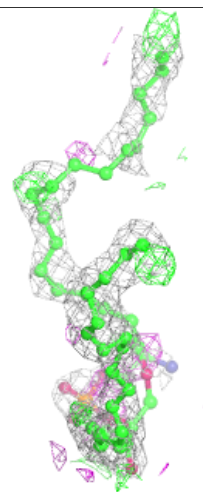
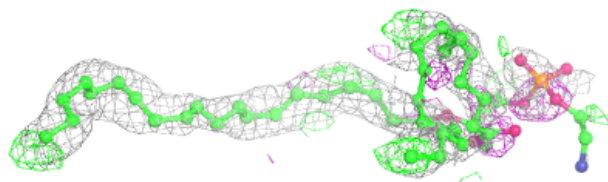
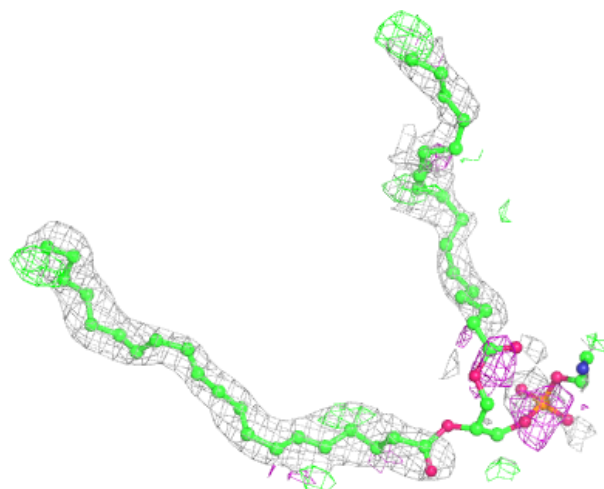
**Electron density around CHD W 1060:**

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



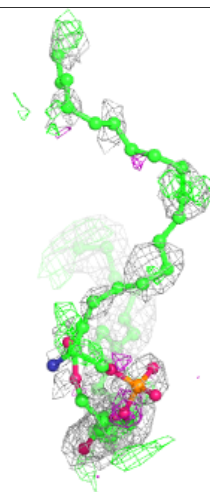
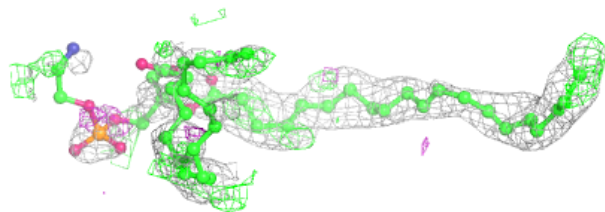
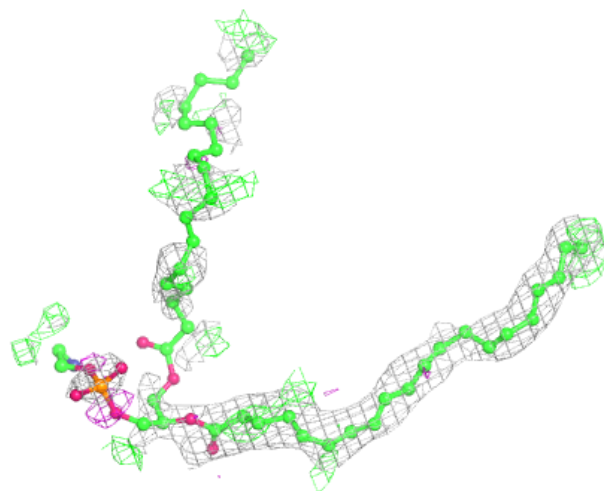
**Electron density around PEK T 263:**

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



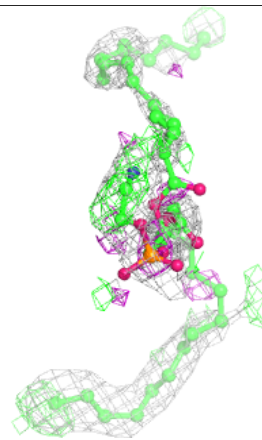
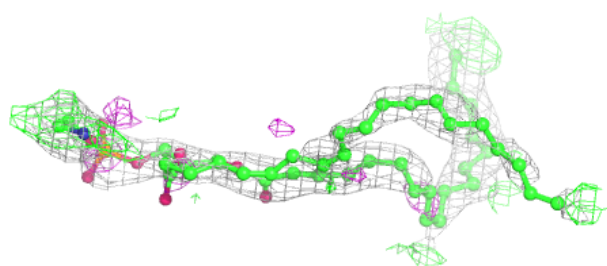
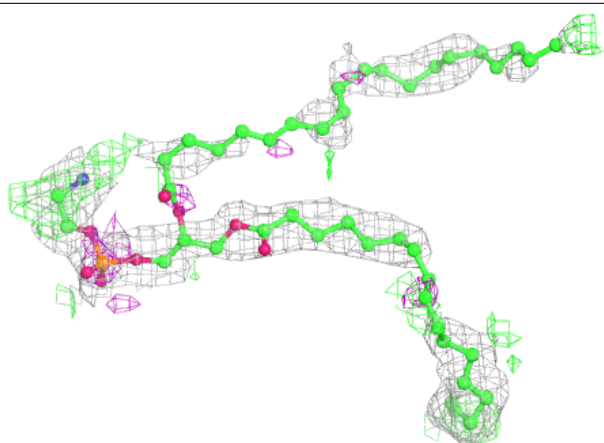
**Electron density around PEK G 1263:**

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



**Electron density around PEK P 1265:**

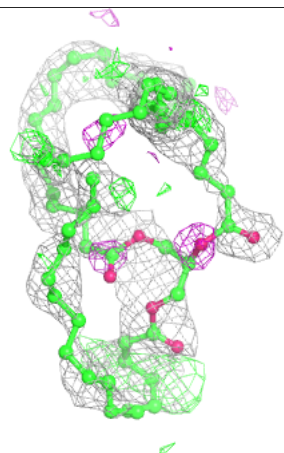
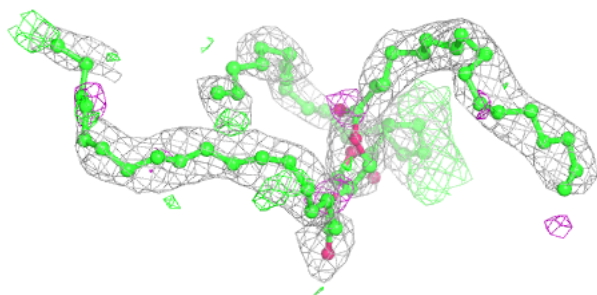
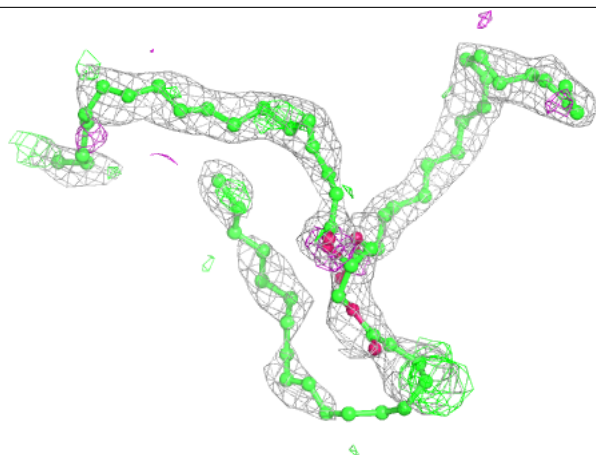
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



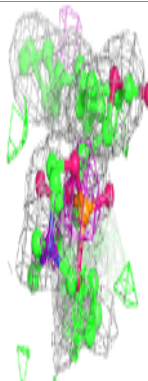
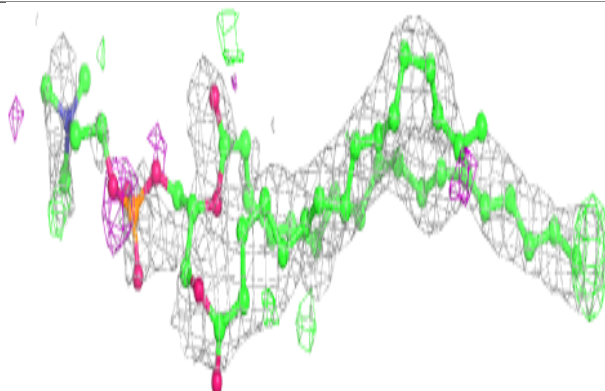
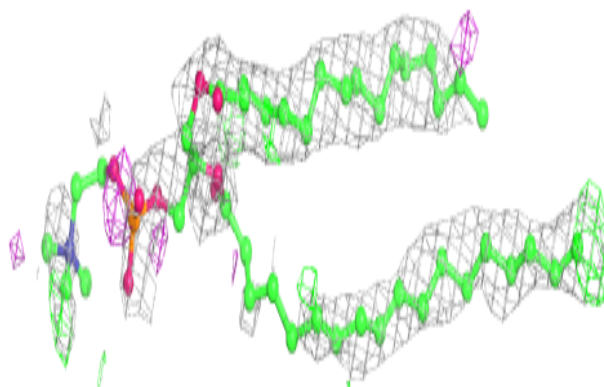


