



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 06:11 PM BST

PDB ID : 5IY5  
Title : Electron transfer complex of cytochrome c and cytochrome c oxidase at 2.0 angstrom resolution  
Authors : Shimada, S.; Baba, J.; Aoe, S.; Shimada, A.; Yamashita, E.; Tsukihara, T.  
Deposited on : 2016-03-24  
Resolution : 2.00 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.

---

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 : 2.13  
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) : 2.13

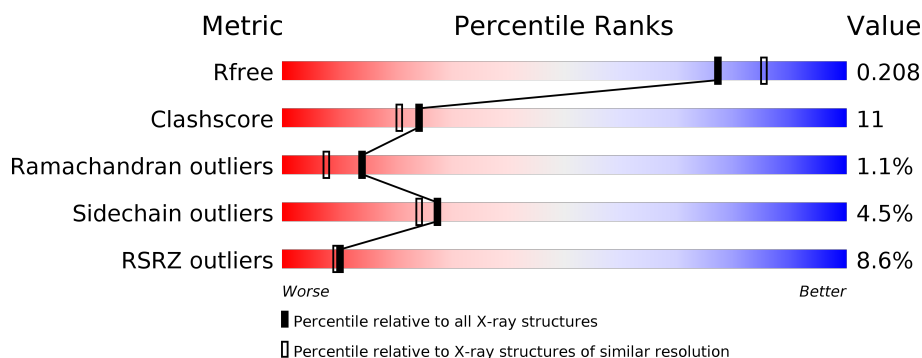
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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>4%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>.</div> </div> </div>
1	N	514	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>12%</div> <div>.</div> </div> </div>
2	B	227	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>22%</div> <div>.</div> </div> </div>
2	O	227	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>.</div> </div> </div>
3	C	259	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>13%</div> <div>.</div> </div> </div>
3	P	259	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>14%</div> </div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	144	
4	Q	144	
5	E	105	
5	R	105	
6	F	98	
6	S	98	
7	G	84	
7	T	84	
8	H	79	
8	U	79	
9	I	73	
9	V	73	
10	J	58	
10	W	58	
11	K	49	
11	X	49	
12	L	46	
12	Y	46	
13	M	43	
13	Z	43	
14	1	105	
14	2	105	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	NA	C	302	-	-	-	X
17	NA	P	302	-	-	-	X
18	HEA	A	605	X	-	-	-
18	HEA	N	606	X	-	-	-
24	CHD	W	101	-	-	-	X
26	CDL	G	101	-	-	X	-
26	CDL	T	101	-	-	X	-
27	UNL	C	310	-	-	X	-
27	UNL	N	601	-	-	X	-
27	UNL	P	308	-	-	X	-
27	UNL	P	310	-	-	X	-
28	PSC	V	101	-	-	X	-
29	ZN	S	101	-	-	X	-
9	SAC	I	1	-	X	-	-
9	SAC	V	1	-	-	-	X



## 2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 34765 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	11	0
			4084	2731	628	685	40			
1	N	514	Total	C	N	O	S	0	8	0
			4065	2717	627	683	38			

- 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	2	0
			1836	1192	283	343	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	6	0
			2149	1437	343	355	14			
3	P	259	Total	C	N	O	S	0	5	0
			2143	1433	342	354	14			

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

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	1	0
			1203	782	199	218	4			

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

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

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

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

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

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

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

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

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

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

- Molecule 10 is a protein called Cytochrome c oxidase subunit 7A1, mitochondrial.

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

*Continued on next page...*

*Continued from previous page...*

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

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

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, mitochondrial.

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, mitochondrial.

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 a protein called Cytochrome c.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	1	105	Total	C	N	O	S	0	0	0
			826	526	144	152	4			
14	2	105	Total	C	N	O	S	0	0	0
			826	526	144	152	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	0	ACE	-	acetylation	UNP P00004
2	0	ACE	-	acetylation	UNP P00004

- Molecule 15 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

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

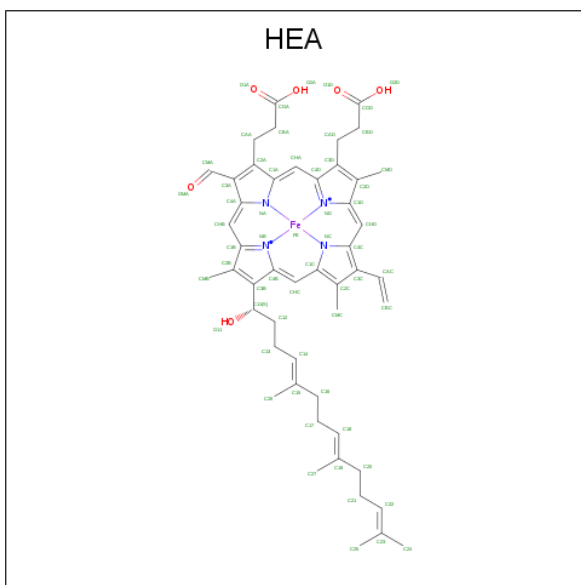
- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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).

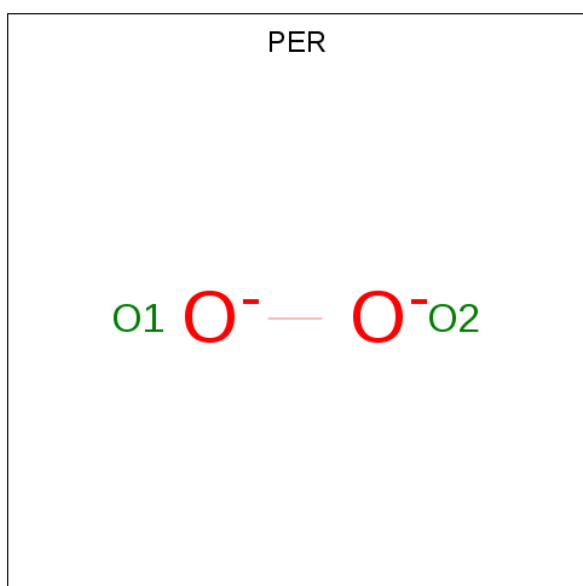
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	P	1	Total Na 1 1	0	0
17	A	1	Total Na 1 1	0	0
17	C	1	Total Na 1 1	0	0
17	N	1	Total Na 1 1	0	0

- Molecule 18 is HEME-A (three-letter code: HEA) (formula:  $C_{49}H_{56}FeN_4O_6$ ).



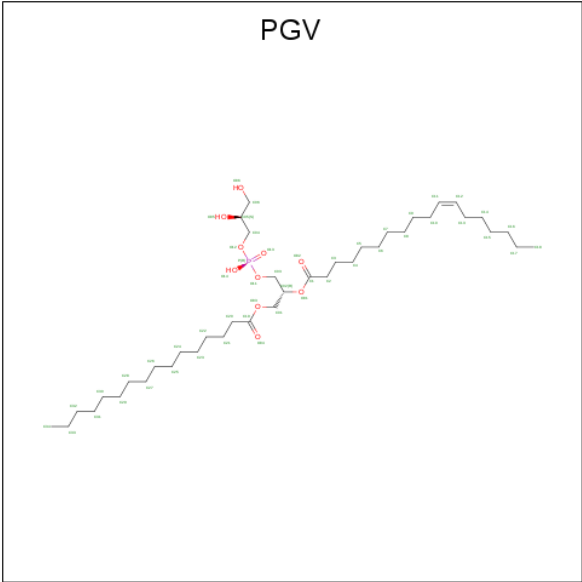
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
18	A	1	Total	C	Fe	N	O	0	1
			69	58	1	4	6		
18	A	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		
18	N	1	Total	C	Fe	N	O	0	1
			69	58	1	4	6		
18	N	1	Total	C	Fe	N	O	0	0
			60	49	1	4	6		

- Molecule 19 is PEROXIDE ION (three-letter code: PER) (formula: O<sub>2</sub>).



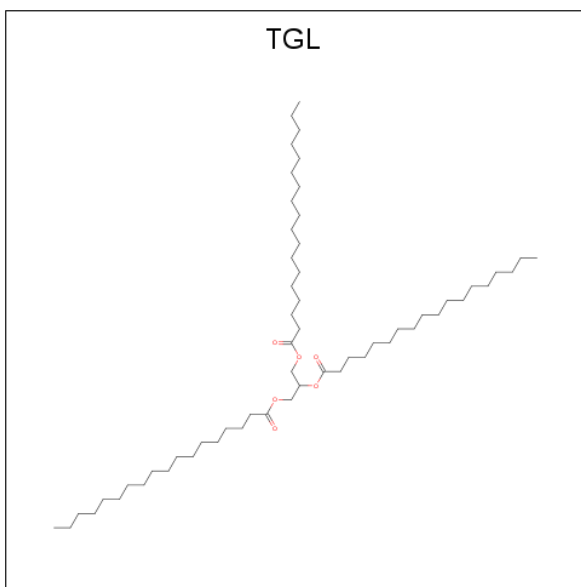
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
19	A	1	Total	O	0	0
			2	2		
19	N	1	Total	O	0	0
			2	2		

- 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).



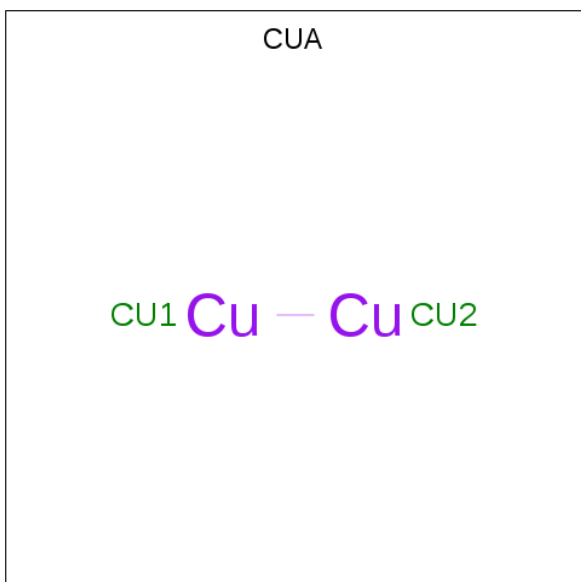
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	A	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	C	1	Total	C	O	P	0	0
			51	40	10	1		
20	N	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0
			51	40	10	1		
20	P	1	Total	C	O	P	0	0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

- Molecule 21 is TRISTEAROYLGLYCEROL (three-letter code: TGL) (formula: C<sub>57</sub>H<sub>110</sub>O<sub>6</sub>).



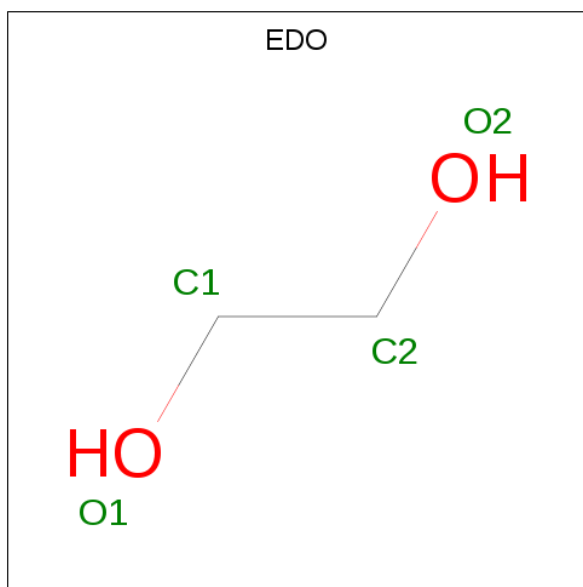
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	B	1	Total	C	O	0	0
			63	57	6		
21	D	1	Total	C	O	0	0
			63	57	6		
21	L	1	Total	C	O	0	0
			63	57	6		
21	N	1	Total	C	O	0	0
			63	57	6		
21	Q	1	Total	C	O	0	0
			63	57	6		

- Molecule 22 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu<sub>2</sub>).



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

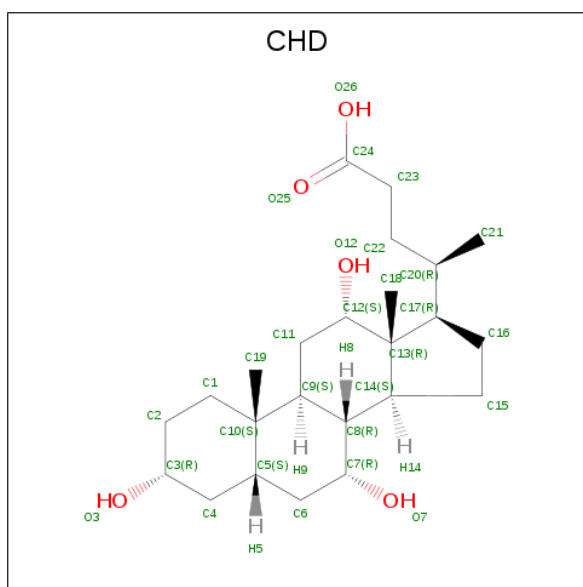
- Molecule 23 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
23	B	1	Total C O 4 2 2	0	0
23	C	1	Total C O 4 2 2	0	0
23	E	1	Total C O 4 2 2	0	0
23	F	1	Total C O 4 2 2	0	0
23	G	1	Total C O 4 2 2	0	0
23	I	1	Total C O 4 2 2	0	0
23	N	1	Total C O 4 2 2	0	0
23	N	1	Total C O 4 2 2	0	0
23	S	1	Total C O 4 2 2	0	0

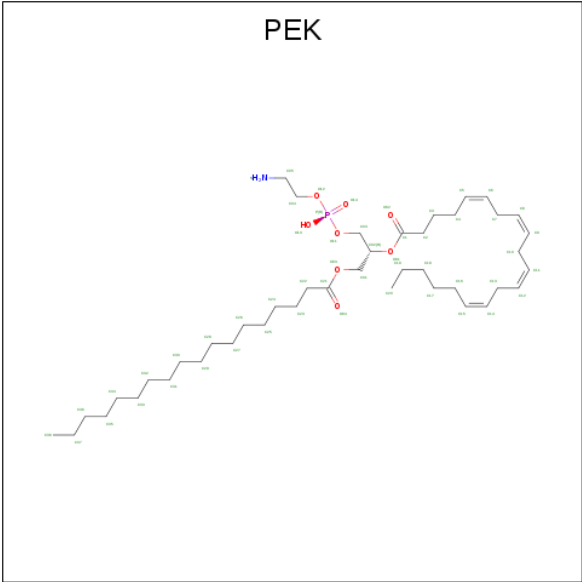
- Molecule 24 is CHOLIC ACID (three-letter code: CHD) (formula: C<sub>24</sub>H<sub>40</sub>O<sub>5</sub>).





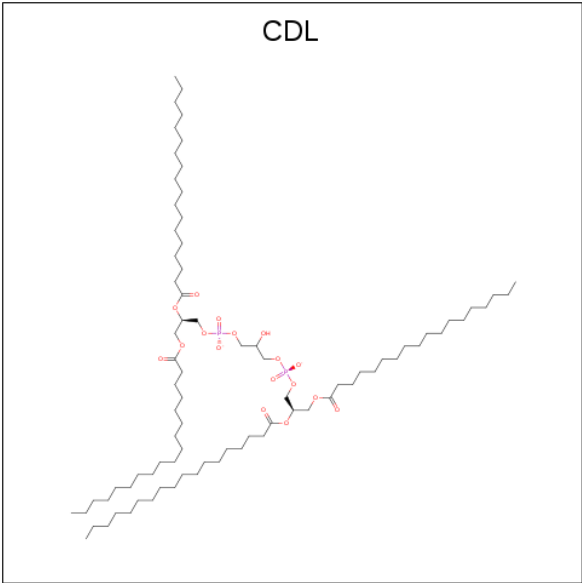
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
24	C	1	Total C O 29 24 5	0	0
24	C	1	Total C O 29 24 5	0	0
24	G	1	Total C O 29 24 5	0	0
24	J	1	Total C O 29 24 5	0	0
24	P	1	Total C O 29 24 5	0	0
24	P	1	Total C O 29 24 5	0	0
24	T	1	Total C O 29 24 5	0	0
24	W	1	Total C O 29 24 5	0	0

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



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

- Molecule 26 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



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

Continued on next page...

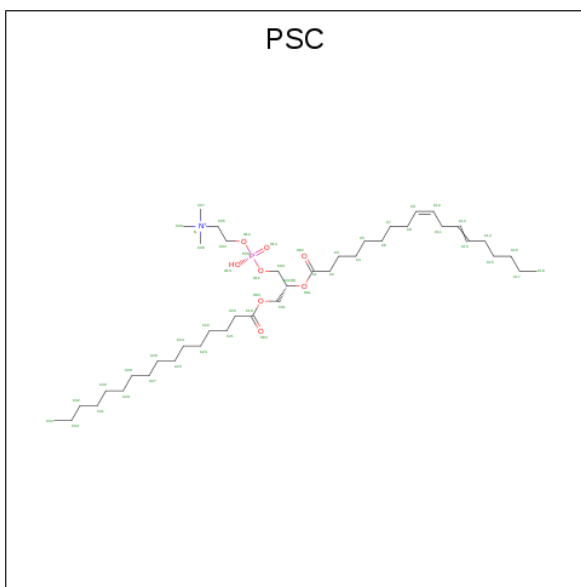
*Continued from previous page...*

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

- Molecule 27 is UNKNOWN LIGAND (three-letter code: UNL) (formula: ).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	P	3	Total	C	0	0
			43	43		
27	J	1	Total	C	0	0
			10	10		
27	C	3	Total	C	0	0
			42	42		
27	W	1	Total	C	0	0
			9	9		
27	T	1	Total	C	0	0
			18	18		
27	N	4	Total	C	0	0
			63	63		
27	Y	1	Total	C	0	0
			10	10		
27	L	1	Total	C	0	0
			10	10		

- Molecule 28 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).

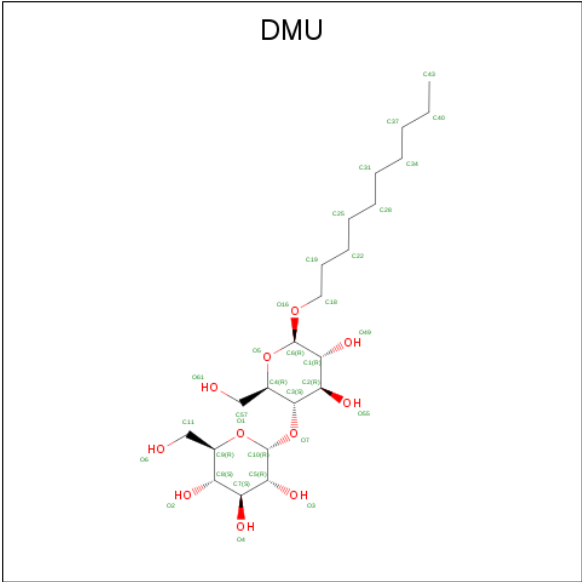


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
28	E	1	Total	C	N	O	P	0	0
			52	42	1	8	1		
28	V	1	Total	C	N	O	P	0	0
			52	42	1	8	1		

- Molecule 29 is ZINC ION (three-letter code: ZN) (formula: Zn).

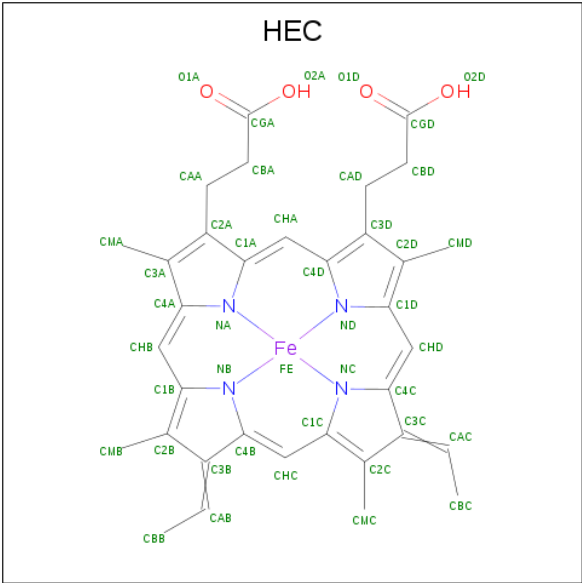
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	S	1	Total	Zn	0	0
			1	1		
29	F	1	Total	Zn	0	0
			1	1		

- Molecule 30 is DECYL-BETA-D-MALTOPYRANOSIDE (three-letter code: DMU) (formula: C<sub>22</sub>H<sub>42</sub>O<sub>11</sub>).



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

- Molecule 31 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
31	1	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
31	2	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 32 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
32	A	252	Total O 252 252	0	0
32	B	193	Total O 193 193	0	0
32	C	137	Total O 137 137	0	0
32	D	122	Total O 122 122	0	0
32	E	119	Total O 119 119	0	0
32	F	97	Total O 97 97	0	0
32	G	60	Total O 60 60	0	0
32	H	76	Total O 76 76	0	0
32	I	49	Total O 49 49	0	0
32	J	30	Total O 30 30	0	0
32	K	29	Total O 29 29	0	0
32	L	33	Total O 33 33	0	0
32	M	26	Total O 26 26	0	0
32	N	229	Total O 229 229	0	0
32	O	141	Total O 141 141	0	0
32	P	110	Total O 110 110	0	0
32	Q	99	Total O 99 99	0	0
32	R	83	Total O 83 83	0	0
32	S	95	Total O 95 95	0	0
32	T	41	Total O 41 41	0	0
32	U	54	Total O 54 54	0	0

*Continued on next page...*

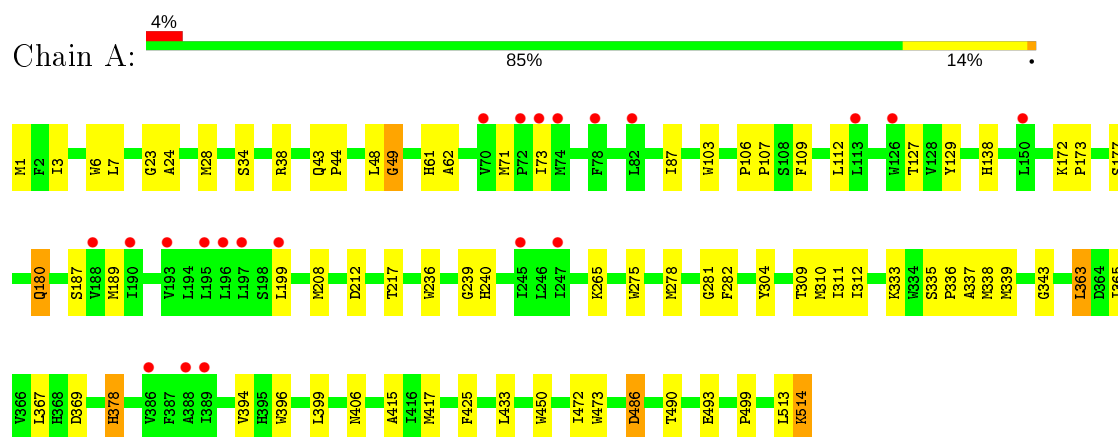
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
32	V	17	Total 17	O 17	0	0
32	W	10	Total 10	O 10	0	0
32	X	17	Total 17	O 17	0	0
32	Y	21	Total 21	O 21	0	0
32	Z	16	Total 16	O 16	0	0
32	1	53	Total 53	O 53	0	0
32	2	28	Total 28	O 28	0	0

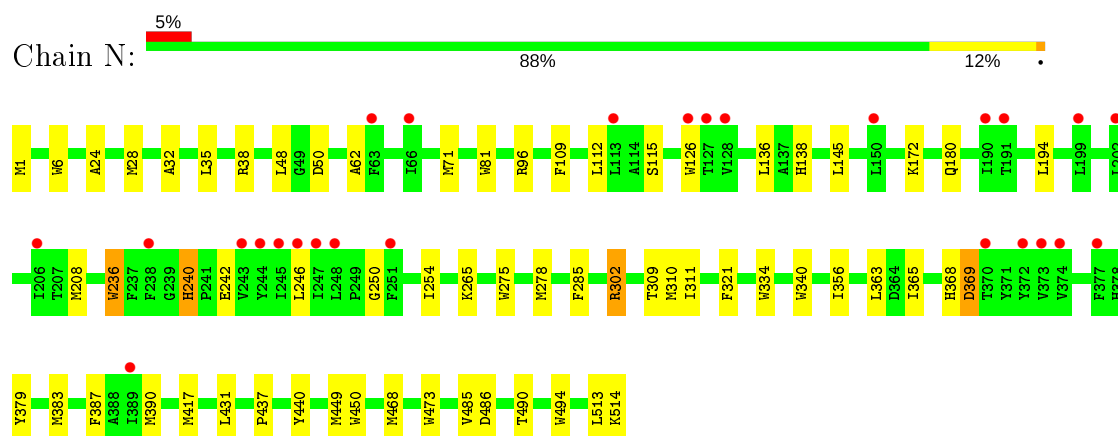
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

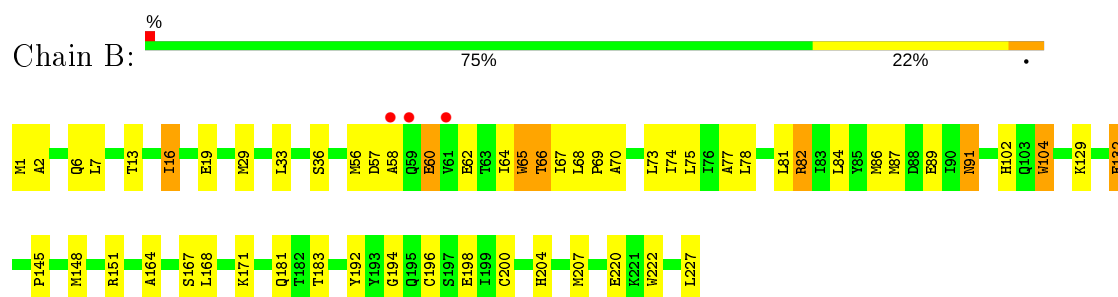
#### • Molecule 1: Cytochrome c oxidase subunit 1



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

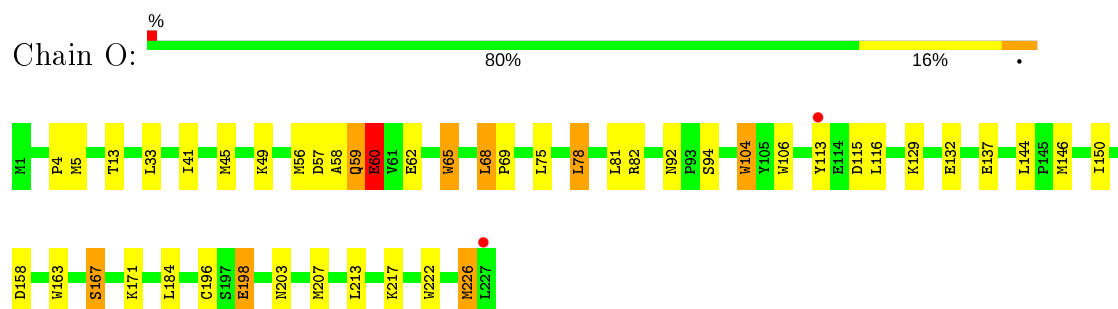


#### • Molecule 2: Cytochrome c oxidase subunit 2

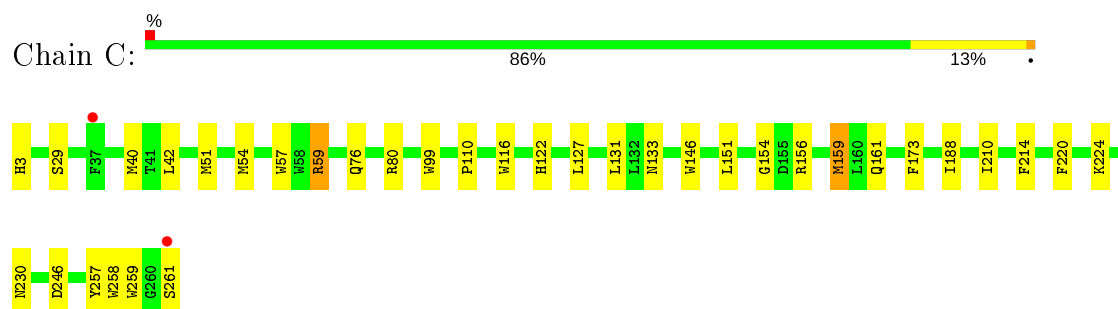




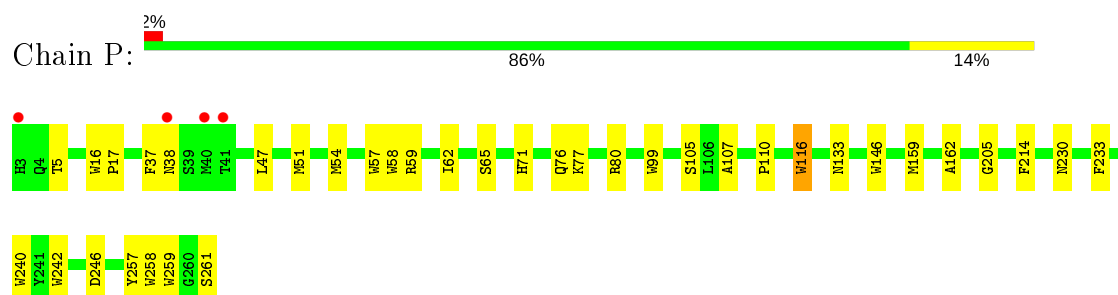
- Molecule 2: Cytochrome c oxidase subunit 2



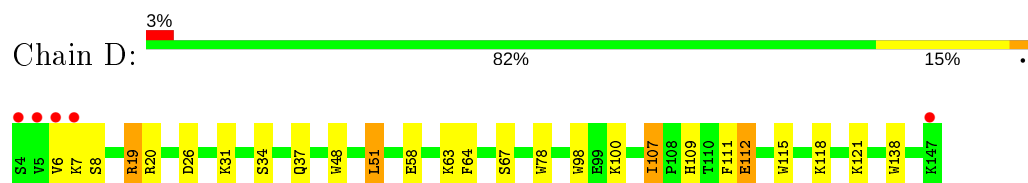
- Molecule 3: Cytochrome c oxidase subunit 3



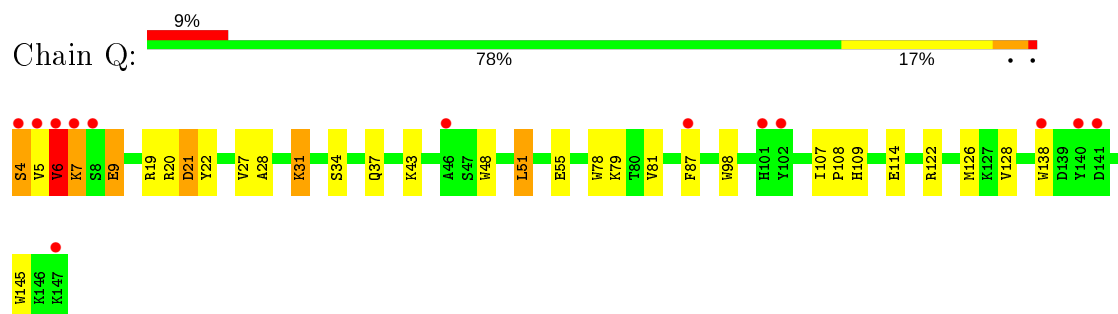
- Molecule 3: Cytochrome c oxidase subunit 3



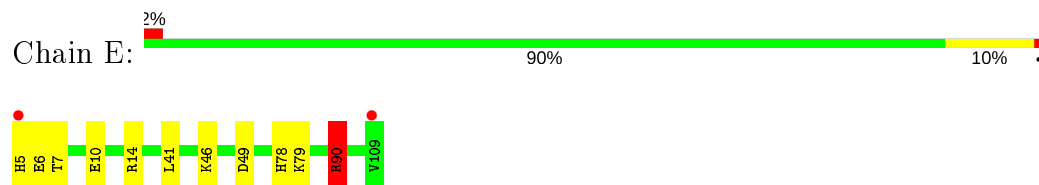
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



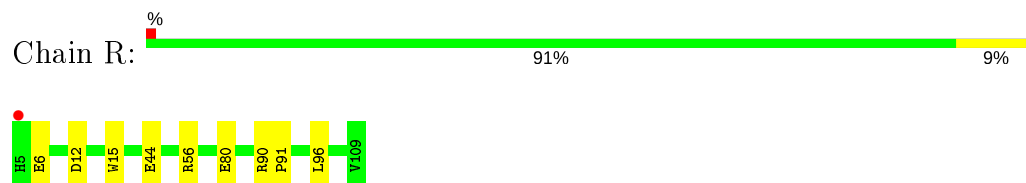
- Molecule 4: Cytochrome c oxidase subunit 4 isoform 1, mitochondrial



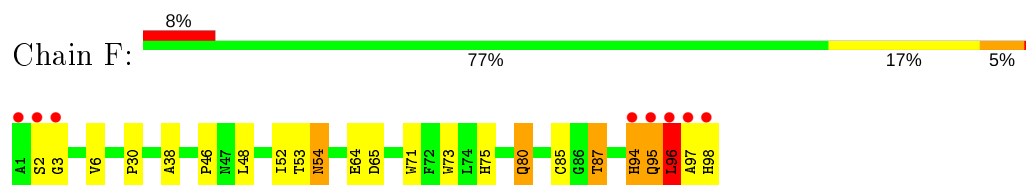
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



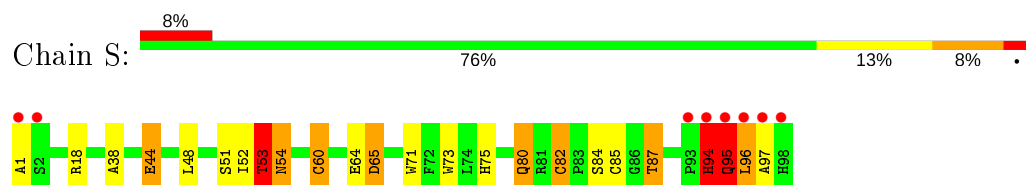
- Molecule 5: Cytochrome c oxidase subunit 5A, mitochondrial



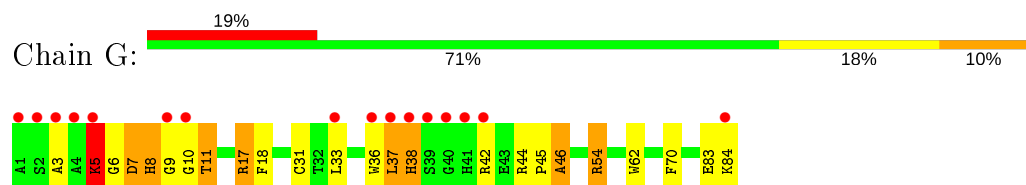
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



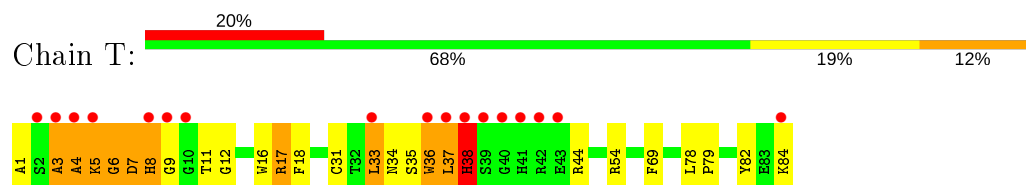
- Molecule 6: Cytochrome c oxidase subunit 5B, mitochondrial



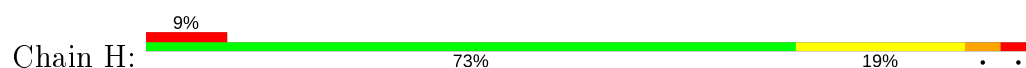
- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

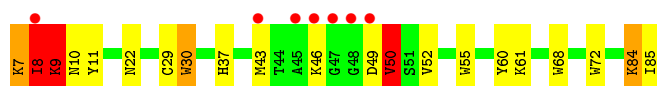


- Molecule 7: Cytochrome c oxidase subunit 6A2, mitochondrial

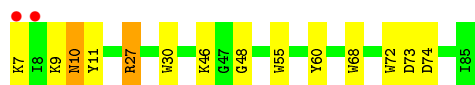
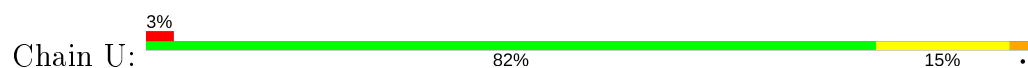


- Molecule 8: Cytochrome c oxidase subunit 6B1

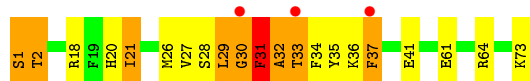




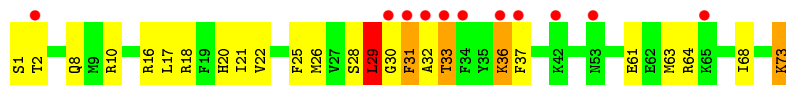
- Molecule 8: Cytochrome c oxidase subunit 6B1



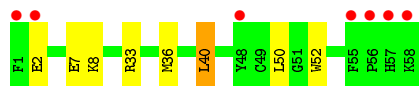
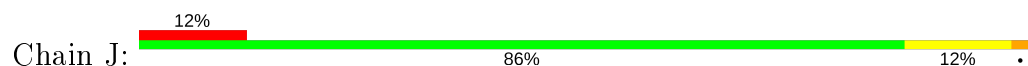
- Molecule 9: Cytochrome c oxidase subunit 6C



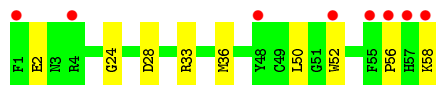
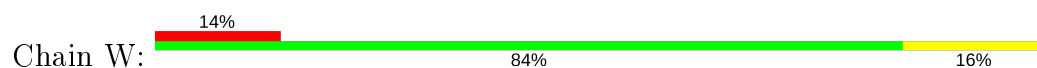
- Molecule 9: Cytochrome c oxidase subunit 6C



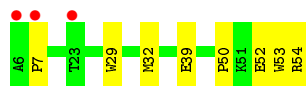
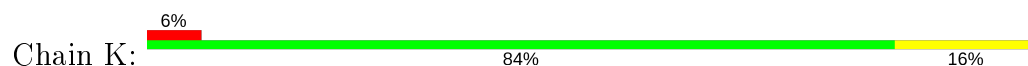
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



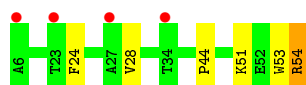
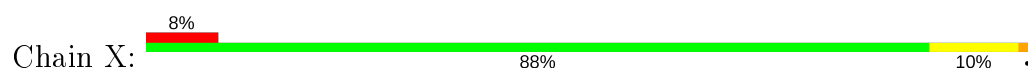
- Molecule 10: Cytochrome c oxidase subunit 7A1, mitochondrial



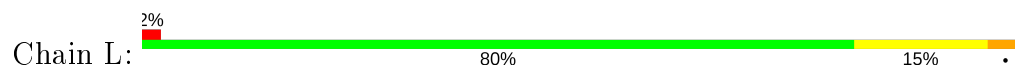
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



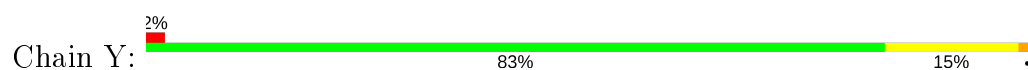
- Molecule 11: Cytochrome c oxidase subunit 7B, mitochondrial



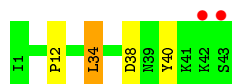
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



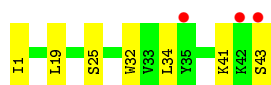
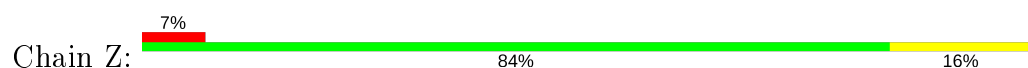
- Molecule 12: Cytochrome c oxidase subunit 7C, mitochondrial



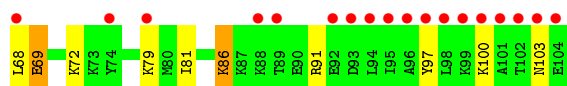
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial



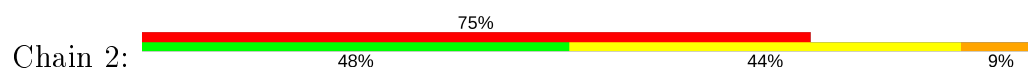
- Molecule 13: Cytochrome c oxidase subunit 8B, mitochondrial

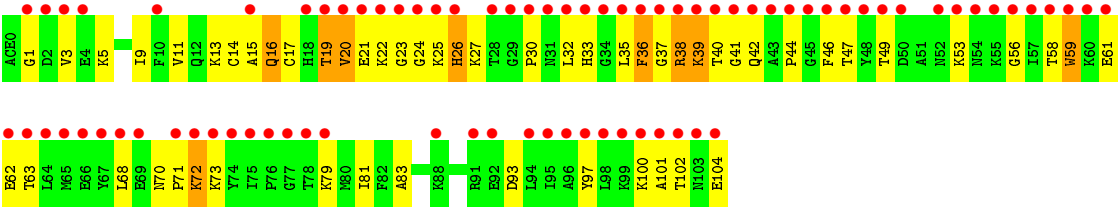


- Molecule 14: Cytochrome c



- Molecule 14: Cytochrome c





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.29Å 183.87Å 148.93Å 90.00° 102.12° 90.00°	Depositor
Resolution (Å)	40.00 – 2.00 49.35 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.00-2.00) 99.4 (49.35-2.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0048	Depositor
R, $R_{free}$	0.167 , 0.207 0.168 , 0.208	Depositor DCC
$R_{free}$ test set	19990 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.586	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 72.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	34765	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.47% 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: CDL, ZN, CHD, ACE, PSC, SAC, NA, HEC, MG, PER, EDO, PGV, TPO, CU, DMU, CUA, PEK, FME, UNL, TGL, 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	1.31	11/4244 (0.3%)	1.04	9/5793 (0.2%)
1	N	1.20	9/4214 (0.2%)	0.94	5/5754 (0.1%)
2	B	1.26	6/1878 (0.3%)	1.09	4/2558 (0.2%)
2	O	0.99	6/1860 (0.3%)	0.96	1/2534 (0.0%)
3	C	1.20	5/2247 (0.2%)	0.87	1/3070 (0.0%)
3	P	1.15	7/2238 (0.3%)	0.86	0/3058
4	D	1.21	7/1229 (0.6%)	1.13	8/1658 (0.5%)
4	Q	1.09	5/1240 (0.4%)	0.97	2/1672 (0.1%)
5	E	1.04	0/871	0.99	5/1182 (0.4%)
5	R	1.01	1/871 (0.1%)	0.89	0/1182
6	F	1.17	3/765 (0.4%)	1.04	2/1038 (0.2%)
6	S	1.15	4/765 (0.5%)	1.15	5/1038 (0.5%)
7	G	1.17	2/690 (0.3%)	1.01	3/937 (0.3%)
7	T	1.20	1/690 (0.1%)	1.09	5/937 (0.5%)
8	H	1.25	7/682 (1.0%)	1.19	4/921 (0.4%)
8	U	1.05	4/682 (0.6%)	0.99	4/921 (0.4%)
9	I	1.09	0/605	1.09	2/802 (0.2%)
9	V	0.86	0/605	0.96	1/802 (0.1%)
10	J	0.96	1/471 (0.2%)	0.88	1/636 (0.2%)
10	W	0.87	1/471 (0.2%)	0.86	0/636
11	K	1.13	1/398 (0.3%)	0.96	0/546
11	X	0.94	1/398 (0.3%)	0.86	0/546
12	L	1.15	0/393	0.90	0/526
12	Y	1.05	0/393	0.95	1/526 (0.2%)
13	M	1.05	0/345	1.01	1/470 (0.2%)
13	Z	1.01	1/345 (0.3%)	1.01	2/470 (0.4%)
14	1	0.73	1/840 (0.1%)	0.78	0/1120
14	2	0.68	1/840 (0.1%)	0.74	0/1120
All	All	1.14	85/31270 (0.3%)	0.98	66/42453 (0.2%)