**Electron density around TGL N 1522:**

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

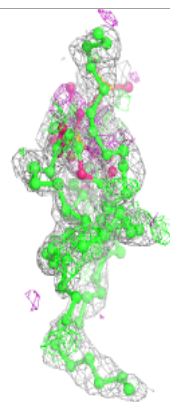
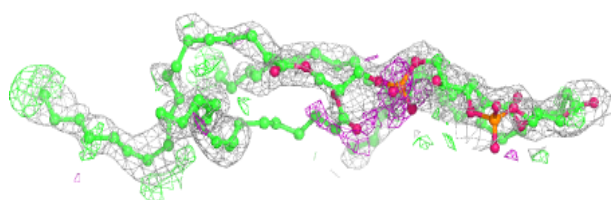
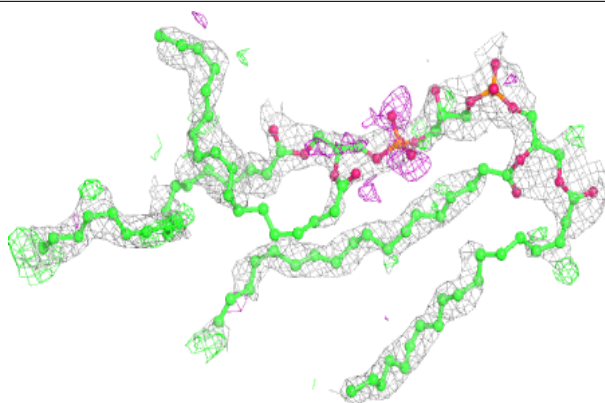
**Electron density around PSC O 1230:**

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

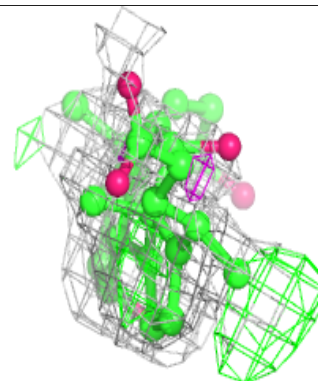
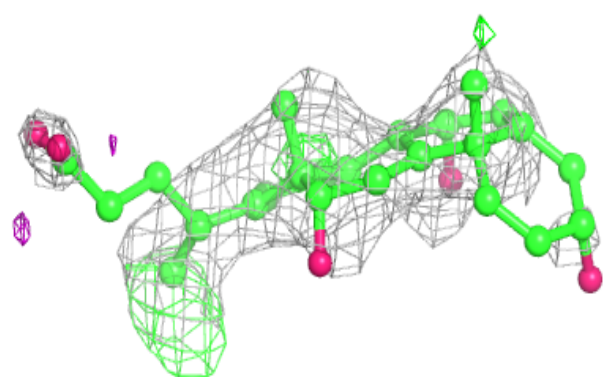
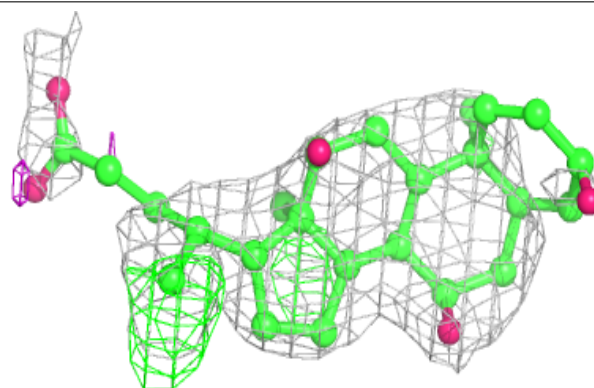


**Electron density around CDL G 269:**

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

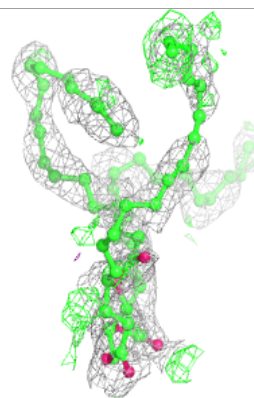
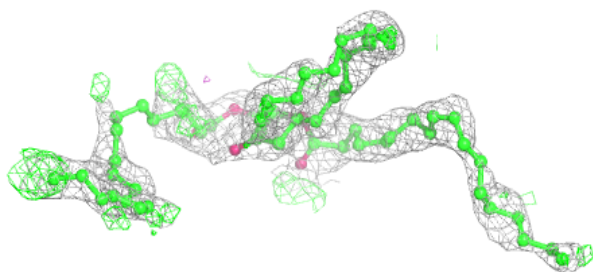
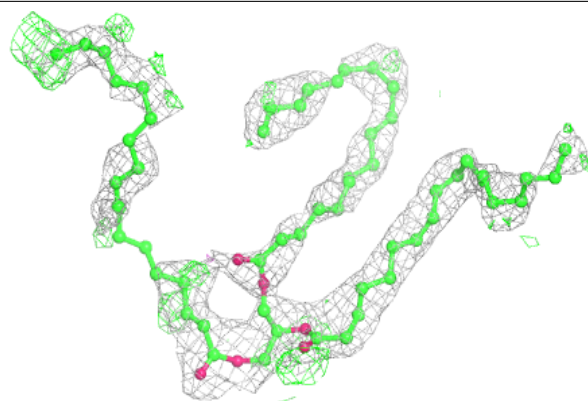
**Electron density around CHD J 60:**

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

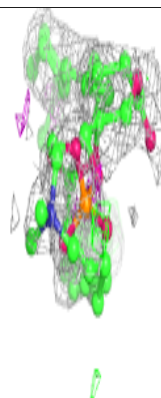
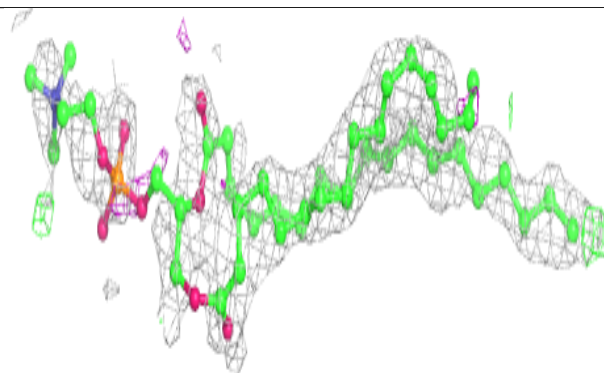
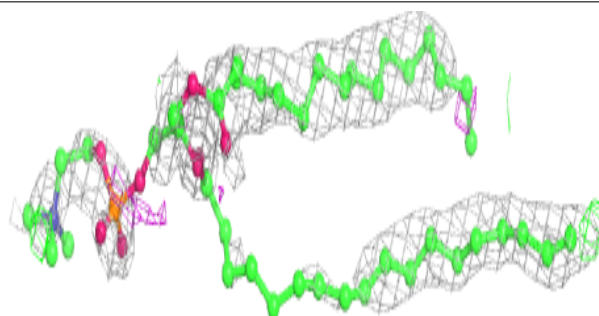


**Electron density around TGL Q 1523:**

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

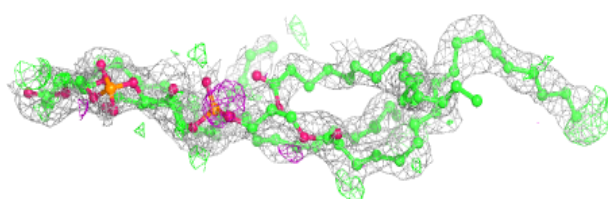
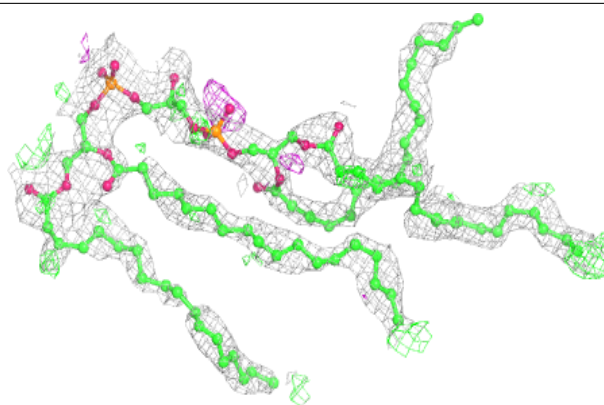
**Electron density around PSC B 230:**

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

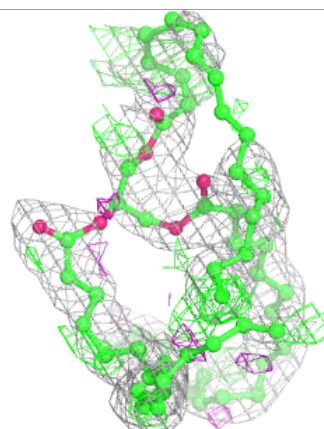
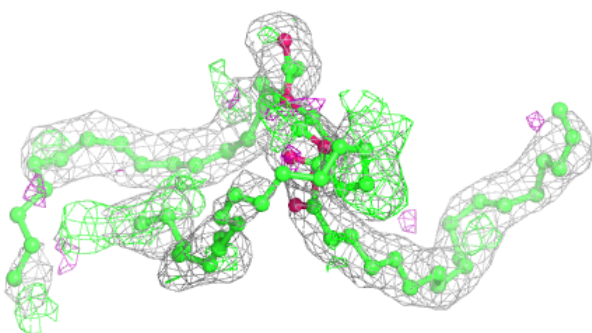
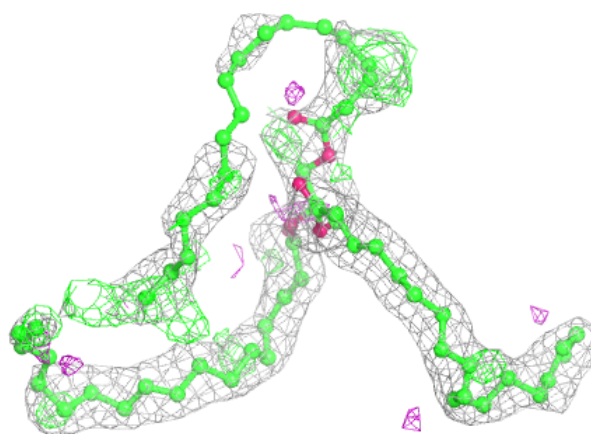


**Electron density around CDL T 1269:**

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

**Electron density around TGL L 522:**

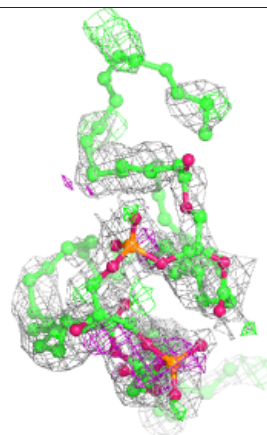
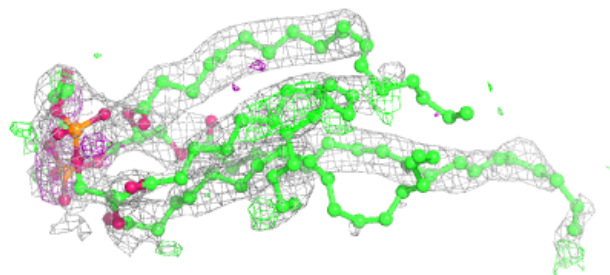
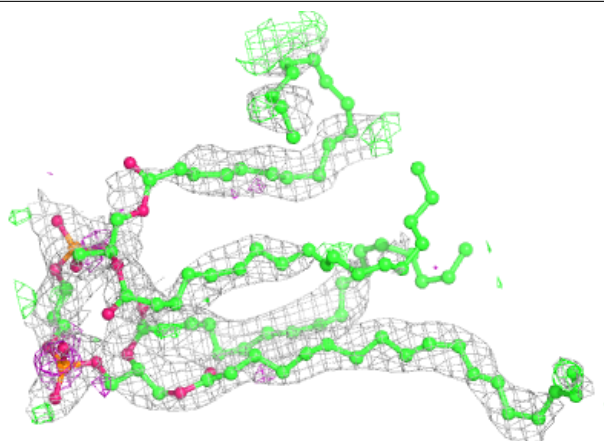
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



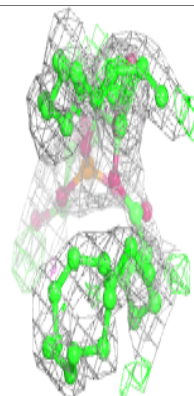
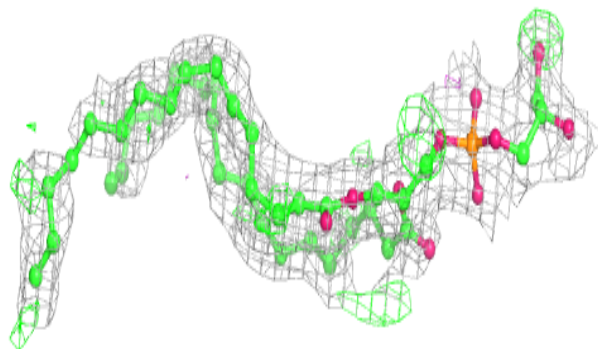
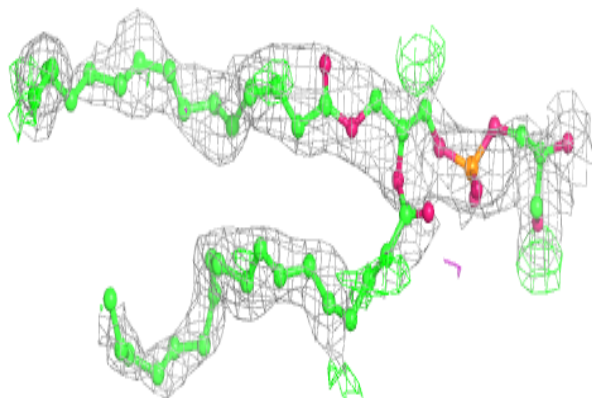


**Electron density around CDL P 1270:**

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

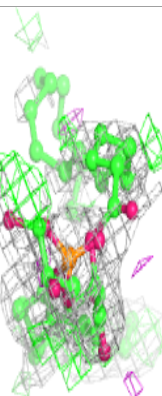
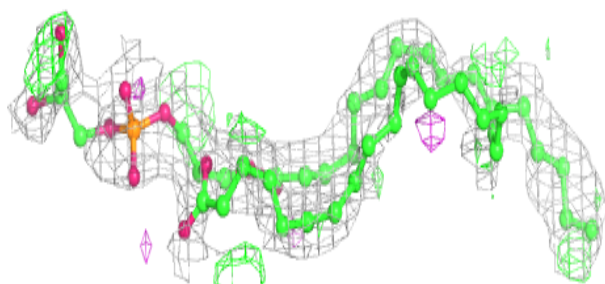
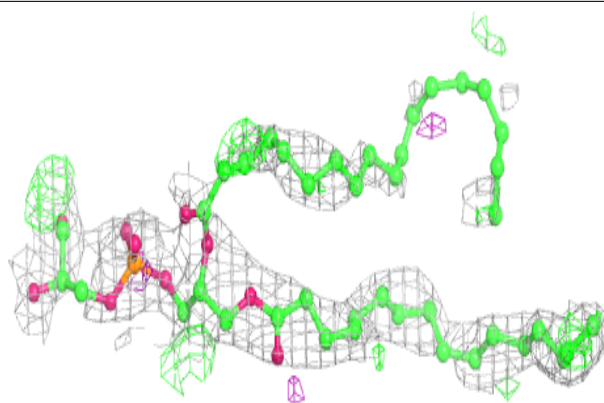
**Electron density around PGV C 268:**

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

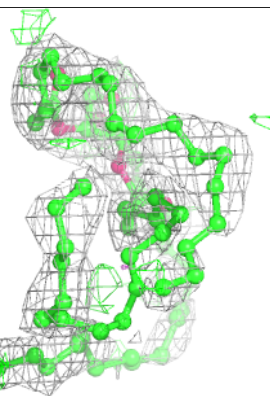
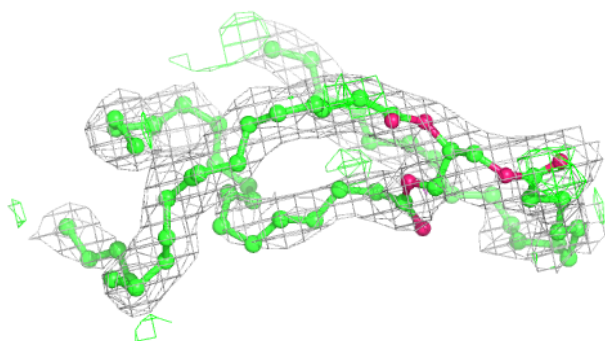
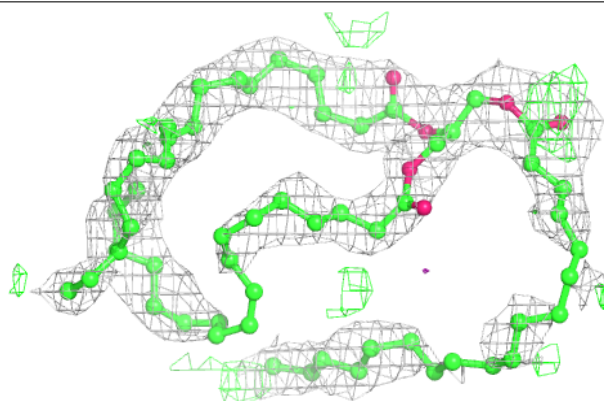