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
1	N	0	1
6	S	0	2
8	H	0	2
9	V	0	2
All	All	0	8

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	116	TRP	CD2-CE2	8.38	1.51	1.41
2	B	132	GLU	CD-OE2	8.22	1.34	1.25
6	S	60	CYS	CB-SG	8.20	1.96	1.82
2	B	167	SER	CB-OG	-8.05	1.31	1.42
1	N	236	TRP	CD2-CE2	7.79	1.50	1.41
1	N	275	TRP	CD2-CE2	7.66	1.50	1.41
4	D	115	TRP	CD2-CE2	7.58	1.50	1.41
3	C	116	TRP	CD2-CE2	7.46	1.50	1.41
1	A	396	TRP	CD2-CE2	7.42	1.50	1.41
2	B	65	TRP	CD2-CE2	7.40	1.50	1.41
2	O	106	TRP	CD2-CE2	7.02	1.49	1.41
3	P	242	TRP	CD2-CE2	7.02	1.49	1.41
3	C	99	TRP	CD2-CE2	6.78	1.49	1.41
6	F	73	TRP	CD2-CE2	6.65	1.49	1.41
1	A	473	TRP	CD2-CE2	6.63	1.49	1.41
1	A	49	GLY	C-O	6.61	1.34	1.23
8	H	9	LYS	C-O	6.61	1.35	1.23
7	G	36	TRP	CD2-CE2	6.59	1.49	1.41
6	S	71	TRP	CD2-CE2	6.58	1.49	1.41
8	H	8	ILE	N-CA	6.50	1.59	1.46
3	P	57	TRP	CD2-CE2	6.42	1.49	1.41
1	A	378	HIS	CG-CD2	6.36	1.46	1.35
1	N	340	TRP	CD2-CE2	6.34	1.49	1.41
1	A	61	HIS	CG-CD2	6.31	1.46	1.35
1	A	275	TRP	CD2-CE2	6.30	1.49	1.41
4	D	138	TRP	CD2-CE2	6.28	1.48	1.41
3	P	259	TRP	CD2-CE2	6.24	1.48	1.41
14	1	59	TRP	CD2-CE2	6.22	1.48	1.41
6	F	71	TRP	CD2-CE2	6.22	1.48	1.41

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	259	TRP	CD2-CE2	6.20	1.48	1.41
8	H	72	TRP	CD2-CE2	6.08	1.48	1.41
4	D	98	TRP	CD2-CE2	6.05	1.48	1.41
8	U	72	TRP	CD2-CE2	6.04	1.48	1.41
4	Q	145	TRP	CD2-CE2	5.98	1.48	1.41
3	P	99	TRP	CD2-CE2	5.97	1.48	1.41
8	U	55	TRP	CD2-CE2	5.88	1.48	1.41
3	P	58	TRP	CD2-CE2	5.87	1.48	1.41
6	S	73	TRP	CD2-CE2	5.86	1.48	1.41
3	C	57	TRP	CD2-CE2	5.84	1.48	1.41
7	G	62	TRP	CD2-CE2	5.81	1.48	1.41
7	T	36	TRP	CD2-CE2	5.78	1.48	1.41
1	A	450	TRP	CD2-CE2	5.78	1.48	1.41
1	A	6	TRP	CD2-CE2	5.77	1.48	1.41
1	N	81	TRP	CD2-CE2	5.75	1.48	1.41
11	K	29	TRP	CD2-CE2	5.72	1.48	1.41
8	U	68	TRP	CD2-CE2	5.66	1.48	1.41
1	N	473	TRP	CD2-CE2	5.65	1.48	1.41
4	Q	138	TRP	CD2-CE2	5.64	1.48	1.41
4	D	112	GLU	CD-OE1	5.63	1.31	1.25
2	B	222	TRP	CD2-CE2	5.61	1.48	1.41
4	Q	22	TYR	CG-CD1	5.60	1.46	1.39
8	U	30	TRP	CD2-CE2	5.59	1.48	1.41
1	N	126	TRP	CD2-CE2	5.58	1.48	1.41
11	X	53	TRP	CD2-CE2	5.57	1.48	1.41
4	Q	9	GLU	CD-OE2	5.56	1.31	1.25
4	D	48	TRP	CD2-CE2	5.55	1.48	1.41
2	O	104	TRP	CD2-CE2	5.55	1.48	1.41
5	R	15	TRP	CD2-CE2	5.51	1.48	1.41
1	A	493	GLU	CD-OE2	-5.47	1.19	1.25
2	O	65	TRP	CD2-CE2	5.46	1.48	1.41
10	W	52	TRP	CD2-CE2	5.37	1.47	1.41
1	N	494	TRP	CD2-CE2	5.33	1.47	1.41
2	B	198	GLU	CD-OE2	-5.31	1.19	1.25
6	F	94	HIS	CB-CG	5.30	1.59	1.50
2	O	163	TRP	CD2-CE2	5.29	1.47	1.41
8	H	30	TRP	CG-CD1	5.27	1.44	1.36
8	H	30	TRP	CD2-CE2	5.27	1.47	1.41
1	N	334	TRP	CD2-CE2	5.25	1.47	1.41
10	J	52	TRP	CD2-CE2	5.23	1.47	1.41
8	H	68	TRP	CD2-CE2	5.20	1.47	1.41
2	O	222	TRP	CD2-CE2	5.19	1.47	1.41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	67	SER	CB-OG	5.17	1.49	1.42
6	S	82	CYS	CB-SG	-5.17	1.73	1.81
8	H	55	TRP	CD2-CE2	5.16	1.47	1.41
3	C	258	TRP	CD2-CE2	5.11	1.47	1.41
2	O	198	GLU	C-O	5.11	1.33	1.23
3	P	240	TRP	CD2-CE2	5.09	1.47	1.41
1	N	6	TRP	CD2-CE2	5.08	1.47	1.41
1	A	187	SER	CA-CB	5.08	1.60	1.52
4	Q	98	TRP	CD2-CE2	5.08	1.47	1.41
1	A	103	TRP	CD2-CE2	5.08	1.47	1.41
4	D	115	TRP	CG-CD1	5.04	1.43	1.36
13	Z	32	TRP	CD2-CE2	5.03	1.47	1.41
2	B	104	TRP	CD2-CE2	5.03	1.47	1.41
14	2	59	TRP	CD2-CE2	5.03	1.47	1.41

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	20	ARG	NE-CZ-NH2	-11.62	114.49	120.30
2	B	82	ARG	NE-CZ-NH2	11.54	126.07	120.30
1	A	71	MET	CG-SD-CE	-11.09	82.46	100.20
1	A	486	ASP	CB-CG-OD1	10.23	127.51	118.30
5	E	90	ARG	NE-CZ-NH1	9.99	125.29	120.30
8	H	9	LYS	CA-CB-CG	-9.89	91.63	113.40
8	H	8	ILE	CG1-CB-CG2	9.71	132.77	111.40
4	D	20	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	A	486	ASP	CB-CG-OD2	-8.95	110.25	118.30
5	E	90	ARG	NE-CZ-NH2	-8.82	115.89	120.30
4	D	19	ARG	NE-CZ-NH2	8.12	124.36	120.30
9	I	21	ILE	CG1-CB-CG2	-7.64	94.60	111.40
8	U	27	ARG	NE-CZ-NH2	-7.38	116.61	120.30
2	B	82	ARG	NE-CZ-NH1	-7.26	116.67	120.30
8	H	9	LYS	O-C-N	7.16	134.15	122.70
2	O	82	ARG	NE-CZ-NH2	-7.04	116.78	120.30
7	G	17	ARG	NE-CZ-NH2	-6.89	116.86	120.30
6	F	96	LEU	CB-CG-CD2	-6.87	99.32	111.00
1	N	71	MET	CG-SD-CE	-6.86	89.23	100.20
7	T	12	GLY	N-CA-C	6.74	129.95	113.10
7	T	5	LYS	CD-CE-NZ	6.61	126.91	111.70
4	D	51	LEU	CB-CG-CD2	6.49	122.04	111.00
13	Z	19	LEU	CA-CB-CG	6.40	130.02	115.30
6	S	60	CYS	O-C-N	6.27	132.73	122.70

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	U	73	ASP	CB-CG-OD1	6.05	123.75	118.30
8	H	9	LYS	CB-CG-CD	-6.04	95.91	111.60
7	T	33	LEU	CA-CB-CG	5.99	129.08	115.30
6	S	18	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	A	189	MET	CA-CB-CG	-5.92	103.23	113.30
5	E	14	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	49	GLY	N-CA-C	-5.89	98.39	113.10
6	S	65	ASP	CB-CG-OD2	-5.84	113.05	118.30
5	E	49	ASP	CB-CG-OD1	5.83	123.55	118.30
8	U	27	ARG	NE-CZ-NH1	5.78	123.19	120.30
7	T	17	ARG	CB-CG-CD	-5.77	96.61	111.60
5	E	14	ARG	NE-CZ-NH1	5.75	123.18	120.30
4	Q	51	LEU	CB-CG-CD1	5.68	120.66	111.00
2	B	167	SER	CB-CA-C	-5.66	99.34	110.10
1	A	212	ASP	CB-CG-OD2	5.66	123.39	118.30
4	D	51	LEU	CB-CG-CD1	5.63	120.58	111.00
13	M	34	LEU	CB-CG-CD1	5.61	120.53	111.00
9	I	31	PHE	N-CA-C	-5.60	95.88	111.00
1	A	208	MET	CG-SD-CE	5.58	109.13	100.20
7	G	17	ARG	CB-CG-CD	-5.58	97.09	111.60
4	D	26	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	N	96	ARG	NE-CZ-NH2	-5.54	117.53	120.30
6	F	3	GLY	N-CA-C	-5.53	99.27	113.10
9	V	29	LEU	CA-CB-CG	5.51	127.97	115.30
3	C	59	ARG	NE-CZ-NH2	-5.50	117.55	120.30
4	D	19	ARG	NE-CZ-NH1	-5.47	117.56	120.30
1	A	363	LEU	CB-CG-CD2	5.46	120.29	111.00
10	J	40	LEU	CB-CG-CD2	5.45	120.27	111.00
7	G	54	ARG	NE-CZ-NH2	-5.44	117.58	120.30
8	U	74	ASP	CB-CG-OD1	5.43	123.19	118.30
6	S	60	CYS	CA-C-N	-5.37	105.39	117.20
2	B	168	LEU	CB-CG-CD1	-5.35	101.91	111.00
1	N	302	ARG	NE-CZ-NH1	-5.34	117.63	120.30
7	T	17	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	199	LEU	CB-CG-CD2	-5.25	102.07	111.00
4	D	19	ARG	CB-CA-C	-5.18	100.04	110.40
12	Y	20	ARG	NE-CZ-NH1	5.17	122.88	120.30
6	S	53	THR	CB-CA-C	-5.13	97.75	111.60
1	N	208	MET	CG-SD-CE	5.11	108.38	100.20
1	N	50	ASP	CB-CG-OD1	5.10	122.89	118.30
4	Q	20	ARG	NE-CZ-NH2	-5.07	117.77	120.30
13	Z	19	LEU	CB-CG-CD2	-5.04	102.43	111.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	HIS	Sidechain
8	H	8	ILE	Peptide
8	H	9	LYS	Peptide
1	N	240	HIS	Sidechain
6	S	94	HIS	Peptide
6	S	95	GLN	Peptide
9	V	32	ALA	Peptide
9	V	33	THR	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	4084	0	4069	63	0
1	N	4065	0	4046	44	0
2	B	1836	0	1843	43	0
2	O	1824	0	1833	40	0
3	C	2149	0	2075	24	0
3	P	2143	0	2067	29	0
4	D	1195	0	1183	16	0
4	Q	1203	0	1196	30	0
5	E	852	0	845	8	0
5	R	852	0	845	5	0
6	F	748	0	728	25	0
6	S	748	0	729	25	0
7	G	675	0	643	20	0
7	T	675	0	644	26	0
8	H	662	0	623	36	0
8	U	662	0	623	7	0
9	I	601	0	613	39	0
9	V	601	0	613	19	0
10	J	460	0	459	7	0
10	W	460	0	459	12	0
11	K	384	0	366	5	0
11	X	384	0	366	8	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	L	380	0	380	12	0
12	Y	380	0	380	6	0
13	M	335	0	352	1	0
13	Z	335	0	352	4	0
14	1	826	0	849	25	0
14	2	826	0	848	40	0
15	A	1	0	0	0	0
15	N	1	0	0	0	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
17	A	1	0	0	0	0
17	C	1	0	0	0	0
17	N	1	0	0	0	0
17	P	1	0	0	0	0
18	A	129	0	88	9	0
18	N	129	0	88	10	0
19	A	2	0	0	0	0
19	N	2	0	0	1	0
20	A	102	0	152	9	0
20	C	102	0	152	14	0
20	N	51	0	76	1	0
20	P	102	0	152	10	0
21	B	63	0	110	6	0
21	D	63	0	110	12	0
21	L	63	0	110	20	0
21	N	63	0	110	2	0
21	Q	63	0	110	10	0
22	B	2	0	0	0	0
22	O	2	0	0	0	0
23	B	4	0	6	0	0
23	C	4	0	6	0	0
23	E	4	0	6	1	0
23	F	4	0	6	0	0
23	G	4	0	6	0	0
23	I	4	0	6	0	0
23	N	8	0	12	0	0
23	S	4	0	6	0	0
24	C	58	0	78	4	0
24	G	29	0	39	0	0
24	J	29	0	38	5	0
24	P	58	0	78	2	0
24	T	29	0	39	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	W	29	0	37	5	0
25	C	53	0	77	7	0
25	P	53	0	77	3	0
26	C	100	0	156	15	0
26	G	100	0	156	23	0
26	P	100	0	156	12	0
26	T	100	0	156	24	0
27	C	42	0	0	4	0
27	J	10	0	0	1	0
27	L	10	0	0	1	0
27	N	63	0	0	2	0
27	P	43	0	0	6	0
27	T	18	0	0	1	0
27	W	9	0	0	1	0
27	Y	10	0	0	1	0
28	E	52	0	80	19	0
28	V	52	0	80	21	0
29	F	1	0	0	0	0
29	S	1	0	0	2	0
30	M	33	0	42	1	0
30	Z	33	0	42	1	0
31	1	43	0	31	4	0
31	2	43	0	30	4	0
32	1	53	0	0	6	0
32	2	28	0	0	7	0
32	A	252	0	0	19	0
32	B	193	0	0	6	0
32	C	137	0	0	7	0
32	D	122	0	0	7	0
32	E	119	0	0	6	0
32	F	97	0	0	2	2
32	G	60	0	0	11	0
32	H	76	0	0	7	0
32	I	49	0	0	5	0
32	J	30	0	0	3	0
32	K	29	0	0	1	0
32	L	33	0	0	1	0
32	M	26	0	0	2	0
32	N	229	0	0	6	0
32	O	141	0	0	3	0
32	P	110	0	0	9	0
32	Q	99	0	0	7	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	R	83	0	0	1	0
32	S	95	0	0	5	0
32	T	41	0	0	3	0
32	U	54	0	0	4	2
32	V	17	0	0	2	0
32	W	10	0	0	0	0
32	X	17	0	0	3	0
32	Y	21	0	0	0	0
32	Z	16	0	0	0	0
All	All	34765	0	32733	716	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (716) 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)
27:C:310:UNL:C4	27:C:310:UNL:C6	1.76	1.36
32:A:927:HOH:O	26:T:101:CDL:H412	1.17	1.28
5:E:79:LYS:HE3	32:E:387:HOH:O	1.31	1.24
27:W:102:UNL:C5	27:W:102:UNL:C4	2.17	1.23
1:A:486:ASP:OD2	4:D:19:ARG:HD2	1.32	1.21
19:N:607:PER:O2	19:N:607:PER:O1	1.54	1.21
9:I:29:LEU:O	9:I:32:ALA:N	1.71	1.20
32:P:475:HOH:O	10:W:58:LYS:HE2	1.38	1.20
24:J:101:CHD:H212	32:J:221:HOH:O	1.41	1.17
28:V:101:PSC:H343	28:V:101:PSC:H12	1.22	1.14
28:E:201:PSC:C01	28:E:201:PSC:H221	1.79	1.13
32:C:526:HOH:O	26:G:101:CDL:H551	0.98	1.12
9:I:29:LEU:O	9:I:32:ALA:CA	1.98	1.12
32:A:927:HOH:O	26:T:101:CDL:C40	1.97	1.12
28:E:201:PSC:H221	28:E:201:PSC:O03	1.37	1.10
26:P:306:CDL:OB3	32:P:401:HOH:O	1.65	1.10
14:1:17:CYS:SG	31:1:201:HEC:HAC	1.78	1.09
8:H:7:LYS:O	8:H:8:ILE:CG2	2.01	1.09
21:L:101:TGL:HC41	21:L:101:TGL:OC1	1.29	1.08
26:G:101:CDL:CB2	32:G:244:HOH:O	2.00	1.07
6:F:94:HIS:HB2	6:F:96:LEU:HB2	1.09	1.06
8:H:7:LYS:O	8:H:8:ILE:HB	1.47	1.06
27:P:310:UNL:C5	27:P:310:UNL:C4	2.33	1.06
27:C:310:UNL:C5	27:C:310:UNL:C6	2.33	1.06

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:220:GLU:OE2	32:B:401:HOH:O	1.73	1.05
1:A:282:PHE:HA	7:T:4:ALA:HB3	1.36	1.05
9:I:26:MET:O	9:I:30:GLY:CA	2.05	1.05
8:H:7:LYS:O	8:H:8:ILE:CB	2.05	1.04
28:E:201:PSC:H343	28:E:201:PSC:H12	1.40	1.04
20:A:607:PGV:H22	32:A:701:HOH:O	1.57	1.04
27:L:102:UNL:C10	27:L:102:UNL:C4	2.35	1.04
3:C:133:ASN:ND2	32:C:402:HOH:O	1.89	1.04
28:V:101:PSC:H22	32:V:212:HOH:O	1.58	1.03
9:V:29:LEU:O	9:V:31:PHE:N	1.91	1.03
4:D:6:VAL:HG21	4:D:31:LYS:NZ	1.75	1.01
21:D:201:TGL:HA91	21:D:201:TGL:H231	1.40	1.00
9:I:26:MET:O	9:I:30:GLY:HA3	1.61	1.00
9:I:31:PHE:CZ	9:I:32:ALA:O	2.15	1.00
10:W:33:ARG:HG2	24:W:101:CHD:H152	1.42	0.99
8:H:9:LYS:N	8:H:9:LYS:HD3	1.49	0.98
6:F:85:CYS:SG	6:F:87:THR:HG23	2.02	0.98
26:C:306:CDL:O1	32:C:401:HOH:O	1.83	0.97
8:H:7:LYS:O	8:H:8:ILE:HG22	1.62	0.97
8:H:8:ILE:N	32:H:101:HOH:O	1.94	0.96
2:O:226:MET:CE	2:O:226:MET:HA	1.96	0.96
25:C:303:PEK:H161	25:C:303:PEK:H11	1.47	0.94
7:G:11:TPO:O	32:G:201:HOH:O	1.87	0.94
3:P:133:ASN:ND2	32:P:402:HOH:O	2.02	0.93
2:B:29:MET:HG3	9:I:31:PHE:HZ	1.33	0.92
26:G:101:CDL:HB21	32:G:244:HOH:O	1.62	0.91
32:A:927:HOH:O	26:T:101:CDL:C41	1.82	0.91
3:P:37:PHE:CE1	10:W:58:LYS:HG3	2.05	0.91
6:F:30:PRO:O	6:F:96:LEU:HD21	1.70	0.91
26:P:306:CDL:H1	32:P:403:HOH:O	1.70	0.91
9:I:29:LEU:O	9:I:32:ALA:CB	2.19	0.90
1:N:514:LYS:HE2	32:S:258:HOH:O	1.70	0.90
32:P:493:HOH:O	6:S:1:ALA:HB1	1.67	0.90
21:L:101:TGL:CC4	21:L:101:TGL:OC1	2.16	0.90
4:Q:21:ASP:HB2	32:Q:301:HOH:O	1.72	0.90
2:O:58:ALA:O	2:O:62:GLU:HG3	1.71	0.90
6:F:75:HIS:H	6:F:80:GLN:HE22	1.19	0.89
6:S:85:CYS:SG	6:S:87:THR:HG23	2.13	0.88
14:2:81:ILE:HD12	32:2:328:HOH:O	1.74	0.87
26:G:101:CDL:H241	26:G:101:CDL:H522	1.55	0.87
12:L:2:HIS:CD2	12:L:3:TYR:H	1.93	0.87