**Electron density around PGV P 1268:**

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

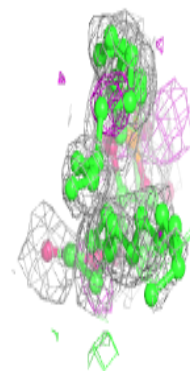
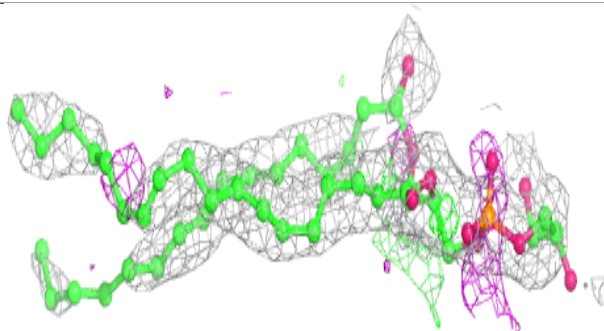
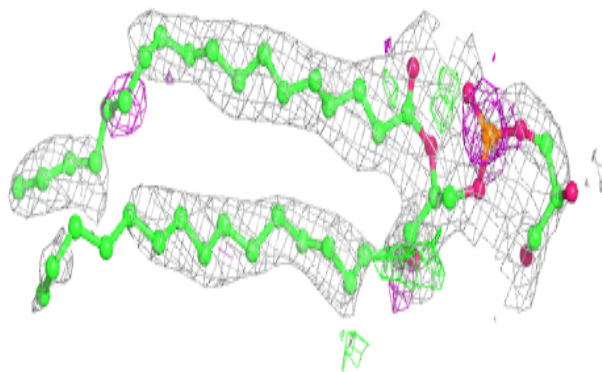
**Electron density around TGL N 1521:**

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

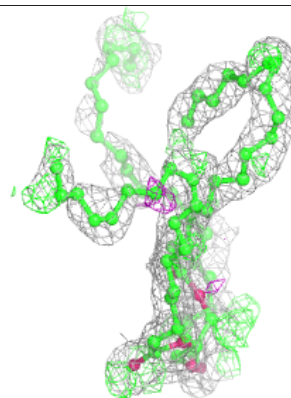
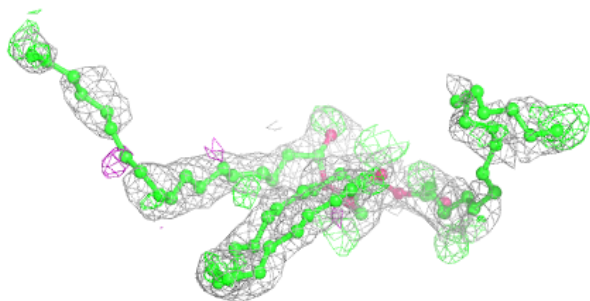
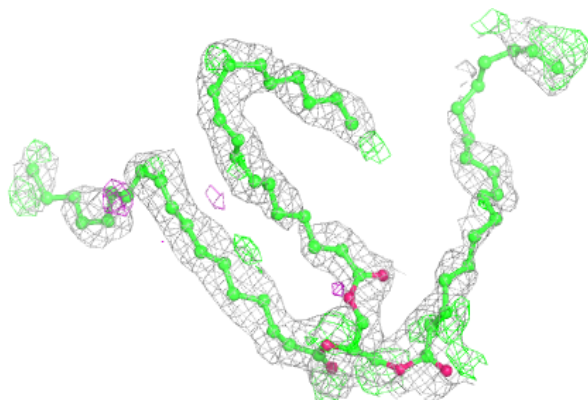


**Electron density around PGV N 1524:**

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

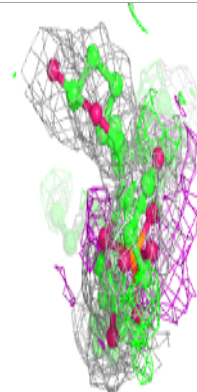
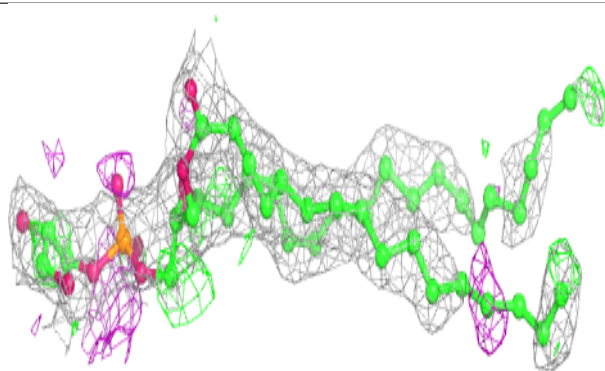
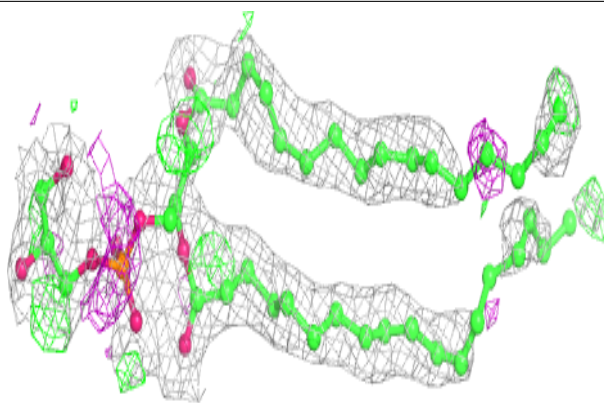
**Electron density around TGL D 523:**

$2mF_o-DF_c$  (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:**

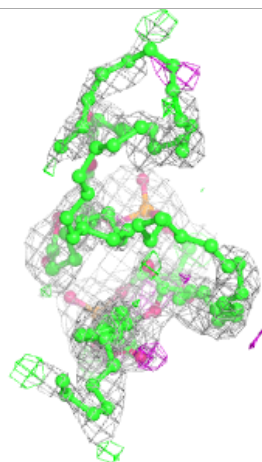
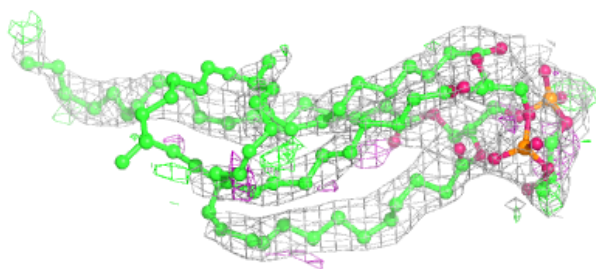
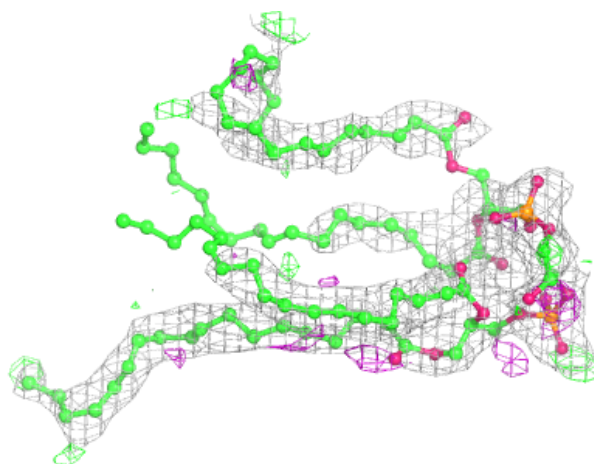
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





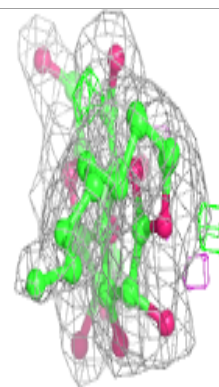
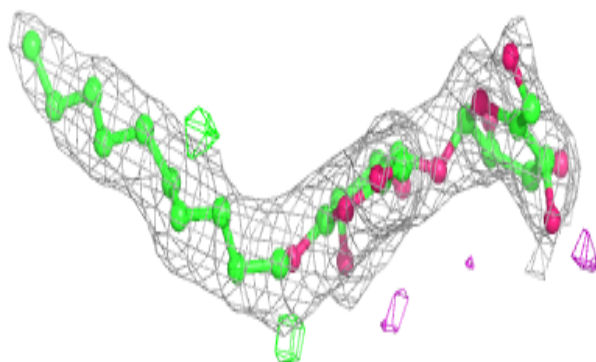
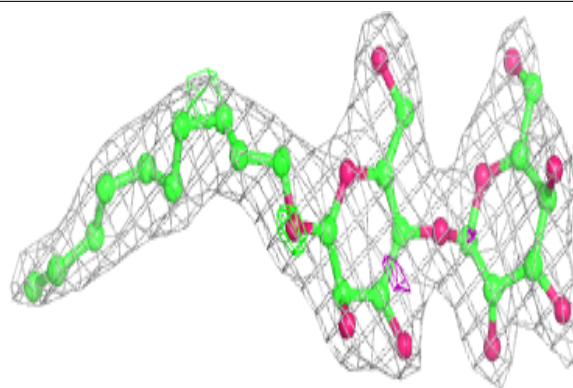
**Electron density around CDL C 270:**

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

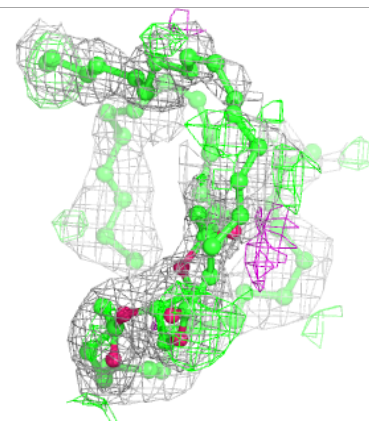
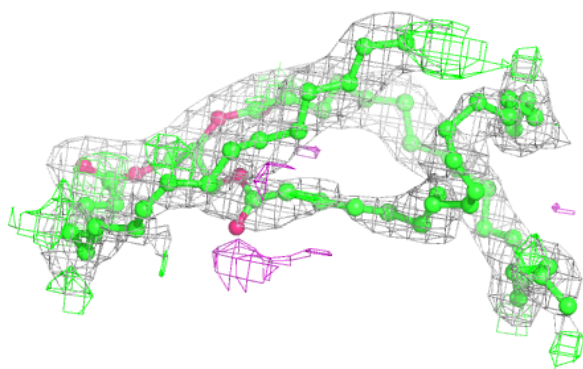
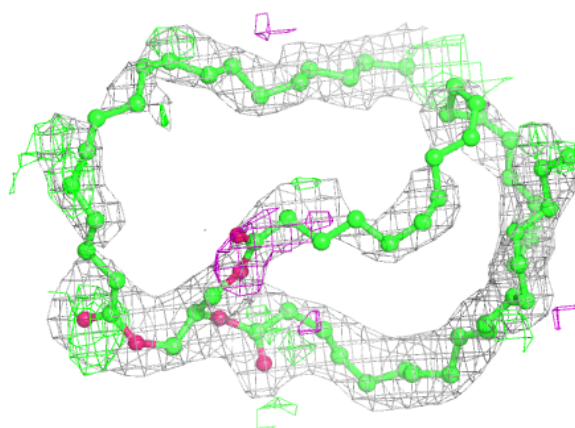


**Electron density around DMU Z 1526:**

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

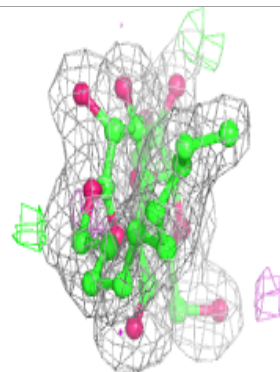
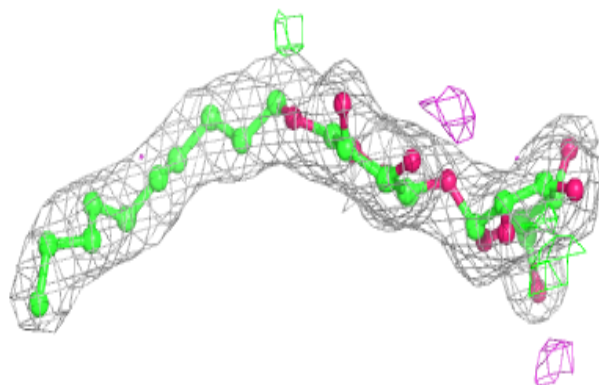
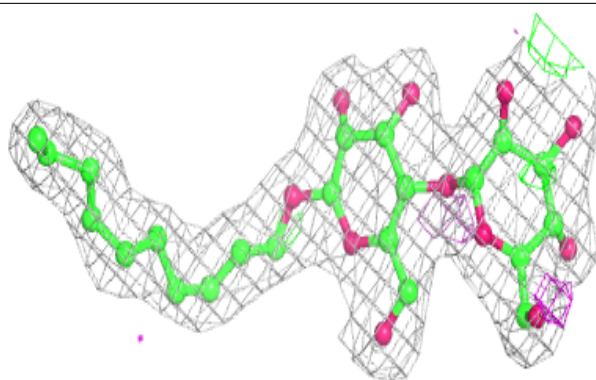
**Electron density around TGL A 521:**

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

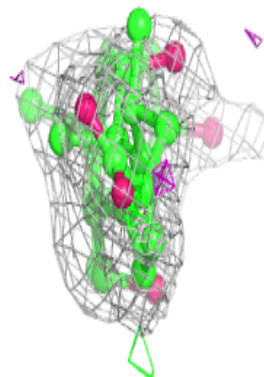
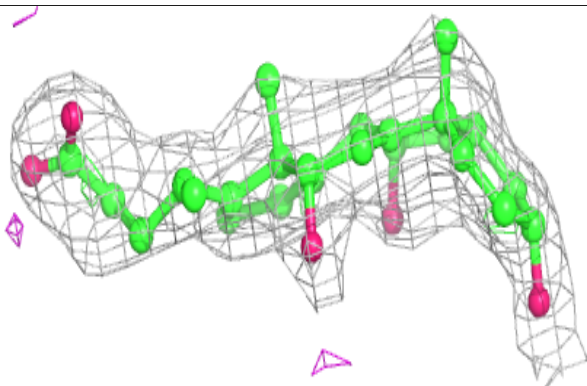
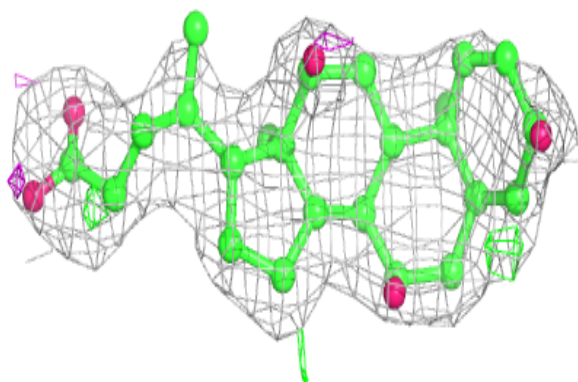


**Electron density around DMU M 526:**

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

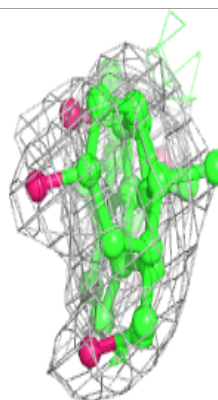
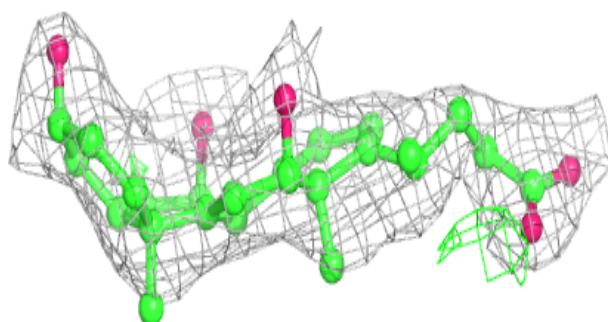
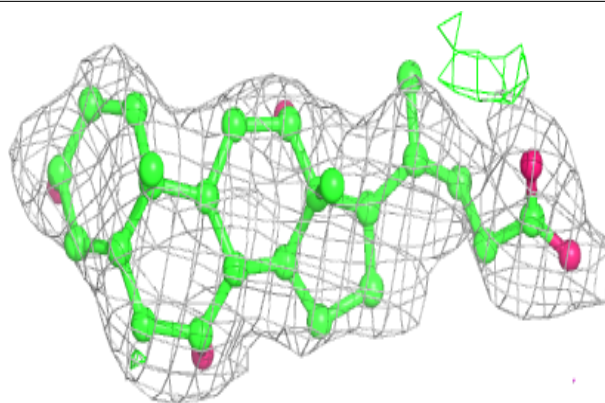
**Electron density around CHD C 271:**