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:B:301:TGL:H302	21:B:301:TGL:H121	1.56	0.87
9:I:29:LEU:O	9:I:32:ALA:HB2	1.75	0.86
1:A:417[B]:MET:HE3	32:A:921:HOH:O	1.75	0.86
20:P:305:PGV:H062	32:U:103:HOH:O	1.76	0.86
12:L:20:ARG:HH21	21:L:101:TGL:HC52	1.39	0.86
3:P:37:PHE:CD1	10:W:58:LYS:HG3	2.11	0.85
27:Y:101:UNL:C4	27:Y:101:UNL:C5	2.54	0.85
6:F:30:PRO:O	6:F:96:LEU:CD2	2.24	0.85
1:A:282:PHE:HA	7:T:4:ALA:CB	2.07	0.84
26:G:101:CDL:HA21	26:G:101:CDL:H111	1.57	0.84
26:G:101:CDL:HB22	32:G:244:HOH:O	1.70	0.84
9:I:33:THR:HG22	9:I:37:PHE:HB3	1.57	0.84
28:E:201:PSC:O03	28:E:201:PSC:C22	2.23	0.84
6:F:94:HIS:CB	6:F:96:LEU:HB2	2.02	0.84
8:H:84:LYS:HA	8:H:84:LYS:HZ3	1.42	0.83
27:C:310:UNL:C5	27:C:310:UNL:C4	2.56	0.83
11:X:54:ARG:HH21	11:X:54:ARG:HG3	1.43	0.83
20:P:304:PGV:H151	20:P:304:PGV:H11	1.58	0.83
6:F:94:HIS:HB2	6:F:96:LEU:CB	2.02	0.83
2:B:16:ILE:HD13	32:B:549:HOH:O	1.79	0.82
9:I:30:GLY:O	9:I:31:PHE:C	2.16	0.82
9:I:26:MET:O	9:I:30:GLY:N	2.12	0.81
6:S:75:HIS:H	6:S:80:GLN:HE22	1.23	0.81
4:D:6:VAL:HG21	4:D:31:LYS:HZ1	1.41	0.81
3:P:205:GLY:HA3	25:P:303:PEK:H161	1.63	0.81
4:Q:31:LYS:HE3	32:Q:376:HOH:O	1.80	0.81
20:A:607:PGV:H211	32:M:216:HOH:O	1.80	0.80
8:U:46:LYS:HE3	32:U:143:HOH:O	1.80	0.80
14:2:20:VAL:HG12	14:2:102:THR:HG22	1.64	0.80
2:B:81:LEU:HD12	26:T:101:CDL:H351	1.64	0.80
6:S:64:GLU:O	6:S:65:ASP:HB2	1.81	0.79
32:N:737:HOH:O	21:Q:201:TGL:HB32	1.83	0.79
28:V:101:PSC:H291	28:V:101:PSC:H331	1.65	0.79
11:X:54:ARG:HH21	11:X:54:ARG:CG	1.96	0.79
24:P:307:CHD:H231	32:P:504:HOH:O	1.83	0.79
20:A:608:PGV:H343	25:C:303:PEK:H383	1.65	0.78
21:L:101:TGL:C36	21:L:101:TGL:H312	2.13	0.78
14:2:3:VAL:HG13	14:2:97:TYR:HA	1.65	0.78
12:L:2:HIS:HD2	12:L:3:TYR:H	1.30	0.78
20:P:305:PGV:C06	32:U:103:HOH:O	2.31	0.78
32:N:725:HOH:O	3:P:77:LYS:HE3	1.83	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:6:GLY:O	7:G:7:ASP:HB2	1.83	0.78
1:N:417:MET:HE3	32:N:928:HOH:O	1.83	0.78
27:J:102:UNL:C6	27:J:102:UNL:C10	2.62	0.77
12:L:24:MET:HG3	32:L:223:HOH:O	1.83	0.77
2:B:29:MET:HG3	9:I:31:PHE:CZ	2.17	0.77
4:Q:21:ASP:CB	32:Q:301:HOH:O	2.29	0.77
1:A:514:LYS:HA	6:F:38:ALA:HB3	1.67	0.77
12:L:20:ARG:NH2	21:L:101:TGL:HC52	1.99	0.77
14:2:70:ASN:HB3	14:2:73:LYS:HB3	1.67	0.76
6:F:94:HIS:HD2	6:F:97:ALA:H	1.33	0.76
1:A:28:MET:CE	18:A:604[B]:HEA:H271	2.15	0.76
14:2:21:GLU:OE2	14:2:24:GLY:HA3	1.86	0.76
14:2:19:THR:HG23	14:2:27:LYS:HD2	1.67	0.76
4:Q:21:ASP:CG	32:Q:301:HOH:O	2.23	0.75
7:G:38:HIS:NE2	26:G:101:CDL:H122	2.01	0.75
9:I:31:PHE:CE1	9:I:32:ALA:O	2.38	0.75
9:V:10:ARG:HD3	28:V:101:PSC:H063	1.67	0.75
2:B:58:ALA:O	2:B:62:GLU:HG3	1.87	0.75
14:1:81:ILE:CG2	32:1:346:HOH:O	2.34	0.74
6:F:94:HIS:O	32:F:201:HOH:O	2.06	0.74
4:D:78:TRP:HB3	21:D:201:TGL:HB22	1.69	0.74
4:D:100:LYS:NZ	32:D:301:HOH:O	2.21	0.73
28:E:201:PSC:C34	28:E:201:PSC:H12	2.14	0.73
1:N:28:MET:HE1	18:N:605[B]:HEA:C27	2.18	0.73
2:O:116:LEU:HD11	2:O:226:MET:HG2	1.69	0.73
2:O:56:MET:HB3	28:V:101:PSC:H211	1.70	0.73
9:I:2:THR:N	32:I:201:HOH:O	1.94	0.73
14:1:17:CYS:SG	31:1:201:HEC:C3C	2.75	0.73
26:P:306:CDL:OB9	26:P:306:CDL:H521	1.87	0.73
2:O:226:MET:HA	2:O:226:MET:HE2	1.70	0.73
2:B:19:GLU:OE2	2:B:82:ARG:NH1	2.22	0.72
8:H:43:MET:CE	8:H:49:ASP:H	2.02	0.72
9:I:31:PHE:CD2	9:I:32:ALA:N	2.57	0.72
4:D:6:VAL:HG21	4:D:31:LYS:HZ2	1.51	0.72
28:E:201:PSC:H011	28:E:201:PSC:H221	1.71	0.72
14:2:71:PRO:HD2	14:2:83:ALA:O	1.89	0.72
1:A:28:MET:CE	18:A:604[B]:HEA:C27	2.68	0.72
2:O:226:MET:HA	2:O:226:MET:HE3	1.71	0.72
2:O:57:ASP:H	28:V:101:PSC:H202	1.55	0.71
8:H:84:LYS:HZ2	8:H:85:ILE:H	1.36	0.71
4:Q:87:PHE:HB2	32:X:113:HOH:O	1.90	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:194:LEU:HD22	1:N:285:PHE:HE2	1.53	0.71
8:H:8:ILE:C	8:H:9:LYS:HD3	2.11	0.71
28:E:201:PSC:H343	28:E:201:PSC:C12	2.18	0.71
9:I:29:LEU:C	9:I:32:ALA:H	1.94	0.71
20:A:608:PGV:H183	25:C:303:PEK:H322	1.72	0.70
26:G:101:CDL:H271	27:N:601:UNL:C17	2.21	0.70
14:1:17:CYS:SG	31:1:201:HEC:CBC	2.76	0.70
28:V:101:PSC:H343	28:V:101:PSC:C12	2.13	0.70
2:B:66:THR:HG22	2:B:67:ILE:HD13	1.72	0.70
14:2:16:GLN:H	14:2:16:GLN:HE21	1.38	0.70
8:H:7:LYS:C	32:H:101:HOH:O	2.26	0.69
4:Q:19[B]:ARG:HD3	4:Q:21:ASP:OD1	1.92	0.69
3:P:37:PHE:HE1	10:W:58:LYS:HG3	1.57	0.69
14:2:32:LEU:HD22	14:2:35:LEU:HD22	1.74	0.69
4:Q:28:ALA:O	4:Q:31:LYS:HD2	1.93	0.69
9:I:31:PHE:O	9:I:34:PHE:N	2.18	0.69
9:V:31:PHE:C	9:V:31:PHE:CD1	2.66	0.69
21:D:201:TGL:H122	21:D:201:TGL:HB81	1.75	0.68
7:T:34:ASN:O	7:T:38:HIS:HB3	1.92	0.68
20:A:608:PGV:H343	25:C:303:PEK:C38	2.23	0.68
1:A:282:PHE:CA	7:T:4:ALA:HB3	2.19	0.68
2:B:57:ASP:H	28:E:201:PSC:H211	1.58	0.68
1:A:239:GLY:CA	32:A:900:HOH:O	2.42	0.68
6:S:60:CYS:HG	29:S:101:ZN:ZN	1.05	0.68
12:L:14:SER:H	21:L:101:TGL:HC31	1.60	0.67
1:N:28:MET:HE1	18:N:605[B]:HEA:H271	1.75	0.67
2:O:116:LEU:HD11	2:O:226:MET:CG	2.24	0.67
1:A:304:TYR:HD1	26:T:101:CDL:HB32	1.59	0.67
1:A:337:ALA:HB2	1:A:394:VAL:HG23	1.76	0.67
26:T:101:CDL:H271	27:T:102:UNL:C17	2.24	0.67
6:F:64:GLU:O	6:F:65:ASP:HB2	1.95	0.67
28:V:101:PSC:H072	32:V:201:HOH:O	1.94	0.67
12:Y:26:THR:HG23	13:Z:25:SER:HB3	1.77	0.67
7:T:38:HIS:O	7:T:38:HIS:CD2	2.48	0.67
21:B:301:TGL:H342	21:B:301:TGL:H211	1.76	0.66
8:H:84:LYS:HA	8:H:84:LYS:NZ	2.09	0.66
1:N:28:MET:CE	18:N:605[B]:HEA:H271	2.25	0.66
26:C:306:CDL:OB9	26:C:306:CDL:H522	1.96	0.66
9:I:30:GLY:C	9:I:32:ALA:N	2.38	0.66
9:V:73:LYS:NZ	9:V:73:LYS:HB3	2.08	0.66
2:B:145:PRO:HG2	2:B:148:MET:HE2	1.77	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:514:LYS:HA	6:S:38:ALA:HB3	1.77	0.66
4:Q:34:SER:H	4:Q:37:GLN:NE2	1.94	0.66
26:T:101:CDL:H382	26:T:101:CDL:H152	1.78	0.66
14:1:86:LYS:HA	14:1:86:LYS:HE3	1.77	0.66
2:B:64:ILE:HG22	32:B:554:HOH:O	1.95	0.66
1:A:28:MET:HE2	18:A:604[B]:HEA:C27	2.24	0.66
1:N:145:LEU:HD11	27:P:310:UNL:C6	2.26	0.66
1:A:172:LYS:HZ1	7:T:9:GLY:HA3	1.60	0.65
32:A:927:HOH:O	26:T:101:CDL:H401	1.76	0.65
28:V:101:PSC:C28	28:V:101:PSC:H322	2.27	0.65
4:Q:4:SER:N	4:Q:31:LYS:H	1.95	0.65
7:G:45:PRO:O	7:G:46:ALA:CB	2.44	0.65
12:L:25:MET:HG2	21:L:101:TGL:HA62	1.78	0.65
14:1:19:THR:HG23	14:1:27:LYS:HD2	1.79	0.64
14:2:26:HIS:CD2	14:2:26:HIS:H	2.15	0.64
1:A:28:MET:HE2	18:A:604[B]:HEA:H273	1.79	0.64
6:F:94:HIS:O	6:F:95:GLN:HB3	1.94	0.64
7:T:7:ASP:O	7:T:8:HIS:HB2	1.97	0.64
28:V:101:PSC:H012	28:V:101:PSC:P	2.37	0.64
1:A:239:GLY:HA3	32:A:900:HOH:O	1.98	0.64
9:I:33:THR:HG22	9:I:37:PHE:CB	2.27	0.64
8:U:9:LYS:O	8:U:10:ASN:HB2	1.97	0.64
31:2:201:HEC:HBC1	32:2:317:HOH:O	1.97	0.64
4:D:109:HIS:HD2	32:D:355:HOH:O	1.80	0.64
11:X:54:ARG:NH2	11:X:54:ARG:HG3	2.06	0.64
21:D:201:TGL:HA91	21:D:201:TGL:C23	2.17	0.63
9:I:73:LYS:N	9:I:73:LYS:HD3	2.12	0.63
3:P:80[B]:ARG:HH22	27:P:308:UNL:C1	2.10	0.63
31:2:201:HEC:CBC	32:2:317:HOH:O	2.46	0.63
3:C:220:PHE:HB2	26:C:306:CDL:H711	1.81	0.63
7:T:17:ARG:HD3	32:T:205:HOH:O	1.98	0.63
20:C:305:PGV:C06	8:H:22:ASN:HD22	2.12	0.63
5:R:44:GLU:OE1	32:R:201:HOH:O	2.15	0.63
1:N:28:MET:CE	18:N:605[B]:HEA:C27	2.77	0.63
21:N:608:TGL:H221	21:N:608:TGL:HA72	1.79	0.63
6:S:94:HIS:O	6:S:95:GLN:HB2	1.99	0.63
1:A:339:MET:HE2	32:D:392:HOH:O	1.99	0.63
2:B:57:ASP:H	28:E:201:PSC:C21	2.11	0.62
3:C:51[A]:MET:SD	26:C:306:CDL:H612	2.38	0.62
2:B:68:LEU:HD23	28:E:201:PSC:H171	1.80	0.62
14:2:30:PRO:HD3	14:2:46:PHE:CE2	2.33	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:L:101:TGL:HA92	21:L:101:TGL:C23	2.29	0.62
32:A:892:HOH:O	12:L:2:HIS:HE1	1.81	0.62
1:A:278[B]:MET:HE1	7:T:6:GLY:H	1.65	0.62
6:S:60:CYS:SG	29:S:101:ZN:ZN	1.88	0.62
14:1:7:LYS:HG3	14:1:97:TYR:CE1	2.35	0.62
14:2:16:GLN:H	14:2:16:GLN:NE2	1.96	0.62
4:Q:43:LYS:HE3	4:Q:55:GLU:OE1	1.98	0.62
4:Q:9:GLU:OE1	4:Q:9:GLU:HA	2.00	0.62
28:V:101:PSC:H281	28:V:101:PSC:H322	1.82	0.62
32:B:554:HOH:O	28:E:201:PSC:H151	2.00	0.62
26:G:101:CDL:C27	27:N:601:UNL:C17	2.76	0.62
9:I:30:GLY:O	9:I:32:ALA:N	2.32	0.62
8:H:84:LYS:NZ	8:H:85:ILE:H	1.97	0.61
2:O:57:ASP:N	28:V:101:PSC:H202	2.15	0.61
26:G:101:CDL:OB2	26:G:101:CDL:H142	1.99	0.61
2:O:116:LEU:CD1	2:O:226:MET:CG	2.79	0.61
2:O:198:GLU:OE2	32:O:401:HOH:O	2.16	0.61
14:2:22:LYS:HA	14:2:33:HIS:HB2	1.82	0.61
4:Q:34:SER:H	4:Q:37:GLN:HE21	1.46	0.61
26:T:101:CDL:OA7	26:T:101:CDL:H322	1.99	0.61
7:T:37:LEU:O	7:T:38:HIS:CB	2.49	0.61
1:A:310:MET:CE	2:B:77:ALA:HB2	2.31	0.61
10:W:33:ARG:HG2	24:W:101:CHD:C15	2.25	0.61
2:B:86:MET:O	2:B:89:GLU:HG2	2.00	0.61
2:O:196:CYS:HB2	2:O:207:MET:HG3	1.83	0.61
7:G:38:HIS:NE2	26:G:101:CDL:H362	2.16	0.60
20:N:612:PGV:H61	3:P:54:MET:HG2	1.83	0.60
14:2:5:LYS:HD3	14:2:93:ASP:OD2	2.02	0.60
7:G:84:LYS:N	32:G:203:HOH:O	2.19	0.60
3:C:3:HIS:HA	32:C:410:HOH:O	2.01	0.60
10:J:7:GLU:HG3	32:J:220:HOH:O	2.01	0.60
1:N:486:ASP:OD2	4:Q:19[A]:ARG:NE	2.34	0.60
26:T:101:CDL:H311	26:T:101:CDL:CA5	2.31	0.60
26:P:306:CDL:H222	26:P:306:CDL:H262	1.84	0.60
7:G:7:ASP:O	7:G:8:HIS:HB2	2.02	0.60
1:N:265:LYS:HB2	1:N:490:THR:HG21	1.83	0.59
20:P:304:PGV:C15	20:P:304:PGV:H11	2.27	0.59
26:G:101:CDL:H201	26:G:101:CDL:HB32	1.84	0.59
21:Q:201:TGL:HG2	21:Q:201:TGL:HB32	1.83	0.59
2:O:116:LEU:CD1	2:O:226:MET:HG2	2.33	0.59
7:G:17:ARG:HD3	32:G:208:HOH:O	2.01	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:9:LYS:HB3	32:H:102:HOH:O	2.03	0.59
7:G:9:GLY:HA3	1:N:172:LYS:HZ1	1.68	0.59
3:C:224:LYS:HE3	26:C:306:CDL:HB32	1.85	0.59
26:G:101:CDL:H371	2:O:81:LEU:HD12	1.85	0.59
3:C:210:ILE:HG12	20:C:304:PGV:H132	1.85	0.58
12:Y:26:THR:HG23	13:Z:25:SER:CB	2.33	0.58
1:A:282:PHE:HZ	26:T:101:CDL:H752	1.68	0.58
1:A:278[B]:MET:CE	7:T:5:LYS:HB3	2.33	0.58
21:L:101:TGL:HA92	21:L:101:TGL:H231	1.85	0.58
32:P:493:HOH:O	6:S:1:ALA:CB	2.35	0.58
6:F:96:LEU:C	6:F:98:HIS:H	2.07	0.58
26:T:101:CDL:OB4	26:T:101:CDL:H1	2.03	0.58
7:G:5:LYS:HA	1:N:278[B]:MET:CE	2.34	0.58
20:C:305:PGV:H061	8:H:22:ASN:ND2	2.18	0.57
9:I:31:PHE:HE1	9:I:35:TYR:CB	2.17	0.57
1:A:112:LEU:HD23	1:A:112:LEU:C	2.24	0.57
21:D:201:TGL:OB1	21:D:201:TGL:HG32	2.04	0.57
2:B:56:MET:HA	28:E:201:PSC:H212	1.87	0.57
9:I:28:SER:O	9:I:31:PHE:HD2	1.88	0.57
1:A:304:TYR:CD1	26:T:101:CDL:HB32	2.40	0.57
1:N:32:ALA:HB3	12:Y:36:PRO:HG2	1.86	0.57
25:C:303:PEK:H161	25:C:303:PEK:C11	2.28	0.57
20:C:304:PGV:H12	26:C:306:CDL:H622	1.86	0.57
1:A:278[B]:MET:SD	7:T:5:LYS:HB3	2.45	0.57
11:X:24:PHE:O	11:X:28:VAL:HG12	2.05	0.57
6:F:85:CYS:SG	6:F:87:THR:CG2	2.87	0.56
32:A:858:HOH:O	6:F:96:LEU:CD1	2.53	0.56
21:Q:201:TGL:HC21	21:Q:201:TGL:HG11	1.88	0.56
1:A:177:SER:H	1:A:180:GLN:NE2	2.04	0.56
4:Q:27:VAL:HG21	4:Q:31:LYS:HE2	1.87	0.56
1:A:265:LYS:HB2	1:A:490:THR:HG21	1.87	0.56
1:A:28:MET:HE1	18:A:604[B]:HEA:H271	1.86	0.56
8:H:43:MET:HE2	8:H:49:ASP:H	1.70	0.56
8:H:9:LYS:CD	8:H:9:LYS:N	2.41	0.56
1:A:514:LYS:HE2	32:F:237:HOH:O	2.06	0.56
7:T:3:ALA:O	7:T:4:ALA:HB2	2.06	0.56
24:C:307:CHD:O7	24:C:307:CHD:H41	2.06	0.55
14:1:48:TYR:HB2	14:1:53:LYS:HG3	1.87	0.55
2:B:196:CYS:HB2	2:B:207:MET:HG3	1.89	0.55
1:A:406:ASN:HD21	20:A:607:PGV:H31	1.71	0.55
21:Q:201:TGL:CC2	21:Q:201:TGL:HG11	2.36	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:LYS:HA	6:F:38:ALA:CB	2.35	0.55
2:B:84:LEU:HA	2:B:87:MET:HE2	1.87	0.55
4:D:121:LYS:HE2	11:K:52:GLU:OE2	2.07	0.55
26:G:101:CDL:H111	26:G:101:CDL:CA2	2.32	0.55
1:N:194:LEU:HD22	1:N:285:PHE:CE2	2.39	0.55
6:S:64:GLU:O	6:S:65:ASP:CB	2.48	0.55
4:Q:109:HIS:HD2	32:Q:371:HOH:O	1.89	0.55
21:D:201:TGL:CA3	32:D:392:HOH:O	2.54	0.55
6:F:94:HIS:CD2	6:F:97:ALA:H	2.19	0.55
9:I:33:THR:HA	9:I:36:LYS:HB3	1.89	0.55
24:P:301:CHD:H212	24:P:301:CHD:H12	1.88	0.55
21:D:201:TGL:HA31	32:D:392:HOH:O	2.06	0.54
28:E:201:PSC:H072	32:I:221:HOH:O	2.07	0.54
3:P:47:LEU:O	3:P:51[B]:MET:HG3	2.07	0.54
31:2:201:HEC:HBC2	31:2:201:HEC:HHD	1.88	0.54
26:G:101:CDL:O1	32:G:202:HOH:O	2.18	0.54
6:S:60:CYS:SG	6:S:85:CYS:SG	3.05	0.54
14:1:19:THR:CG2	14:1:27:LYS:HD2	2.37	0.54
1:A:365:ILE:HD11	32:A:899:HOH:O	2.06	0.54
9:I:30:GLY:C	9:I:32:ALA:H	2.09	0.54
6:S:53:THR:CG2	32:S:292:HOH:O	2.55	0.54
32:A:858:HOH:O	6:F:96:LEU:HD11	2.07	0.54
6:F:94:HIS:CG	6:F:95:GLN:N	2.75	0.54
9:V:17:LEU:CD2	28:V:101:PSC:H271	2.38	0.54
2:O:104:TRP:CG	2:O:203:ASN:HB2	2.43	0.54
8:U:9:LYS:O	8:U:10:ASN:CB	2.55	0.54
32:A:911:HOH:O	26:T:101:CDL:H131	2.07	0.54
2:B:57:ASP:H	28:E:201:PSC:C20	2.21	0.54
9:V:31:PHE:CD1	9:V:31:PHE:O	2.60	0.54
11:X:54:ARG:NH2	11:X:54:ARG:CG	2.64	0.54
4:Q:9:GLU:HB3	32:S:275:HOH:O	2.07	0.53
1:A:177:SER:H	1:A:180:GLN:HE21	1.56	0.53
1:A:312[A]:ILE:HD12	32:A:763:HOH:O	2.07	0.53
1:N:379:TYR:O	1:N:383[A]:MET:HB2	2.08	0.53
2:O:59:GLN:O	2:O:60:GLU:HG3	2.09	0.53
14:1:49:THR:HG23	14:1:79:LYS:HD3	1.90	0.53
23:E:202:EDO:H22	32:E:391:HOH:O	2.08	0.53
8:H:49:ASP:O	8:H:50:VAL:HB	2.09	0.53
21:Q:201:TGL:H352	9:V:16:ARG:HE	1.73	0.53
9:V:17:LEU:HD21	28:V:101:PSC:H271	1.90	0.53
1:N:449:MET:SD	2:O:5:MET:HG2	2.49	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:28:ALA:O	4:Q:31:LYS:CD	2.56	0.53
32:N:737:HOH:O	21:Q:201:TGL:HG2	2.08	0.53
28:V:101:PSC:H291	28:V:101:PSC:C33	2.32	0.53
2:B:57:ASP:N	28:E:201:PSC:H211	2.24	0.52
8:H:7:LYS:CA	8:H:7:LYS:HE3	2.39	0.52
2:B:33:LEU:HD11	9:I:29:LEU:HD13	1.91	0.52
26:T:101:CDL:H132	26:T:101:CDL:H342	1.91	0.52
1:A:513:LEU:O	1:A:514:LYS:CB	2.55	0.52
1:N:365:ILE:HD11	32:N:863:HOH:O	2.08	0.52
6:S:85:CYS:SG	6:S:87:THR:CG2	2.94	0.52
8:U:9:LYS:O	8:U:10:ASN:ND2	2.40	0.52
14:1:16:GLN:CB	32:1:338:HOH:O	2.58	0.52
8:H:43:MET:HE3	8:H:49:ASP:H	1.75	0.52
9:I:31:PHE:HE1	9:I:35:TYR:H	1.57	0.52
21:L:101:TGL:CA9	21:L:101:TGL:H231	2.39	0.52
4:D:107:ILE:HD13	11:K:39:GLU:HB2	1.92	0.52
7:T:31:CYS:SG	26:T:101:CDL:H551	2.49	0.52
11:X:54:ARG:HH21	11:X:54:ARG:CB	2.23	0.52
7:G:31:CYS:SG	26:G:101:CDL:H512	2.50	0.52
8:H:8:ILE:C	8:H:9:LYS:O	2.46	0.52
14:1:52:ASN:C	14:1:52:ASN:HD22	2.14	0.52
14:2:68:LEU:HD21	31:2:201:HEC:HMB2	1.92	0.52
2:O:13:THR:OG1	2:O:167:SER:HB2	2.09	0.52
7:T:7:ASP:CG	7:T:8:HIS:N	2.63	0.52
5:E:78:HIS:HD2	32:E:364:HOH:O	1.91	0.51
21:L:101:TGL:C36	21:L:101:TGL:C31	2.88	0.51
14:2:62:GLU:HG2	14:2:63:THR:HG23	1.92	0.51
3:C:161[B]:GLN:HG2	24:C:307:CHD:O7	2.10	0.51
1:N:431:LEU:HD21	1:N:450:TRP:HB2	1.92	0.51
3:P:5:THR:HG21	6:S:96:LEU:HD13	1.92	0.51
3:C:156:ARG:HE	24:C:307:CHD:C24	2.23	0.51
26:C:306:CDL:H262	26:C:306:CDL:H381	1.91	0.51
27:P:310:UNL:C4	27:P:310:UNL:C6	2.89	0.51
3:P:5:THR:CG2	6:S:96:LEU:HD13	2.41	0.51
8:U:7:LYS:HE3	8:U:10:ASN:HD21	1.74	0.51
14:2:36:PHE:CE2	14:2:61:GLU:HG3	2.46	0.51
10:J:2:GLU:HG2	32:J:209:HOH:O	2.11	0.51
1:N:24:ALA:HA	18:N:605[A]:HEA:H22	1.93	0.51
26:P:306:CDL:H201	26:P:306:CDL:H162	1.93	0.51
9:I:29:LEU:O	9:I:32:ALA:HA	2.05	0.51
6:S:82:CYS:C	6:S:84:SER:N	2.63	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLY:HA2	21:D:201:TGL:H201	1.93	0.51
8:H:10:ASN:N	32:H:102:HOH:O	1.98	0.51
32:A:950:HOH:O	14:1:81:ILE:HG21	2.10	0.51
14:2:30:PRO:HD3	14:2:46:PHE:CZ	2.46	0.51
1:A:310:MET:HE1	2:B:77:ALA:HB2	1.93	0.50
9:I:1:SAC:H2A1	9:I:1:SAC:CB	2.40	0.50
8:H:7:LYS:HA	8:H:7:LYS:HE3	1.93	0.50
26:G:101:CDL:H372	2:O:78:LEU:HD12	1.94	0.50
4:D:107:ILE:HD11	4:D:111:PHE:CB	2.42	0.50
24:J:101:CHD:H21	24:J:101:CHD:H61	1.94	0.50
4:D:118:LYS:HB3	11:K:53:TRP:HB3	1.94	0.50
9:V:61:GLU:OE1	9:V:64:ARG:NH2	2.45	0.50
20:C:305:PGV:H061	8:H:22:ASN:HD22	1.76	0.50
1:N:309:THR:HG22	18:N:606:HEA:HMB2	1.92	0.50
26:T:101:CDL:H791	26:T:101:CDL:H832	1.93	0.50
26:C:306:CDL:HB21	10:J:8:LYS:HD2	1.92	0.50
14:2:3:VAL:O	14:2:97:TYR:HB2	2.11	0.50
14:2:42:GLN:O	14:2:44:PRO:HD3	2.11	0.50
14:2:9:ILE:O	14:2:13:LYS:HG2	2.11	0.50
1:N:514:LYS:HA	6:S:38:ALA:CB	2.41	0.50
2:O:137:GLU:OE1	4:Q:122:ARG:NH1	2.37	0.50
20:C:305:PGV:H11	3:P:258:TRP:HH2	1.76	0.50
3:P:59:ARG:HG3	26:P:306:CDL:HA22	1.92	0.50
9:I:33:THR:O	9:I:34:PHE:C	2.49	0.50
2:O:68:LEU:HB3	2:O:69:PRO:HD3	1.94	0.50
2:O:56:MET:CB	28:V:101:PSC:H211	2.41	0.50
12:Y:46:LYS:O	12:Y:47:LYS:HB2	2.11	0.50
14:1:72:LYS:HD2	32:1:334:HOH:O	2.12	0.50
1:A:49:GLY:HA3	32:A:908:HOH:O	2.10	0.50
14:2:3:VAL:HG11	14:2:100:LYS:HD2	1.94	0.49
20:C:304:PGV:H172	26:C:306:CDL:H631	1.93	0.49
21:L:101:TGL:H362	21:L:101:TGL:C31	2.42	0.49
6:F:46:PRO:O	6:F:48:LEU:HD22	2.12	0.49
2:O:58:ALA:O	2:O:62:GLU:CG	2.53	0.49
26:C:306:CDL:OB9	26:C:306:CDL:HB4	2.11	0.49
8:H:46:LYS:HA	8:H:46:LYS:HE2	1.94	0.49
2:B:70:ALA:HB1	26:T:101:CDL:H441	1.95	0.49
2:O:116:LEU:CD1	2:O:226:MET:HG3	2.42	0.49
10:W:36:MET:HB3	24:W:101:CHD:C18	2.42	0.49
3:C:146:TRP:CZ2	7:G:17:ARG:HG3	2.48	0.49
6:F:52:ILE:HA	6:F:94:HIS:HB3	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:2:13:LYS:HE3	32:2:311:HOH:O	2.13	0.49
4:D:34:SER:H	4:D:37:GLN:NE2	2.11	0.49
14:1:16:GLN:HB3	32:1:338:HOH:O	2.12	0.49
1:A:333:LYS:HE2	32:M:212:HOH:O	2.11	0.49
8:H:9:LYS:N	32:H:101:HOH:O	2.18	0.48
9:V:33:THR:O	9:V:36:LYS:N	2.46	0.48
14:1:47:THR:HB	32:1:332:HOH:O	2.12	0.48
1:A:24:ALA:HB2	18:A:604[B]:HEA:H253	1.95	0.48
28:E:201:PSC:H21	28:E:201:PSC:H222	1.95	0.48
9:I:31:PHE:CE2	9:I:32:ALA:O	2.64	0.48
14:2:72:LYS:NZ	14:2:83:ALA:HA	2.29	0.48
21:B:301:TGL:H301	21:B:301:TGL:HA72	1.96	0.48
2:B:86:MET:HB3	32:B:536:HOH:O	2.14	0.48
26:G:101:CDL:H172	26:G:101:CDL:H402	1.95	0.48
1:N:240:HIS:C	1:N:240:HIS:CD2	2.86	0.48
10:W:36:MET:HG2	24:W:101:CHD:H183	1.94	0.48
7:T:31:CYS:SG	26:T:101:CDL:H532	2.54	0.48
4:D:63:LYS:HG2	4:D:64:PHE:CE2	2.49	0.48
9:I:33:THR:O	9:I:36:LYS:N	2.47	0.48
1:N:485:VAL:HG22	13:Z:1:ILE:HG13	1.95	0.48
14:2:32:LEU:O	14:2:102:THR:HB	2.13	0.47
1:A:309:THR:HG22	18:A:605:HEA:HMB2	1.96	0.47
7:G:11:TPO:HG22	32:G:210:HOH:O	2.13	0.47
3:P:246:ASP:HB2	32:P:485:HOH:O	2.13	0.47
12:Y:47:LYS:HD2	12:Y:47:LYS:OXT	2.14	0.47
9:I:61:GLU:OE1	9:I:64:ARG:NE	2.40	0.47
21:L:101:TGL:H363	21:L:101:TGL:H312	1.92	0.47
3:P:107:ALA:HB2	20:P:305:PGV:H031	1.96	0.47
2:B:129[A]:LYS:NZ	2:B:132:GLU:OE1	2.43	0.47
8:H:9:LYS:HG3	8:H:11:TYR:H	1.80	0.47
6:S:53:THR:HG22	32:S:292:HOH:O	2.14	0.47
7:G:37:LEU:HD23	26:G:101:CDL:H381	1.96	0.47
8:H:7:LYS:C	8:H:8:ILE:HG22	2.34	0.47
3:P:37:PHE:CE2	27:P:310:UNL:C1	2.98	0.47
28:V:101:PSC:O02	28:V:101:PSC:H011	2.15	0.47
7:G:10:GLY:N	32:G:205:HOH:O	2.47	0.47
9:I:33:THR:HA	9:I:36:LYS:HE3	1.95	0.47
1:N:437:PRO:HG2	1:N:440:TYR:CZ	2.49	0.47
2:O:41:ILE:O	2:O:45:MET:HG2	2.15	0.47
4:Q:78:TRP:N	21:Q:201:TGL:HB22	2.30	0.47
7:T:3:ALA:O	32:T:201:HOH:O	2.20	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Q:201:TGL:H362	9:V:20:HIS:CE1	2.49	0.47
26:C:306:CDL:HB21	10:J:8:LYS:CD	2.45	0.47
14:1:3:VAL:HG13	14:1:97:TYR:HA	1.97	0.47
14:2:16:GLN:N	14:2:16:GLN:NE2	2.63	0.47
14:2:49:THR:O	14:2:53:LYS:HB2	2.14	0.47
20:P:304:PGV:C11	20:P:304:PGV:C15	2.92	0.47
7:T:44:ARG:HD2	7:T:82:TYR:CE1	2.50	0.47
8:H:52:VAL:HG11	8:U:48:GLY:HA3	1.97	0.46
1:N:468:MET:HE3	18:N:605[B]:HEA:H22	1.96	0.46
4:Q:19[B]:ARG:CD	4:Q:21:ASP:OD1	2.61	0.46
9:V:63:MET:HB3	9:V:68:ILE:HD11	1.98	0.46
14:1:3:VAL:HG21	14:1:100:LYS:HE2	1.97	0.46
21:D:201:TGL:HA32	32:D:392:HOH:O	2.16	0.46
8:H:43:MET:HE3	8:H:49:ASP:N	2.31	0.46
2:O:33:LEU:HD12	9:V:28:SER:HB3	1.96	0.46
20:P:304:PGV:C11	20:P:304:PGV:H151	2.37	0.46
3:C:110:PRO:HB3	8:H:30:TRP:CE3	2.50	0.46
3:C:76:GLN:NE2	3:C:80[A]:ARG:HH21	2.13	0.46
3:C:131:LEU:HD11	26:G:101:CDL:H552	1.96	0.46
3:C:133:ASN:HB3	3:C:173:PHE:CE2	2.50	0.46
26:G:101:CDL:H212	1:N:311:ILE:CD1	2.44	0.46
14:2:11:VAL:HA	14:2:15:ALA:HB2	1.96	0.46
20:C:305:PGV:H321	7:T:1:ALA:HB2	1.96	0.46
3:P:16:TRP:N	3:P:17:PRO:CD	2.78	0.46
4:Q:6:VAL:HG12	4:Q:7:LYS:H	1.79	0.46
6:S:51:SER:O	6:S:94:HIS:N	2.49	0.46
21:D:201:TGL:CG3	21:D:201:TGL:OB1	2.64	0.46
28:E:201:PSC:H011	28:E:201:PSC:C22	2.44	0.46
1:A:87:ILE:O	1:A:173:PRO:HD3	2.16	0.46
26:C:306:CDL:O1	26:C:306:CDL:OA3	2.34	0.46
1:N:28:MET:CE	18:N:605[B]:HEA:H273	2.46	0.46
32:A:911:HOH:O	26:T:101:CDL:H151	2.15	0.46
1:A:310:MET:HB3	2:B:73:LEU:HD22	1.97	0.46
12:L:46:LYS:O	12:L:47:LYS:HB2	2.15	0.46
2:B:13:THR:HG21	2:B:192:TYR:CZ	2.51	0.45
7:G:44:ARG:HA	7:G:45:PRO:HD3	1.87	0.45
2:B:145:PRO:HG2	2:B:148:MET:CE	2.43	0.45
21:B:301:TGL:H101	21:B:301:TGL:HA62	1.98	0.45
20:P:305:PGV:H041	32:U:103:HOH:O	2.15	0.45
5:E:90:ARG:HD3	32:E:370:HOH:O	2.16	0.45
9:I:31:PHE:HE1	9:I:35:TYR:HB3	1.81	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:20:ARG:HH22	21:L:101:TGL:HC72	1.82	0.45
11:X:44:PRO:HG3	32:X:115:HOH:O	2.15	0.45
1:A:399:LEU:O	1:A:499:PRO:HA	2.16	0.45
1:A:217:THR:HG22	3:C:188:ILE:HG12	1.99	0.45
5:E:46:LYS:HG2	32:E:333:HOH:O	2.16	0.45
21:L:101:TGL:H362	21:L:101:TGL:H312	1.93	0.45
21:D:201:TGL:H362	9:I:20:HIS:CE1	2.51	0.45
1:N:368:HIS:CD2	1:N:369:ASP:HB2	2.51	0.45
1:N:390:MET:HE1	1:N:468:MET:SD	2.57	0.45
28:V:101:PSC:C34	28:V:101:PSC:H12	2.16	0.45
1:A:378:HIS:CG	1:A:425:PHE:CE1	3.05	0.45
1:A:43:GLN:HB2	1:A:44:PRO:HD2	1.98	0.45
20:A:607:PGV:C2	32:A:701:HOH:O	2.35	0.45
2:B:129[A]:LYS:NZ	32:B:407:HOH:O	2.49	0.45
24:C:301:CHD:O7	20:C:305:PGV:H42	2.17	0.45
6:F:53:THR:OG1	6:F:54:ASN:N	2.43	0.45
8:H:43:MET:CE	8:H:49:ASP:N	2.77	0.45
1:N:250:GLY:O	1:N:254:ILE:HG12	2.17	0.45
2:O:116:LEU:HD11	2:O:226:MET:HG3	1.98	0.45
3:P:146:TRP:CD2	3:P:162:ALA:HB2	2.51	0.45
1:A:311:ILE:CD1	26:T:101:CDL:H201	2.47	0.45
1:A:310:MET:HE3	2:B:77:ALA:HB2	1.98	0.45
9:V:33:THR:HA	9:V:37:PHE:HD2	1.82	0.45
5:E:6:GLU:O	28:E:201:PSC:H081	2.17	0.45
7:G:45:PRO:O	7:G:46:ALA:HB3	2.17	0.45
12:Y:35:ALA:HB3	12:Y:36:PRO:HD3	1.99	0.45
14:1:40:THR:HG22	14:1:59:TRP:CE2	2.52	0.45
6:S:44:GLU:CD	6:S:44:GLU:H	2.19	0.45
7:T:37:LEU:O	7:T:38:HIS:HB2	2.16	0.44
14:1:16:GLN:HB2	32:1:338:HOH:O	2.17	0.44
20:C:305:PGV:H032	32:C:502:HOH:O	2.17	0.44
14:1:25:LYS:HZ3	14:1:26:HIS:H	1.64	0.44
14:2:11:VAL:O	14:2:15:ALA:HB3	2.18	0.44
1:N:321:PHE:CE2	28:V:101:PSC:H162	2.53	0.44
28:E:201:PSC:H041	32:I:221:HOH:O	2.18	0.44
6:S:53:THR:HG23	32:S:292:HOH:O	2.17	0.44
2:B:58:ALA:O	2:B:62:GLU:CG	2.61	0.44
21:L:101:TGL:HC81	21:L:101:TGL:HC22	2.00	0.44
2:O:144:LEU:HD22	2:O:150:ILE:HD13	1.99	0.44
1:A:278[B]:MET:HE1	7:T:5:LYS:HB3	2.00	0.44
2:O:129:LYS:HE2	32:O:516:HOH:O	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:P:306:CDL:H471	26:P:306:CDL:H441	1.80	0.44
3:P:47:LEU:O	3:P:51[A]:MET:HG2	2.18	0.44
21:Q:201:TGL:H231	21:Q:201:TGL:HA91	1.99	0.44
5:R:12:ASP:OD2	5:R:44:GLU:HG3	2.18	0.44
1:A:281:GLY:O	7:T:4:ALA:HB1	2.18	0.44
2:O:4:PRO:HG2	32:X:115:HOH:O	2.17	0.44
2:O:146:MET:HA	2:O:213:LEU:HD12	2.00	0.43
3:P:62:ILE:CD1	26:P:306:CDL:H522	2.48	0.43
1:A:367:LEU:HD21	1:A:433:LEU:HD23	2.01	0.43
20:A:608:PGV:H311	25:C:303:PEK:H382	2.00	0.43
3:C:54:MET:HE1	20:C:304:PGV:H141	2.01	0.43
8:H:37:HIS:HD2	32:H:127:HOH:O	2.00	0.43
1:N:309:THR:CG2	18:N:606:HEA:HMB2	2.49	0.43
3:P:37:PHE:HE1	10:W:58:LYS:CG	2.27	0.43
26:C:306:CDL:C19	26:C:306:CDL:H602	2.49	0.43
5:E:41:LEU:HA	32:I:228:HOH:O	2.17	0.43
20:C:305:PGV:C06	8:H:22:ASN:ND2	2.76	0.43
10:J:33:ARG:HG2	24:J:101:CHD:H151	1.99	0.43
4:Q:48:TRP:HB2	5:R:96:LEU:O	2.18	0.43
6:S:82:CYS:C	6:S:84:SER:H	2.21	0.43
21:N:608:TGL:CA7	21:N:608:TGL:H221	2.47	0.43
26:T:101:CDL:H241	26:T:101:CDL:H542	2.00	0.43
14:2:35:LEU:O	14:2:37:GLY:N	2.52	0.43
2:B:227:LEU:HD23	2:B:227:LEU:HA	1.75	0.43
3:C:210:ILE:HD13	20:C:304:PGV:H302	1.99	0.43
1:A:23:GLY:HA3	1:A:73:ILE:HG13	1.99	0.43
5:E:79:LYS:HD2	32:E:412:HOH:O	2.19	0.43
10:J:40:LEU:HD12	24:J:101:CHD:H183	2.01	0.43
20:P:304:PGV:H312	20:P:304:PGV:H282	1.86	0.43
4:Q:114:GLU:HG3	11:X:51:LYS:HE3	2.01	0.43
9:V:18:ARG:NH2	28:V:101:PSC:C7	2.82	0.43
1:N:136[A]:LEU:HD11	32:2:328:HOH:O	2.18	0.43
1:N:310:MET:HE2	1:N:356:ILE:HG23	1.99	0.43
2:O:150:ILE:HD12	2:O:184:LEU:HD22	2.01	0.43
14:1:100:LYS:HE3	14:1:100:LYS:HB3	1.73	0.43
2:B:102:HIS:O	2:B:104:TRP:HA	2.19	0.43
21:L:101:TGL:H232	21:L:101:TGL:H261	1.67	0.43
9:V:29:LEU:O	9:V:31:PHE:CA	2.65	0.43
4:D:34:SER:H	4:D:37:GLN:HE21	1.67	0.43
25:C:303:PEK:H041	7:G:70:PHE:HB2	2.01	0.43
1:N:302:ARG:HD2	1:N:302:ARG:HH11	1.70	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:132:GLU:HB3	2:O:137:GLU:HG3	2.00	0.43
25:P:303:PEK:H31	25:P:303:PEK:H71	2.00	0.43
9:I:2:THR:CA	32:I:201:HOH:O	2.59	0.42
5:R:90:ARG:HB3	5:R:91:PRO:HD3	2.01	0.42
14:2:26:HIS:ND1	14:2:46:PHE:HB2	2.33	0.42
14:2:58:THR:HG22	14:2:59:TRP:N	2.34	0.42
2:B:7:LEU:HD11	21:B:301:TGL:H152	2.01	0.42
2:O:92:ASN:HD22	2:O:92:ASN:N	2.18	0.42
4:Q:78:TRP:CE2	4:Q:79:LYS:HG3	2.54	0.42
3:C:151:LEU:HB2	3:C:159:MET:HG3	2.00	0.42
26:G:101:CDL:HA22	32:G:244:HOH:O	2.19	0.42
2:B:68:LEU:HB3	2:B:69:PRO:HD3	2.02	0.42
2:B:74:ILE:HG12	26:T:101:CDL:H402	2.02	0.42
6:S:96:LEU:O	6:S:97:ALA:HB3	2.19	0.42
26:T:101:CDL:H152	26:T:101:CDL:H362	2.00	0.42
14:2:38:ARG:NH2	14:2:38:ARG:HB2	2.35	0.42
26:P:306:CDL:OB6	26:P:306:CDL:HB22	2.20	0.42
4:Q:126:MET:HG3	4:Q:128:VAL:HG23	2.01	0.42
4:Q:19[A]:ARG:HG2	32:Q:385:HOH:O	2.19	0.42
4:Q:81:VAL:HG11	21:Q:201:TGL:HB62	2.02	0.42
6:S:52:ILE:CG2	6:S:96:LEU:HB2	2.50	0.42
10:W:24:GLY:N	10:W:28:ASP:OD2	2.50	0.42
1:A:106:PRO:HB2	1:A:107:PRO:HD3	2.01	0.42
6:F:94:HIS:CG	6:F:95:GLN:H	2.38	0.42
6:F:94:HIS:HD2	6:F:97:ALA:N	2.11	0.42
9:I:27:VAL:O	9:I:31:PHE:N	2.49	0.42
1:N:48:LEU:O	13:Z:41:LYS:HE2	2.20	0.42
2:O:57:ASP:O	2:O:60:GLU:OE2	2.38	0.42
8:U:9:LYS:HG3	8:U:11:TYR:H	1.84	0.42
9:V:25:PHE:O	9:V:29:LEU:HB2	2.20	0.42
14:2:16:GLN:NE2	32:2:303:HOH:O	2.51	0.42
14:2:49:THR:CG2	14:2:79:LYS:HG2	2.50	0.42
4:D:107:ILE:HD11	4:D:111:PHE:HB2	2.01	0.42
26:P:306:CDL:H612	26:P:306:CDL:H642	1.65	0.42
6:S:54:ASN:HD22	6:S:54:ASN:H	1.66	0.42
3:P:37:PHE:HD1	10:W:58:LYS:HG3	1.71	0.42
1:A:309:THR:CG2	18:A:605:HEA:HMB2	2.50	0.42
2:B:164:ALA:O	2:B:194:GLY:HA3	2.20	0.42
1:N:112:LEU:HD23	1:N:112:LEU:C	2.40	0.42
3:P:257:TYR:O	3:P:261:SER:HB3	2.20	0.42
25:P:303:PEK:H221	7:T:69:PHE:CD1	2.54	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:P:306:CDL:CB5	26:P:306:CDL:HA21	2.49	0.42
9:V:63:MET:HB3	9:V:68:ILE:CD1	2.50	0.42
2:B:2:ALA:HA	2:B:6:GLN:OE1	2.18	0.42
3:C:42:LEU:HD23	3:C:42:LEU:HA	1.79	0.42
30:M:101:DMU:H30	30:M:101:DMU:O1	2.19	0.42
1:N:242:GLU:O	1:N:246:LEU:HG	2.20	0.42
3:P:76:GLN:HE21	3:P:233:PHE:HB2	1.84	0.42
9:V:22:VAL:O	9:V:26:MET:HG2	2.20	0.42
14:1:86:LYS:CA	14:1:86:LYS:HE3	2.45	0.42
1:A:472:ILE:HG21	21:L:101:TGL:HA91	2.02	0.42
5:E:7:THR:OG1	5:E:10:GLU:HG3	2.20	0.42
11:K:50:PRO:HD2	32:K:105:HOH:O	2.19	0.42
14:2:97:TYR:CE1	14:2:101:ALA:HB2	2.55	0.41
2:B:148:MET:HB3	2:B:148:MET:HE3	1.63	0.41
2:B:91:ASN:OD1	2:B:183:THR:HG21	2.20	0.41
3:C:122:HIS:CE1	32:C:498:HOH:O	2.73	0.41
31:1:201:HEC:HBC3	31:1:201:HEC:HMC1	2.02	0.41
1:A:3:ILE:HG12	1:A:7:LEU:HD22	2.02	0.41
20:C:305:PGV:H161	32:T:241:HOH:O	2.21	0.41
2:O:129:LYS:HE3	2:O:129:LYS:HB3	1.61	0.41
3:P:105:SER:HA	3:P:116:TRP:CE3	2.56	0.41
3:P:51[B]:MET:HE1	20:P:304:PGV:H172	2.02	0.41
3:P:146:TRP:HB2	7:T:16:TRP:HB3	2.02	0.41
1:A:513:LEU:HA	1:A:513:LEU:HD23	1.87	0.41
11:K:32:MET:O	11:K:32:MET:HG2	2.19	0.41
12:L:2:HIS:HD2	12:L:3:TYR:N	2.08	0.41
2:O:49:LYS:HE3	32:O:437:HOH:O	2.20	0.41
7:T:3:ALA:O	7:T:4:ALA:CB	2.68	0.41
14:2:59:TRP:CE3	14:2:59:TRP:HA	2.56	0.41
2:B:151:ARG:HD3	2:B:181:GLN:HE21	1.84	0.41
3:C:257:TYR:O	3:C:261:SER:HB3	2.21	0.41
7:G:31:CYS:SG	26:G:101:CDL:H532	2.61	0.41
26:P:306:CDL:CA2	32:P:403:HOH:O	2.67	0.41
8:H:7:LYS:N	32:H:101:HOH:O	2.53	0.41
2:O:78:LEU:HA	2:O:78:LEU:HD12	1.84	0.41
4:Q:107:ILE:HB	4:Q:108:PRO:CD	2.51	0.41
10:W:36:MET:HB3	24:W:101:CHD:H183	2.02	0.41
1:A:48:LEU:HB2	32:A:721:HOH:O	2.20	0.41
2:B:200:CYS:SG	2:B:204:HIS:HA	2.61	0.41
9:I:29:LEU:O	9:I:30:GLY:C	2.59	0.41
10:J:36:MET:HG2	24:J:101:CHD:H162	2.02	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:383[A]:MET:O	1:N:387:PHE:HB2	2.21	0.41
3:P:65:SER:HB3	3:P:71:HIS:CE1	2.56	0.41
26:C:306:CDL:H602	26:C:306:CDL:H201	2.02	0.41
1:N:136[B]:LEU:HD11	32:N:925:HOH:O	2.21	0.41
21:L:101:TGL:H122	21:L:101:TGL:H291	1.71	0.41
1:N:236:TRP:CH2	18:N:606:HEA:HBD1	2.56	0.41
24:T:103:CHD:H12	24:T:103:CHD:H212	2.02	0.41
3:C:154:GLY:HA2	6:F:6:VAL:HB	2.02	0.41
3:C:246:ASP:HB2	32:C:477:HOH:O	2.20	0.41
30:Z:101:DMU:H15	30:Z:101:DMU:H9	1.98	0.41
14:2:16:GLN:HG3	32:2:316:HOH:O	2.21	0.41
2:O:116:LEU:HD13	2:O:226:MET:CG	2.51	0.41
1:A:127:THR:HB	1:A:129:TYR:CE1	2.56	0.41
2:B:36:SER:HB3	21:B:301:TGL:C13	2.51	0.41
14:1:69:GLU:HG3	14:1:91:ARG:CZ	2.50	0.40
14:2:104:GLU:HA	14:2:104:GLU:OE1	2.21	0.40
1:A:335:SER:HB2	1:A:336:PRO:HD2	2.03	0.40
1:A:236:TRP:CH2	18:A:605:HEA:HBD1	2.56	0.40
3:C:59:ARG:HG3	26:C:306:CDL:H512	2.03	0.40
1:A:415:ALA:HB1	21:D:201:TGL:H121	2.03	0.40
7:T:78:LEU:HB3	7:T:79:PRO:HD2	2.03	0.40
2:O:68:LEU:CD2	28:V:101:PSC:H172	2.50	0.40
4:Q:48:TRP:CH2	5:R:56:ARG:HA	2.56	0.40
14:1:68:LEU:HD23	14:1:68:LEU:HA	1.89	0.40
14:2:3:VAL:CG1	14:2:97:TYR:HA	2.45	0.40
3:C:29:SER:HB2	27:C:310:UNL:C4	2.51	0.40
7:G:10:GLY:HA3	32:G:205:HOH:O	2.21	0.40
12:L:25:MET:HG2	21:L:101:TGL:CA6	2.48	0.40
1:N:513:LEU:HA	1:N:513:LEU:HD23	1.83	0.40
3:P:80[B]:ARG:NH2	27:P:308:UNL:C1	2.81	0.40
4:Q:31:LYS:HG3	32:Q:399:HOH:O	2.21	0.40
20:A:607:PGV:H231	13:M:12:PRO:HG3	2.03	0.40
4:D:112:GLU:HB3	32:D:363:HOH:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:F:266:HOH:O	32:U:148:HOH:O[1_455]	2.11	0.09
32:F:276:HOH:O	32:U:141:HOH:O[1_455]	2.14	0.06



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	524/514 (102%)	510 (97%)	14 (3%)	0	100	100
1	N	520/514 (101%)	504 (97%)	16 (3%)	0	100	100
2	B	227/227 (100%)	217 (96%)	9 (4%)	1 (0%)	34	30
2	O	225/227 (99%)	216 (96%)	8 (4%)	1 (0%)	34	30
3	C	263/259 (102%)	259 (98%)	4 (2%)	0	100	100
3	P	262/259 (101%)	256 (98%)	5 (2%)	1 (0%)	34	30
4	D	142/144 (99%)	135 (95%)	7 (5%)	0	100	100
4	Q	143/144 (99%)	136 (95%)	5 (4%)	2 (1%)	11	5
5	E	103/105 (98%)	102 (99%)	1 (1%)	0	100	100
5	R	103/105 (98%)	102 (99%)	1 (1%)	0	100	100
6	F	96/98 (98%)	90 (94%)	4 (4%)	2 (2%)	7	2
6	S	96/98 (98%)	90 (94%)	3 (3%)	3 (3%)	4	1
7	G	81/84 (96%)	65 (80%)	10 (12%)	6 (7%)	1	0
7	T	81/84 (96%)	64 (79%)	10 (12%)	7 (9%)	1	0
8	H	77/79 (98%)	70 (91%)	4 (5%)	3 (4%)	3	1
8	U	77/79 (98%)	73 (95%)	3 (4%)	1 (1%)	12	6
9	I	71/73 (97%)	67 (94%)	1 (1%)	3 (4%)	3	1
9	V	71/73 (97%)	65 (92%)	4 (6%)	2 (3%)	5	1
10	J	56/58 (97%)	56 (100%)	0	0	100	100
10	W	56/58 (97%)	55 (98%)	0	1 (2%)	8	3
11	K	47/49 (96%)	47 (100%)	0	0	100	100
11	X	47/49 (96%)	44 (94%)	3 (6%)	0	100	100
12	L	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
12	Y	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
13	M	41/43 (95%)	38 (93%)	3 (7%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	Z	41/43 (95%)	41 (100%)	0	0	100	100
14	1	103/105 (98%)	90 (87%)	11 (11%)	2 (2%)	8	3
14	2	103/105 (98%)	81 (79%)	15 (15%)	7 (7%)	1	0
All	All	3744/3768 (99%)	3557 (95%)	145 (4%)	42 (1%)	14	8

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	2	SER
6	F	96	LEU
7	G	3	ALA
7	G	7	ASP
7	G	8	HIS
7	G	46	ALA
8	H	8	ILE
8	H	9	LYS
8	H	50	VAL
9	I	2	THR
9	I	32	ALA
3	P	38	ASN
6	S	96	LEU
7	T	4	ALA
7	T	7	ASP
7	T	8	HIS
7	T	38	HIS
8	U	10	ASN
9	V	30	GLY
10	W	56	PRO
14	2	25	LYS
14	2	36	PHE
14	2	39	LYS
2	B	60	GLU
7	G	5	LYS
2	O	60	GLU
6	S	94	HIS
7	T	3	ALA
14	1	24	GLY
7	G	38	HIS
6	S	95	GLN
7	T	37	LEU
14	2	56	GLY

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	Q	5	VAL
7	T	6	GLY
9	V	29	LEU
4	Q	6	VAL
14	1	37	GLY
14	2	1	GLY
9	I	30	GLY
14	2	23	GLY
14	2	41	GLY

### 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	437/426 (103%)	429 (98%)	8 (2%)	59	63
1	N	433/426 (102%)	425 (98%)	8 (2%)	59	63
2	B	212/210 (101%)	204 (96%)	8 (4%)	33	31
2	O	210/210 (100%)	196 (93%)	14 (7%)	16	11
3	C	230/224 (103%)	225 (98%)	5 (2%)	52	55
3	P	229/224 (102%)	225 (98%)	4 (2%)	60	65
4	D	128/128 (100%)	123 (96%)	5 (4%)	32	30
4	Q	129/128 (101%)	123 (95%)	6 (5%)	26	22
5	E	92/92 (100%)	90 (98%)	2 (2%)	52	55
5	R	92/92 (100%)	90 (98%)	2 (2%)	52	55
6	F	81/81 (100%)	77 (95%)	4 (5%)	25	21
6	S	81/81 (100%)	75 (93%)	6 (7%)	13	9
7	G	67/67 (100%)	60 (90%)	7 (10%)	7	4
7	T	67/67 (100%)	60 (90%)	7 (10%)	7	4
8	H	71/71 (100%)	63 (89%)	8 (11%)	6	3
8	U	71/71 (100%)	69 (97%)	2 (3%)	43	44
9	I	57/57 (100%)	50 (88%)	7 (12%)	4	2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	V	57/57 (100%)	51 (90%)	6 (10%)	7	4
10	J	49/49 (100%)	48 (98%)	1 (2%)	55	58
10	W	49/49 (100%)	47 (96%)	2 (4%)	30	28
11	K	39/39 (100%)	37 (95%)	2 (5%)	24	19
11	X	39/39 (100%)	38 (97%)	1 (3%)	46	48
12	L	39/39 (100%)	36 (92%)	3 (8%)	13	8
12	Y	39/39 (100%)	36 (92%)	3 (8%)	13	8
13	M	37/37 (100%)	34 (92%)	3 (8%)	11	7
13	Z	37/37 (100%)	35 (95%)	2 (5%)	22	18
14	1	86/86 (100%)	78 (91%)	8 (9%)	9	5
14	2	86/86 (100%)	75 (87%)	11 (13%)	4	2
All	All	3244/3212 (101%)	3099 (96%)	145 (4%)	27	24

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	109	PHE
1	A	138	HIS
1	A	180	GLN
1	A	338	MET
1	A	363	LEU
1	A	369	ASP
1	A	514	LYS
2	B	16	ILE
2	B	60	GLU
2	B	65	TRP
2	B	66	THR
2	B	75	LEU
2	B	78	LEU
2	B	91	ASN
2	B	171	LYS
3	C	40	MET
3	C	127	LEU
3	C	159	MET
3	C	214	PHE
3	C	230	ASN
4	D	7	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	D	8	SER
4	D	51	LEU
4	D	58	GLU
4	D	107	ILE
5	E	5	HIS
5	E	90	ARG
6	F	54	ASN
6	F	80	GLN
6	F	87	THR
6	F	95	GLN
7	G	5	LYS
7	G	18	PHE
7	G	33	LEU
7	G	37	LEU
7	G	42	ARG
7	G	54	ARG
7	G	83	GLU
8	H	7	LYS
8	H	8	ILE
8	H	9	LYS
8	H	29	CYS
8	H	50	VAL
8	H	60	TYR
8	H	61	LYS
8	H	84	LYS
9	I	18	ARG
9	I	21	ILE
9	I	29	LEU
9	I	31	PHE
9	I	33	THR
9	I	37	PHE
9	I	41	GLU
10	J	50	LEU
11	K	7	PRO
11	K	54	ARG
12	L	2	HIS
12	L	5	GLU
12	L	47	LYS
13	M	34	LEU
13	M	38	ASP
13	M	40	TYR
1	N	35	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	N	38	ARG
1	N	109	PHE
1	N	115	SER
1	N	138	HIS
1	N	180	GLN
1	N	363	LEU
1	N	369	ASP
2	O	59	GLN
2	O	60	GLU
2	O	65	TRP
2	O	68	LEU
2	O	75	LEU
2	O	78	LEU
2	O	94	SER
2	O	113	TYR
2	O	115	ASP
2	O	158	ASP
2	O	167	SER
2	O	171	LYS
2	O	217	LYS
2	O	226	MET
3	P	110	PRO
3	P	159	MET
3	P	214	PHE
3	P	230	ASN
4	Q	4	SER
4	Q	6	VAL
4	Q	7	LYS
4	Q	21	ASP
4	Q	31	LYS
4	Q	51	LEU
5	R	6	GLU
5	R	80	GLU
6	S	44	GLU
6	S	48	LEU
6	S	53	THR
6	S	54	ASN
6	S	80	GLN
6	S	87	THR
7	T	18	PHE
7	T	33	LEU
7	T	35	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
7	T	36	TRP
7	T	38	HIS
7	T	54	ARG
7	T	84	LYS
8	U	27	ARG
8	U	60	TYR
9	V	2	THR
9	V	8	GLN
9	V	21	ILE
9	V	31	PHE
9	V	36	LYS
9	V	73	LYS
10	W	2	GLU
10	W	50	LEU
11	X	54	ARG
12	Y	2	HIS
12	Y	5	GLU
12	Y	20	ARG
13	Z	34	LEU
13	Z	43	SER
14	1	14	CYS
14	1	20	VAL
14	1	25	LYS
14	1	38	ARG
14	1	52	ASN
14	1	69	GLU
14	1	86	LYS
14	1	103	ASN
14	2	14	CYS
14	2	16	GLN
14	2	17	CYS
14	2	19	THR
14	2	20	VAL
14	2	26	HIS
14	2	38	ARG
14	2	39	LYS
14	2	40	THR
14	2	47	THR
14	2	72	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	98	ASN
1	A	178	GLN
1	A	180	GLN
1	A	512	ASN
2	B	10	GLN
2	B	181	GLN
2	B	195	GLN
3	C	50	ASN
3	C	68	GLN
3	C	76	GLN
4	D	37	GLN
4	D	109	HIS
5	E	94	ASN
6	F	54	ASN
6	F	80	GLN
6	F	94	HIS
6	F	95	GLN
6	F	98	HIS
7	G	8	HIS
8	H	22	ASN
9	I	20	HIS
10	J	29	ASN
12	L	2	HIS
1	N	4	ASN
1	N	80	ASN
1	N	98	ASN
1	N	178	GLN
1	N	180	GLN
1	N	413	HIS
1	N	512	ASN
2	O	10	GLN
2	O	22	HIS
2	O	92	ASN
2	O	181	GLN
2	O	195	GLN
3	P	3	HIS
3	P	68	GLN
3	P	70	HIS
3	P	76	GLN
4	Q	37	GLN
4	Q	101	HIS
5	R	94	ASN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
6	S	54	ASN
6	S	80	GLN
7	T	38	HIS
8	U	10	ASN
8	U	12	GLN
8	U	37	HIS
9	V	20	HIS
10	W	29	ASN
14	1	103	ASN
14	2	16	GLN
14	2	26	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	FME	N	1	1	8,9,10	0.82	0	7,9,11	6.36	5 (71%)
7	TPO	T	11	7	8,10,11	2.15	2 (25%)	10,14,16	1.27	1 (10%)
7	TPO	G	11	7	8,10,11	1.80	2 (25%)	10,14,16	1.05	0
1	FME	A	1	1	8,9,10	1.47	1 (12%)	7,9,11	5.60	5 (71%)
9	SAC	I	1	9	7,8,9	2.23	2 (28%)	8,9,11	2.36	3 (37%)
2	FME	O	1	2	8,9,10	0.83	0	7,9,11	0.96	0
9	SAC	V	1	9	7,8,9	2.50	2 (28%)	8,9,11	1.76	3 (37%)
2	FME	B	1	2	8,9,10	2.62	3 (37%)	7,9,11	8.29	5 (71%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.  
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	N	1	1	-	4/7/9/11	-
7	TPO	T	11	7	-	6/9/11/13	-
7	TPO	G	11	7	-	4/9/11/13	-
1	FME	A	1	1	-	4/7/9/11	-
9	SAC	I	1	9	-	6/7/8/10	-
2	FME	O	1	2	-	0/7/9/11	-
9	SAC	V	1	9	-	2/7/8/10	-
2	FME	B	1	2	-	1/7/9/11	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	FME	CA-N	5.44	1.54	1.46
9	V	1	SAC	OAC-C1A	4.88	1.34	1.23
9	I	1	SAC	OAC-C1A	4.72	1.33	1.23
9	V	1	SAC	CA-N	4.17	1.52	1.46
2	B	1	FME	O1-CN	-3.92	1.10	1.22
1	A	1	FME	CA-N	3.68	1.51	1.46
7	T	11	TPO	P-O1P	3.58	1.62	1.50
7	T	11	TPO	P-OG1	3.35	1.65	1.59
9	I	1	SAC	CA-N	3.20	1.50	1.46
7	G	11	TPO	P-O1P	3.13	1.60	1.50
7	G	11	TPO	P-OG1	3.10	1.65	1.59
2	B	1	FME	CB-CA	2.66	1.58	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	FME	CA-N-CN	-20.68	91.02	122.82
1	N	1	FME	CA-N-CN	-15.59	98.84	122.82
1	A	1	FME	CA-N-CN	-13.93	101.39	122.82
2	B	1	FME	O1-CN-N	5.84	140.65	125.27
9	I	1	SAC	CA-N-C1A	4.65	131.72	123.15
1	N	1	FME	CE-SD-CG	3.93	113.91	100.40
9	I	1	SAC	C2A-C1A-N	3.44	121.92	116.10
2	B	1	FME	C-CA-N	3.13	115.39	109.73
1	A	1	FME	CE-SD-CG	3.08	111.00	100.40
1	N	1	FME	O1-CN-N	2.92	132.96	125.27
1	N	1	FME	C-CA-N	-2.85	104.58	109.73