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

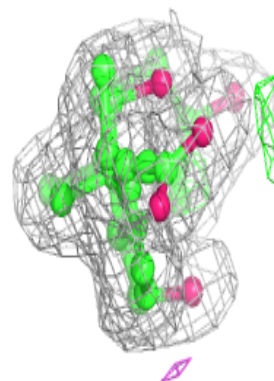
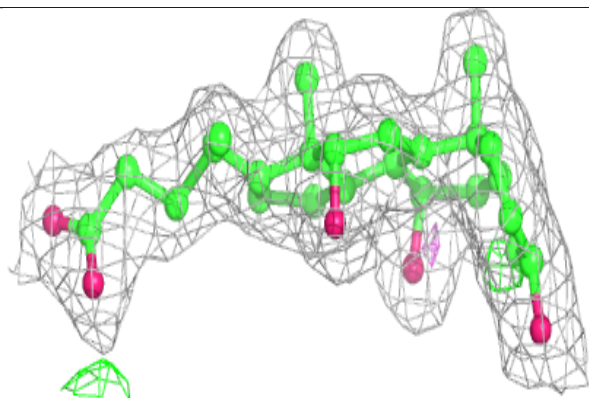
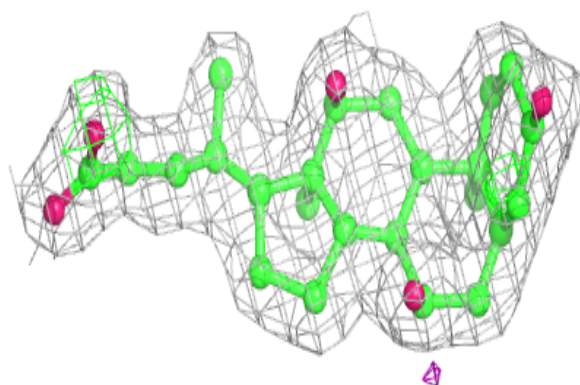


**Electron density around CHD P 1271:**

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

**Electron density around CHD P 1525:**

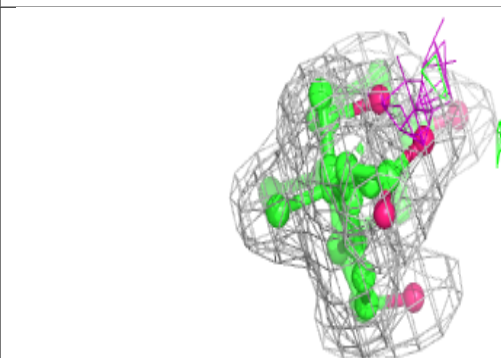
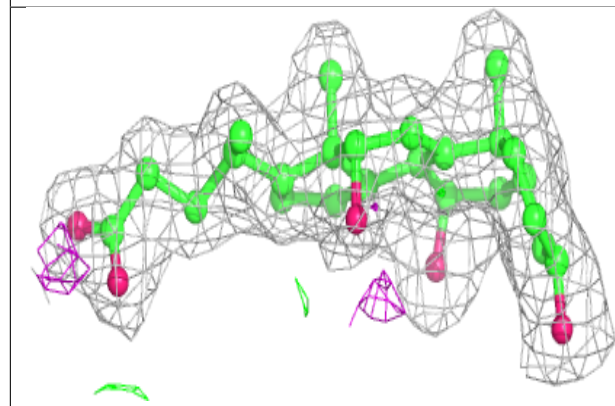
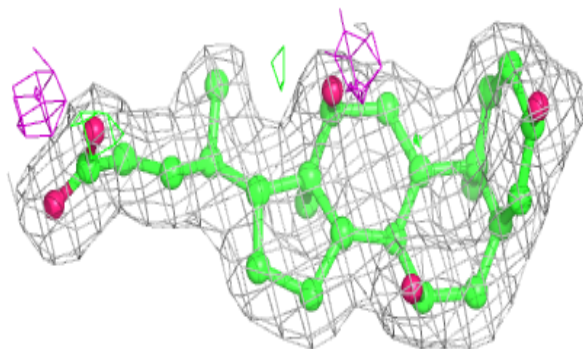
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



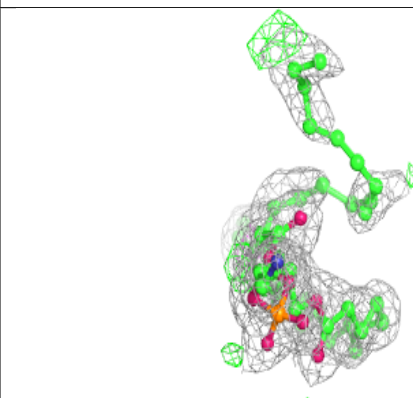
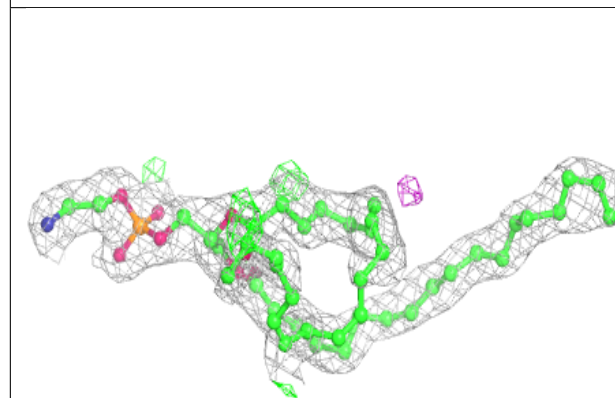
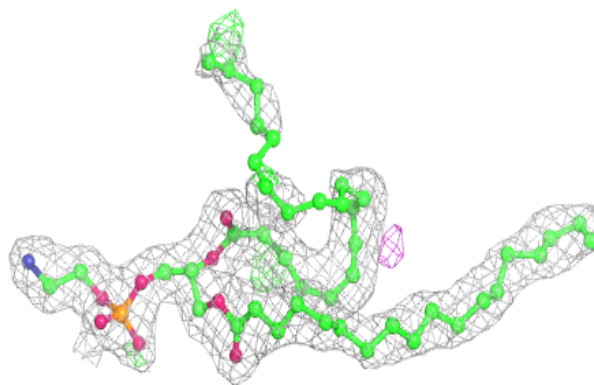


**Electron density around CHD C 525:**

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

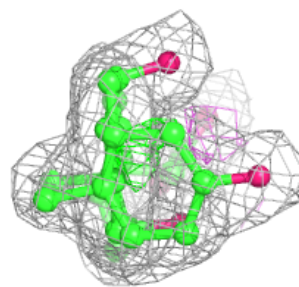
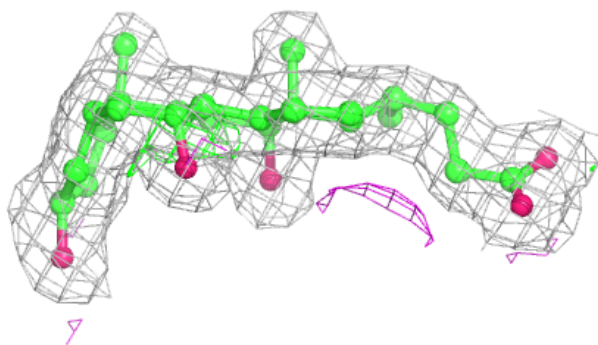
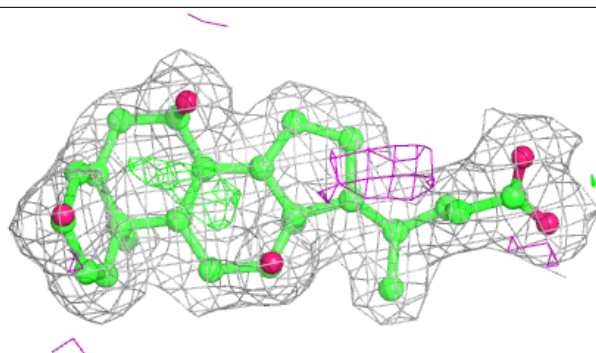
**Electron density around PEK P 1264:**

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

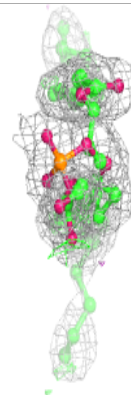
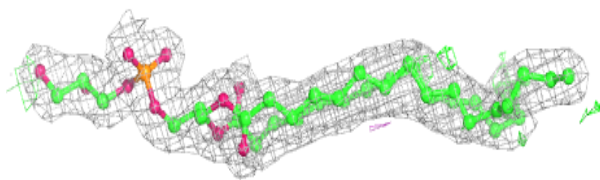
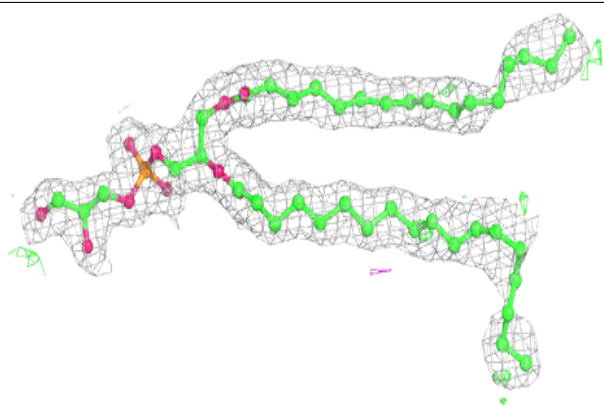


**Electron density around CHD O 229:**

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

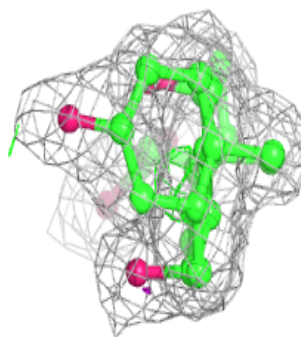
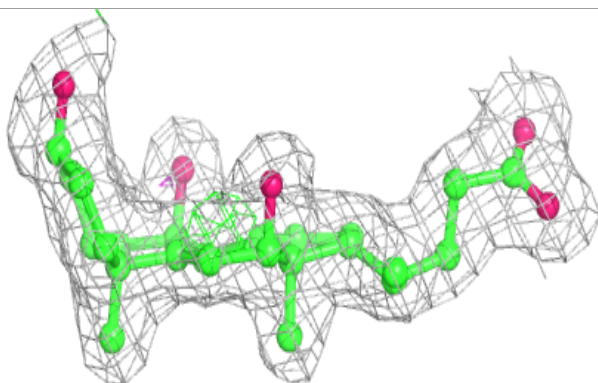
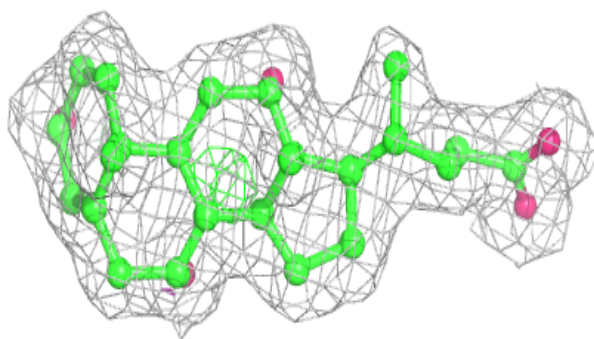
**Electron density around PGV C 267:**

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

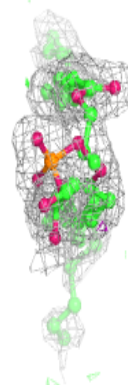
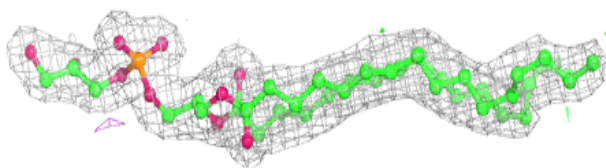
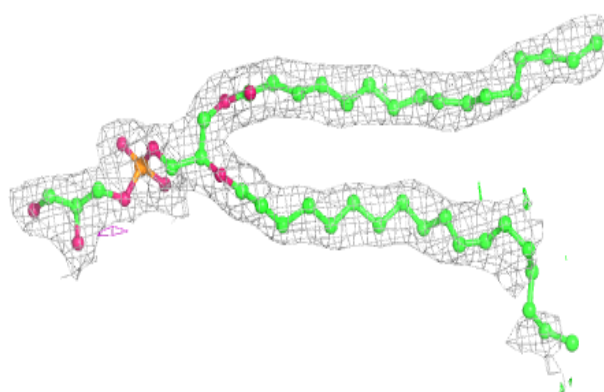


**Electron density around CHD B 1086:**

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

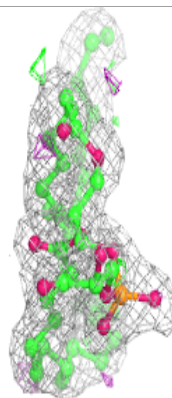
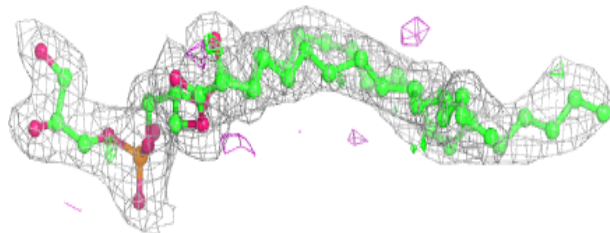
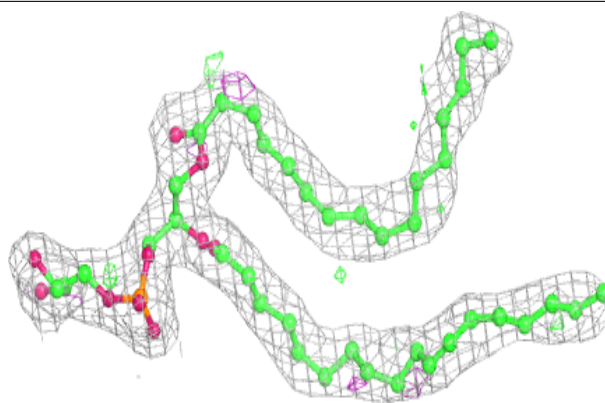
**Electron density around PGV P 1267:**

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

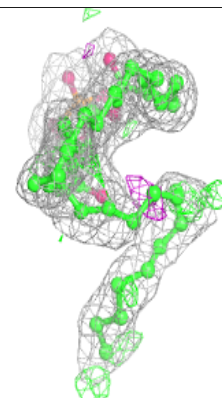
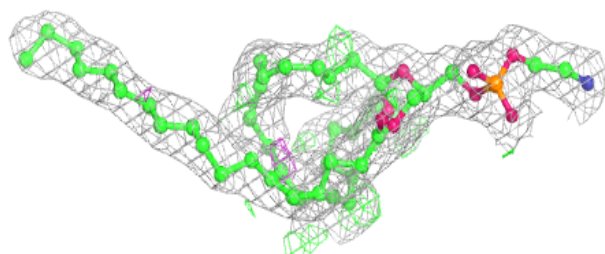
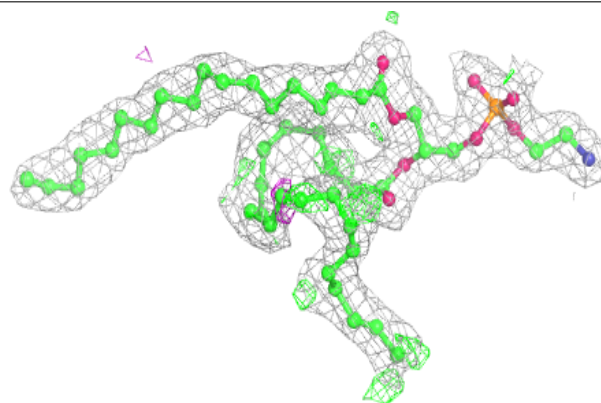


**Electron density around PGV N 1266:**

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

**Electron density around PEK G 264:**

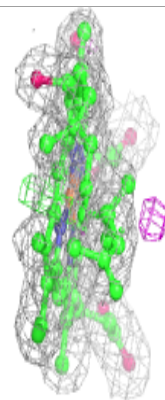
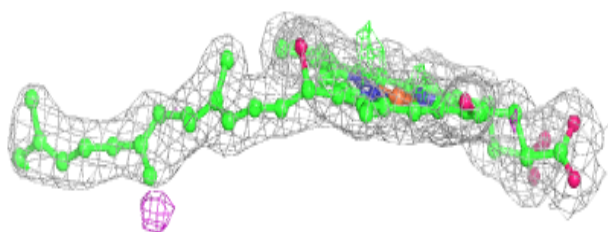
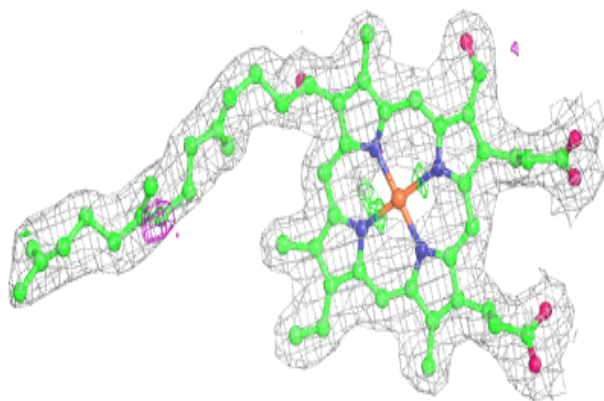
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