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	T	11	TPO	P-OG1-CB	2.58	131.00	123.21
1	A	1	FME	CG-CB-CA	-2.55	105.87	112.95
9	V	1	SAC	C2A-C1A-N	2.54	120.40	116.10
9	V	1	SAC	CA-N-C1A	2.51	127.78	123.15
1	N	1	FME	CG-CB-CA	-2.42	106.21	112.95
9	V	1	SAC	C-CA-N	2.31	113.91	109.73
1	A	1	FME	O1-CN-N	2.20	131.07	125.27
2	B	1	FME	O-C-CA	-2.15	119.13	124.78
2	B	1	FME	CG-CB-CA	-2.07	107.21	112.95
9	I	1	SAC	OAC-C1A-N	-2.02	118.25	121.95
1	A	1	FME	O-C-CA	-2.01	119.51	124.78

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	N	1	FME	O1-CN-N-CA
1	N	1	FME	N-CA-CB-CG
7	T	11	TPO	N-CA-CB-CG2
7	T	11	TPO	N-CA-CB-OG1
7	T	11	TPO	C-CA-CB-CG2
7	T	11	TPO	CA-CB-OG1-P
7	G	11	TPO	N-CA-CB-OG1
7	G	11	TPO	CA-CB-OG1-P
1	A	1	FME	O1-CN-N-CA
1	A	1	FME	N-CA-CB-CG
9	I	1	SAC	CB-CA-N-C1A
9	I	1	SAC	O-C-CA-CB
9	I	1	SAC	C-CA-CB-OG
2	B	1	FME	O1-CN-N-CA
9	I	1	SAC	C2A-C1A-N-CA
9	I	1	SAC	OAC-C1A-N-CA
9	V	1	SAC	C2A-C1A-N-CA
9	V	1	SAC	OAC-C1A-N-CA
1	N	1	FME	CB-CG-SD-CE
9	I	1	SAC	N-CA-CB-OG
1	A	1	FME	CB-CG-SD-CE
7	G	11	TPO	N-CA-CB-CG2
7	T	11	TPO	CB-OG1-P-O1P
1	N	1	FME	C-CA-CB-CG
1	A	1	FME	C-CA-CB-CG
7	T	11	TPO	CB-OG1-P-O3P

*Continued on next page...*

*Continued from previous page...*

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

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	11	TPO	2	0
9	I	1	SAC	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 76 ligands modelled in this entry, 15 are unknown and 10 are monoatomic - leaving 51 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	$\# Z  > 2$
18	HEA	N	606	1,19	44,67,67	1.31	5 (11%)	37,103,103	1.89	8 (21%)
22	CUA	B	302	2	0,1,1	0.00	-	-		
24	CHD	G	102	-	29,32,32	1.16	2 (6%)	48,51,51	2.05	13 (27%)
26	CDL	C	306	-	99,99,99	1.39	12 (12%)	105,111,111	1.41	10 (9%)
20	PGV	N	612	-	50,50,50	0.85	1 (2%)	53,56,56	1.21	4 (7%)
21	TGL	D	201	-	62,62,62	1.39	6 (9%)	65,65,65	1.51	8 (12%)
20	PGV	P	304	-	50,50,50	0.82	2 (4%)	53,56,56	1.17	6 (11%)
20	PGV	A	607	-	50,50,50	1.12	2 (4%)	53,56,56	1.05	5 (9%)
24	CHD	P	301	-	29,32,32	1.08	2 (6%)	48,51,51	1.92	13 (27%)
28	PSC	V	101	-	51,51,51	1.21	3 (5%)	57,59,59	1.31	5 (8%)
21	TGL	B	301	-	62,62,62	1.45	8 (12%)	65,65,65	1.87	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	HEA	N	605[A]	-	44,67,67	1.01	2 (4%)	37,103,103	2.12	14 (37%)
26	CDL	G	101	-	99,99,99	1.44	12 (12%)	105,111,111	1.35	13 (12%)
18	HEA	N	605[B]	-	44,67,67	1.00	2 (4%)	37,103,103	2.15	16 (43%)
20	PGV	C	304	-	50,50,50	0.80	2 (4%)	53,56,56	1.33	7 (13%)
24	CHD	C	307	-	29,32,32	0.90	1 (3%)	48,51,51	3.61	26 (54%)
24	CHD	T	103	-	29,32,32	1.10	2 (6%)	48,51,51	2.05	18 (37%)
23	EDO	N	614	-	3,3,3	0.41	0	2,2,2	0.47	0
20	PGV	A	608	-	50,50,50	1.06	4 (8%)	53,56,56	1.28	6 (11%)
25	PEK	P	303	-	52,52,52	0.99	3 (5%)	55,57,57	0.96	2 (3%)
24	CHD	P	307	-	29,32,32	0.58	0	48,51,51	2.48	19 (39%)
23	EDO	C	311	-	3,3,3	0.61	0	2,2,2	0.29	0
23	EDO	I	101	-	3,3,3	0.63	0	2,2,2	0.28	0
23	EDO	N	613	-	3,3,3	0.57	0	2,2,2	0.37	0
28	PSC	E	201	-	51,51,51	1.32	3 (5%)	57,59,59	1.51	9 (15%)
23	EDO	S	102	-	3,3,3	0.64	0	2,2,2	0.79	0
30	DMU	Z	101	-	34,34,34	0.75	1 (2%)	45,45,45	1.07	5 (11%)
23	EDO	G	103	-	3,3,3	0.84	0	2,2,2	0.68	0
20	PGV	P	305	-	50,50,50	1.29	2 (4%)	53,56,56	1.39	6 (11%)
23	EDO	B	303	-	3,3,3	0.78	0	2,2,2	0.48	0
26	CDL	P	306	-	99,99,99	1.41	12 (12%)	105,111,111	1.22	10 (9%)
24	CHD	J	101	-	29,32,32	0.85	1 (3%)	48,51,51	2.19	16 (33%)
18	HEA	A	604[B]	-	44,67,67	1.08	2 (4%)	37,103,103	2.05	10 (27%)
21	TGL	N	608	-	62,62,62	1.48	8 (12%)	65,65,65	2.09	14 (21%)
19	PER	N	607	18,15	0,1,1	0.00	-	-		
19	PER	A	606	18,15	0,1,1	0.00	-	-		
18	HEA	A	604[A]	-	44,67,67	1.09	3 (6%)	37,103,103	2.14	10 (27%)
23	EDO	E	202	-	3,3,3	0.50	0	2,2,2	0.73	0
21	TGL	Q	201	-	62,62,62	1.40	6 (9%)	65,65,65	1.29	9 (13%)
25	PEK	C	303	-	52,52,52	0.96	2 (3%)	55,57,57	1.20	5 (9%)
26	CDL	T	101	-	99,99,99	1.43	12 (12%)	105,111,111	1.48	15 (14%)
24	CHD	W	101	-	29,32,32	0.87	2 (6%)	48,51,51	3.20	22 (45%)
20	PGV	C	305	-	50,50,50	1.40	3 (6%)	53,56,56	1.42	7 (13%)
24	CHD	C	301	-	29,32,32	1.32	4 (13%)	48,51,51	1.82	12 (25%)
23	EDO	F	102	-	3,3,3	0.45	0	2,2,2	0.54	0
30	DMU	M	101	-	34,34,34	0.74	0	45,45,45	1.77	9 (20%)
31	HEC	2	201	14	26,50,50	1.53	4 (15%)	18,82,82	0.95	1 (5%)
31	HEC	1	201	14	26,50,50	1.35	3 (11%)	18,82,82	1.95	6 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	TGL	L	101	-	62,62,62	1.56	6 (9%)	65,65,65	1.58	14 (21%)
18	HEA	A	605	1,19	44,67,67	1.15	4 (9%)	37,103,103	1.88	8 (21%)
22	CUA	O	301	2	0,1,1	0.00	-	-	-	-

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
18	HEA	N	606	1,19	2/2/7/16	1/24/76/76	-
24	CHD	C	301	-	-	0/7/74/74	0/4/4/4
24	CHD	G	102	-	-	1/7/74/74	0/4/4/4
26	CDL	C	306	-	-	62/110/110/110	-
20	PGV	N	612	-	-	9/55/55/55	-
21	TGL	D	201	-	-	38/65/65/65	-
20	PGV	P	304	-	-	12/55/55/55	-
20	PGV	A	607	-	-	30/55/55/55	-
24	CHD	P	301	-	-	0/7/74/74	0/4/4/4
28	PSC	V	101	-	-	35/55/55/55	-
21	TGL	B	301	-	-	33/65/65/65	-
18	HEA	N	605[A]	-	-	1/24/76/76	-
26	CDL	G	101	-	-	58/110/110/110	-
18	HEA	N	605[B]	-	-	3/24/76/76	-
20	PGV	C	304	-	-	19/55/55/55	-
24	CHD	C	307	-	-	6/7/74/74	0/4/4/4
24	CHD	T	103	-	-	0/7/74/74	0/4/4/4
23	EDO	N	614	-	-	1/1/1/1	-
20	PGV	A	608	-	-	12/55/55/55	-
25	PEK	P	303	-	-	20/56/56/56	-
24	CHD	P	307	-	-	3/7/74/74	1/4/4/4
23	EDO	C	311	-	-	1/1/1/1	-
23	EDO	I	101	-	-	0/1/1/1	-
23	EDO	N	613	-	-	0/1/1/1	-
28	PSC	E	201	-	-	36/55/55/55	-
23	EDO	S	102	-	-	0/1/1/1	-
30	DMU	Z	101	-	-	4/19/59/59	0/2/2/2
23	EDO	G	103	-	-	0/1/1/1	-

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	PGV	P	305	-	-	31/55/55/55	-
26	CDL	P	306	-	-	67/110/110/110	-
24	CHD	J	101	-	-	5/7/74/74	0/4/4/4
18	HEA	A	604[B]	-	-	2/24/76/76	-
21	TGL	N	608	-	-	34/65/65/65	-
18	HEA	A	604[A]	-	-	1/24/76/76	-
23	EDO	E	202	-	-	1/1/1/1	-
21	TGL	Q	201	-	-	35/65/65/65	-
25	PEK	C	303	-	-	20/56/56/56	-
26	CDL	T	101	-	-	61/110/110/110	-
24	CHD	W	101	-	-	6/7/74/74	0/4/4/4
20	PGV	C	305	-	-	30/55/55/55	-
23	EDO	B	303	-	-	1/1/1/1	-
23	EDO	F	102	-	-	0/1/1/1	-
30	DMU	M	101	-	-	6/19/59/59	0/2/2/2
31	HEC	2	201	14	-	3/6/54/54	-
31	HEC	1	201	14	-	0/6/54/54	-
21	TGL	L	101	-	-	46/65/65/65	-
18	HEA	A	605	1,19	2/2/7/16	1/24/76/76	-

All (149) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	L	101	TGL	OG2-CB1	7.00	1.54	1.34
20	C	305	PGV	O01-C1	5.88	1.50	1.34
21	L	101	TGL	OG3-CC1	5.77	1.50	1.33
28	E	201	PSC	O01-C1	5.63	1.50	1.34
28	V	101	PSC	O01-C1	5.60	1.50	1.34
26	G	101	CDL	OB6-CB5	5.47	1.49	1.34
21	N	608	TGL	OG2-CB1	5.40	1.49	1.34
26	C	306	CDL	OB8-CB7	5.36	1.49	1.33
20	P	305	PGV	O03-C19	5.29	1.48	1.33
21	N	608	TGL	OG1-CA1	5.28	1.48	1.33
26	T	101	CDL	OB6-CB5	5.28	1.49	1.34
21	D	201	TGL	OG1-CA1	5.22	1.48	1.33
26	C	306	CDL	OA6-CA5	5.21	1.49	1.34
20	C	305	PGV	O03-C19	5.19	1.48	1.33
20	P	305	PGV	O01-C1	5.16	1.48	1.34
21	B	301	TGL	OG3-CC1	5.15	1.48	1.33

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	Q	201	TGL	OG2-CB1	5.13	1.48	1.34
26	P	306	CDL	OA8-CA7	5.11	1.48	1.33
26	T	101	CDL	OA8-CA7	5.07	1.48	1.33
26	T	101	CDL	OA6-CA5	5.07	1.48	1.34
20	A	607	PGV	O03-C19	5.05	1.48	1.33
21	N	608	TGL	OG3-CC1	5.04	1.48	1.33
26	G	101	CDL	OB8-CB7	5.03	1.48	1.33
21	Q	201	TGL	OG3-CC1	5.02	1.48	1.33
21	D	201	TGL	OG2-CB1	5.02	1.48	1.34
26	P	306	CDL	OA6-CA5	5.01	1.48	1.34
26	C	306	CDL	OA8-CA7	4.94	1.47	1.33
21	B	301	TGL	OG1-CA1	4.93	1.47	1.33
26	P	306	CDL	OB8-CB7	4.92	1.47	1.33
21	Q	201	TGL	OG1-CA1	4.88	1.47	1.33
26	G	101	CDL	OA8-CA7	4.77	1.47	1.33
21	L	101	TGL	OG1-CA1	4.76	1.47	1.33
21	D	201	TGL	OG3-CC1	4.69	1.47	1.33
28	E	201	PSC	O03-C19	4.69	1.47	1.33
26	P	306	CDL	OB6-CB5	4.68	1.47	1.34
26	T	101	CDL	OB8-CB7	4.66	1.46	1.33
26	G	101	CDL	OA6-CA5	4.59	1.47	1.34
20	N	612	PGV	O03-C19	4.55	1.46	1.33
25	P	303	PEK	O01-C1	4.40	1.46	1.34
25	C	303	PEK	O01-C1	4.33	1.46	1.34
21	B	301	TGL	OG2-CB1	4.30	1.46	1.34
20	A	607	PGV	O01-C1	4.24	1.46	1.34
31	1	201	HEC	CBC-CAC	-4.20	1.33	1.49
31	2	201	HEC	CBB-CAB	-4.09	1.34	1.49
31	2	201	HEC	CBC-CAC	-4.05	1.34	1.49
31	1	201	HEC	CBB-CAB	-3.99	1.34	1.49
20	A	608	PGV	O03-C19	3.94	1.44	1.33
21	B	301	TGL	OC1-CC1	-3.88	1.11	1.22
28	V	101	PSC	O03-C19	3.79	1.44	1.33
26	C	306	CDL	OB6-CB5	3.77	1.44	1.34
18	N	606	HEA	C3B-C11	-3.76	1.50	1.52
28	E	201	PSC	C13-C12	3.74	1.53	1.31
28	V	101	PSC	C13-C12	3.71	1.53	1.31
31	2	201	HEC	C3B-C4B	3.62	1.49	1.43
26	P	306	CDL	C59-C58	-3.43	1.32	1.51
24	G	102	CHD	C4-C3	3.36	1.58	1.51
25	P	303	PEK	O03-C21	3.33	1.43	1.33
21	L	101	TGL	C20-CA9	-3.30	1.33	1.51

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	306	CDL	C59-C58	-3.22	1.33	1.51
20	P	304	PGV	O01-C1	3.17	1.43	1.34
26	P	306	CDL	C82-C81	-3.16	1.33	1.51
26	T	101	CDL	C59-C58	-3.15	1.33	1.51
21	N	608	TGL	C20-CA9	-3.11	1.34	1.51
21	L	101	TGL	C10-CB9	-3.11	1.34	1.51
26	C	306	CDL	C79-C78	-3.10	1.34	1.51
20	C	304	PGV	O03-C19	3.09	1.42	1.33
26	C	306	CDL	C62-C61	-3.09	1.34	1.51
26	C	306	CDL	C19-C18	-3.08	1.34	1.51
31	2	201	HEC	C3B-C2B	-3.08	1.37	1.40
21	Q	201	TGL	C15-CC9	-3.06	1.34	1.51
26	G	101	CDL	C42-C41	-3.05	1.34	1.51
24	T	103	CHD	C4-C3	3.04	1.57	1.51
26	P	306	CDL	C79-C78	-3.04	1.34	1.51
26	T	101	CDL	C19-C18	-3.03	1.34	1.51
26	G	101	CDL	C22-C21	-3.03	1.34	1.51
26	G	101	CDL	C62-C61	-3.01	1.34	1.51
21	D	201	TGL	C10-CB9	-3.00	1.34	1.51
26	C	306	CDL	C82-C81	-2.99	1.34	1.51
26	C	306	CDL	C22-C21	-2.99	1.34	1.51
26	P	306	CDL	C19-C18	-2.99	1.34	1.51
25	C	303	PEK	O03-C21	2.99	1.42	1.33
21	D	201	TGL	C15-CC9	-2.98	1.34	1.51
26	T	101	CDL	C62-C61	-2.97	1.34	1.51
18	N	606	HEA	O11-C11	2.96	1.49	1.42
26	P	306	CDL	C62-C61	-2.95	1.35	1.51
21	N	608	TGL	C15-CC9	-2.94	1.35	1.51
26	P	306	CDL	C39-C38	-2.94	1.35	1.51
26	C	306	CDL	C42-C41	-2.94	1.35	1.51
26	P	306	CDL	C22-C21	-2.93	1.35	1.51
26	P	306	CDL	C42-C41	-2.93	1.35	1.51
26	T	101	CDL	C39-C38	-2.92	1.35	1.51
21	B	301	TGL	C15-CC9	-2.92	1.35	1.51
21	Q	201	TGL	C10-CB9	-2.92	1.35	1.51
26	G	101	CDL	C19-C18	-2.92	1.35	1.51
26	G	101	CDL	C39-C38	-2.91	1.35	1.51
21	B	301	TGL	C20-CA9	-2.91	1.35	1.51
26	T	101	CDL	C82-C81	-2.90	1.35	1.51
26	G	101	CDL	C82-C81	-2.88	1.35	1.51
20	P	304	PGV	O03-C19	2.84	1.41	1.33
24	G	102	CHD	C13-C14	-2.83	1.50	1.55

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	101	CDL	C79-C78	-2.82	1.35	1.51
26	G	101	CDL	C59-C58	-2.82	1.35	1.51
26	T	101	CDL	C22-C21	-2.80	1.35	1.51
21	N	608	TGL	C10-CB9	-2.79	1.35	1.51
26	T	101	CDL	C42-C41	-2.77	1.36	1.51
31	I	201	HEC	C3B-C4B	2.77	1.48	1.43
20	A	608	PGV	O01-C1	2.77	1.42	1.34
21	D	201	TGL	C20-CA9	-2.77	1.36	1.51
24	C	301	CHD	C8-C7	2.73	1.58	1.53
26	T	101	CDL	C79-C78	-2.71	1.36	1.51
21	L	101	TGL	C15-CC9	-2.70	1.36	1.51
18	N	606	HEA	CAA-C2A	2.69	1.56	1.52
24	P	301	CHD	C18-C13	2.64	1.58	1.54
26	C	306	CDL	C39-C38	-2.64	1.36	1.51
18	N	605[A]	HEA	O11-C11	2.63	1.48	1.42
18	N	605[B]	HEA	O11-C11	2.63	1.48	1.42
18	N	606	HEA	C1C-CHC	2.62	1.48	1.41
24	P	301	CHD	C8-C7	2.57	1.57	1.53
30	Z	101	DMU	O16-C6	2.54	1.44	1.40
24	C	301	CHD	C11-C9	2.52	1.57	1.53
18	N	605[A]	HEA	C3B-C11	-2.52	1.50	1.52
18	N	605[B]	HEA	C3B-C11	-2.52	1.50	1.52
18	A	605	HEA	C3A-C2A	-2.50	1.36	1.40
21	Q	201	TGL	C20-CA9	-2.50	1.37	1.51
21	B	301	TGL	C10-CB9	-2.50	1.37	1.51
24	C	301	CHD	C16-C17	2.48	1.59	1.54
18	A	605	HEA	C18-C19	2.45	1.38	1.33
24	T	103	CHD	C11-C9	2.44	1.57	1.53
18	A	605	HEA	CMC-C2C	2.44	1.56	1.51
20	C	305	PGV	C01-C02	2.41	1.58	1.50
21	N	608	TGL	OC1-CC1	-2.39	1.15	1.22
20	A	608	PGV	O03-C01	2.31	1.50	1.45
25	P	303	PEK	O03-C01	-2.27	1.40	1.45
18	N	606	HEA	C18-C19	2.27	1.38	1.33
24	W	101	CHD	C20-C17	2.23	1.58	1.54
20	C	304	PGV	O01-C1	2.22	1.40	1.34
18	A	604[A]	HEA	C22-C23	2.21	1.38	1.32
18	A	604[B]	HEA	C3C-CAC	2.20	1.52	1.47
18	A	604[A]	HEA	C3C-CAC	2.20	1.52	1.47
20	A	608	PGV	O01-C02	-2.19	1.41	1.46
24	C	301	CHD	C18-C13	2.18	1.57	1.54
18	A	604[B]	HEA	C14-C15	2.08	1.38	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	A	604[A]	HEA	C14-C15	2.08	1.38	1.33
21	N	608	TGL	OG2-CG2	2.07	1.51	1.46
24	J	101	CHD	C2-C3	2.07	1.56	1.51
24	C	307	CHD	C11-C12	2.07	1.56	1.53
21	B	301	TGL	OG1-CG1	-2.05	1.40	1.45
18	A	605	HEA	C16-C15	2.05	1.55	1.51
24	W	101	CHD	C13-C17	2.05	1.59	1.55

All (394) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	307	CHD	C10-C9-C8	10.37	122.96	111.82
24	W	101	CHD	C17-C13-C12	9.83	126.64	117.67
24	C	307	CHD	C6-C5-C4	-7.51	102.55	111.19
24	W	101	CHD	C13-C17-C20	7.48	128.43	119.50
24	C	307	CHD	C4-C5-C10	7.22	120.33	112.66
24	G	102	CHD	C6-C7-C8	6.79	118.73	111.48
21	B	301	TGL	CG2-OG2-CB1	6.74	134.38	117.79
21	N	608	TGL	CG2-OG2-CB1	6.60	134.03	117.79
21	D	201	TGL	OG2-CB1-CB2	6.52	125.56	111.50
28	E	201	PSC	O01-C1-C2	6.43	125.35	111.50
24	C	307	CHD	C15-C14-C8	6.42	127.30	118.33
24	C	307	CHD	C19-C10-C1	-6.40	97.94	108.26
24	W	101	CHD	C15-C14-C8	6.24	127.05	118.33
24	C	307	CHD	C11-C9-C8	-6.05	102.02	110.88
26	T	101	CDL	OB6-CB5-C51	5.97	124.36	111.50
21	N	608	TGL	OG3-CC1-CC2	5.87	130.33	111.91
24	P	307	CHD	C9-C10-C5	5.85	116.79	108.58
24	W	101	CHD	C1-C10-C5	5.81	116.36	107.77
21	L	101	TGL	OG2-CB1-CB2	5.79	123.98	111.50
24	C	307	CHD	C11-C12-C13	5.77	117.16	111.24
21	B	301	TGL	CG3-OG3-CC1	5.76	138.47	117.12
24	C	301	CHD	C15-C14-C13	5.69	109.13	103.55
24	C	307	CHD	C6-C7-C8	-5.65	105.45	111.48
26	C	306	CDL	CB4-OB6-CB5	-5.63	103.92	117.79
24	P	307	CHD	C10-C9-C8	5.61	117.84	111.82
18	N	606	HEA	CAD-CBD-CGD	-5.57	103.33	112.67
24	G	102	CHD	C6-C5-C4	-5.56	104.78	111.19
24	J	101	CHD	C13-C17-C20	5.56	126.13	119.50
24	T	103	CHD	C18-C13-C12	-5.54	103.42	109.07
18	N	605[A]	HEA	C13-C12-C11	-5.53	106.05	114.35
18	N	605[B]	HEA	C13-C12-C11	-5.53	106.05	114.35

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	B	301	TGL	OG2-CG2-CG1	5.49	128.27	108.40
18	A	604[B]	HEA	CAA-CBA-CGA	-5.48	103.47	112.67
18	A	604[A]	HEA	CAA-CBA-CGA	-5.48	103.47	112.67
26	G	101	CDL	OB6-CB5-C51	5.47	123.30	111.50
20	P	305	PGV	O01-C1-C2	5.46	123.26	111.50
24	W	101	CHD	C17-C13-C14	-5.43	94.62	100.09
24	P	307	CHD	C9-C11-C12	-5.33	107.27	114.30
21	B	301	TGL	OG2-CB1-CB2	5.28	122.89	111.50
24	W	101	CHD	C14-C8-C7	5.27	118.80	111.81
26	T	101	CDL	OA6-CA5-C11	5.24	122.80	111.50
24	W	101	CHD	C14-C8-C9	-5.22	102.55	109.71
24	J	101	CHD	C22-C20-C17	5.22	121.07	110.28
24	C	307	CHD	C11-C9-C10	5.22	119.11	113.73
21	N	608	TGL	OG1-CA1-CA2	5.19	128.20	111.91
18	A	604[B]	HEA	C13-C12-C11	-5.16	106.60	114.35
18	A	604[A]	HEA	C13-C12-C11	-5.16	106.60	114.35
18	N	606	HEA	C1B-C2B-C3B	-5.15	103.42	107.00
21	N	608	TGL	OG2-CB1-CB2	5.10	122.50	111.50
20	C	305	PGV	O01-C1-C2	5.10	122.49	111.50
28	V	101	PSC	O01-C1-C2	5.07	122.42	111.50
20	P	305	PGV	O03-C19-C20	5.03	127.70	111.91
24	W	101	CHD	C6-C5-C4	-4.84	105.61	111.19
24	P	301	CHD	C22-C23-C24	-4.81	103.26	113.59
18	A	605	HEA	C13-C12-C11	-4.76	107.20	114.35
26	C	306	CDL	OA6-CA5-C11	4.74	121.72	111.50
24	C	301	CHD	C21-C20-C22	-4.72	102.96	110.36
18	A	605	HEA	CAD-CBD-CGD	-4.69	104.80	112.67
24	P	301	CHD	C15-C14-C13	4.69	108.15	103.55
20	N	612	PGV	O03-C19-C20	4.51	126.07	111.91
30	M	101	DMU	C18-O16-C6	-4.51	106.37	113.84
21	N	608	TGL	OG3-CC1-OC1	-4.45	112.36	123.59
31	I	201	HEC	CBD-CAD-C3D	-4.42	104.33	112.49
24	P	307	CHD	C14-C8-C9	-4.39	103.69	109.71
21	N	608	TGL	CG3-OG3-CC1	4.32	133.13	117.12
30	M	101	DMU	O2-C8-C9	-4.29	98.63	109.30
24	W	101	CHD	C18-C13-C12	-4.24	104.75	109.07
24	C	307	CHD	C21-C20-C22	-4.17	103.83	110.36
18	N	605[A]	HEA	C20-C21-C22	-4.13	98.32	111.88
24	P	307	CHD	C16-C17-C13	4.12	107.59	103.55
18	A	605	HEA	C1B-C2B-C3B	-4.12	104.13	107.00
24	P	307	CHD	C4-C5-C10	4.06	116.97	112.66
26	G	101	CDL	OA6-CA5-C11	4.04	120.22	111.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	M	101	DMU	O1-C9-C11	4.02	116.42	106.44
18	A	604[A]	HEA	C27-C19-C20	4.01	122.03	115.27
26	T	101	CDL	CA4-OA6-CA5	4.00	127.65	117.79
21	N	608	TGL	OG1-CA1-OA1	-3.99	113.52	123.59
24	W	101	CHD	C6-C7-C8	3.98	115.73	111.48
18	A	605	HEA	CMC-C2C-C3C	3.98	132.12	124.68
24	P	307	CHD	C14-C8-C7	3.98	117.08	111.81
28	V	101	PSC	C21-C20-C19	-3.96	99.21	113.62
24	C	307	CHD	C14-C8-C9	-3.96	104.28	109.71
24	C	307	CHD	C15-C14-C13	3.95	107.43	103.55
24	J	101	CHD	C16-C17-C20	3.95	118.26	112.15
20	N	612	PGV	O03-C19-O04	-3.92	113.69	123.59
21	L	101	TGL	OG3-CC1-CC2	3.92	124.22	111.91
30	M	101	DMU	O3-C5-C7	3.92	119.40	110.35
24	T	103	CHD	C13-C17-C20	-3.90	114.84	119.50
26	C	306	CDL	OB8-CB7-C71	3.86	124.01	111.91
20	C	305	PGV	O03-C19-C20	3.85	123.98	111.91
24	J	101	CHD	C17-C13-C14	-3.81	96.25	100.09
24	W	101	CHD	C1-C10-C9	-3.79	105.39	111.35
21	B	301	TGL	OG1-CA1-CA2	3.79	123.80	111.91
18	A	604[B]	HEA	C27-C19-C20	3.76	121.60	115.27
26	P	306	CDL	OB8-CB7-C71	3.76	123.70	111.91
24	T	103	CHD	C22-C23-C24	-3.75	105.53	113.59
24	C	307	CHD	C21-C20-C17	3.73	118.63	112.92
24	G	102	CHD	O12-C12-C13	-3.72	104.74	111.03
24	J	101	CHD	C15-C14-C13	3.72	107.20	103.55
24	C	307	CHD	C1-C2-C3	3.72	115.24	110.47
24	P	307	CHD	C15-C14-C8	3.70	123.50	118.33
18	A	605	HEA	CMC-C2C-C1C	-3.70	122.78	128.46
24	J	101	CHD	C14-C8-C7	3.67	116.67	111.81
25	C	303	PEK	O03-C21-O04	-3.65	114.39	123.59
24	P	301	CHD	C9-C11-C12	-3.63	109.50	114.30
20	A	608	PGV	O03-C19-O04	-3.63	114.44	123.59
21	N	608	TGL	OG2-CG2-CG3	3.61	121.47	108.40
20	A	608	PGV	O01-C1-O02	-3.60	115.01	123.70
18	N	605[A]	HEA	C1B-C2B-C3B	-3.59	104.50	107.00
18	N	605[B]	HEA	C1B-C2B-C3B	-3.59	104.50	107.00
20	C	305	PGV	C01-O03-C19	3.59	130.41	117.12
18	A	604[B]	HEA	C13-C14-C15	-3.58	119.04	127.66
18	A	604[A]	HEA	C13-C14-C15	-3.58	119.04	127.66
26	T	101	CDL	OA8-CA7-C31	3.58	123.14	111.91
21	N	608	TGL	CG3-CG2-CG1	-3.57	103.36	111.79

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	608	PGV	O01-C1-C2	3.57	119.19	111.50
21	Q	201	TGL	OG1-CA1-CA2	3.55	123.04	111.91
24	P	307	CHD	C22-C23-C24	-3.54	105.97	113.59
21	Q	201	TGL	OG3-CC1-CC2	3.53	123.00	111.91
20	C	304	PGV	O01-C1-O02	-3.53	115.17	123.70
24	P	301	CHD	C13-C14-C8	-3.53	110.23	114.74
25	C	303	PEK	O03-C01-C02	-3.53	98.17	108.43
24	C	307	CHD	C14-C8-C7	3.52	116.48	111.81
20	C	304	PGV	O03-C19-O04	-3.52	114.71	123.59
24	C	307	CHD	C9-C10-C5	3.51	113.50	108.58
24	W	101	CHD	C10-C9-C8	3.50	115.58	111.82
18	N	605[A]	HEA	CAD-CBD-CGD	-3.50	106.79	112.67
18	N	605[B]	HEA	CAD-CBD-CGD	-3.50	106.79	112.67
24	G	102	CHD	C18-C13-C12	-3.50	105.51	109.07
31	1	201	HEC	CMC-C2C-C3C	3.48	129.91	125.82
24	J	101	CHD	C4-C3-C2	3.45	114.67	110.55
18	A	604[B]	HEA	C26-C15-C16	-3.42	109.51	115.27
18	A	604[A]	HEA	C26-C15-C16	-3.42	109.51	115.27
24	W	101	CHD	C4-C5-C10	3.37	116.24	112.66
24	T	103	CHD	C15-C14-C13	3.37	106.85	103.55
21	L	101	TGL	CG2-OG2-CB1	3.36	126.07	117.79
25	P	303	PEK	C2-C3-C4	3.36	119.21	113.23
24	P	307	CHD	C1-C10-C9	-3.35	106.09	111.35
24	P	307	CHD	O7-C7-C8	3.34	116.89	109.43
24	W	101	CHD	C6-C5-C10	3.33	116.19	112.66
18	A	604[A]	HEA	C21-C20-C19	3.31	123.87	112.98
25	C	303	PEK	C01-O03-C21	3.31	129.37	117.12
18	A	604[A]	HEA	C20-C19-C18	-3.29	114.45	121.12
18	N	605[A]	HEA	CAA-CBA-CGA	-3.29	107.15	112.67
18	N	605[B]	HEA	CAA-CBA-CGA	-3.29	107.15	112.67
24	T	103	CHD	C4-C3-C2	3.28	114.47	110.55
21	B	301	TGL	OG3-CC1-CC2	3.28	122.20	111.91
20	P	304	PGV	O01-C1-C2	3.28	118.56	111.50
18	N	605[A]	HEA	C3C-C4C-NC	3.27	113.44	109.21
18	N	605[B]	HEA	C3C-C4C-NC	3.27	113.44	109.21
21	N	608	TGL	OG3-CG3-CG2	3.27	117.95	108.43
26	P	306	CDL	OA6-CA5-C11	3.26	118.54	111.50
24	P	307	CHD	C23-C22-C20	-3.26	110.33	114.72
21	D	201	TGL	OG3-CC1-CC2	3.25	122.11	111.91
24	T	103	CHD	C9-C8-C7	3.24	115.75	111.88
20	C	305	PGV	C02-O01-C1	3.23	125.75	117.79
31	1	201	HEC	CMC-C2C-C1C	-3.22	123.52	128.46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	606	HEA	C27-C19-C20	3.21	120.68	115.27
24	G	102	CHD	C13-C17-C20	-3.20	115.67	119.50
26	G	101	CDL	CB6-OB8-CB7	3.20	128.98	117.12
21	D	201	TGL	OG1-CG1-CG2	3.20	117.75	108.43
24	J	101	CHD	C10-C9-C8	3.18	115.23	111.82
21	Q	201	TGL	OG2-CB1-CB2	3.18	118.34	111.50
21	D	201	TGL	OG1-CA1-CA2	3.17	121.86	111.91
21	N	608	TGL	OG2-CG2-CG1	3.17	119.86	108.40
26	C	306	CDL	CA6-OA8-CA7	3.15	128.77	117.12
30	M	101	DMU	O3-C5-C10	-3.14	102.43	110.05
24	C	301	CHD	C17-C13-C14	-3.13	96.94	100.09
18	A	605	HEA	CBA-CAA-C2A	-3.13	106.72	112.48
24	P	301	CHD	C17-C13-C14	-3.10	96.96	100.09
18	N	606	HEA	C20-C19-C18	-3.10	114.84	121.12
24	P	301	CHD	C1-C10-C5	3.09	112.34	107.77
24	J	101	CHD	C1-C2-C3	3.08	114.41	110.47
24	C	307	CHD	C23-C22-C20	-3.07	110.58	114.72
18	N	605[A]	HEA	CMB-C2B-C3B	3.05	130.67	124.69
18	N	605[B]	HEA	CMB-C2B-C3B	3.05	130.67	124.69
24	P	301	CHD	C6-C7-C8	3.05	114.74	111.48
24	C	301	CHD	C5-C4-C3	-3.04	108.30	112.76
21	Q	201	TGL	OG1-CG1-CG2	3.03	117.25	108.43
20	A	608	PGV	O03-C19-C20	3.03	121.41	111.91
26	T	101	CDL	OA8-CA6-CA4	3.02	117.22	108.43
18	N	605[B]	HEA	C27-C19-C20	3.01	120.34	115.27
28	E	201	PSC	O01-C1-O02	-3.00	116.45	123.70
24	J	101	CHD	C9-C11-C12	-3.00	110.34	114.30
25	P	303	PEK	O01-C1-C2	2.99	117.94	111.50
21	L	101	TGL	CG3-OG3-CC1	2.98	128.15	117.12
25	C	303	PEK	O01-C1-C2	2.98	117.92	111.50
24	P	301	CHD	C11-C12-C13	2.97	114.30	111.24
20	C	304	PGV	O01-C1-C2	2.97	117.90	111.50
24	C	301	CHD	C11-C9-C8	2.97	115.22	110.88
26	P	306	CDL	OB6-CB5-C51	2.93	117.82	111.50
24	P	307	CHD	O7-C7-C6	-2.90	102.74	109.94
26	C	306	CDL	C52-C51-CB5	-2.88	103.14	113.62
24	C	307	CHD	C18-C13-C12	2.88	112.00	109.07
21	D	201	TGL	OG2-CB1-OB1	-2.88	116.74	123.70
21	L	101	TGL	OB1-CB1-CB2	-2.86	112.56	123.73
21	L	101	TGL	OG1-CG1-CG2	2.86	116.76	108.43
26	T	101	CDL	OB8-CB6-CB4	2.86	116.75	108.43
24	T	103	CHD	O3-C3-C2	-2.81	103.00	110.16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	C	307	CHD	C16-C17-C13	2.81	106.31	103.55
31	I	201	HEC	C3B-C4B-NB	-2.81	105.64	110.94
20	A	607	PGV	O03-C19-C20	2.81	120.72	111.91
28	V	101	PSC	C28-C27-C26	-2.80	100.20	114.42
24	J	101	CHD	C23-C22-C20	-2.79	110.97	114.72
21	L	101	TGL	OG1-CA1-CA2	2.78	120.63	111.91
26	C	306	CDL	OB6-CB5-C51	2.78	117.48	111.50
26	P	306	CDL	OA8-CA7-C31	2.77	120.60	111.91
21	B	301	TGL	OB1-CB1-CB2	-2.76	112.96	123.73
26	G	101	CDL	OB8-CB7-C71	2.76	120.56	111.91
24	J	101	CHD	C1-C10-C5	2.76	111.84	107.77
26	G	101	CDL	OA6-CA5-OA7	-2.75	117.05	123.70
18	N	605[A]	HEA	C16-C15-C14	-2.75	115.55	121.12
18	N	605[B]	HEA	C16-C15-C14	-2.75	115.55	121.12
28	E	201	PSC	C28-C27-C26	-2.75	100.47	114.42
24	J	101	CHD	C13-C14-C8	-2.75	111.23	114.74
20	A	607	PGV	C01-O03-C19	2.71	127.17	117.12
24	T	103	CHD	C14-C13-C12	2.71	109.92	107.40
24	W	101	CHD	C11-C12-C13	2.69	114.01	111.24
30	M	101	DMU	C10-C5-C7	-2.69	104.39	110.00
24	G	102	CHD	C1-C2-C3	2.68	113.91	110.47
24	J	101	CHD	C15-C14-C8	2.68	122.07	118.33
21	N	608	TGL	OB1-CB1-CB2	-2.66	113.35	123.73
28	E	201	PSC	O03-C19-C20	2.65	120.24	111.91
24	P	307	CHD	C4-C3-C2	2.65	113.72	110.55
24	T	103	CHD	C6-C5-C4	-2.63	108.16	111.19
26	C	306	CDL	OA8-CA7-C31	2.63	120.17	111.91
20	C	304	PGV	O03-C19-C20	2.63	120.15	111.91
24	C	307	CHD	C22-C23-C24	-2.63	107.95	113.59
24	C	301	CHD	C11-C12-C13	2.62	113.94	111.24
20	C	304	PGV	C27-C26-C25	-2.61	101.17	114.42
21	Q	201	TGL	OG3-CC1-OC1	-2.61	117.01	123.59
24	C	307	CHD	O7-C7-C8	2.61	115.25	109.43
20	P	305	PGV	O03-C19-O04	-2.60	117.02	123.59
26	T	101	CDL	CB6-CB4-CB3	-2.60	105.64	111.79
18	A	605	HEA	CAA-CBA-CGA	-2.60	108.31	112.67
21	Q	201	TGL	OG1-CA1-OA1	-2.60	117.04	123.59
26	G	101	CDL	CB4-OB6-CB5	2.59	124.17	117.79
24	G	102	CHD	C1-C10-C9	-2.58	107.30	111.35
18	N	605[A]	HEA	C26-C15-C16	2.57	119.59	115.27
18	N	605[B]	HEA	C26-C15-C16	2.57	119.59	115.27
26	G	101	CDL	OA8-CA7-C31	2.57	119.96	111.91

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	W	101	CHD	C2-C1-C10	2.57	117.18	112.78
24	W	101	CHD	O7-C7-C6	-2.56	103.59	109.94
21	L	101	TGL	C11-C10-CB9	2.56	127.43	114.42
24	T	103	CHD	O12-C12-C11	-2.56	103.91	109.12
24	C	301	CHD	C23-C22-C20	-2.56	111.27	114.72
24	T	103	CHD	C9-C10-C5	2.55	112.17	108.58
26	G	101	CDL	C83-C82-C81	2.55	127.36	114.42
28	E	201	PSC	C31-C30-C29	-2.54	101.54	114.42
18	N	605[B]	HEA	C17-C18-C19	2.53	133.76	127.66
20	P	304	PGV	O03-C19-O04	-2.52	117.23	123.59
18	A	604[B]	HEA	CMC-C2C-C3C	2.52	129.40	124.68
18	A	604[A]	HEA	CMC-C2C-C3C	2.52	129.40	124.68
24	W	101	CHD	C9-C10-C5	2.51	112.11	108.58
18	A	604[B]	HEA	C20-C19-C18	-2.51	116.03	121.12
24	C	301	CHD	C16-C15-C14	-2.50	100.18	105.13
30	Z	101	DMU	O1-C9-C11	2.50	112.64	106.44
24	P	307	CHD	C19-C10-C5	-2.49	106.14	110.36
24	C	301	CHD	C18-C13-C12	2.49	111.60	109.07
24	G	102	CHD	C19-C10-C1	-2.48	104.26	108.26
20	P	305	PGV	O03-C01-C02	2.48	115.66	108.43
18	A	604[B]	HEA	C3C-C4C-NC	2.48	112.42	109.21
18	A	604[A]	HEA	C3C-C4C-NC	2.48	112.42	109.21
20	A	608	PGV	O14-P-O13	2.47	124.45	112.24
20	P	304	PGV	O14-P-O13	2.47	124.45	112.24
18	N	606	HEA	C16-C15-C14	2.47	126.11	121.12
18	N	606	HEA	CAA-CBA-CGA	-2.45	108.55	112.67
24	P	307	CHD	C15-C14-C13	2.45	105.96	103.55
20	A	607	PGV	O01-C1-C2	2.43	116.74	111.50
24	T	103	CHD	C1-C10-C5	2.42	111.35	107.77
26	G	101	CDL	OB8-CB7-OB9	-2.42	117.49	123.59
21	L	101	TGL	OG2-CG2-CG3	2.42	117.16	108.40
18	A	604[B]	HEA	C17-C18-C19	-2.42	121.84	127.66
30	M	101	DMU	O1-C9-C8	-2.42	105.30	109.69
24	T	103	CHD	C23-C22-C20	-2.41	111.47	114.72
24	T	103	CHD	C5-C4-C3	-2.41	109.22	112.76
24	P	301	CHD	C13-C17-C20	-2.40	116.63	119.50
26	P	306	CDL	OB8-CB7-OB9	-2.40	117.55	123.59
26	T	101	CDL	C82-C81-C80	2.39	126.56	114.42
21	N	608	TGL	OG1-CG1-CG2	2.39	115.39	108.43
28	E	201	PSC	O01-C02-C03	2.38	117.03	108.40
20	N	612	PGV	O01-C1-O02	-2.37	117.97	123.70
21	Q	201	TGL	C11-C10-CB9	2.37	126.44	114.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	605[A]	HEA	CMB-C2B-C1B	-2.37	124.83	128.46
18	N	605[B]	HEA	CMB-C2B-C1B	-2.37	124.83	128.46
24	C	307	CHD	C9-C11-C12	-2.36	111.19	114.30
18	N	605[A]	HEA	CBA-CAA-C2A	2.36	116.82	112.48
18	N	605[B]	HEA	CBA-CAA-C2A	2.36	116.82	112.48
24	C	307	CHD	O12-C12-C13	-2.36	107.05	111.03
20	C	305	PGV	O03-C01-C02	2.36	115.29	108.43
24	C	301	CHD	C16-C17-C13	2.35	105.86	103.55
20	P	304	PGV	C02-O01-C1	2.35	123.57	117.79
26	T	101	CDL	OB8-CB7-OB9	-2.34	117.67	123.59
30	Z	101	DMU	O5-C4-C57	2.34	112.26	106.44
20	A	607	PGV	C5-C4-C3	-2.34	102.53	114.42
25	C	303	PEK	O13-P-O14	2.34	123.79	112.24
24	W	101	CHD	C18-C13-C17	2.33	114.86	111.21
20	P	304	PGV	O01-C1-O02	-2.33	118.06	123.70
30	M	101	DMU	O4-C7-C8	-2.33	104.97	110.35
26	P	306	CDL	C56-C55-C54	-2.33	102.62	114.42
26	P	306	CDL	CA6-OA8-CA7	2.32	125.72	117.12
24	G	102	CHD	C2-C1-C10	2.32	116.76	112.78
30	M	101	DMU	O4-C7-C5	2.31	115.69	110.35
24	W	101	CHD	C14-C13-C12	-2.30	105.26	107.40
28	V	101	PSC	C25-C24-C23	-2.30	102.75	114.42
21	B	301	TGL	OG3-CC1-OC1	-2.30	117.80	123.59
20	A	608	PGV	O03-C01-C02	2.29	115.11	108.43
26	P	306	CDL	OB8-CB6-CB4	-2.29	101.76	108.43
24	G	102	CHD	O7-C7-C6	-2.29	104.26	109.94
18	N	605[B]	HEA	C25-C23-C24	2.29	119.66	114.60
18	N	605[A]	HEA	CBD-CAD-C3D	-2.28	108.28	112.49
18	N	605[B]	HEA	CBD-CAD-C3D	-2.28	108.28	112.49
26	P	306	CDL	C54-C53-C52	-2.28	102.86	114.42
31	2	201	HEC	C3B-C4B-NB	-2.26	106.67	110.94
30	Z	101	DMU	C1-C2-C3	2.26	114.84	109.68
21	D	201	TGL	OG3-CG3-CG2	2.26	115.00	108.43
24	T	103	CHD	C6-C7-C8	2.26	113.89	111.48
26	G	101	CDL	C60-C59-C58	2.25	125.86	114.42
24	P	301	CHD	C18-C13-C14	2.25	114.73	111.21
21	L	101	TGL	CA5-CA4-CA3	-2.25	103.00	114.42
24	P	301	CHD	C14-C13-C12	-2.25	105.31	107.40
28	E	201	PSC	C02-O01-C1	2.24	123.32	117.79
21	L	101	TGL	CC4-CC3-CC2	-2.24	105.14	113.19
26	T	101	CDL	OA6-CA5-OA7	-2.24	118.29	123.70
24	C	307	CHD	C16-C17-C20	2.23	115.60	112.15

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	J	101	CHD	C11-C12-C13	2.22	113.52	111.24
21	D	201	TGL	C21-C20-CA9	2.21	125.66	114.42
24	W	101	CHD	C9-C11-C12	-2.20	111.39	114.30
21	Q	201	TGL	C21-C20-CA9	2.20	125.60	114.42
24	P	307	CHD	C21-C20-C22	-2.20	106.91	110.36
24	W	101	CHD	C19-C10-C5	-2.20	106.63	110.36
21	B	301	TGL	OG1-CA1-OA1	-2.20	118.04	123.59
20	P	305	PGV	O01-C1-O02	-2.20	118.39	123.70
18	N	605[A]	HEA	C21-C20-C19	2.19	120.19	112.98
20	C	305	PGV	O01-C02-C01	2.19	116.34	108.40
24	C	307	CHD	C2-C1-C10	2.19	116.53	112.78
21	L	101	TGL	OG3-CG3-CG2	2.18	114.79	108.43
24	C	301	CHD	C13-C14-C8	-2.18	111.96	114.74
24	C	301	CHD	C22-C23-C24	-2.17	108.92	113.59
26	C	306	CDL	C83-C82-C81	2.17	125.44	114.42
20	P	304	PGV	C22-C21-C20	-2.17	105.39	113.19
20	P	305	PGV	O04-C19-C20	-2.17	115.27	123.73
26	C	306	CDL	C39-C38-C37	2.16	125.40	114.42
28	V	101	PSC	C29-C28-C27	-2.16	103.47	114.42
24	C	307	CHD	C5-C4-C3	2.16	115.92	112.76
24	P	307	CHD	C5-C4-C3	-2.16	109.59	112.76
20	C	304	PGV	C03-C02-C01	-2.15	106.70	111.79
28	E	201	PSC	C21-C20-C19	-2.15	105.80	113.62
26	C	306	CDL	C40-C39-C38	2.14	125.28	114.42
24	G	102	CHD	C18-C13-C14	2.14	114.55	111.21
30	Z	101	DMU	C7-C8-C9	2.13	114.05	110.24
24	T	103	CHD	C1-C10-C9	-2.13	108.00	111.35
26	P	306	CDL	C82-C81-C80	2.13	125.24	114.42
26	T	101	CDL	C83-C82-C81	2.13	125.23	114.42
18	N	606	HEA	C16-C17-C18	2.13	118.88	111.88
26	T	101	CDL	OB7-CB5-C51	-2.13	115.44	123.73
24	P	301	CHD	C14-C8-C7	-2.12	108.99	111.81
24	T	103	CHD	C13-C14-C8	-2.12	112.03	114.74
26	T	101	CDL	OA6-CA4-CA6	2.12	116.08	108.40
24	P	307	CHD	O3-C3-C4	-2.12	105.63	109.85
26	G	101	CDL	CA6-OA8-CA7	2.11	124.95	117.12
20	A	607	PGV	C8-C9-C10	-2.11	104.58	113.79
26	G	101	CDL	C82-C81-C80	2.11	125.15	114.42
24	J	101	CHD	C14-C8-C9	-2.10	106.82	109.71
21	N	608	TGL	C10-CB9-CB8	2.10	125.10	114.42
18	N	605[A]	HEA	O11-C11-C3B	-2.09	105.97	112.00
18	N	605[B]	HEA	O11-C11-C3B	-2.09	105.97	112.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	N	606	HEA	C3C-C4C-NC	2.09	111.91	109.21
28	E	201	PSC	C03-C02-C01	-2.09	106.86	111.79
18	A	605	HEA	C3C-C4C-NC	2.08	111.90	109.21
24	T	103	CHD	C19-C10-C1	-2.08	104.91	108.26
31	1	201	HEC	C3C-C4C-NC	-2.08	107.02	110.94
21	B	301	TGL	C10-CB9-CB8	2.08	124.98	114.42
20	N	612	PGV	O01-C1-C2	2.08	115.98	111.50
20	C	305	PGV	C21-C20-C19	2.07	121.14	113.62
21	L	101	TGL	C16-C15-CC9	2.07	124.91	114.42
20	C	304	PGV	O14-P-O13	2.06	122.42	112.24
21	L	101	TGL	OC1-CC1-CC2	-2.05	115.73	123.73
18	A	604[B]	HEA	C21-C22-C23	-2.05	120.74	127.75
21	Q	201	TGL	OG2-CB1-OB1	-2.05	118.75	123.70
24	P	301	CHD	C23-C22-C20	2.05	117.48	114.72
26	G	101	CDL	C80-C79-C78	2.05	124.83	114.42
26	T	101	CDL	C79-C78-C77	2.04	124.80	114.42
24	G	102	CHD	C4-C3-C2	2.04	112.99	110.55
21	B	301	TGL	C16-C15-CC9	2.04	124.79	114.42
18	A	604[A]	HEA	C16-C17-C18	2.04	118.57	111.88
21	D	201	TGL	C16-C15-CC9	2.03	124.74	114.42
21	B	301	TGL	CA3-CA2-CA1	-2.03	106.24	113.62
26	T	101	CDL	C63-C62-C61	2.02	124.70	114.42
21	B	301	TGL	C15-CC9-CC8	2.02	124.66	114.42
18	N	605[B]	HEA	C21-C22-C23	-2.02	120.86	127.75
31	1	201	HEC	CMB-C2B-C1B	-2.01	125.37	128.46
24	G	102	CHD	C15-C14-C13	2.01	105.52	103.55
30	Z	101	DMU	O55-C2-C1	-2.00	105.72	110.35

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
18	N	606	HEA	ND
18	N	606	HEA	NB
18	A	605	HEA	ND
18	A	605	HEA	NB

All (735) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
26	C	306	CDL	CA2-C1-CB2-OB2
26	C	306	CDL	CA3-OA5-PA1-OA3
26	C	306	CDL	CA3-OA5-PA1-OA4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
26	C	306	CDL	OA7-CA5-OA6-CA4
26	C	306	CDL	CB3-OB5-PB2-OB2
26	C	306	CDL	C51-CB5-OB6-CB4
28	V	101	PSC	C03-O11-P-O12
28	V	101	PSC	C03-O11-P-O13
28	V	101	PSC	C03-O11-P-O14
28	V	101	PSC	C2-C1-O01-C02
28	V	101	PSC	C11-C12-C13-C14
26	G	101	CDL	CA2-OA2-PA1-OA3
26	G	101	CDL	CA2-OA2-PA1-OA4
26	G	101	CDL	C11-CA5-OA6-CA4
26	G	101	CDL	CB3-OB5-PB2-OB2
18	N	605[B]	HEA	C16-C17-C18-C19
18	N	605[B]	HEA	C19-C20-C21-C22
21	B	301	TGL	OB1-CB1-OG2-CG2
21	B	301	TGL	OG1-CG1-CG2-OG2
20	P	305	PGV	C03-O11-P-O12
20	P	305	PGV	C03-O11-P-O13
20	P	305	PGV	C03-O11-P-O14
20	P	305	PGV	O01-C02-C03-O11
20	P	305	PGV	O12-C04-C05-C06
20	P	305	PGV	C04-C05-C06-O06
26	P	306	CDL	CB2-OB2-PB2-OB3
26	P	306	CDL	CB2-OB2-PB2-OB4
26	P	306	CDL	CB3-OB5-PB2-OB3
26	P	306	CDL	CB3-OB5-PB2-OB4
24	J	101	CHD	C13-C17-C20-C22
24	J	101	CHD	C16-C17-C20-C21
24	J	101	CHD	C20-C22-C23-C24
21	N	608	TGL	OB1-CB1-OG2-CG2
21	N	608	TGL	OG1-CG1-CG2-OG2
21	N	608	TGL	CC2-CC1-OG3-CG3
21	N	608	TGL	OC1-CC1-OG3-CG3
21	Q	201	TGL	CB2-CB1-OG2-CG2
21	Q	201	TGL	OB1-CB1-OG2-CG2
26	T	101	CDL	CA2-OA2-PA1-OA3
26	T	101	CDL	CA3-OA5-PA1-OA3
26	T	101	CDL	CA3-OA5-PA1-OA4
26	T	101	CDL	C11-CA5-OA6-CA4
26	T	101	CDL	OA9-CA7-OA8-CA6
26	T	101	CDL	C31-CA7-OA8-CA6
26	T	101	CDL	C1-CB2-OB2-PB2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
26	T	101	CDL	CB3-OB5-PB2-OB3
21	D	201	TGL	OG1-CG1-CG2-OG2
21	D	201	TGL	CC2-CC1-OG3-CG3
21	D	201	TGL	OC1-CC1-OG3-CG3
28	E	201	PSC	C03-O11-P-O13
28	E	201	PSC	C04-O12-P-O13
28	E	201	PSC	C04-O12-P-O14
28	E	201	PSC	O12-C04-C05-N
28	E	201	PSC	C2-C1-O01-C02
28	E	201	PSC	C9-C10-C11-C12
24	W	101	CHD	C13-C17-C20-C22
24	W	101	CHD	C16-C17-C20-C21
24	W	101	CHD	C16-C17-C20-C22
20	C	305	PGV	C04-O12-P-O13
20	C	305	PGV	O01-C02-C03-O11
31	2	201	HEC	C2A-CAA-CBA-CGA
21	L	101	TGL	CB2-CB1-OG2-CG2
21	L	101	TGL	OB1-CB1-OG2-CG2
28	V	101	PSC	O04-C19-O03-C01
21	Q	201	TGL	OC1-CC1-OG3-CG3
21	Q	201	TGL	CC2-CC1-OG3-CG3
24	J	101	CHD	C16-C17-C20-C22
26	C	306	CDL	OB7-CB5-OB6-CB4
28	V	101	PSC	O02-C1-O01-C02
28	E	201	PSC	O02-C1-O01-C02
28	V	101	PSC	C20-C19-O03-C01
26	C	306	CDL	C11-CA5-OA6-CA4
21	N	608	TGL	CB2-CB1-OG2-CG2
26	P	306	CDL	C61-C62-C63-C64
20	A	607	PGV	C20-C19-O03-C01
26	T	101	CDL	C71-CB7-OB8-CB6
20	A	607	PGV	C10-C11-C12-C13
20	C	304	PGV	C10-C11-C12-C13
25	C	303	PEK	C13-C14-C15-C16
26	T	101	CDL	C79-C80-C81-C82
26	G	101	CDL	OA7-CA5-OA6-CA4
26	T	101	CDL	OA7-CA5-OA6-CA4
20	A	607	PGV	O04-C19-O03-C01
26	C	306	CDL	O1-C1-CB2-OB2
26	G	101	CDL	O1-C1-CA2-OA2
20	P	305	PGV	O12-C04-C05-O05
28	E	201	PSC	C20-C19-O03-C01

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	B	301	TGL	CB2-CB1-OG2-CG2
20	P	305	PGV	C2-C1-O01-C02
28	V	101	PSC	C26-C27-C28-C29
26	T	101	CDL	C22-C23-C24-C25
20	P	304	PGV	C28-C29-C30-C31
30	Z	101	DMU	C19-C22-C25-C28
21	D	201	TGL	CA9-C20-C21-C22
21	B	301	TGL	C15-C16-C17-C18
24	W	101	CHD	C17-C20-C22-C23
26	P	306	CDL	C58-C59-C60-C61
26	G	101	CDL	CB4-CB3-OB5-PB2
26	T	101	CDL	OB9-CB7-OB8-CB6
28	E	201	PSC	O04-C19-O03-C01
21	L	101	TGL	C12-C13-C14-C29
18	N	605[B]	HEA	C15-C16-C17-C18
18	A	604[B]	HEA	C19-C20-C21-C22
18	A	604[A]	HEA	C19-C20-C21-C22
26	T	101	CDL	C51-CB5-OB6-CB4
26	T	101	CDL	C17-C18-C19-C20
28	E	201	PSC	C04-C05-N-C06
21	B	301	TGL	CC2-CC1-OG3-CG3
28	E	201	PSC	C6-C7-C8-C9
20	C	305	PGV	C1-C2-C3-C4
30	M	101	DMU	O6-C11-C9-O1
24	C	307	CHD	C17-C20-C22-C23
26	T	101	CDL	O1-C1-CB2-OB2
28	V	101	PSC	C29-C30-C31-C32
20	P	305	PGV	O02-C1-O01-C02
21	L	101	TGL	C23-C24-C25-C26
21	B	301	TGL	OC1-CC1-OG3-CG3
24	P	307	CHD	C17-C20-C22-C23
24	C	307	CHD	C21-C20-C22-C23
21	N	608	TGL	CA1-CA2-CA3-CA4
26	T	101	CDL	CB7-C71-C72-C73
21	L	101	TGL	C20-C21-C22-C23
24	J	101	CHD	C13-C17-C20-C21
26	C	306	CDL	CB7-C71-C72-C73
26	G	101	CDL	CB5-C51-C52-C53
21	B	301	TGL	CB1-CB2-CB3-CB4
26	P	306	CDL	CA7-C31-C32-C33
21	D	201	TGL	CC1-CC2-CC3-CC4
21	L	101	TGL	CA2-CA1-OG1-CG1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
24	P	307	CHD	C21-C20-C22-C23
28	V	101	PSC	C19-C20-C21-C22
21	D	201	TGL	CB1-CB2-CB3-CB4
30	M	101	DMU	O6-C11-C9-C8
21	N	608	TGL	C10-C11-C12-C13
24	W	101	CHD	C21-C20-C22-C23
21	L	101	TGL	CA9-C20-C21-C22
26	T	101	CDL	OB7-CB5-OB6-CB4
24	W	101	CHD	C13-C17-C20-C21
26	T	101	CDL	CA5-C11-C12-C13
20	A	608	PGV	C10-C11-C12-C13
25	P	303	PEK	C7-C8-C9-C10
28	E	201	PSC	C11-C10-C9-C8
26	C	306	CDL	CA3-OA5-PA1-OA2
20	A	607	PGV	C03-O11-P-O12
26	G	101	CDL	CA2-OA2-PA1-OA5
26	G	101	CDL	CA3-OA5-PA1-OA2
20	P	305	PGV	C04-O12-P-O11
26	P	306	CDL	CB2-OB2-PB2-OB5
26	P	306	CDL	CB3-OB5-PB2-OB2
26	T	101	CDL	CA3-OA5-PA1-OA2
26	T	101	CDL	CB3-OB5-PB2-OB2
28	E	201	PSC	C03-O11-P-O12
28	E	201	PSC	C04-O12-P-O11
20	C	305	PGV	C04-O12-P-O11
21	Q	201	TGL	C20-C21-C22-C23
26	G	101	CDL	CB2-C1-CA2-OA2
26	T	101	CDL	CA2-C1-CB2-OB2
30	Z	101	DMU	O16-C18-C19-C22
20	N	612	PGV	C26-C27-C28-C29
28	E	201	PSC	C04-C05-N-C07
28	E	201	PSC	C04-C05-N-C08
24	P	307	CHD	C20-C22-C23-C24
21	D	201	TGL	CB9-C10-C11-C12
28	V	101	PSC	C4-C5-C6-C7
26	P	306	CDL	C59-C60-C61-C62
21	Q	201	TGL	CC9-C15-C16-C17
26	C	306	CDL	C59-C60-C61-C62
20	A	607	PGV	C20-C21-C22-C23
25	P	303	PEK	C26-C27-C28-C29
21	Q	201	TGL	CB9-C10-C11-C12
21	Q	201	TGL	C13-C14-C29-C30

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
26	T	101	CDL	C31-C32-C33-C34
21	D	201	TGL	C17-C18-C19-C33
21	D	201	TGL	C18-C19-C33-C34
26	G	101	CDL	C72-C73-C74-C75
20	P	305	PGV	C20-C21-C22-C23
26	P	306	CDL	C21-C22-C23-C24
21	N	608	TGL	CA5-CA6-CA7-CA8
21	D	201	TGL	CG3-CG2-OG2-CB1
26	G	101	CDL	C42-C43-C44-C45
26	G	101	CDL	C76-C77-C78-C79
21	B	301	TGL	CC4-CC5-CC6-CC7
26	P	306	CDL	C37-C38-C39-C40
21	Q	201	TGL	CA7-CA8-CA9-C20
21	Q	201	TGL	CB7-CB8-CB9-C10
26	C	306	CDL	C12-C13-C14-C15
26	C	306	CDL	C20-C21-C22-C23
26	G	101	CDL	C12-C13-C14-C15
20	P	305	PGV	C5-C6-C7-C8
26	P	306	CDL	C56-C57-C58-C59
25	C	303	PEK	C28-C29-C30-C31
26	T	101	CDL	C58-C59-C60-C61
21	D	201	TGL	C23-C24-C25-C26
21	L	101	TGL	CC3-CC4-CC5-CC6
26	C	306	CDL	C82-C83-C84-C85
21	B	301	TGL	C11-C10-CB9-CB8
21	B	301	TGL	C22-C23-C24-C25
20	P	305	PGV	C6-C7-C8-C9
21	Q	201	TGL	CC3-CC4-CC5-CC6
21	Q	201	TGL	C17-C18-C19-C33
26	T	101	CDL	C38-C39-C40-C41
21	L	101	TGL	CB7-CB8-CB9-C10
21	L	101	TGL	C19-C33-C34-C35
25	C	303	PEK	C21-C22-C23-C24
21	L	101	TGL	CC1-CC2-CC3-CC4
20	P	304	PGV	C24-C25-C26-C27
21	B	301	TGL	CA4-CA5-CA6-CA7
20	P	305	PGV	C30-C31-C32-C33
26	P	306	CDL	C62-C63-C64-C65
21	N	608	TGL	CC6-CC7-CC8-CC9
28	E	201	PSC	C27-C28-C29-C30
21	L	101	TGL	OA1-CA1-OG1-CG1
26	C	306	CDL	C76-C77-C78-C79

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
26	G	101	CDL	C19-C20-C21-C22
26	G	101	CDL	C61-C62-C63-C64
26	P	306	CDL	C40-C41-C42-C43
26	P	306	CDL	C81-C82-C83-C84
21	N	608	TGL	CC4-CC5-CC6-CC7
26	C	306	CDL	C13-C14-C15-C16
26	C	306	CDL	C31-C32-C33-C34
26	C	306	CDL	C63-C64-C65-C66
25	P	303	PEK	C28-C29-C30-C31
26	P	306	CDL	C73-C74-C75-C76
21	N	608	TGL	CB7-CB8-CB9-C10
21	N	608	TGL	CC5-CC6-CC7-CC8
21	Q	201	TGL	C10-C11-C12-C13
21	L	101	TGL	CB3-CB4-CB5-CB6
21	L	101	TGL	C21-C22-C23-C24
26	C	306	CDL	C21-C22-C23-C24
26	P	306	CDL	C43-C44-C45-C46
21	N	608	TGL	C23-C24-C25-C26
21	Q	201	TGL	CB6-CB7-CB8-CB9
26	T	101	CDL	C40-C41-C42-C43
30	M	101	DMU	C22-C25-C28-C31
20	A	607	PGV	O02-C1-O01-C02
26	P	306	CDL	OB7-CB5-OB6-CB4
26	P	306	CDL	C51-CB5-OB6-CB4
26	C	306	CDL	C81-C82-C83-C84
28	V	101	PSC	C14-C15-C16-C17
28	E	201	PSC	C1-C2-C3-C4
26	C	306	CDL	C17-C18-C19-C20
20	N	612	PGV	C29-C30-C31-C32
20	P	304	PGV	C25-C26-C27-C28
28	V	101	PSC	C2-C3-C4-C5
21	N	608	TGL	CA3-CA4-CA5-CA6
21	N	608	TGL	C11-C12-C13-C14
21	Q	201	TGL	CA6-CA7-CA8-CA9
26	T	101	CDL	C82-C83-C84-C85
20	C	305	PGV	C28-C29-C30-C31
21	L	101	TGL	CB4-CB5-CB6-CB7
21	L	101	TGL	CC4-CC5-CC6-CC7
26	C	306	CDL	C71-C72-C73-C74
26	G	101	CDL	C82-C83-C84-C85
20	C	304	PGV	C29-C30-C31-C32
21	B	301	TGL	CA9-C20-C21-C22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	N	608	TGL	CA2-CA3-CA4-CA5
21	Q	201	TGL	CA4-CA5-CA6-CA7
25	C	303	PEK	C34-C35-C36-C37
20	A	607	PGV	C14-C15-C16-C17
20	A	607	PGV	C27-C28-C29-C30
20	C	304	PGV	C24-C25-C26-C27
21	Q	201	TGL	CC5-CC6-CC7-CC8
20	C	304	PGV	C14-C15-C16-C17
21	B	301	TGL	CB9-C10-C11-C12
21	N	608	TGL	C12-C13-C14-C29
21	Q	201	TGL	C23-C24-C25-C26
20	A	607	PGV	C23-C24-C25-C26
21	B	301	TGL	CB7-CB8-CB9-C10
21	B	301	TGL	C20-C21-C22-C23
21	L	101	TGL	CB6-CB7-CB8-CB9
26	C	306	CDL	C22-C23-C24-C25
20	A	607	PGV	C29-C30-C31-C32
26	T	101	CDL	C59-C60-C61-C62
20	C	305	PGV	C2-C3-C4-C5
20	C	305	PGV	C6-C7-C8-C9
26	T	101	CDL	C52-C53-C54-C55
21	D	201	TGL	C21-C22-C23-C24
20	P	305	PGV	C23-C24-C25-C26
21	N	608	TGL	C13-C14-C29-C30
26	T	101	CDL	CA7-C31-C32-C33
20	C	305	PGV	C19-C20-C21-C22
20	A	607	PGV	C2-C1-O01-C02
20	P	305	PGV	C26-C27-C28-C29
26	P	306	CDL	C80-C81-C82-C83
20	P	305	PGV	O05-C05-C06-O06
26	G	101	CDL	C14-C15-C16-C17
25	C	303	PEK	C16-C17-C18-C19
26	P	306	CDL	C51-C52-C53-C54
21	Q	201	TGL	CB2-CB3-CB4-CB5
26	P	306	CDL	C82-C83-C84-C85
26	C	306	CDL	C43-C44-C45-C46
26	P	306	CDL	C35-C36-C37-C38
21	D	201	TGL	CA6-CA7-CA8-CA9
23	E	202	EDO	O1-C1-C2-O2
28	V	101	PSC	C30-C31-C32-C33
20	C	305	PGV	C7-C8-C9-C10
20	C	305	PGV	C23-C24-C25-C26

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	L	101	TGL	CB1-CB2-CB3-CB4
26	P	306	CDL	C41-C42-C43-C44
21	D	201	TGL	C21-C20-CA9-CA8
26	G	101	CDL	C11-C12-C13-C14
20	C	305	PGV	C14-C15-C16-C17
21	L	101	TGL	CB2-CB3-CB4-CB5
26	T	101	CDL	C57-C58-C59-C60
20	C	305	PGV	C11-C10-C9-C8
26	C	306	CDL	C71-CB7-OB8-CB6
25	P	303	PEK	C23-C24-C25-C26
26	C	306	CDL	C33-C34-C35-C36
26	T	101	CDL	C71-C72-C73-C74
20	C	304	PGV	C30-C31-C32-C33
28	V	101	PSC	C5-C6-C7-C8
28	V	101	PSC	C28-C29-C30-C31
26	P	306	CDL	C79-C80-C81-C82
26	C	306	CDL	C38-C39-C40-C41
26	P	306	CDL	C23-C24-C25-C26
26	C	306	CDL	C31-CA7-OA8-CA6
26	G	101	CDL	C71-CB7-OB8-CB6
18	A	604[B]	HEA	C15-C16-C17-C18
20	N	612	PGV	C13-C14-C15-C16
26	T	101	CDL	C20-C21-C22-C23
26	G	101	CDL	C51-CB5-OB6-CB4
26	P	306	CDL	C76-C77-C78-C79
20	C	305	PGV	C24-C25-C26-C27
26	T	101	CDL	OB6-CB4-CB6-OB8
26	T	101	CDL	C60-C61-C62-C63
20	P	304	PGV	C29-C30-C31-C32
26	T	101	CDL	C37-C38-C39-C40
20	P	305	PGV	C11-C10-C9-C8
20	P	304	PGV	C1-C2-C3-C4
20	P	304	PGV	C27-C28-C29-C30
26	C	306	CDL	C15-C16-C17-C18
26	C	306	CDL	C41-C42-C43-C44
21	L	101	TGL	C22-C23-C24-C25
26	T	101	CDL	C56-C57-C58-C59
21	B	301	TGL	CC7-CC8-CC9-C15
26	C	306	CDL	OA9-CA7-OA8-CA6
26	G	101	CDL	OB7-CB5-OB6-CB4
26	C	306	CDL	C14-C15-C16-C17
26	C	306	CDL	C56-C57-C58-C59

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	A	607	PGV	C22-C23-C24-C25
21	L	101	TGL	C11-C12-C13-C14
26	C	306	CDL	C1-CA2-OA2-PA1
20	A	607	PGV	C02-C03-O11-P
20	P	304	PGV	C22-C23-C24-C25
20	C	304	PGV	C7-C8-C9-C10
21	D	201	TGL	CC6-CC7-CC8-CC9
26	C	306	CDL	CA7-C31-C32-C33
25	P	303	PEK	C1-C2-C3-C4
26	P	306	CDL	CB7-C71-C72-C73
28	E	201	PSC	C19-C20-C21-C22
28	E	201	PSC	C22-C23-C24-C25
21	L	101	TGL	CA1-CA2-CA3-CA4
26	G	101	CDL	C52-C53-C54-C55
26	T	101	CDL	C63-C64-C65-C66
26	G	101	CDL	CA2-C1-CB2-OB2
20	A	608	PGV	C13-C14-C15-C16
30	M	101	DMU	C25-C28-C31-C34
28	E	201	PSC	C26-C27-C28-C29
20	A	607	PGV	C25-C26-C27-C28
21	N	608	TGL	C29-C30-C31-C32
21	Q	201	TGL	C21-C22-C23-C24
21	B	301	TGL	OG1-CG1-CG2-CG3
20	P	305	PGV	C24-C25-C26-C27
26	P	306	CDL	CA3-CA4-CA6-OA8
21	N	608	TGL	CG1-CG2-CG3-OG3
21	Q	201	TGL	OG1-CG1-CG2-CG3
26	T	101	CDL	CA3-CA4-CA6-OA8
26	T	101	CDL	CB3-CB4-CB6-OB8
28	E	201	PSC	O03-C01-C02-C03
28	E	201	PSC	C2-C3-C4-C5
28	E	201	PSC	C24-C25-C26-C27
25	C	303	PEK	C7-C8-C9-C10
20	P	305	PGV	C31-C32-C33-C34
21	D	201	TGL	C29-C30-C31-C32
21	N	608	TGL	C25-C26-C27-C28
21	N	608	TGL	C14-C29-C30-C31
26	C	306	CDL	C83-C84-C85-C86
26	G	101	CDL	C44-C45-C46-C47
20	C	305	PGV	C25-C26-C27-C28
20	C	304	PGV	C27-C28-C29-C30
26	P	306	CDL	C38-C39-C40-C41

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
26	P	306	CDL	C78-C79-C80-C81
21	B	301	TGL	CB5-CB6-CB7-CB8
21	N	608	TGL	CC2-CC3-CC4-CC5
26	G	101	CDL	C58-C59-C60-C61
30	M	101	DMU	C34-C37-C40-C43
21	B	301	TGL	CA2-CA1-OG1-CG1
20	N	612	PGV	C4-C5-C6-C7
20	P	305	PGV	C15-C16-C17-C18
25	C	303	PEK	C17-C18-C19-C20
28	V	101	PSC	C01-C02-O01-C1
28	E	201	PSC	C01-C02-O01-C1
26	P	306	CDL	C13-C14-C15-C16
28	V	101	PSC	C21-C22-C23-C24
20	C	304	PGV	C15-C16-C17-C18
26	C	306	CDL	OB5-CB3-CB4-OB6
20	C	304	PGV	C26-C27-C28-C29
28	V	101	PSC	C15-C16-C17-C18
21	D	201	TGL	CA5-CA6-CA7-CA8
26	C	306	CDL	OB9-CB7-OB8-CB6
20	C	305	PGV	C27-C28-C29-C30
25	C	303	PEK	C15-C16-C17-C18
26	P	306	CDL	C11-CA5-OA6-CA4
26	P	306	CDL	C31-C32-C33-C34
21	Q	201	TGL	CC7-CC8-CC9-C15
26	G	101	CDL	OB6-CB4-CB6-OB8
21	N	608	TGL	OG2-CG2-CG3-OG3
28	E	201	PSC	C28-C29-C30-C31
26	G	101	CDL	OB9-CB7-OB8-CB6
26	G	101	CDL	C60-C61-C62-C63
20	C	304	PGV	C13-C14-C15-C16
21	N	608	TGL	CA7-CA8-CA9-C20
20	A	607	PGV	C31-C32-C33-C34
20	C	304	PGV	C31-C32-C33-C34
26	T	101	CDL	C64-C65-C66-C67
20	N	612	PGV	C14-C15-C16-C17
20	A	607	PGV	C2-C3-C4-C5
28	V	101	PSC	C27-C28-C29-C30
28	E	201	PSC	C31-C32-C33-C34
20	N	612	PGV	C12-C13-C14-C15
25	C	303	PEK	C4-C5-C6-C7
26	C	306	CDL	C53-C54-C55-C56
21	N	608	TGL	C16-C17-C18-C19

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
26	C	306	CDL	OB5-CB3-CB4-CB6
26	G	101	CDL	OB5-CB3-CB4-CB6
20	P	305	PGV	C01-C02-C03-O11
25	P	303	PEK	C27-C28-C29-C30
21	Q	201	TGL	C11-C12-C13-C14
21	D	201	TGL	CA3-CA4-CA5-CA6
25	C	303	PEK	O12-C04-C05-N
28	V	101	PSC	C25-C26-C27-C28
25	P	303	PEK	C16-C17-C18-C19
26	P	306	CDL	C63-C64-C65-C66
21	D	201	TGL	CC3-CC4-CC5-CC6
26	P	306	CDL	O1-C1-CA2-OA2
21	B	301	TGL	OA1-CA1-OG1-CG1
26	T	101	CDL	C55-C56-C57-C58
21	L	101	TGL	C24-C25-C26-C27
26	C	306	CDL	C34-C35-C36-C37
28	E	201	PSC	C23-C24-C25-C26
21	L	101	TGL	C21-C20-CA9-CA8
20	P	304	PGV	C02-C03-O11-P
28	V	101	PSC	C02-C03-O11-P
21	B	301	TGL	CA5-CA6-CA7-CA8
20	P	305	PGV	C22-C23-C24-C25
21	B	301	TGL	CB3-CB4-CB5-CB6
25	C	303	PEK	C32-C33-C34-C35
26	P	306	CDL	CB3-CB4-CB6-OB8
21	N	608	TGL	OG1-CG1-CG2-CG3
21	D	201	TGL	OG1-CG1-CG2-CG3
21	L	101	TGL	OG1-CG1-CG2-CG3
21	B	301	TGL	C11-C12-C13-C14
21	L	101	TGL	C29-C30-C31-C32
26	G	101	CDL	CA7-C31-C32-C33
20	N	612	PGV	C10-C11-C12-C13
25	P	303	PEK	C4-C5-C6-C7
20	N	612	PGV	C31-C32-C33-C34
26	G	101	CDL	C75-C76-C77-C78
26	T	101	CDL	C41-C42-C43-C44
21	L	101	TGL	C33-C34-C35-C36
28	V	101	PSC	C20-C21-C22-C23
26	P	306	CDL	C15-C16-C17-C18
21	N	608	TGL	CB4-CB5-CB6-CB7
26	G	101	CDL	C37-C38-C39-C40
21	L	101	TGL	C13-C14-C29-C30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	B	301	TGL	CA3-CA4-CA5-CA6
26	C	306	CDL	CB4-CB6-OB8-CB7
26	C	306	CDL	C35-C36-C37-C38
20	A	608	PGV	C31-C32-C33-C34
28	V	101	PSC	C9-C10-C11-C12
28	E	201	PSC	C10-C11-C12-C13
26	G	101	CDL	C23-C24-C25-C26
20	C	305	PGV	O05-C05-C06-O06
21	N	608	TGL	CB1-CB2-CB3-CB4
21	B	301	TGL	C24-C25-C26-C27
21	Q	201	TGL	OG1-CA1-CA2-CA3
21	Q	201	TGL	C19-C33-C34-C35
26	P	306	CDL	OB6-CB4-CB6-OB8
21	Q	201	TGL	OG1-CG1-CG2-OG2
28	E	201	PSC	O03-C01-C02-O01
21	L	101	TGL	OG2-CG2-CG3-OG3
21	D	201	TGL	C11-C12-C13-C14
25	P	303	PEK	C33-C34-C35-C36
25	C	303	PEK	C26-C27-C28-C29
26	C	306	CDL	C79-C80-C81-C82
26	P	306	CDL	C74-C75-C76-C77
30	Z	101	DMU	C18-C19-C22-C25
24	C	307	CHD	C20-C22-C23-C24
26	P	306	CDL	C60-C61-C62-C63
21	L	101	TGL	C11-C10-CB9-CB8
20	C	305	PGV	C01-C02-C03-O11
24	G	102	CHD	C17-C20-C22-C23
21	D	201	TGL	C11-C10-CB9-CB8
21	L	101	TGL	C10-C11-C12-C13
25	C	303	PEK	C10-C11-C12-C13
26	P	306	CDL	C57-C58-C59-C60
20	C	304	PGV	C12-C13-C14-C15
26	P	306	CDL	OA7-CA5-OA6-CA4
28	E	201	PSC	C4-C5-C6-C7
20	A	607	PGV	O03-C01-C02-C03
26	T	101	CDL	CB4-CB3-OB5-PB2
21	D	201	TGL	CG1-CG2-CG3-OG3
20	A	607	PGV	C15-C16-C17-C18
28	V	101	PSC	O01-C02-C03-O11
26	G	101	CDL	OB5-CB3-CB4-OB6
21	Q	201	TGL	CA2-CA3-CA4-CA5
26	T	101	CDL	C54-C55-C56-C57

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
20	P	304	PGV	C11-C12-C13-C14
26	P	306	CDL	CB2-C1-CA2-OA2
20	P	304	PGV	C7-C8-C9-C10
26	P	306	CDL	C75-C76-C77-C78
26	C	306	CDL	OB6-CB4-CB6-OB8
20	A	607	PGV	O03-C01-C02-O01
26	C	306	CDL	C60-C61-C62-C63
26	P	306	CDL	C34-C35-C36-C37
26	C	306	CDL	C16-C17-C18-C19
26	T	101	CDL	C14-C15-C16-C17
26	C	306	CDL	C61-C62-C63-C64
21	D	201	TGL	C25-C26-C27-C28
21	B	301	TGL	CB6-CB7-CB8-CB9
25	P	303	PEK	C10-C11-C12-C13
26	P	306	CDL	C17-C18-C19-C20
21	L	101	TGL	CA4-CA5-CA6-CA7
21	L	101	TGL	C16-C15-CC9-CC8
20	C	305	PGV	C3-C4-C5-C6
26	T	101	CDL	C78-C79-C80-C81
21	L	101	TGL	C17-C18-C19-C33
20	A	608	PGV	C12-C13-C14-C15
26	G	101	CDL	CB2-OB2-PB2-OB5
21	D	201	TGL	CA2-CA3-CA4-CA5
30	M	101	DMU	C19-C22-C25-C28
20	P	305	PGV	C02-C03-O11-P
26	P	306	CDL	CA4-CA3-OA5-PA1
26	C	306	CDL	C36-C37-C38-C39
25	C	303	PEK	C33-C34-C35-C36
26	C	306	CDL	CB3-OB5-PB2-OB3
20	A	607	PGV	C03-O11-P-O13
26	G	101	CDL	CA3-OA5-PA1-OA3
26	G	101	CDL	CB2-OB2-PB2-OB4
26	G	101	CDL	CB3-OB5-PB2-OB4
20	P	305	PGV	C04-O12-P-O13
26	P	306	CDL	CA2-OA2-PA1-OA3
26	T	101	CDL	CB3-OB5-PB2-OB4
20	C	305	PGV	C04-O12-P-O14
26	G	101	CDL	C77-C78-C79-C80
25	P	303	PEK	C22-C21-O03-C01
28	V	101	PSC	C01-C02-C03-O11
26	G	101	CDL	C32-C31-CA7-OA8
24	C	307	CHD	C16-C17-C20-C21