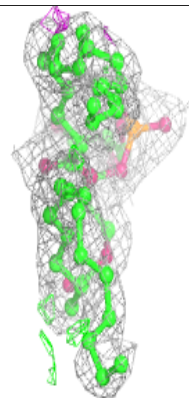
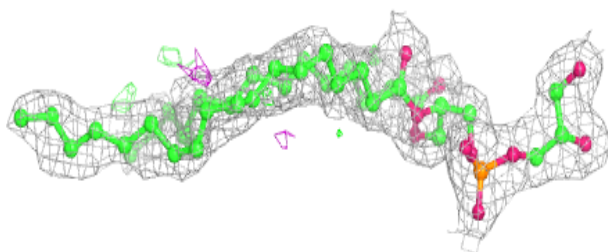
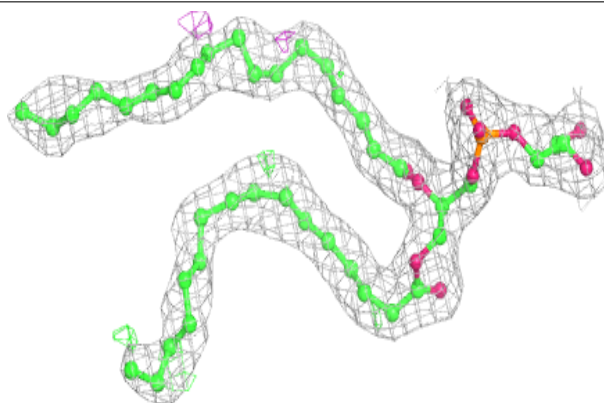


**Electron density around HEA N 515:**

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

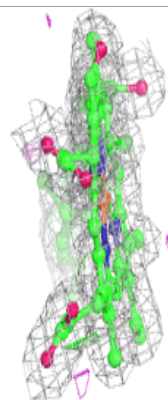
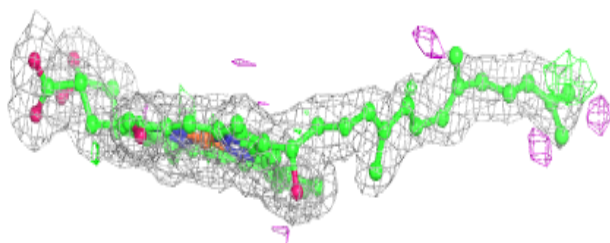
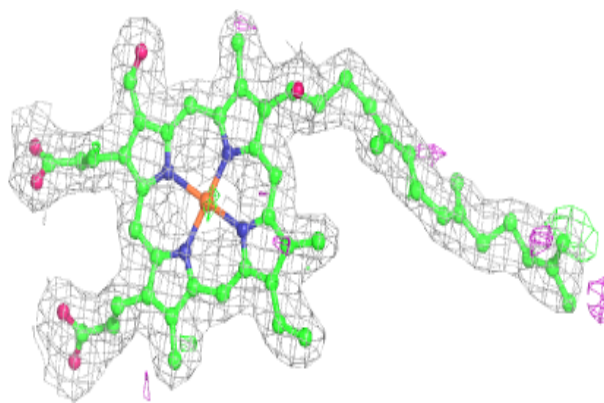
**Electron density around PGV A 522:**

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

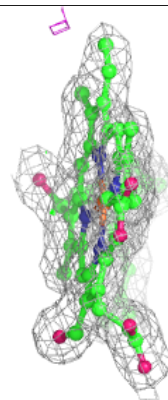
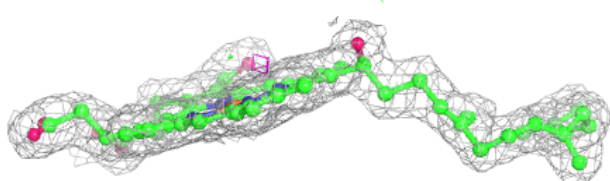
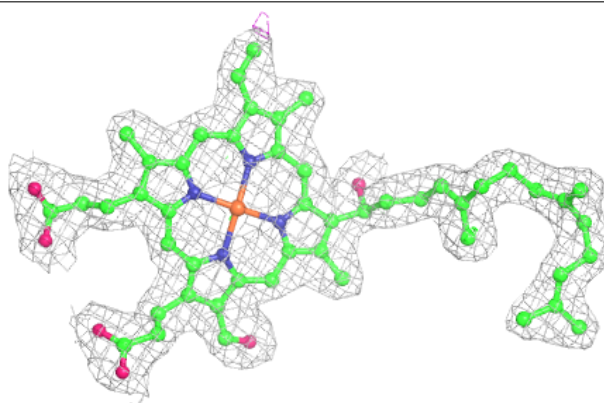


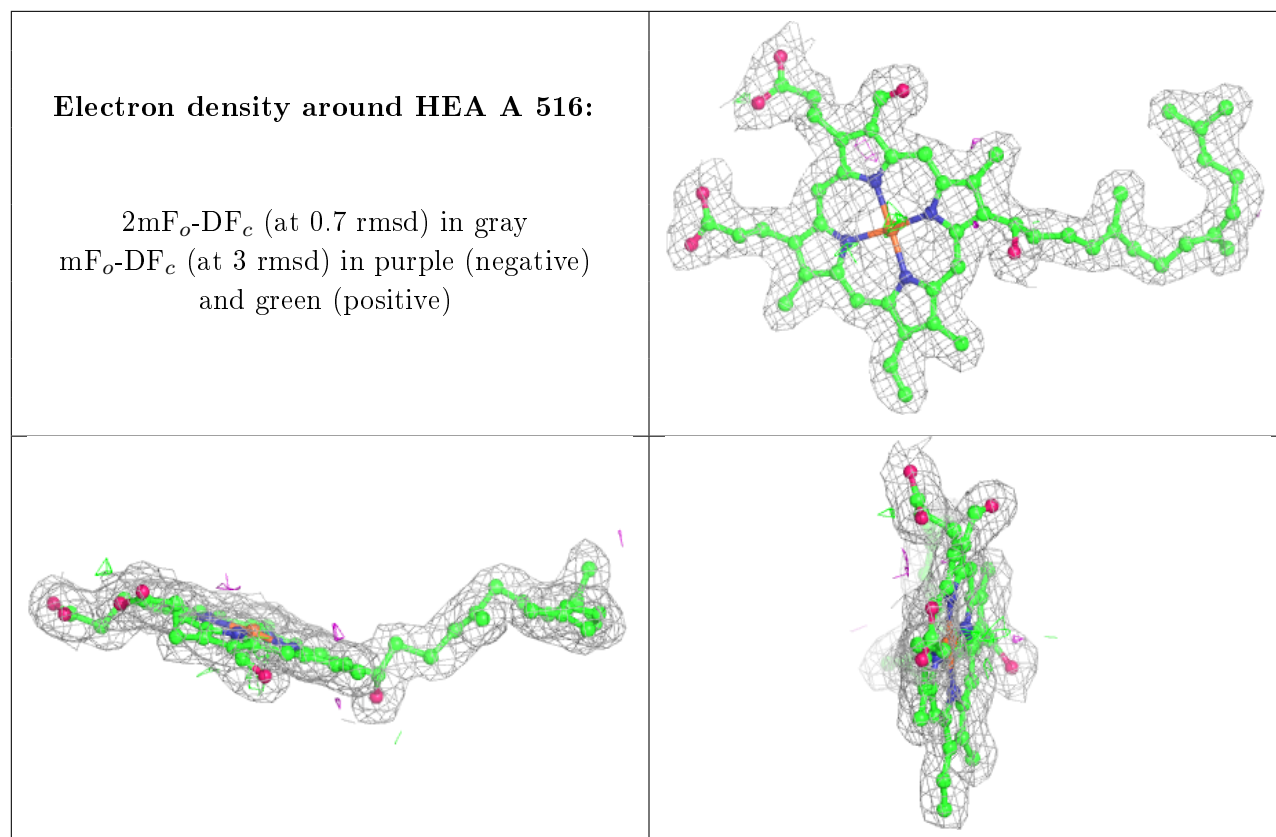
**Electron density around HEA A 515:**

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

**Electron density around HEA 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)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.