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
26	G	101	CDL	C16-C17-C18-C19
28	E	201	PSC	C05-C04-O12-P
28	E	201	PSC	C3-C4-C5-C6
21	L	101	TGL	CA2-CA3-CA4-CA5
20	A	608	PGV	C27-C28-C29-C30
21	B	301	TGL	CA6-CA7-CA8-CA9
25	C	303	PEK	C23-C24-C25-C26
26	G	101	CDL	O1-C1-CB2-OB2
26	G	101	CDL	C59-C60-C61-C62
26	G	101	CDL	CB3-CB4-CB6-OB8
31	2	201	HEC	C1A-C2A-CAA-CBA
31	2	201	HEC	C3A-C2A-CAA-CBA
28	V	101	PSC	O03-C01-C02-O01
26	P	306	CDL	OA6-CA4-CA6-OA8
26	T	101	CDL	OA6-CA4-CA6-OA8
21	D	201	TGL	OG2-CG2-CG3-OG3
26	P	306	CDL	C12-C13-C14-C15
21	Q	201	TGL	C14-C29-C30-C31
20	C	304	PGV	C02-C03-O11-P
25	P	303	PEK	C17-C18-C19-C20
21	D	201	TGL	C20-C21-C22-C23
20	C	304	PGV	C25-C26-C27-C28
20	P	305	PGV	C21-C22-C23-C24
20	P	305	PGV	C27-C28-C29-C30
25	P	303	PEK	C21-C22-C23-C24
21	N	608	TGL	CC7-CC8-CC9-C15
21	D	201	TGL	C10-C11-C12-C13
28	E	201	PSC	O03-C19-C20-C21
20	A	607	PGV	C21-C22-C23-C24
25	C	303	PEK	C24-C25-C26-C27
21	B	301	TGL	CG1-CG2-OG2-CB1
20	A	607	PGV	C01-C02-C03-O11
18	N	606	HEA	C11-C12-C13-C14
20	C	304	PGV	C1-C2-C3-C4
21	Q	201	TGL	CA5-CA6-CA7-CA8
26	P	306	CDL	CB4-CB6-OB8-CB7
20	A	608	PGV	C02-C01-O03-C19
21	B	301	TGL	C21-C22-C23-C24
20	C	305	PGV	C31-C32-C33-C34
21	L	101	TGL	OG1-CG1-CG2-OG2
20	A	607	PGV	C04-O12-P-O11
26	P	306	CDL	CA3-OA5-PA1-OA2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
26	T	101	CDL	CB2-OB2-PB2-OB5
20	C	305	PGV	C03-O11-P-O12
26	C	306	CDL	CA3-CA4-CA6-OA8
21	B	301	TGL	CG1-CG2-CG3-OG3
21	L	101	TGL	CG1-CG2-CG3-OG3
26	T	101	CDL	C12-C13-C14-C15
26	C	306	CDL	C75-C76-C77-C78
25	P	303	PEK	C35-C36-C37-C38
28	E	201	PSC	C14-C15-C16-C17
26	C	306	CDL	C44-C45-C46-C47
20	C	304	PGV	C05-C04-O12-P
20	A	607	PGV	O01-C1-C2-C3
26	G	101	CDL	C81-C82-C83-C84
20	P	304	PGV	C11-C10-C9-C8
20	C	305	PGV	C10-C11-C12-C13
21	Q	201	TGL	CB3-CB4-CB5-CB6
18	N	605[A]	HEA	C19-C20-C21-C22
21	D	201	TGL	CC5-CC6-CC7-CC8
20	A	607	PGV	C11-C10-C9-C8
21	L	101	TGL	C16-C17-C18-C19
26	T	101	CDL	O1-C1-CA2-OA2
26	P	306	CDL	C1-CB2-OB2-PB2
26	T	101	CDL	C1-CA2-OA2-PA1
21	L	101	TGL	CC2-CC3-CC4-CC5
20	P	304	PGV	C31-C32-C33-C34
21	D	201	TGL	CC7-CC8-CC9-C15
21	L	101	TGL	CC5-CC6-CC7-CC8
26	T	101	CDL	C53-C54-C55-C56
21	N	608	TGL	CG1-CG2-OG2-CB1
20	C	305	PGV	C15-C16-C17-C18
28	V	101	PSC	C3-C4-C5-C6
20	A	607	PGV	C9-C10-C11-C12
21	N	608	TGL	C11-C10-CB9-CB8
25	C	303	PEK	C6-C7-C8-C9
25	C	303	PEK	C9-C10-C11-C12
20	P	305	PGV	C25-C26-C27-C28
26	C	306	CDL	C1-CB2-OB2-PB2
20	A	607	PGV	O05-C05-C06-O06
20	A	607	PGV	C7-C8-C9-C10
20	P	305	PGV	C9-C10-C11-C12
26	C	306	CDL	C52-C53-C54-C55
26	G	101	CDL	C31-C32-C33-C34

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	D	201	TGL	C33-C34-C35-C36
21	D	201	TGL	OB1-CB1-OG2-CG2
21	L	101	TGL	CB9-C10-C11-C12
26	G	101	CDL	C51-C52-C53-C54
25	P	303	PEK	C31-C32-C33-C34
26	G	101	CDL	C73-C74-C75-C76
21	L	101	TGL	C14-C29-C30-C31
26	C	306	CDL	C74-C75-C76-C77
26	P	306	CDL	CA5-C11-C12-C13
25	P	303	PEK	C29-C30-C31-C32
28	E	201	PSC	C7-C8-C9-C10
26	P	306	CDL	C42-C43-C44-C45
26	P	306	CDL	C84-C85-C86-C87
26	T	101	CDL	OB5-CB3-CB4-CB6
26	P	306	CDL	C77-C78-C79-C80
26	G	101	CDL	C52-C51-CB5-OB6
21	L	101	TGL	OG1-CA1-CA2-CA3
21	N	608	TGL	CB9-C10-C11-C12
20	C	305	PGV	C05-C04-O12-P
20	A	608	PGV	C14-C15-C16-C17
21	D	201	TGL	C24-C25-C26-C27
21	B	301	TGL	C12-C13-C14-C29
21	Q	201	TGL	C24-C25-C26-C27
20	C	304	PGV	C11-C12-C13-C14
21	D	201	TGL	CA1-CA2-CA3-CA4
30	Z	101	DMU	C31-C34-C37-C40
28	V	101	PSC	C24-C25-C26-C27
28	V	101	PSC	C11-C10-C9-C8
26	P	306	CDL	C24-C25-C26-C27
20	P	305	PGV	C13-C14-C15-C16
26	T	101	CDL	C35-C36-C37-C38
21	D	201	TGL	CC4-CC5-CC6-CC7
26	P	306	CDL	C19-C20-C21-C22
26	T	101	CDL	C32-C31-CA7-OA8
25	P	303	PEK	C30-C31-C32-C33
25	P	303	PEK	O04-C21-O03-C01
20	C	304	PGV	C9-C10-C11-C12
25	C	303	PEK	C14-C15-C16-C17
26	C	306	CDL	CB3-CB4-CB6-OB8
21	Q	201	TGL	OA1-CA1-CA2-CA3
20	A	607	PGV	O01-C02-C03-O11
26	G	101	CDL	C84-C85-C86-C87

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
21	D	201	TGL	OG3-CC1-CC2-CC3
23	N	614	EDO	O1-C1-C2-O2
26	C	306	CDL	C77-C78-C79-C80
21	Q	201	TGL	CC6-CC7-CC8-CC9
20	C	305	PGV	O12-C04-C05-O05
20	A	608	PGV	C4-C5-C6-C7
26	G	101	CDL	C62-C63-C64-C65
26	P	306	CDL	C32-C31-CA7-OA8
28	V	101	PSC	C22-C23-C24-C25
26	G	101	CDL	C39-C40-C41-C42
20	P	305	PGV	C1-C2-C3-C4
25	P	303	PEK	C15-C16-C17-C18
20	A	608	PGV	O03-C19-C20-C21
21	L	101	TGL	OG2-CB1-CB2-CB3
21	L	101	TGL	C25-C26-C27-C28
21	N	608	TGL	CA9-C20-C21-C22
26	P	306	CDL	C22-C23-C24-C25
20	C	305	PGV	C04-C05-C06-O06
21	B	301	TGL	C16-C15-CC9-CC8
20	C	305	PGV	O12-C04-C05-C06
21	B	301	TGL	CC6-CC7-CC8-CC9
26	T	101	CDL	C32-C31-CA7-OA9
28	V	101	PSC	C7-C8-C9-C10
28	V	101	PSC	O03-C01-C02-C03
26	P	306	CDL	C72-C73-C74-C75
24	C	307	CHD	C13-C17-C20-C21
21	D	201	TGL	OC1-CC1-CC2-CC3
18	A	605	HEA	C26-C15-C16-C17
26	P	306	CDL	C32-C31-CA7-OA9
26	C	306	CDL	CB2-OB2-PB2-OB3
26	C	306	CDL	CB3-OB5-PB2-OB4
20	A	607	PGV	C04-O12-P-O13
28	V	101	PSC	C04-O12-P-O13
26	P	306	CDL	CA2-OA2-PA1-OA4
23	C	311	EDO	O1-C1-C2-O2
23	B	303	EDO	O1-C1-C2-O2
21	L	101	TGL	OB1-CB1-CB2-CB3
26	P	306	CDL	OB9-CB7-OB8-CB6
26	G	101	CDL	C55-C56-C57-C58
26	G	101	CDL	C79-C80-C81-C82
20	A	608	PGV	C19-C20-C21-C22
26	T	101	CDL	C12-C11-CA5-OA6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
26	G	101	CDL	C21-C22-C23-C24
21	Q	201	TGL	C15-C16-C17-C18
24	C	307	CHD	C16-C17-C20-C22
26	T	101	CDL	C19-C20-C21-C22
26	C	306	CDL	C52-C51-CB5-OB6
20	C	305	PGV	O01-C1-C2-C3
26	G	101	CDL	C80-C81-C82-C83
20	C	304	PGV	C28-C29-C30-C31
20	N	612	PGV	O03-C19-C20-C21
21	Q	201	TGL	C25-C26-C27-C28
20	A	608	PGV	C11-C10-C9-C8
25	P	303	PEK	C25-C26-C27-C28
26	T	101	CDL	C12-C11-CA5-OA7
20	A	608	PGV	C9-C10-C11-C12
20	C	305	PGV	C9-C10-C11-C12
25	C	303	PEK	C22-C23-C24-C25
20	C	305	PGV	O02-C1-C2-C3
21	D	201	TGL	OG1-CA1-CA2-CA3

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	P	307	CHD	C1-C10-C2-C3-C4-C5

38 monomers are involved in 249 short contacts:

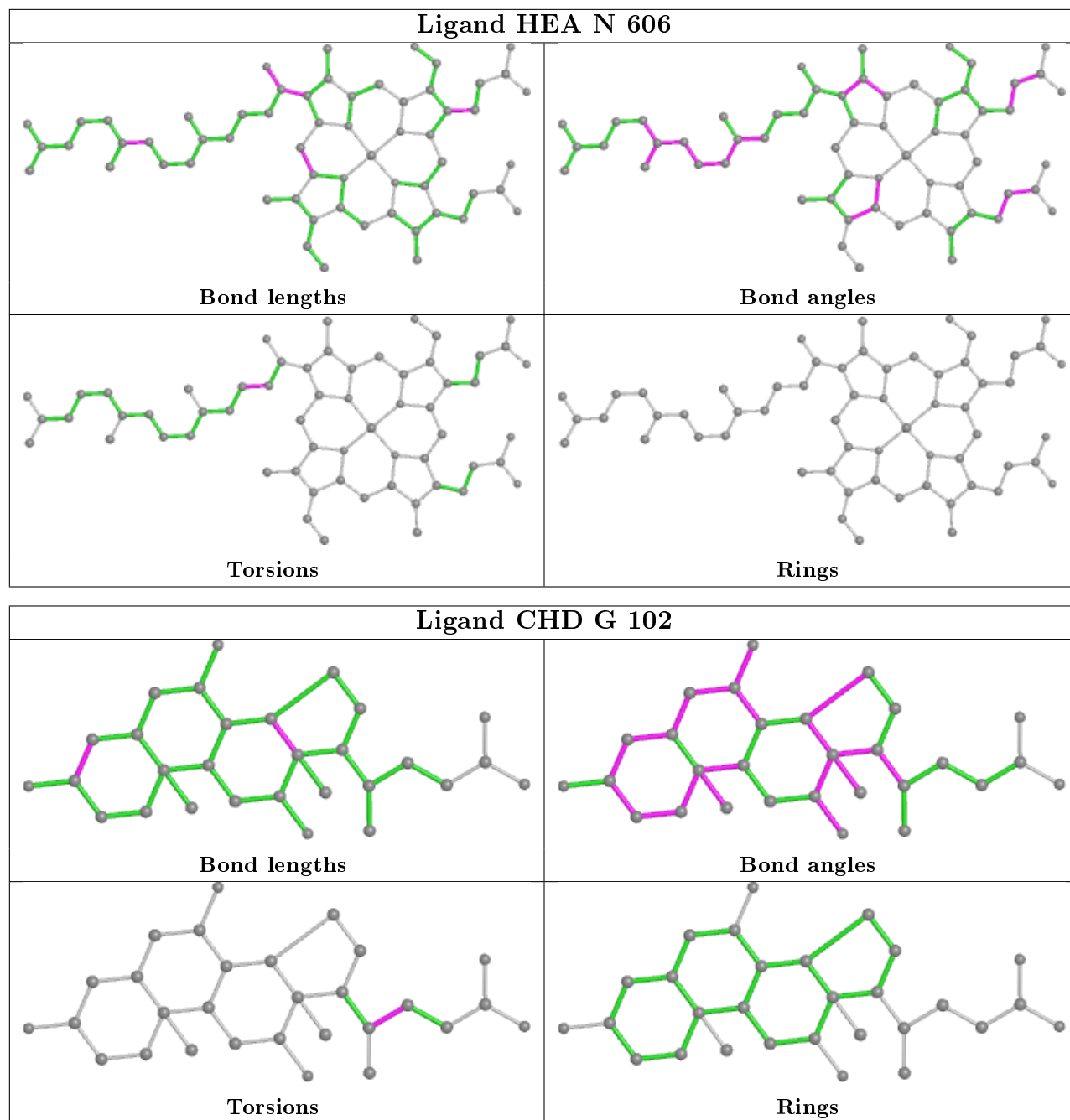
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	N	606	HEA	3	0
26	C	306	CDL	15	0
20	N	612	PGV	1	0
21	D	201	TGL	12	0
20	P	304	PGV	6	0
20	A	607	PGV	5	0
24	P	301	CHD	1	0
28	V	101	PSC	21	0
21	B	301	TGL	6	0
18	N	605[A]	HEA	1	0
26	G	101	CDL	23	0
18	N	605[B]	HEA	6	0
20	C	304	PGV	5	0
24	C	307	CHD	3	0
24	T	103	CHD	1	0

*Continued on next page...*

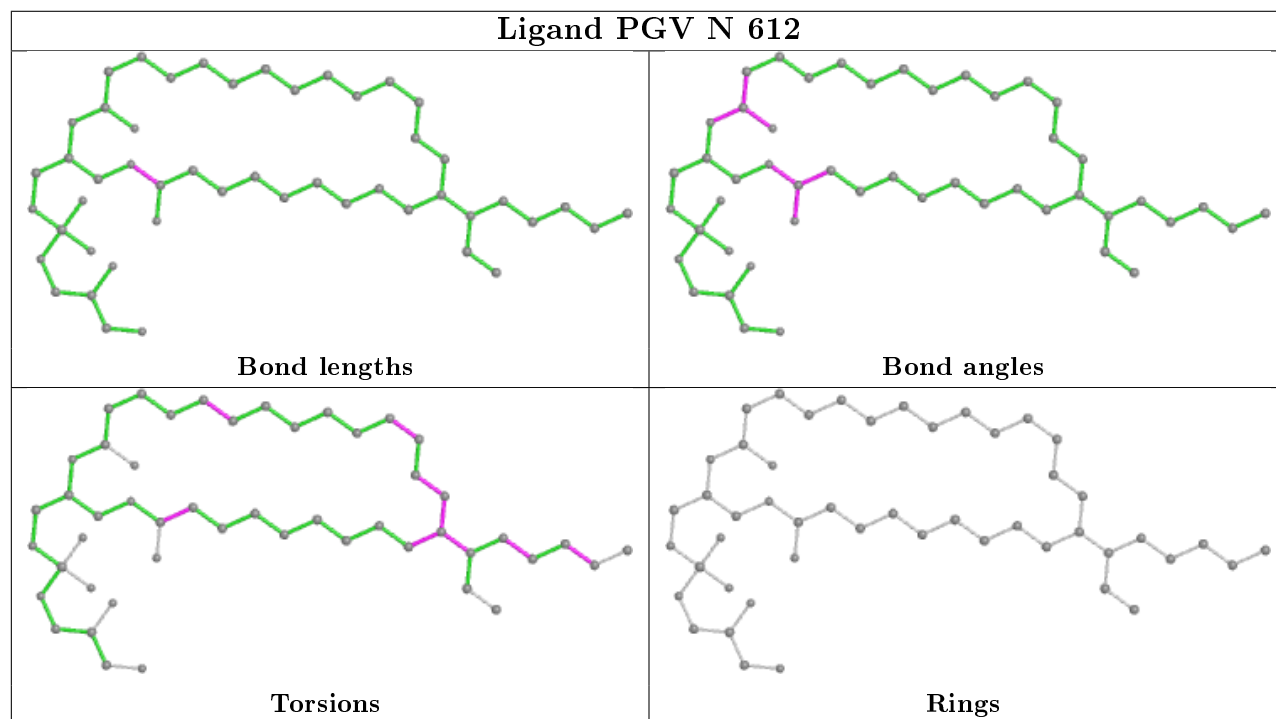
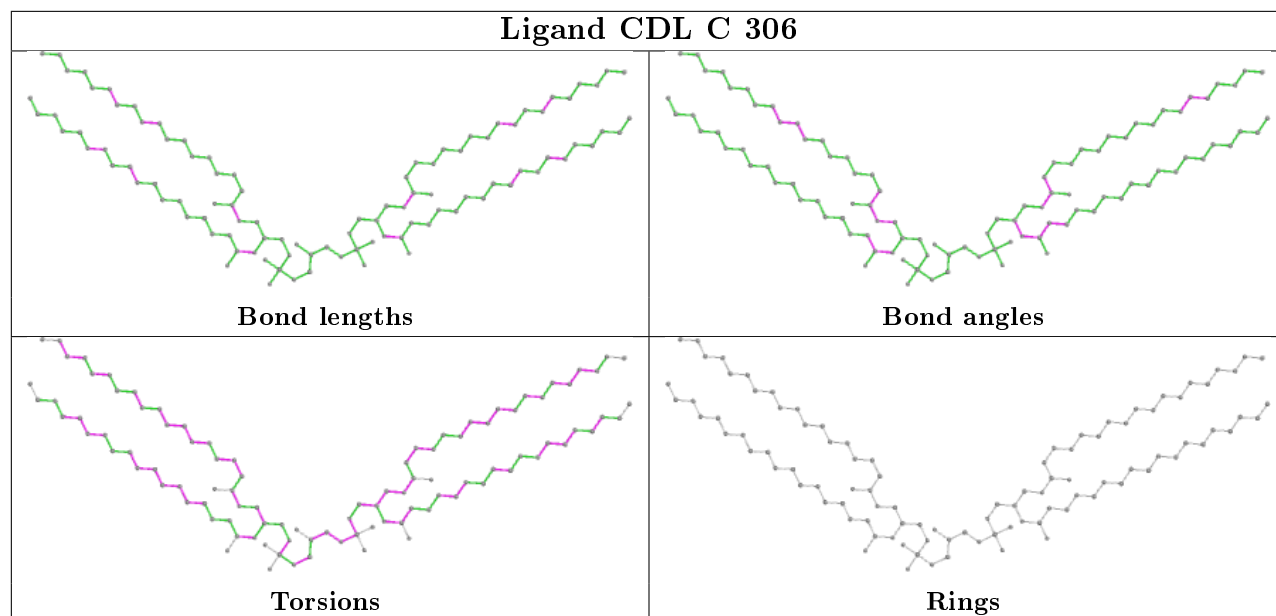
*Continued from previous page...*

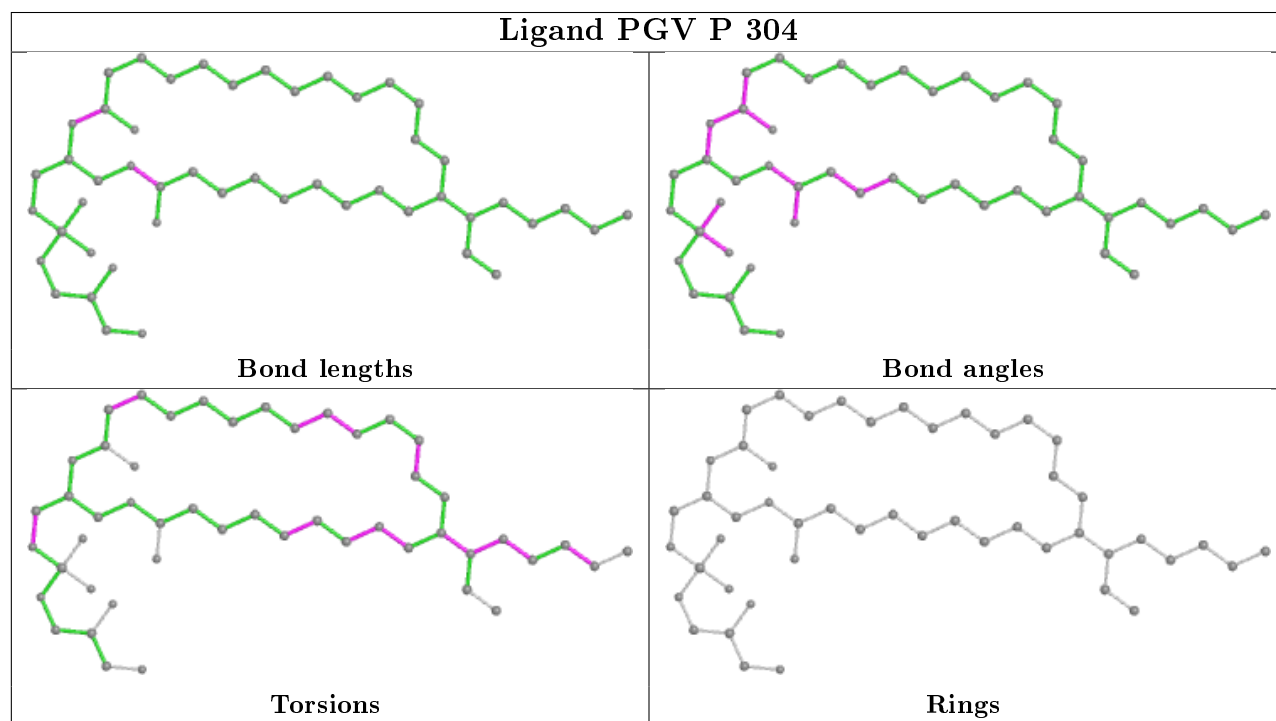
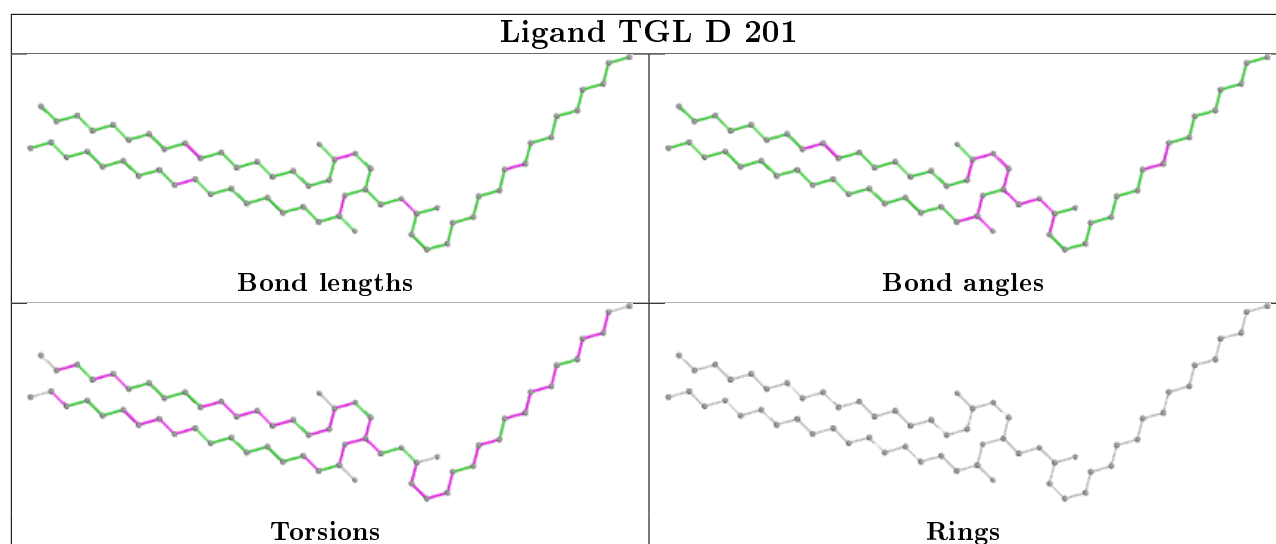
Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	608	PGV	4	0
25	P	303	PEK	3	0
24	P	307	CHD	1	0
28	E	201	PSC	19	0
30	Z	101	DMU	1	0
20	P	305	PGV	4	0
26	P	306	CDL	12	0
24	J	101	CHD	5	0
18	A	604[B]	HEA	6	0
21	N	608	TGL	2	0
19	N	607	PER	1	0
23	E	202	EDO	1	0
21	Q	201	TGL	10	0
25	C	303	PEK	7	0
26	T	101	CDL	24	0
24	W	101	CHD	5	0
20	C	305	PGV	9	0
24	C	301	CHD	1	0
30	M	101	DMU	1	0
31	2	201	HEC	4	0
31	1	201	HEC	4	0
21	L	101	TGL	20	0
18	A	605	HEA	3	0

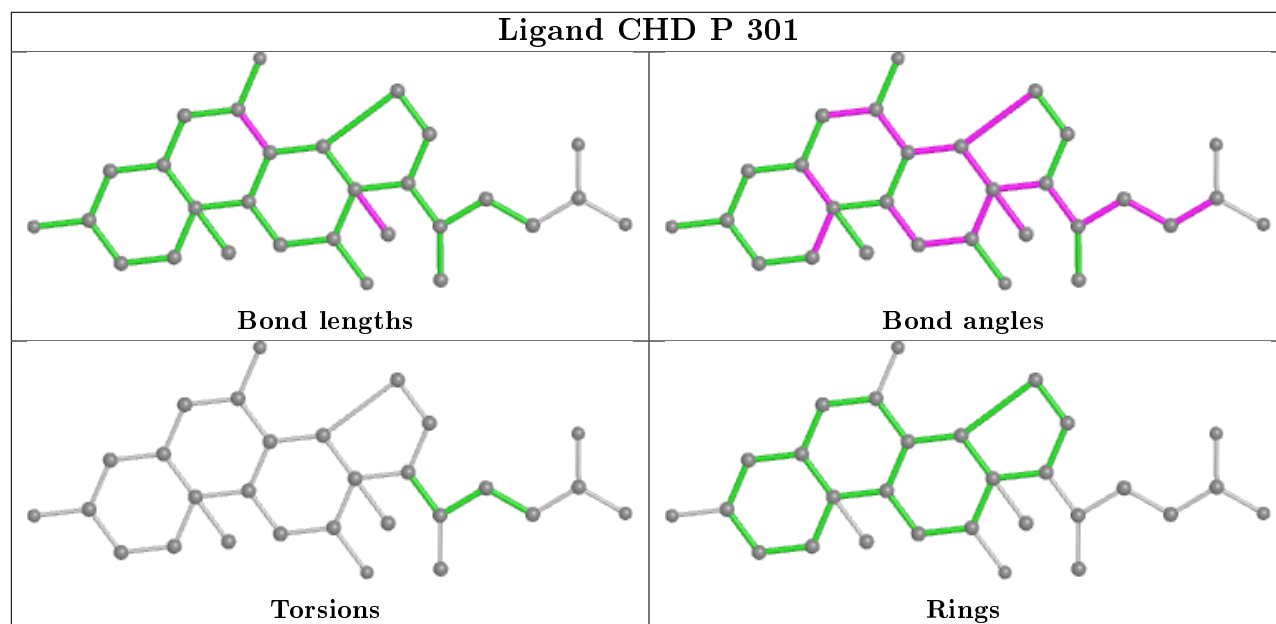
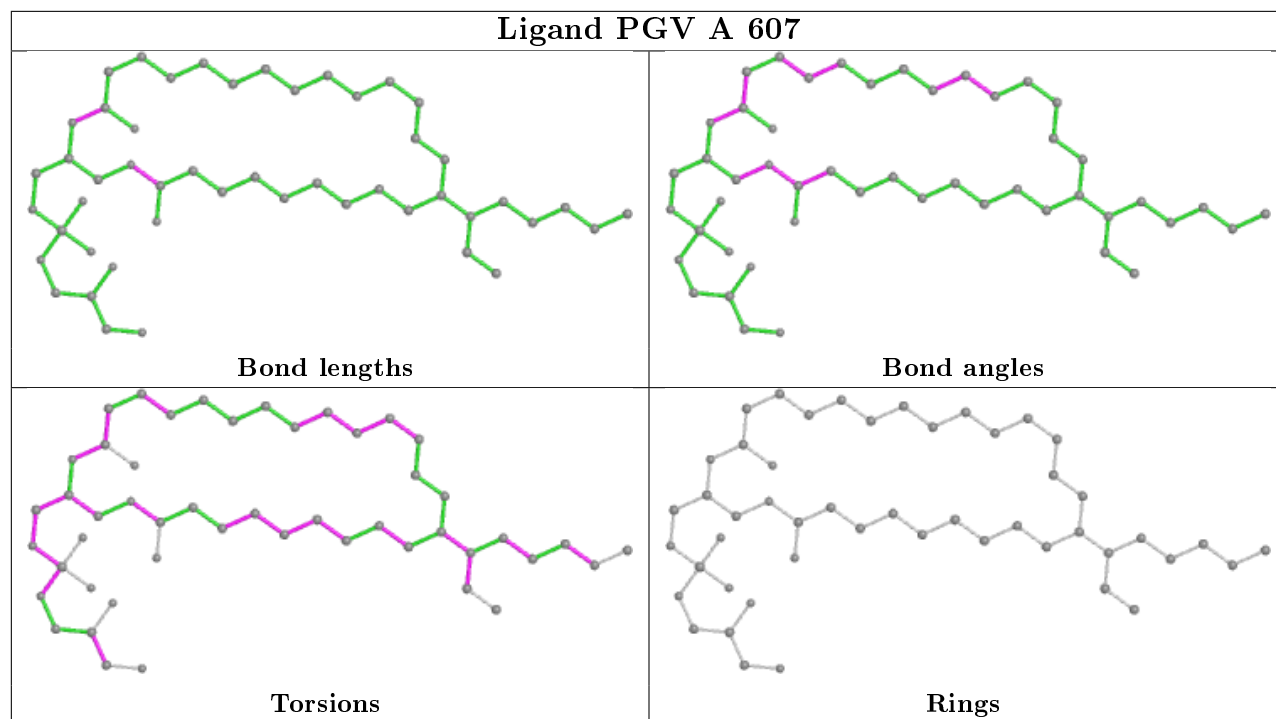
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

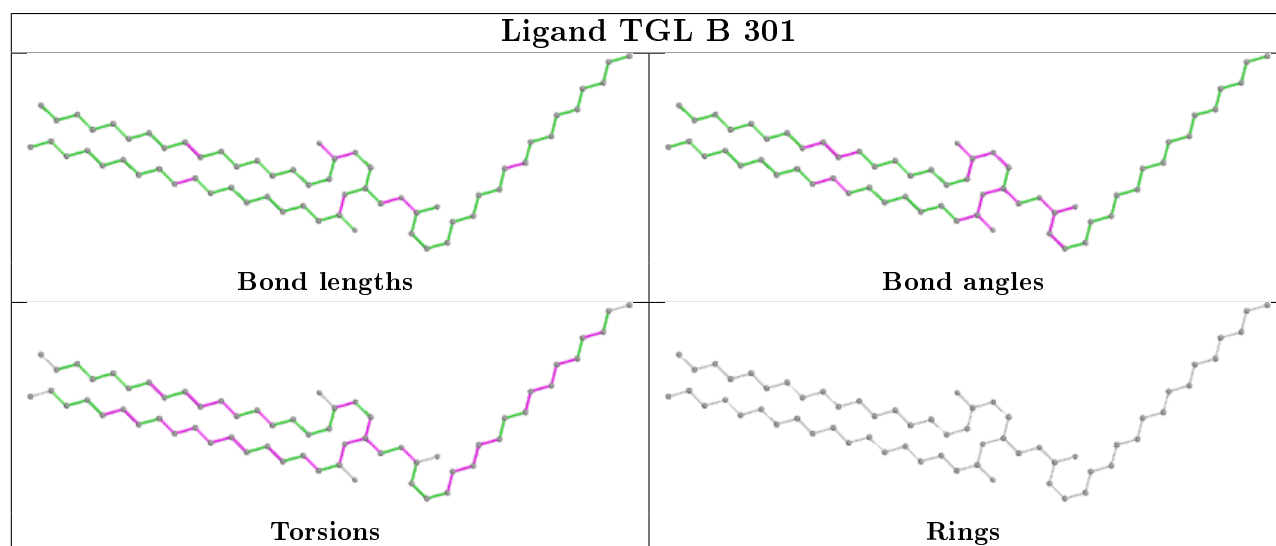
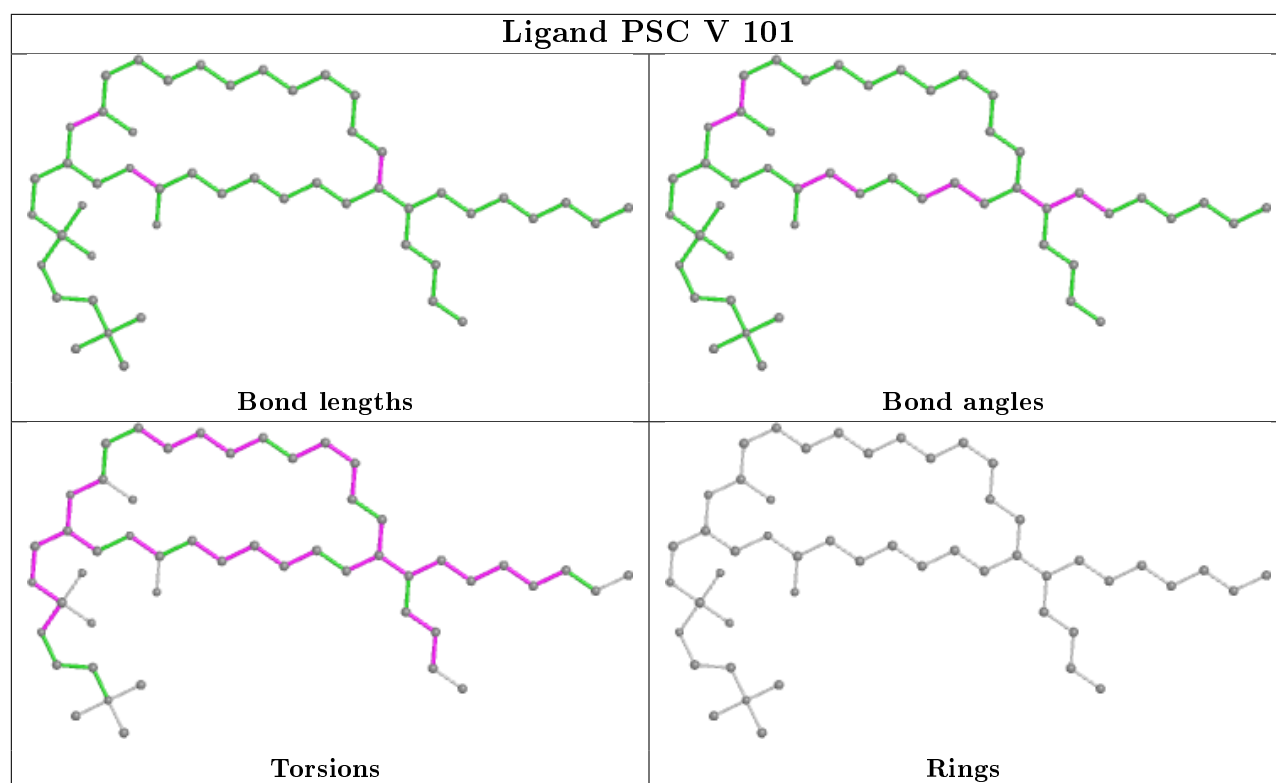


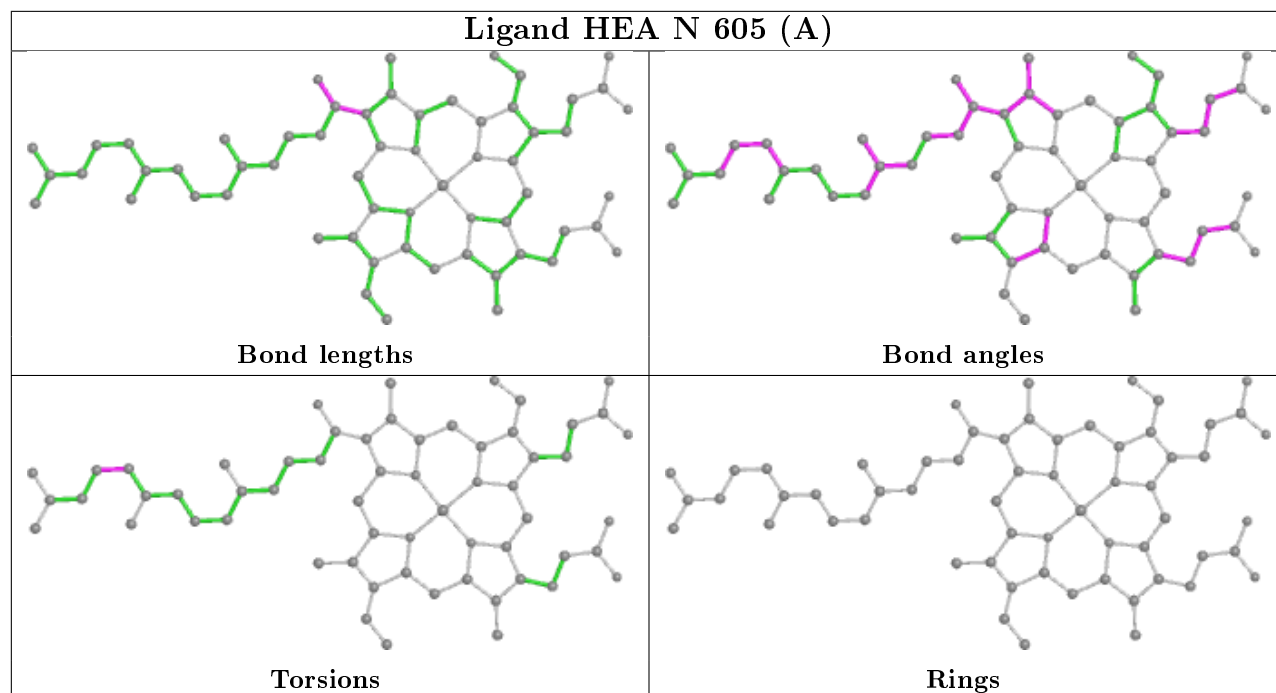
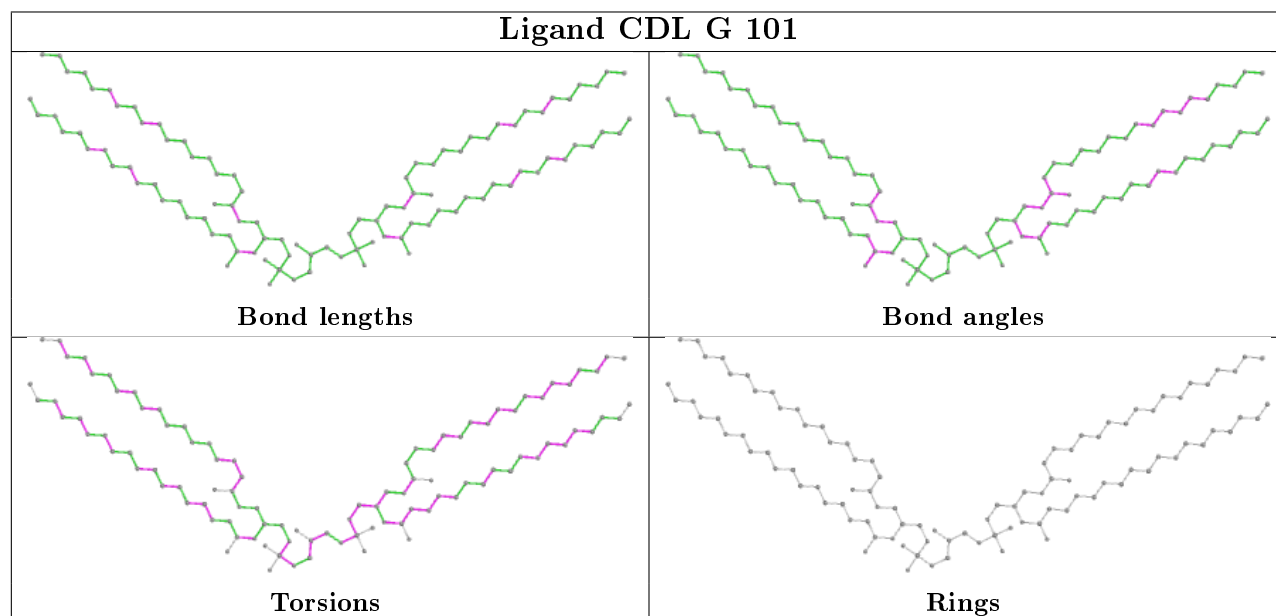


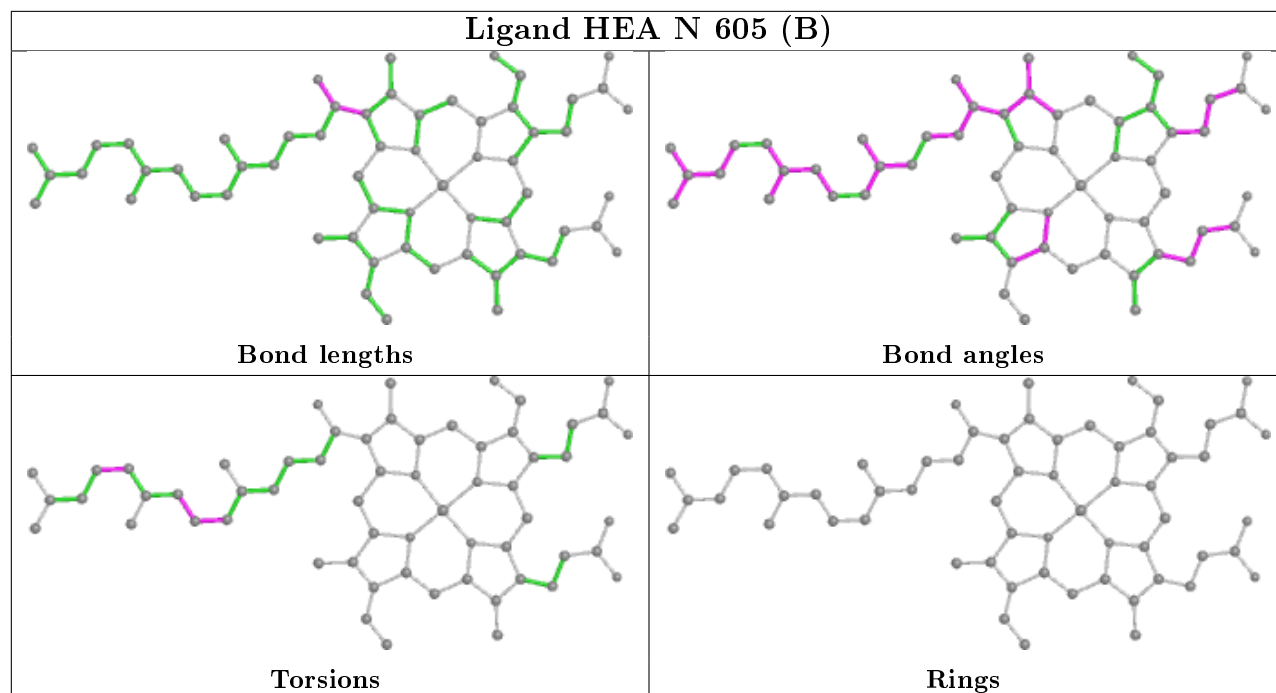
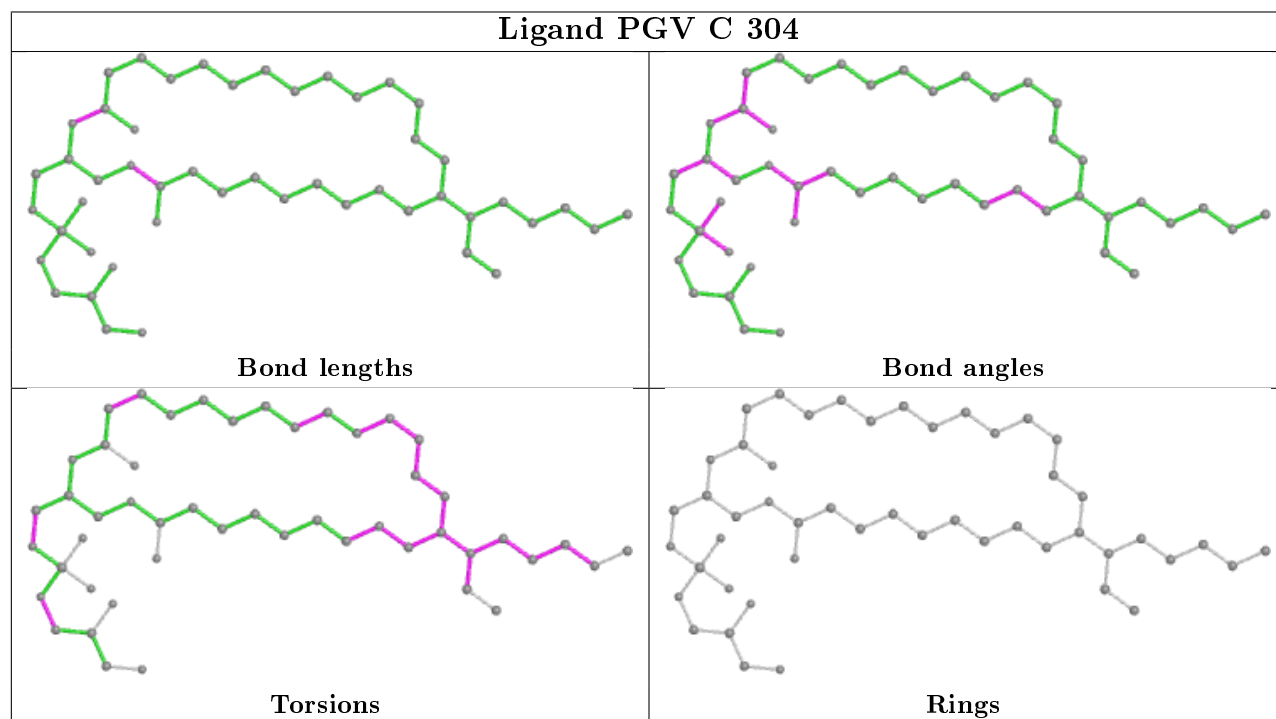


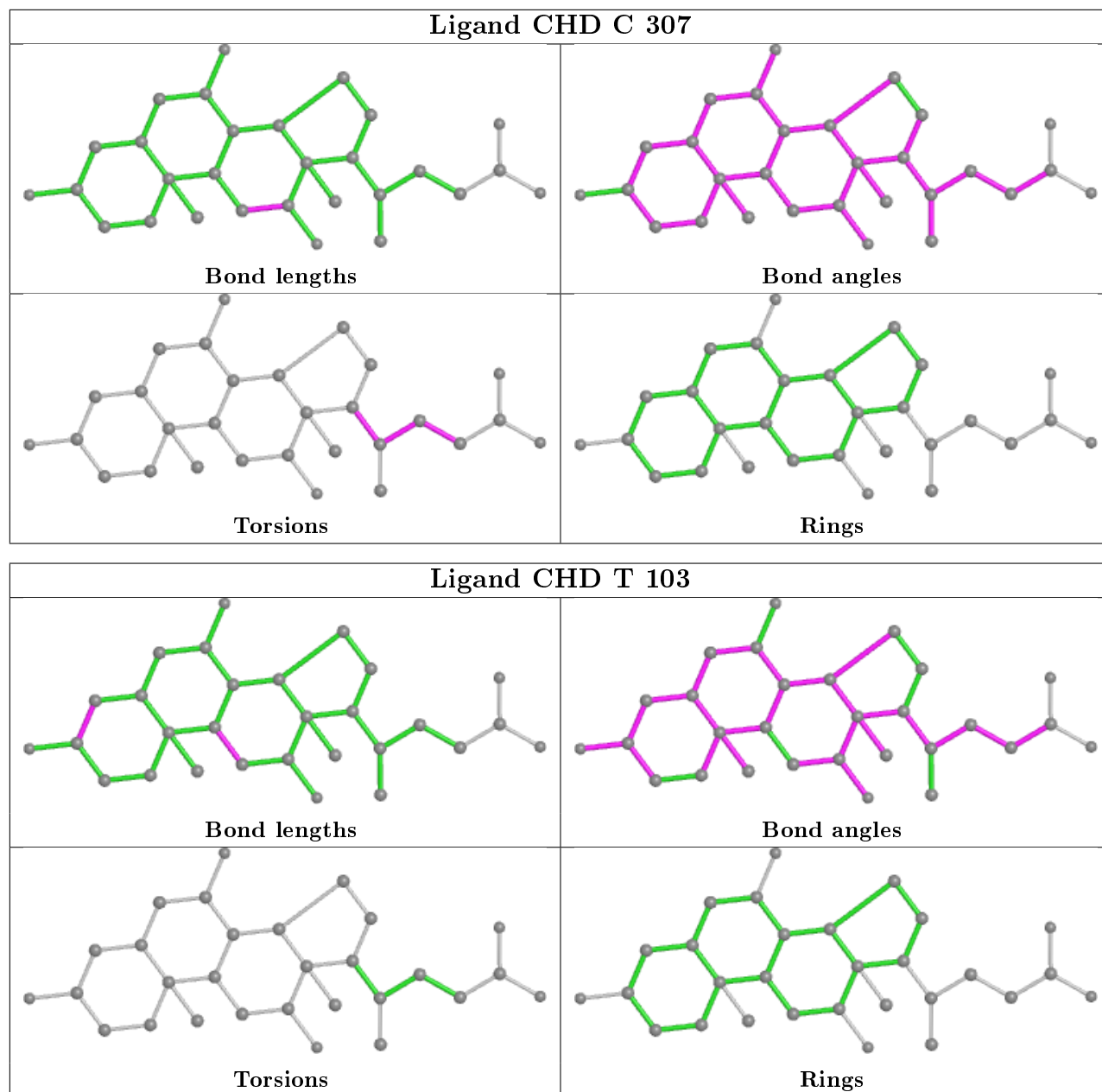


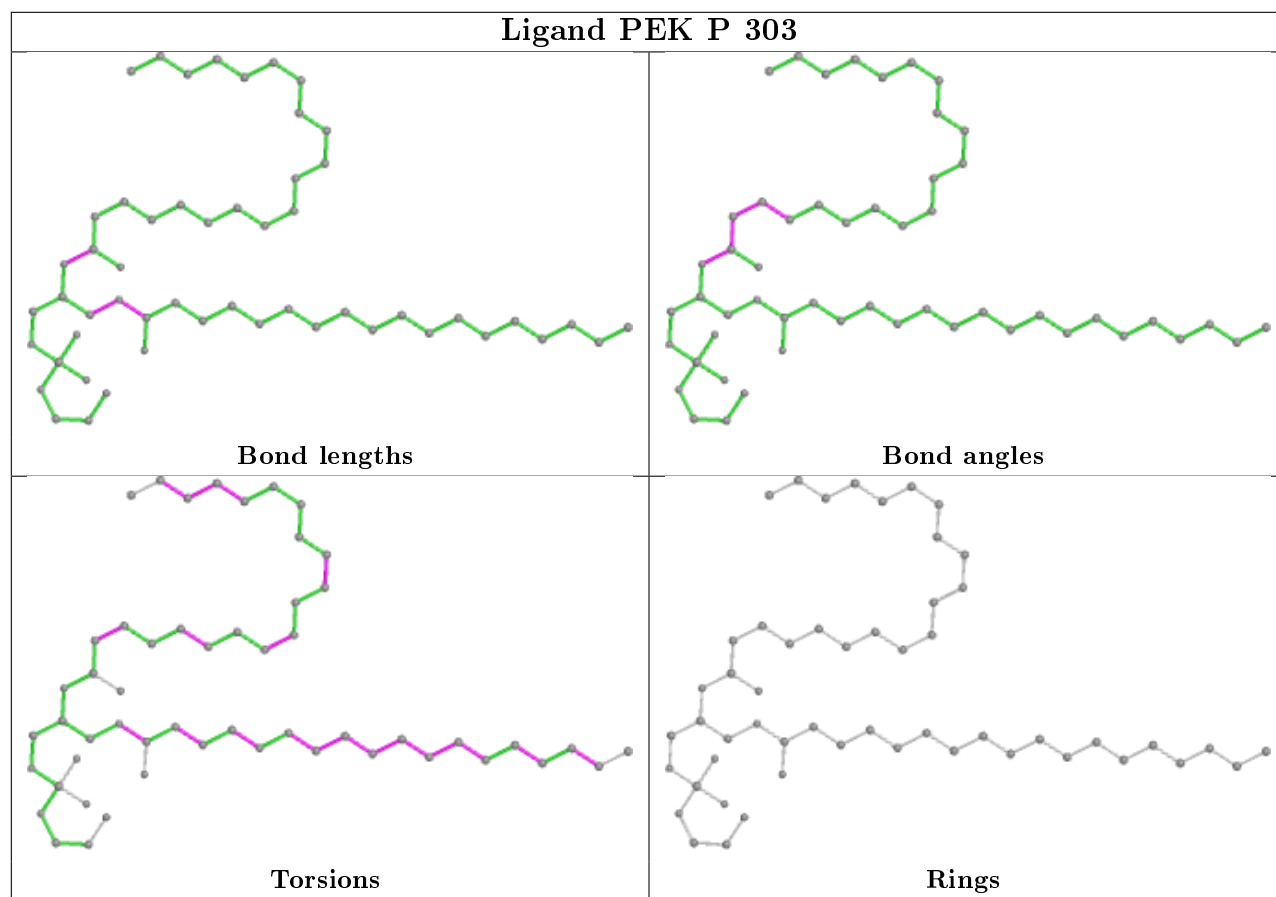
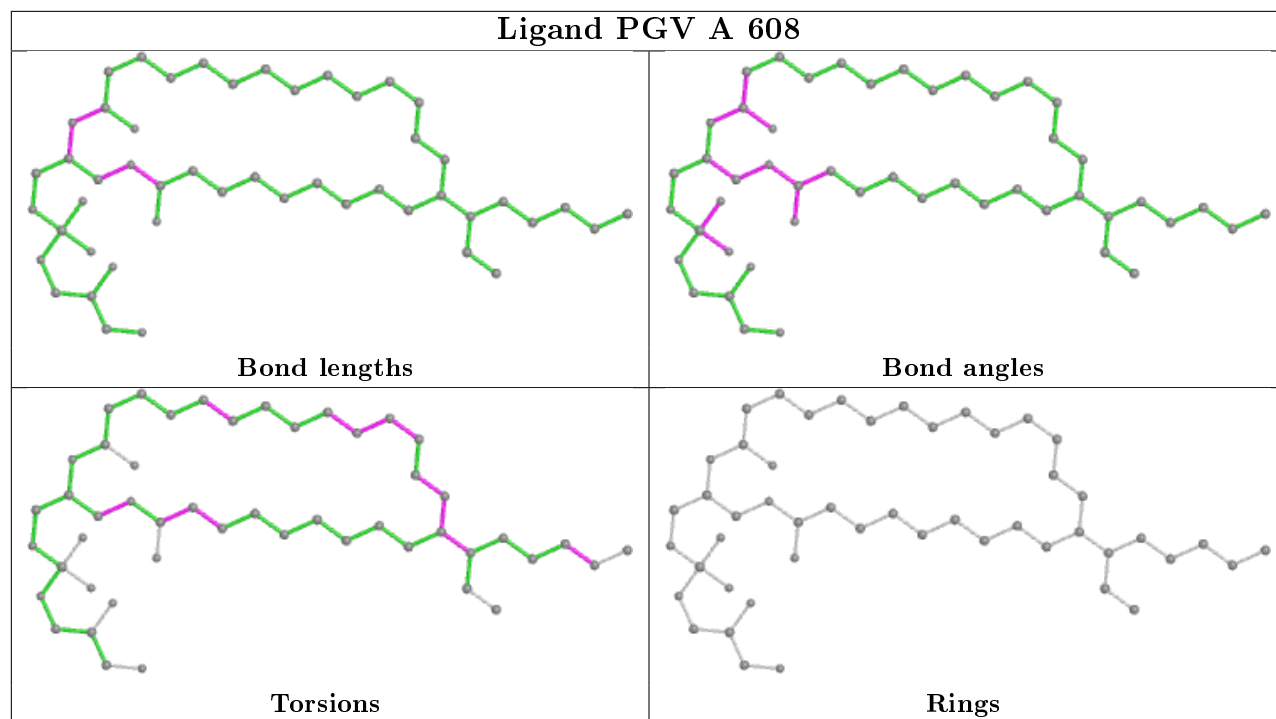




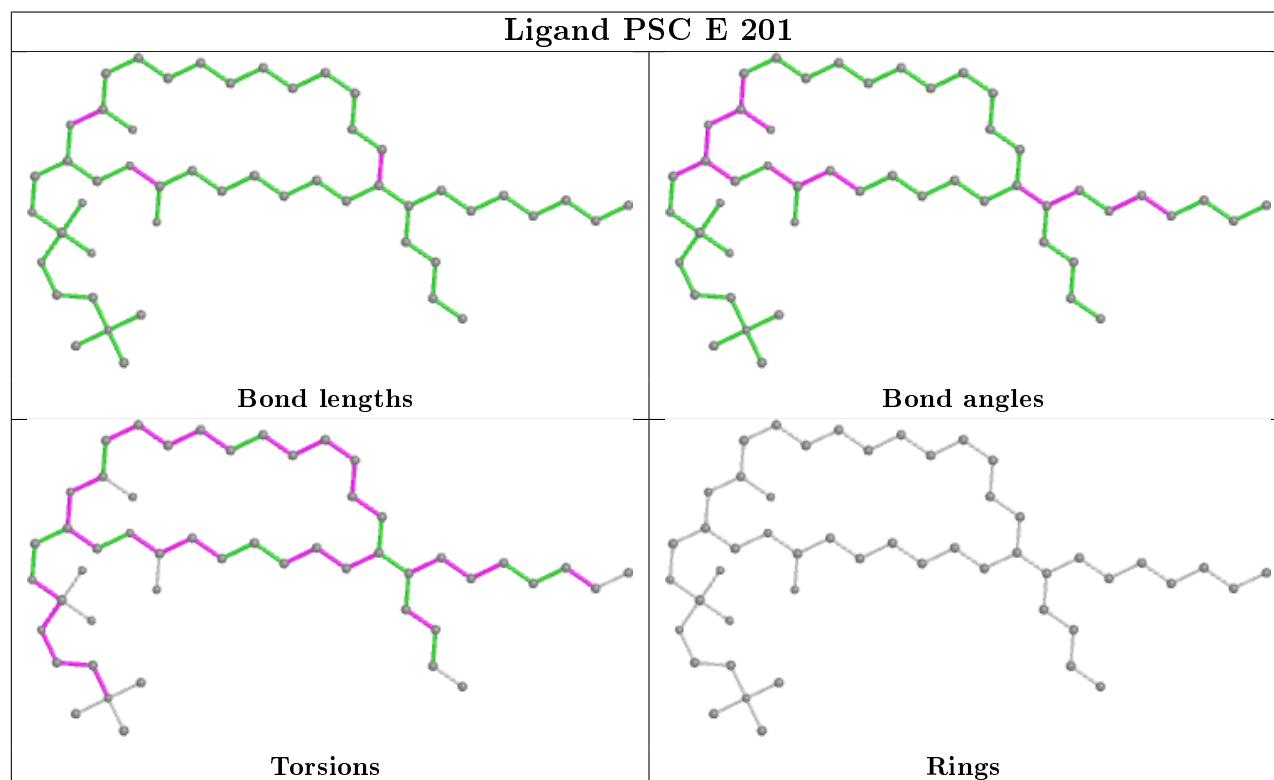
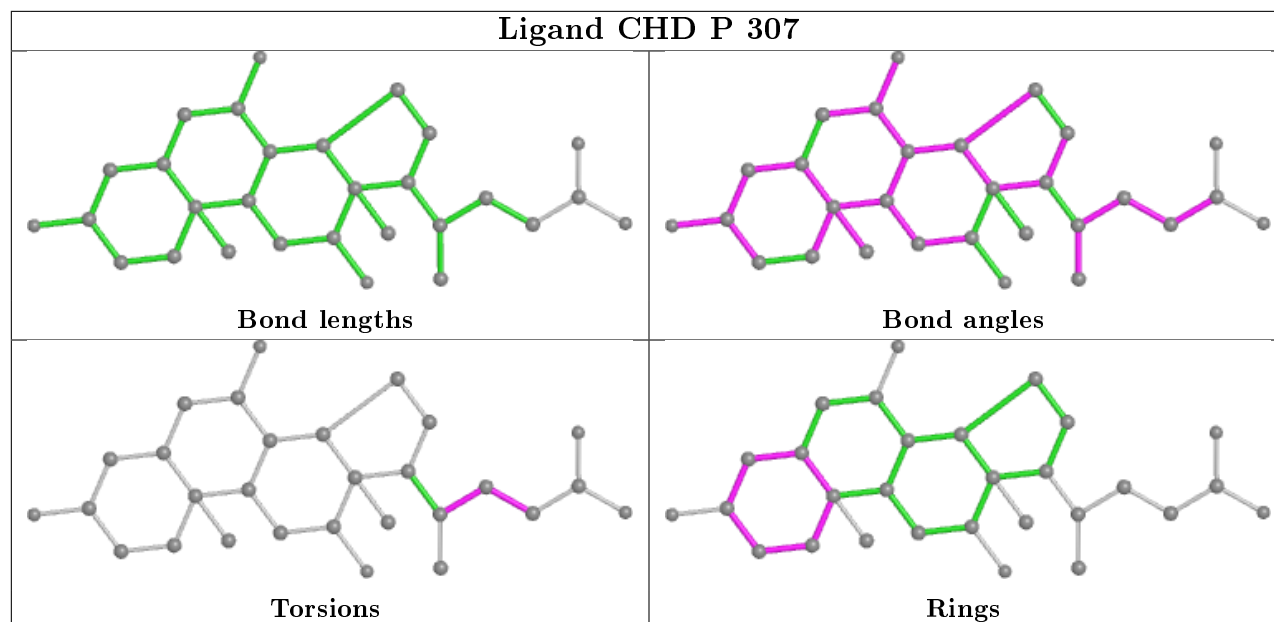
**Ligand HEA N 605 (A)****Ligand CDL G 101**

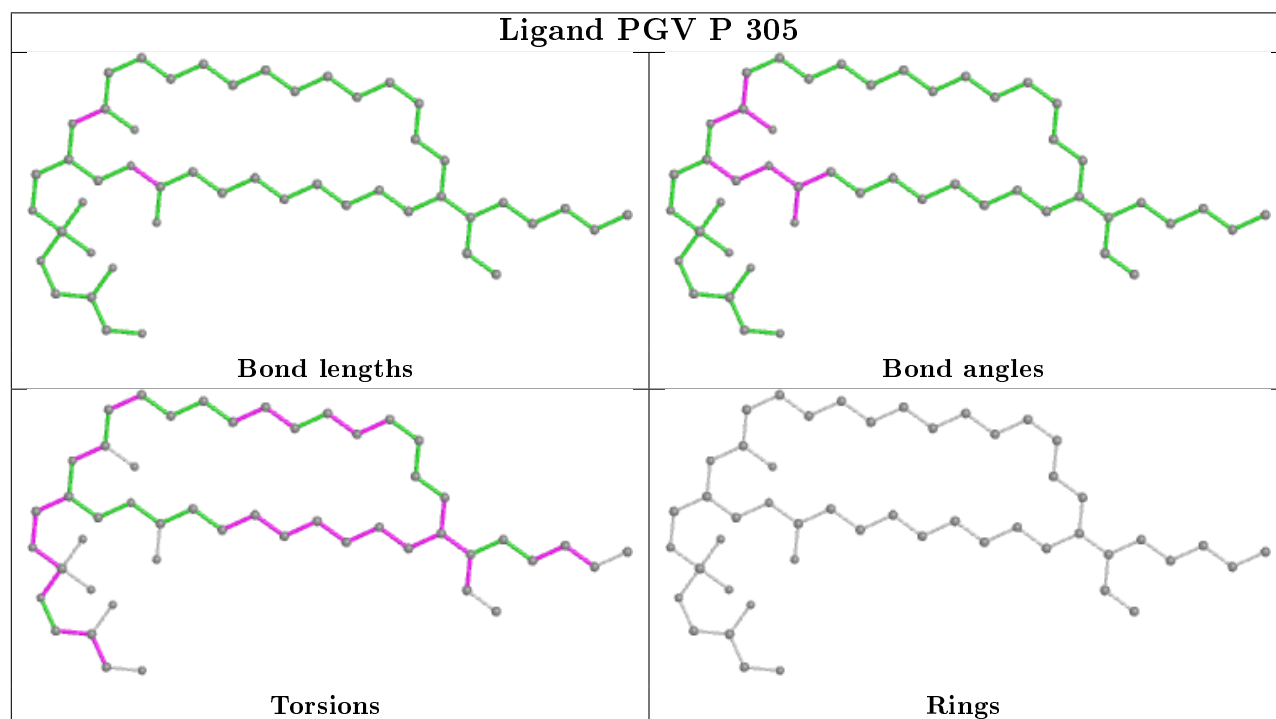
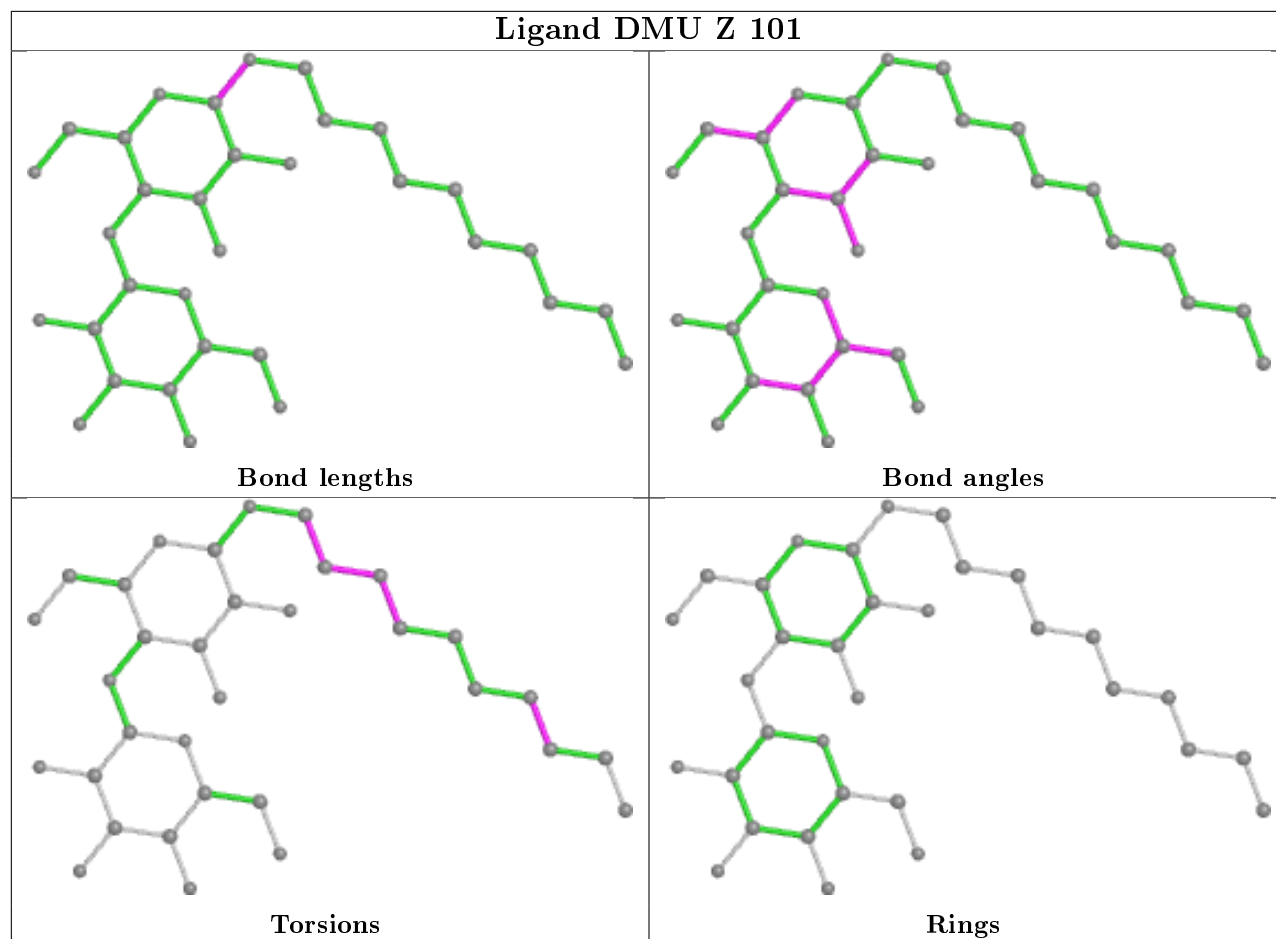
**Ligand HEA N 605 (B)****Ligand PGV C 304**

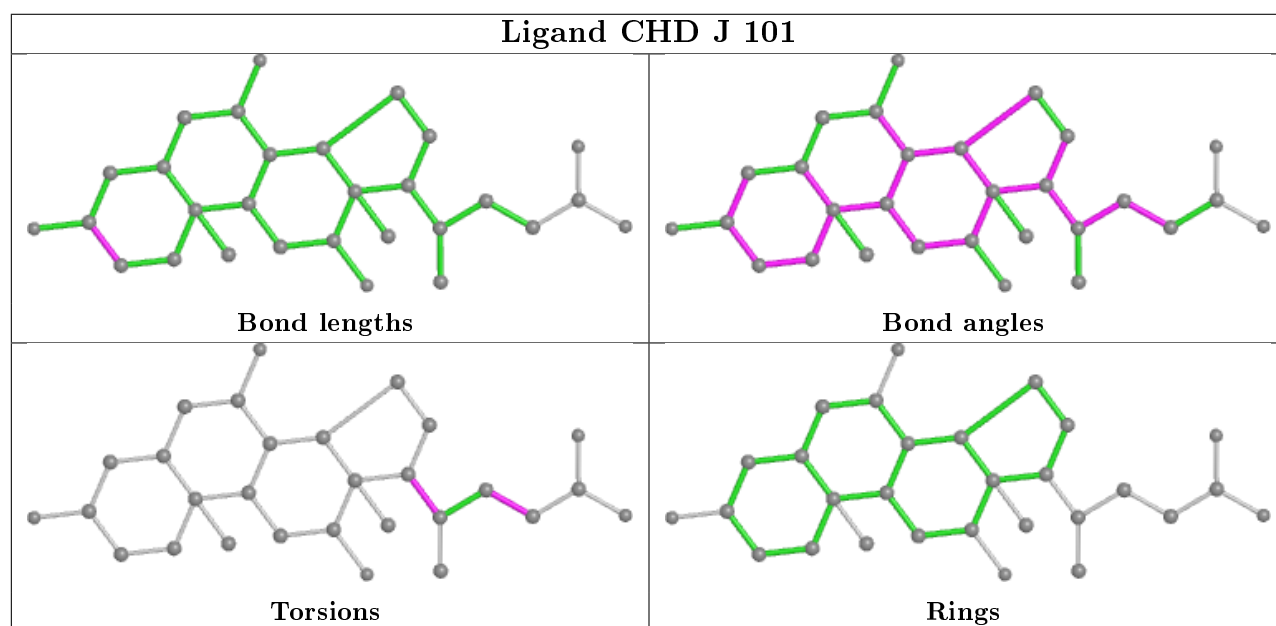
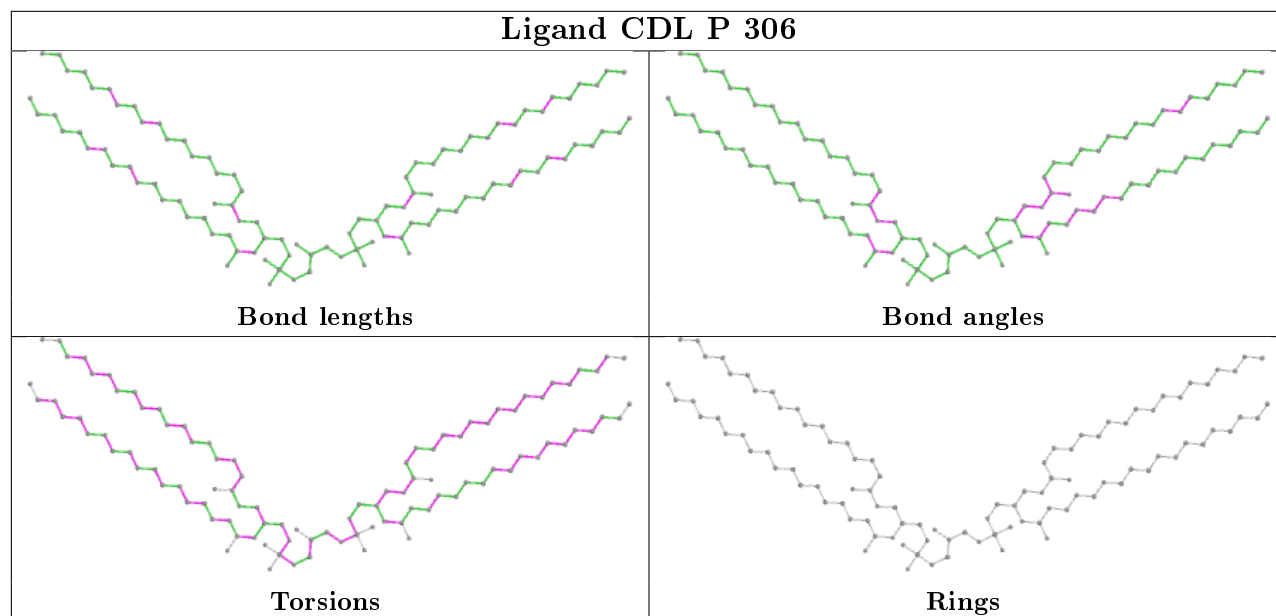


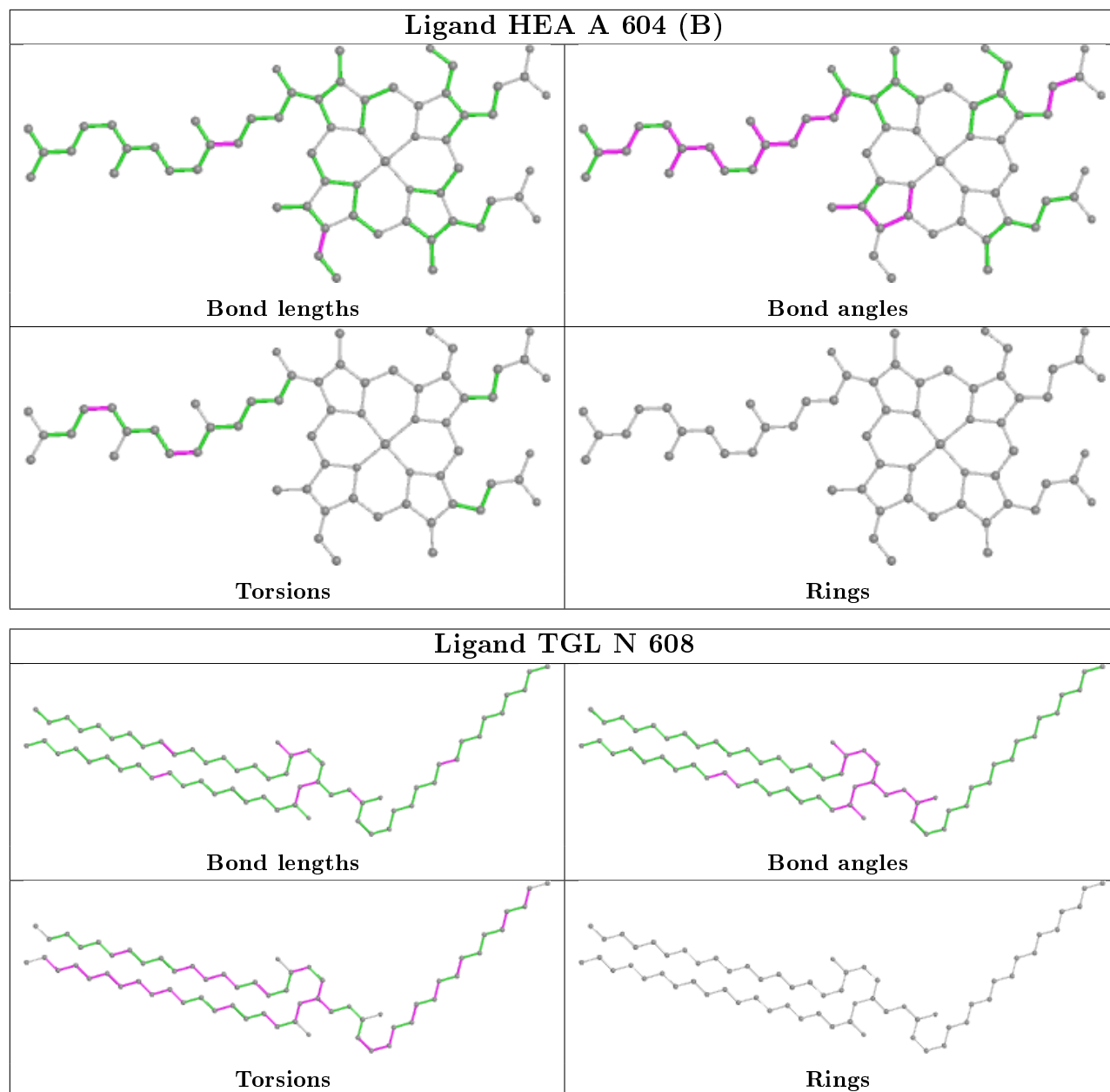


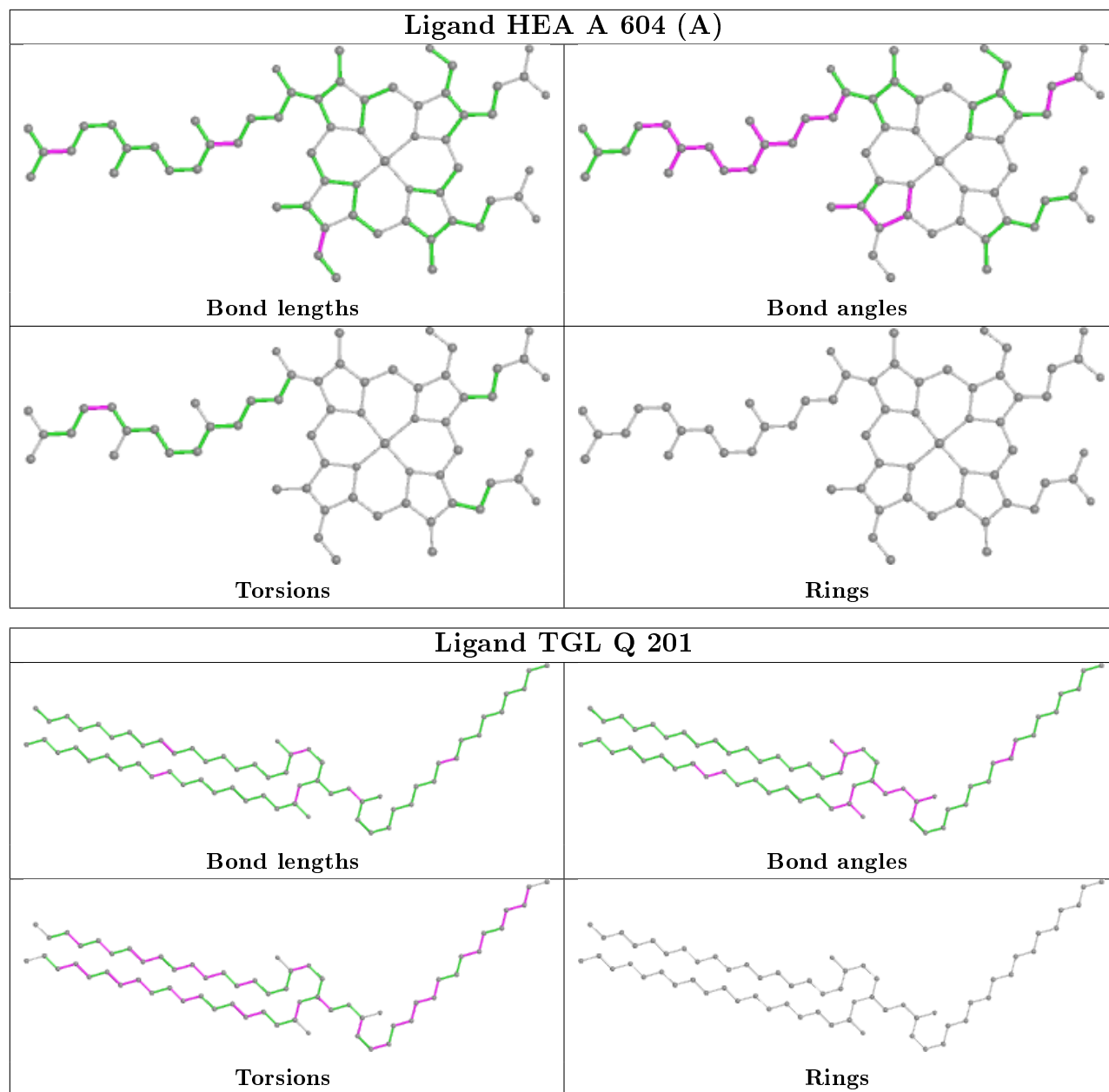


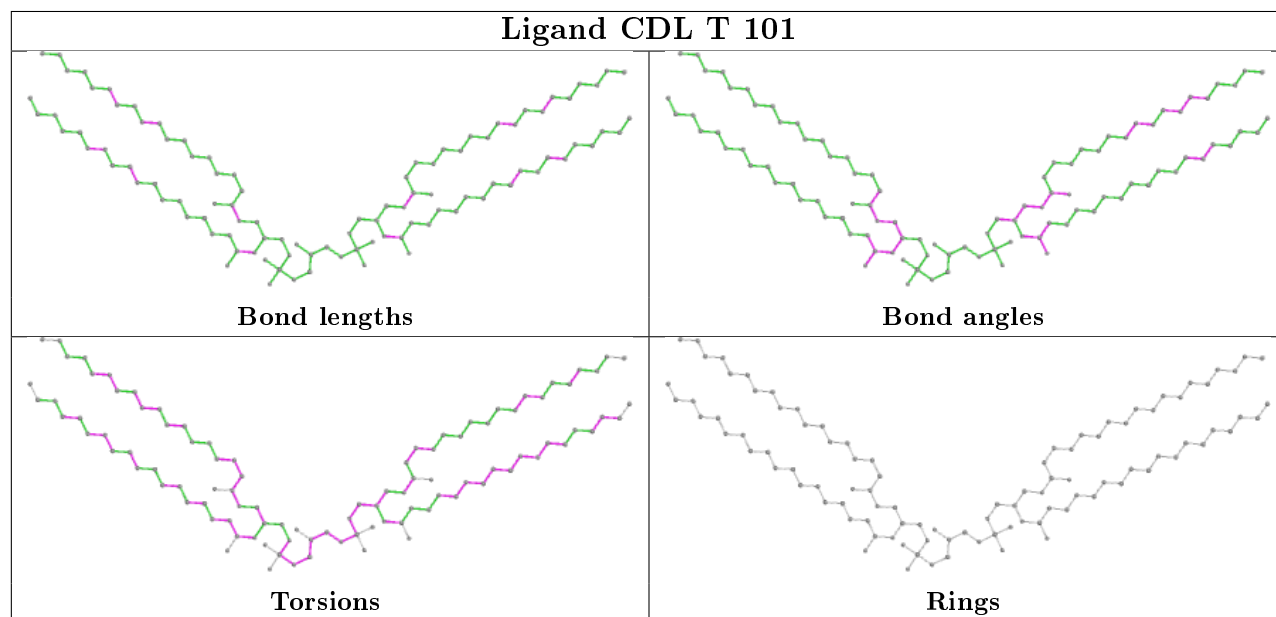
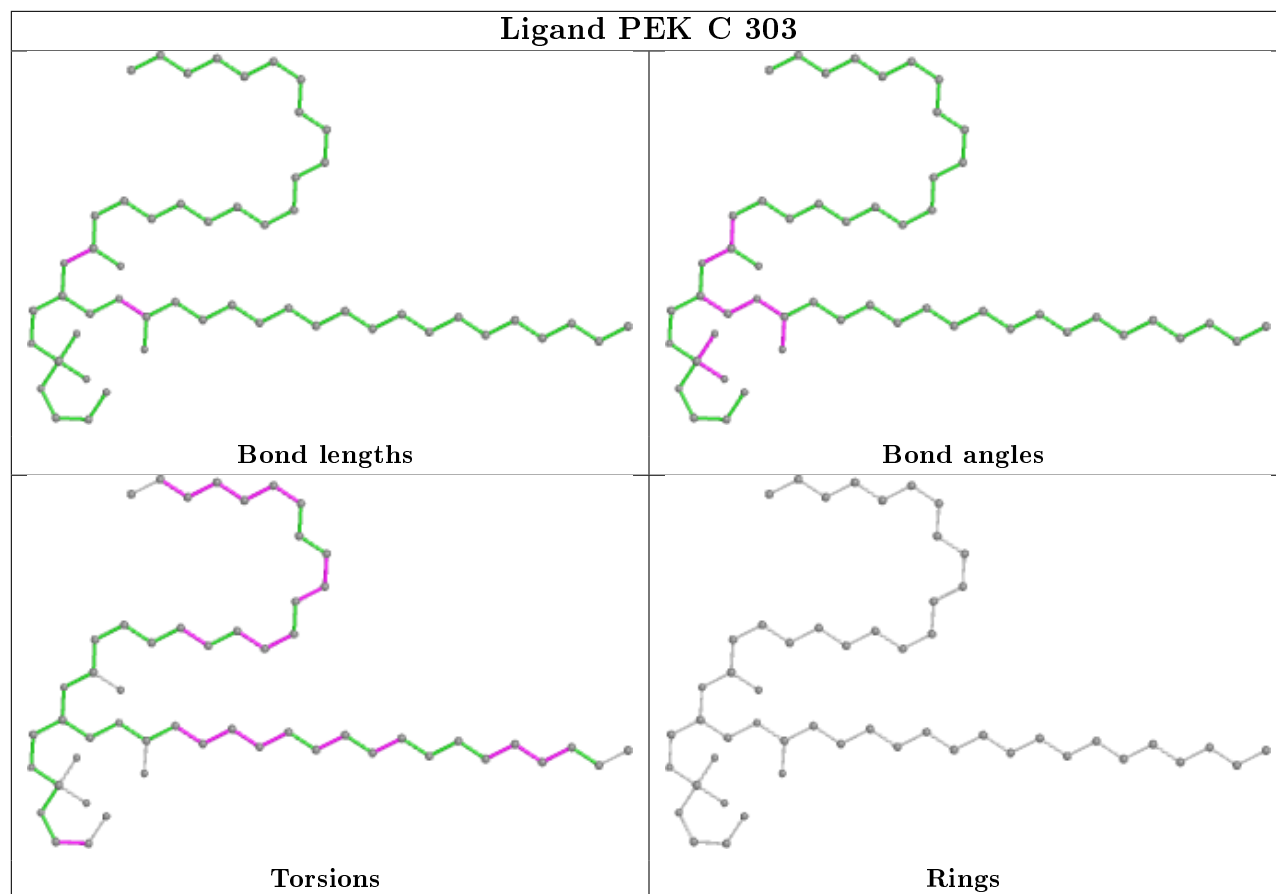


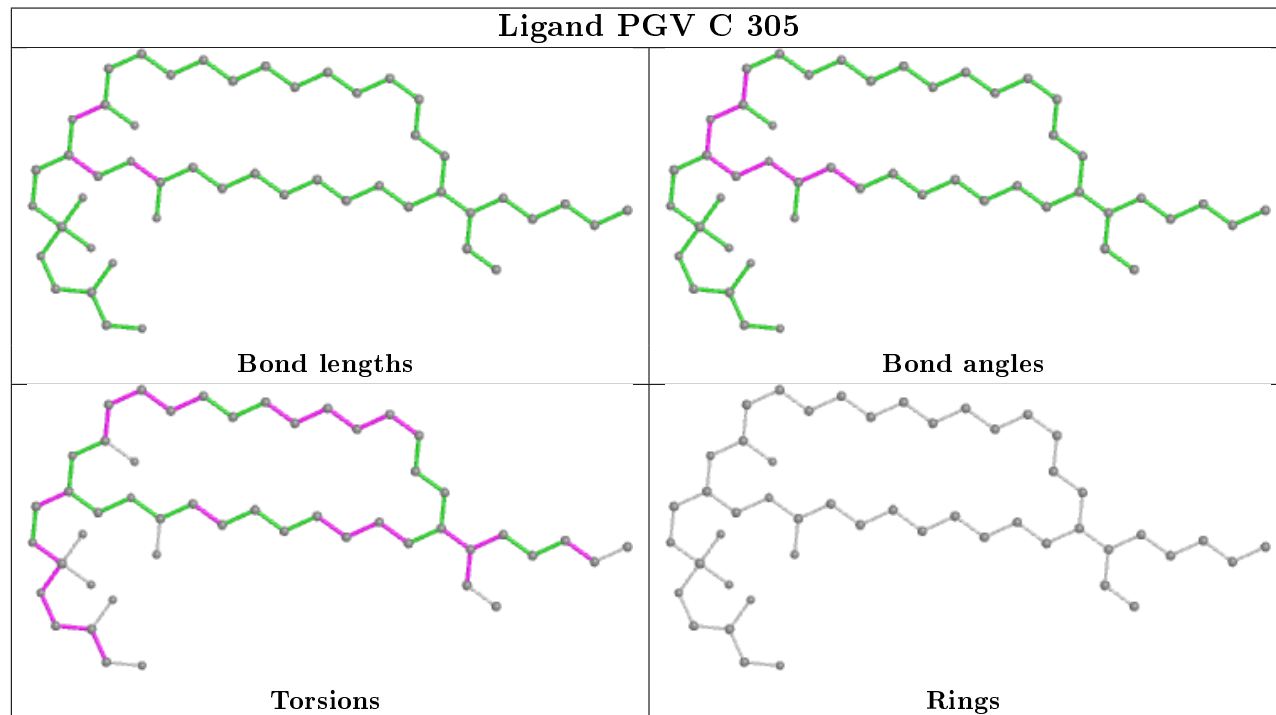
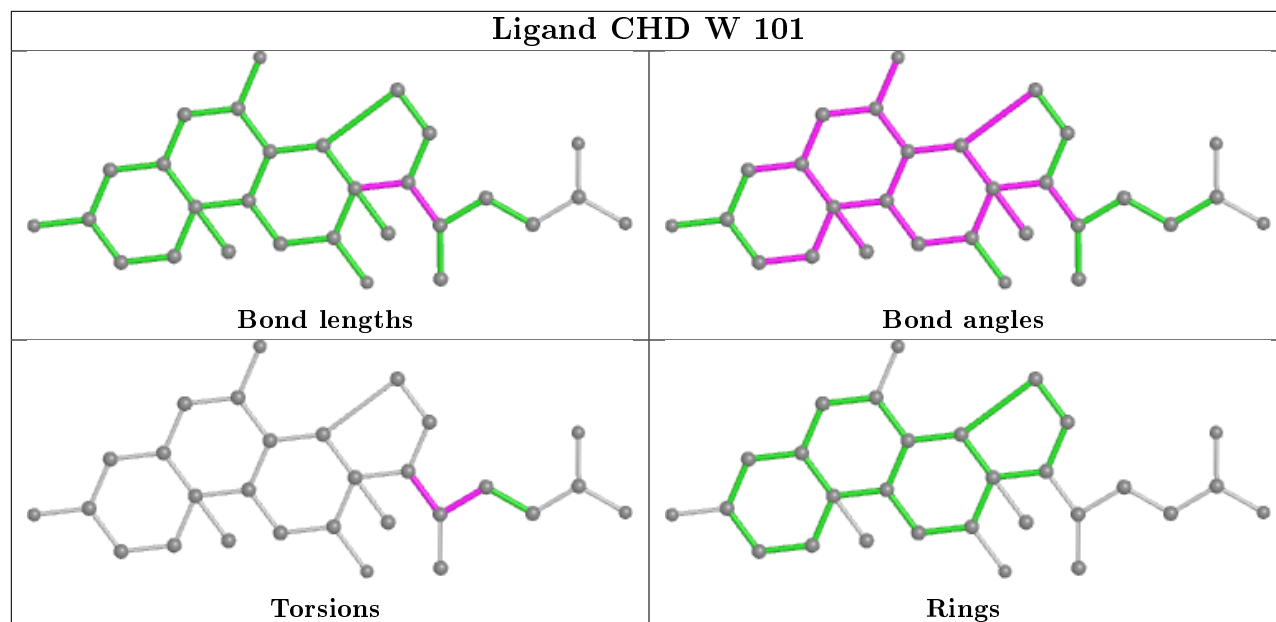


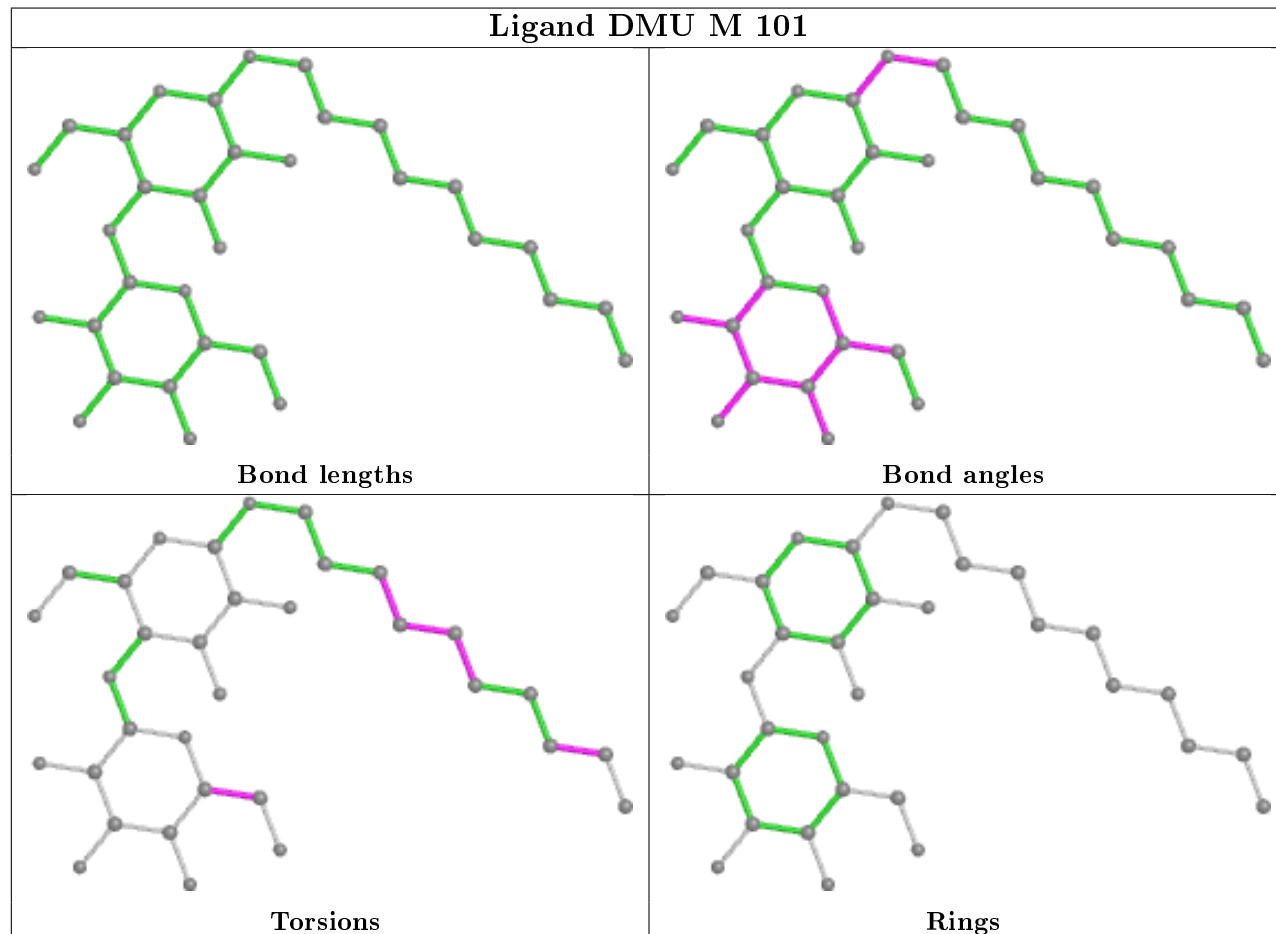
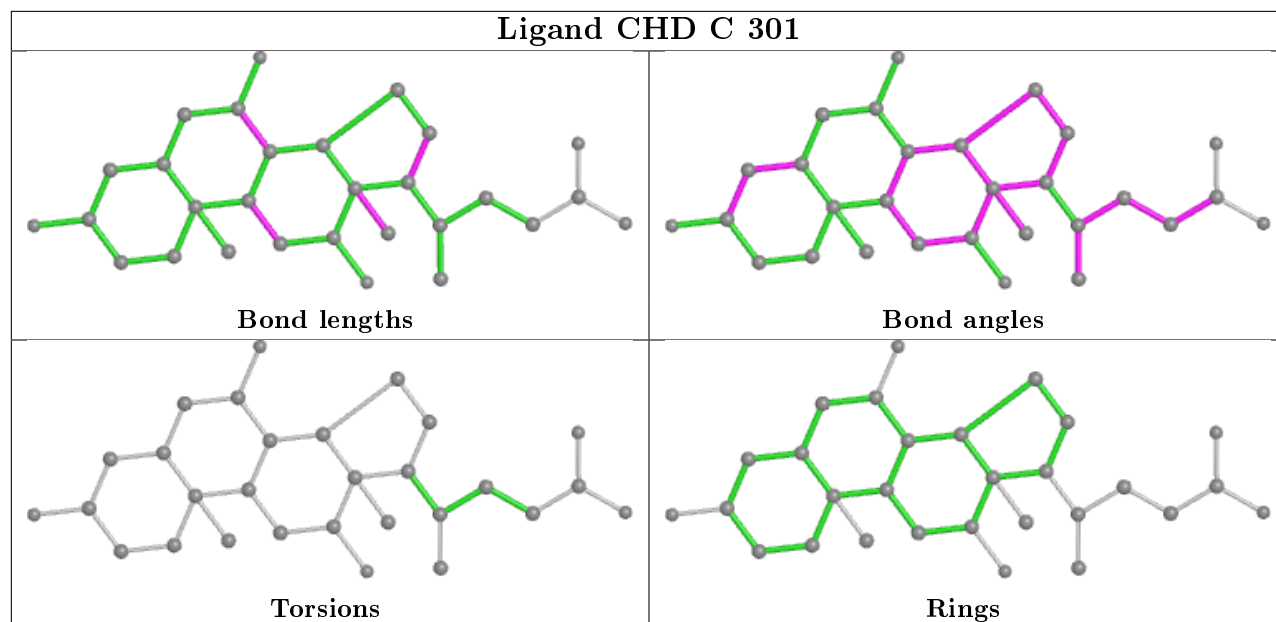






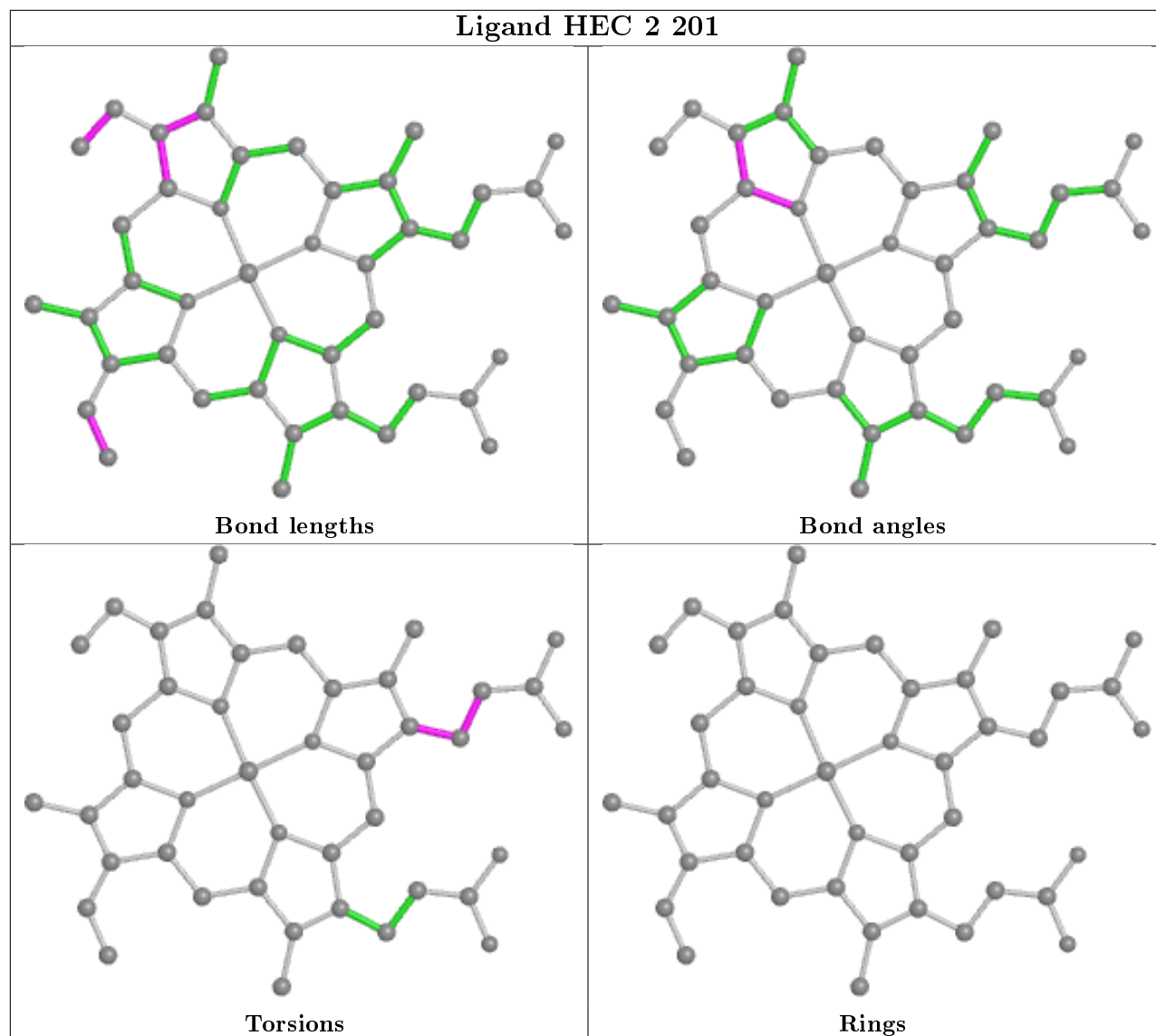




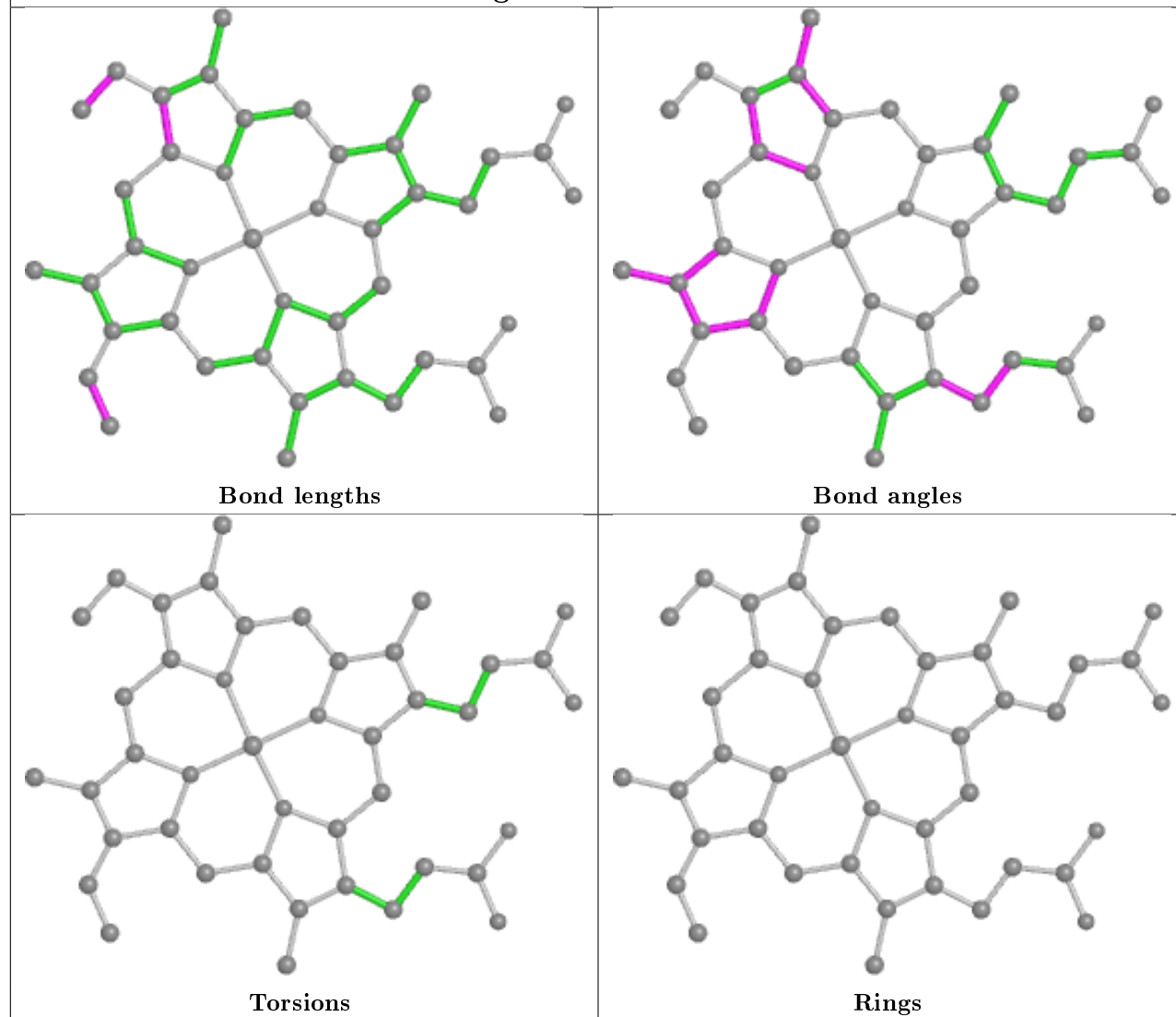




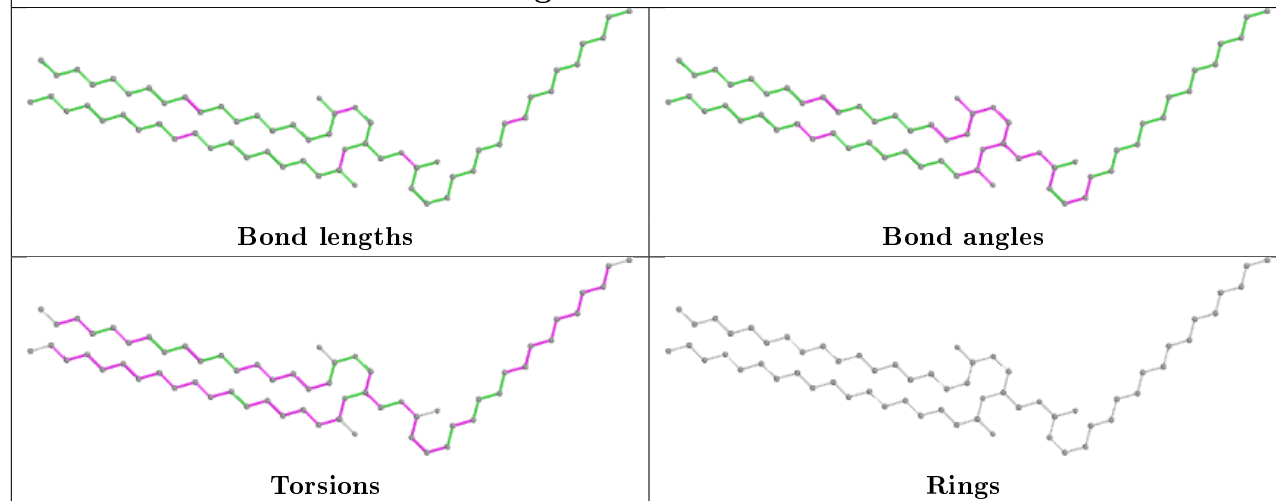
## Ligand HEC 2 201

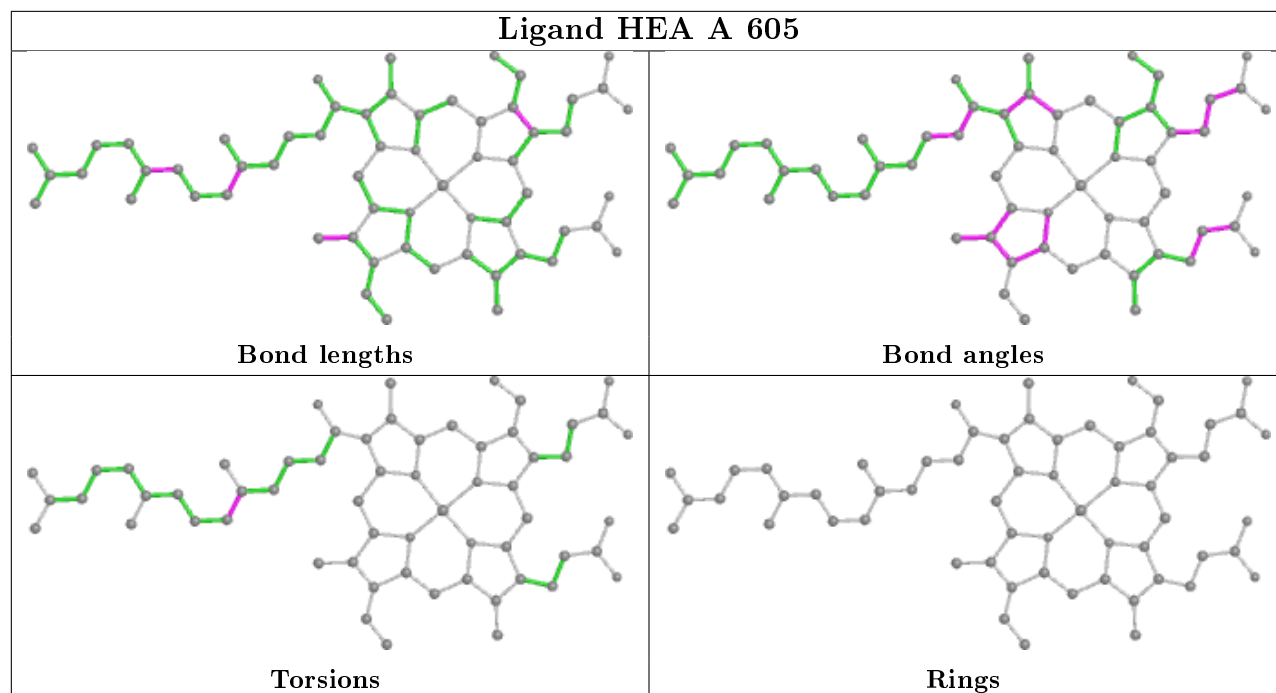


## Ligand HEC 1 201



## Ligand TGL L 101





## 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%)	0.21	21 (4%) 37 36	22, 30, 39, 74	0
1	N	513/514 (99%)	0.23	26 (5%) 28 27	27, 36, 48, 71	0
2	B	226/227 (99%)	-0.34	3 (1%) 77 76	26, 35, 59, 109	0
2	O	226/227 (99%)	-0.15	2 (0%) 84 83	34, 49, 78, 98	0
3	C	259/259 (100%)	-0.54	2 (0%) 86 85	26, 35, 48, 83	0
3	P	259/259 (100%)	-0.55	4 (1%) 73 72	28, 38, 52, 87	0
4	D	144/144 (100%)	-0.53	5 (3%) 44 43	30, 38, 63, 144	0
4	Q	144/144 (100%)	0.16	13 (9%) 9 8	32, 50, 81, 139	0
5	E	105/105 (100%)	-0.42	2 (1%) 66 65	30, 38, 62, 134	0
5	R	105/105 (100%)	-0.61	1 (0%) 82 81	33, 41, 62, 123	0
6	F	98/98 (100%)	-0.05	8 (8%) 11 11	30, 40, 95, 141	0
6	S	98/98 (100%)	0.25	8 (8%) 11 11	32, 45, 106, 141	0
7	G	83/84 (98%)	0.56	16 (19%) 1 0	34, 44, 116, 138	0
7	T	83/84 (98%)	0.80	17 (20%) 1 0	31, 47, 111, 136	0
8	H	79/79 (100%)	-0.11	7 (8%) 9 8	33, 43, 90, 106	0
8	U	79/79 (100%)	-0.18	2 (2%) 57 56	38, 49, 69, 137	0
9	I	72/73 (98%)	-0.15	3 (4%) 36 35	33, 46, 66, 79	0
9	V	72/73 (98%)	0.99	11 (15%) 2 1	36, 63, 85, 111	0
10	J	58/58 (100%)	0.36	7 (12%) 4 3	36, 46, 75, 135	0
10	W	58/58 (100%)	0.72	8 (13%) 2 2	39, 53, 84, 144	0
11	K	49/49 (100%)	-0.15	3 (6%) 21 20	35, 42, 58, 70	0
11	X	49/49 (100%)	0.61	4 (8%) 11 11	47, 58, 77, 78	0
12	L	46/46 (100%)	-0.53	1 (2%) 62 60	30, 38, 59, 104	0
12	Y	46/46 (100%)	-0.50	1 (2%) 62 60	36, 46, 69, 111	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
13	M	43/43 (100%)	-0.20	2 (4%) 31 30	32, 40, 79, 127	0
13	Z	43/43 (100%)	-0.05	3 (6%) 16 15	36, 50, 81, 108	0
14	1	104/105 (99%)	2.81	65 (62%) 0 0	45, 90, 118, 125	0
14	2	104/105 (99%)	4.61	79 (75%) 0 0	67, 115, 139, 147	0
All	All	3758/3768 (99%)	0.17	324 (8%) 10 9	22, 40, 98, 147	0

All (324) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	5	VAL	13.5
4	Q	7	LYS	13.3
6	S	1	ALA	13.3
10	W	57	HIS	12.5
14	2	57	ILE	12.1
14	2	35	LEU	11.9
6	S	98	HIS	11.8
14	2	58	THR	11.3
6	F	1	ALA	10.7
10	J	58	LYS	10.5
14	2	36	PHE	10.4
6	S	97	ALA	10.3
10	J	57	HIS	10.3
14	2	32	LEU	10.2
6	S	96	LEU	10.1
14	2	95	ILE	9.7
4	Q	6	VAL	9.6
14	2	59	TRP	9.3
6	F	98	HIS	9.1
14	2	40	THR	9.0
9	V	30	GLY	8.8
14	2	43	ALA	8.6
14	2	22	LYS	8.4
14	2	64	LEU	8.3
6	F	97	ALA	8.3
7	T	10	GLY	8.3
14	2	46	PHE	8.2
5	E	5	HIS	8.1
14	2	74	TYR	7.9
14	2	33	HIS	7.9
14	2	38	ARG	7.8
7	G	3	ALA	7.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	D	5	VAL	7.6
14	2	103	ASN	7.6
14	1	37	GLY	7.5
14	2	76	PRO	7.5
14	2	104	GLU	7.3
8	U	8	ILE	7.3
14	2	45	GLY	7.1
14	2	39	LYS	7.1
14	1	43	ALA	7.1
6	S	94	HIS	7.1
14	2	1	GLY	7.0
14	2	75	ILE	7.0
14	1	102	THR	7.0
14	1	34	GLY	6.9
14	2	42	GLN	6.7
13	M	43	SER	6.6
14	2	77	GLY	6.5
14	2	21	GLU	6.5
14	2	67	TYR	6.5
14	1	101	ALA	6.5
7	G	40	GLY	6.4
7	T	40	GLY	6.4
6	S	2	SER	6.3
8	U	7	LYS	6.3
10	W	58	LYS	6.2
14	1	42	GLN	6.2
14	2	102	THR	6.2
14	1	58	THR	6.1
14	1	95	ILE	6.1
7	G	10	GLY	6.1
14	1	36	PHE	6.1
14	2	98	LEU	6.1
14	2	101	ALA	6.1
7	T	42	ARG	6.1
14	2	19	THR	6.0
14	2	37	GLY	6.0
14	1	57	ILE	6.0
14	1	53	LYS	5.9
14	2	23	GLY	5.9
14	2	20	VAL	5.8
14	2	61	GLU	5.8
14	2	55	LYS	5.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
14	2	3	VAL	5.8
14	2	97	TYR	5.7
14	1	47	THR	5.7
14	2	96	ALA	5.6
5	R	5	HIS	5.6
9	V	33	THR	5.6
14	1	74	TYR	5.5
4	Q	4	SER	5.5
4	D	4	SER	5.5
7	G	36	TRP	5.5
14	2	34	GLY	5.4
4	D	7	LYS	5.4
7	G	39	SER	5.4
14	2	44	PRO	5.4
14	2	99	LYS	5.3
14	1	24	GLY	5.3
14	2	24	GLY	5.3
14	2	63	THR	5.3
14	1	41	GLY	5.2
14	2	18	HIS	5.2
14	2	56	GLY	5.2
14	2	68	LEU	5.2
7	G	2	SER	5.1
9	V	2	THR	5.1
6	F	2	SER	5.1
14	2	28	THR	5.1
14	1	98	LEU	5.1
14	2	60	LYS	5.1
14	2	78	THR	5.0
14	1	99	LYS	5.0
14	1	46	PHE	4.9
14	1	40	THR	4.9
4	Q	8	SER	4.9
14	1	35	LEU	4.9
8	H	48	GLY	4.9
14	1	3	VAL	4.8
14	2	25	LYS	4.8
14	2	54	ASN	4.7
14	1	33	HIS	4.7
7	T	36	TRP	4.7
14	1	32	LEU	4.7
14	1	59	TRP	4.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
6	F	96	LEU	4.6
4	Q	147	LYS	4.6
7	G	9	GLY	4.6
7	T	84	LYS	4.6
14	2	48	TYR	4.6
7	G	5	LYS	4.5
8	H	45	ALA	4.5
14	1	44	PRO	4.5
14	2	71	PRO	4.5
14	2	62	GLU	4.5
7	T	37	LEU	4.5
14	2	65	MET	4.5
14	2	26	HIS	4.5
7	G	41	HIS	4.4
14	1	54	ASN	4.4
14	1	39	LYS	4.4
7	T	41	HIS	4.4
10	W	55	PHE	4.4
14	1	96	ALA	4.3
7	T	2	SER	4.3
10	W	1	PHE	4.3
14	1	50	ASP	4.3
14	1	62	GLU	4.2
2	O	227	LEU	4.2
14	1	68	LEU	4.2
4	D	6	VAL	4.2
14	2	41	GLY	4.2
14	1	48	TYR	4.2
9	V	32	ALA	4.1
12	Y	47	LYS	4.1
10	J	1	PHE	4.1
14	1	51	ALA	4.1
9	I	30	GLY	4.1
7	T	39	SER	4.1
14	2	47	THR	4.1
2	B	59	GLN	4.0
9	I	37	PHE	4.0
14	1	25	LYS	4.0
10	W	48	TYR	4.0
14	1	38	ARG	4.0
14	1	1	GLY	3.9
14	1	104	GLU	3.9

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
14	2	4	GLU	3.9
8	H	49	ASP	3.8
14	1	49	THR	3.8
10	J	56	PRO	3.8
6	F	95	GLN	3.8
14	2	30	PRO	3.8
14	2	49	THR	3.7
14	2	100	LYS	3.7
14	2	94	LEU	3.7
9	V	37	PHE	3.7
14	2	72	LYS	3.7
6	S	93	PRO	3.7
4	Q	102	TYR	3.7
14	2	15	ALA	3.7
9	V	34	PHE	3.7
4	Q	101	HIS	3.6
7	G	42	ARG	3.6
2	O	113	TYR	3.6
7	T	38	HIS	3.6
14	1	23	GLY	3.5
14	1	56	GLY	3.5
14	2	29	GLY	3.5
3	P	3	HIS	3.5
14	2	66	GLU	3.5
14	1	64	LEU	3.4
11	K	7	PRO	3.4
14	2	52	ASN	3.4
1	A	113[A]	LEU	3.4
14	1	103	ASN	3.4
14	1	100	LYS	3.4
7	T	9	GLY	3.3
14	2	31	ASN	3.3
14	2	2	ASP	3.3
1	N	199	LEU	3.2
7	G	84	LYS	3.2
13	Z	42	LYS	3.2
8	H	8	ILE	3.2
14	1	63	THR	3.2
7	G	4	ALA	3.2
6	S	95	GLN	3.1
14	2	53	LYS	3.1
14	1	60	LYS	3.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
6	F	94	HIS	3.1
13	Z	35	TYR	3.1
1	A	73	ILE	3.1
7	T	3	ALA	3.0
10	W	56	PRO	3.0
14	1	61	GLU	3.0
1	N	374	VAL	3.0
12	L	47	LYS	3.0
14	1	55	LYS	3.0
7	T	8	HIS	2.9
14	1	52	ASN	2.9
7	T	43	GLU	2.9
4	Q	140	TYR	2.9
8	H	47	GLY	2.9
9	I	33	THR	2.8
14	1	97	TYR	2.8
5	E	109	VAL	2.8
10	W	52	TRP	2.8
11	X	6	ALA	2.8
14	2	73	LYS	2.8
14	1	45	GLY	2.8
14	1	22	LYS	2.8
14	2	10	PHE	2.7
14	2	88	LYS	2.7
13	Z	43	SER	2.7
2	B	58	ALA	2.7
7	G	38	HIS	2.7
14	1	66	GLU	2.7
14	1	26	HIS	2.7
14	1	65	MET	2.7
9	V	53	ASN	2.7
1	N	373	VAL	2.6
14	1	2	ASP	2.6
8	H	46	LYS	2.6
7	T	4	ALA	2.6
10	J	2	GLU	2.6
7	G	37	LEU	2.6
14	2	79	LYS	2.6
4	Q	87	PHE	2.6
14	1	4	GLU	2.6
1	N	377	PHE	2.5
4	Q	138	TRP	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
8	H	43	MET	2.5
1	N	63	PHE	2.5
7	G	1	ALA	2.5
10	W	4	ARG	2.5
11	X	27	ALA	2.4
14	1	89	THR	2.4
1	A	82	LEU	2.4
1	N	246	LEU	2.4
1	A	386	VAL	2.4
1	A	70	VAL	2.4
1	N	66	ILE	2.4
14	1	67	TYR	2.4
14	2	92	GLU	2.4
9	V	42	LYS	2.4
3	C	37	PHE	2.4
9	V	65	LYS	2.4
1	N	126	TRP	2.4
14	1	93	ASP	2.4
1	N	127	THR	2.3
6	F	3	GLY	2.3
3	P	41	THR	2.3
1	A	199	LEU	2.3
1	N	238	PHE	2.3
11	X	23	THR	2.3
14	1	6	GLY	2.3
3	P	40	MET	2.2
14	2	50	ASP	2.2
1	A	247	ILE	2.2
1	N	245	ILE	2.2
1	N	247	ILE	2.2
1	N	202	LEU	2.2
3	P	38	ASN	2.2
13	M	42	LYS	2.2
9	V	36	LYS	2.2
9	V	31	PHE	2.2
1	A	389	ILE	2.2
1	A	150	LEU	2.2
1	A	78	PHE	2.2
1	N	372	TYR	2.2
14	1	20	VAL	2.2
14	2	91	ARG	2.2
14	2	69	GLU	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	245	ILE	2.2
1	A	196	LEU	2.2
1	N	128	VAL	2.2
1	A	74	MET	2.2
1	A	197	LEU	2.1
1	N	150	LEU	2.1
14	1	88	LYS	2.1
10	J	55	PHE	2.1
3	C	261	SER	2.1
4	Q	141	ASP	2.1
1	A	195	LEU	2.1
1	N	113[A]	LEU	2.1
11	K	6	ALA	2.1
1	A	190	ILE	2.1
1	N	248	LEU	2.1
1	A	188	VAL	2.1
10	J	48	TYR	2.1
1	N	206	ILE	2.1
1	A	388	ALA	2.1
4	Q	46	ALA	2.1
1	N	251	PHE	2.1
7	T	5	LYS	2.1
14	1	92	GLU	2.0
1	A	72	PRO	2.0
1	N	190	ILE	2.0
7	T	33	LEU	2.0
14	1	94	LEU	2.0
1	N	370	THR	2.0
11	K	23	THR	2.0
11	X	34	THR	2.0
1	N	243	VAL	2.0
2	B	61	VAL	2.0
1	N	244	TYR	2.0
14	1	79	LYS	2.0
1	A	126	TRP	2.0
1	N	191	THR	2.0
1	N	389	ILE	2.0
7	G	33	LEU	2.0
1	A	193	VAL	2.0
4	D	147	LYS	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(Å <sup>2</sup> )	Q<0.9
9	SAC	V	1	9/10	0.31	0.92	131,137,150,153	0
7	TPO	T	11	11/12	0.45	0.35	85,109,117,125	0
7	TPO	G	11	11/12	0.50	0.33	81,97,160,160	0
9	SAC	I	1	9/10	0.75	0.39	98,106,110,119	0
1	FME	A	1	10/11	0.95	0.13	40,52,71,88	0
1	FME	N	1	10/11	0.96	0.17	43,61,73,95	0
2	FME	O	1	10/11	0.98	0.14	49,56,65,78	0
2	FME	B	1	10/11	0.98	0.10	30,35,39,51	0

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
17	NA	P	302	1/1	0.55	0.51	57,57,57,57	0
17	NA	C	302	1/1	0.59	0.57	59,59,59,59	0
26	CDL	G	101	100/100	0.66	0.30	58,103,158,163	0
27	UNL	P	309	16/-	0.68	0.17	70,79,89,95	0
24	CHD	W	101	29/29	0.70	0.43	73,114,126,130	0
26	CDL	T	101	100/100	0.73	0.25	61,95,153,161	0
27	UNL	J	102	10/-	0.73	0.29	61,65,77,92	0
20	PGV	P	305	51/51	0.73	0.24	54,86,135,150	0
21	TGL	Q	201	63/63	0.74	0.21	52,82,104,109	0
20	PGV	C	305	51/51	0.74	0.24	55,80,122,138	0
21	TGL	D	201	63/63	0.76	0.22	47,70,101,105	0
28	PSC	E	201	52/52	0.76	0.26	50,79,162,163	0
27	UNL	N	601	17/-	0.76	0.18	52,60,83,85	0
27	UNL	T	102	18/-	0.76	0.18	47,66,85,92	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
30	DMU	Z	101	33/33	0.76	0.30	55,76,107,113	0
27	UNL	N	609	16/-	0.77	0.32	54,59,79,85	0
27	UNL	C	309	17/-	0.77	0.16	60,71,87,90	0
20	PGV	A	607	51/51	0.77	0.30	44,84,151,159	0
27	UNL	W	102	9/-	0.78	0.24	59,62,79,82	0
21	TGL	L	101	63/63	0.78	0.26	45,70,98,107	0
27	UNL	Y	101	10/-	0.78	0.40	69,76,86,94	0
27	UNL	C	310	7/-	0.79	0.34	41,64,76,83	0
26	CDL	P	306	100/100	0.79	0.27	49,97,149,159	0
27	UNL	L	102	10/-	0.80	0.27	61,75,82,86	0
28	PSC	V	101	52/52	0.82	0.23	49,77,145,166	0
24	CHD	C	307	29/29	0.82	0.26	73,85,93,99	0
26	CDL	C	306	100/100	0.83	0.23	51,86,124,152	0
21	TGL	N	608	63/63	0.83	0.19	51,73,104,115	0
23	EDO	I	101	4/4	0.83	0.14	55,59,63,72	0
24	CHD	J	101	29/29	0.84	0.32	61,75,106,109	0
27	UNL	N	611	12/-	0.84	0.16	48,56,68,69	0
23	EDO	E	202	4/4	0.85	0.33	57,61,68,79	0
27	UNL	C	308	18/-	0.85	0.20	55,66,77,81	0
27	UNL	P	310	7/-	0.85	0.27	53,60,76,88	0
27	UNL	N	610	18/-	0.85	0.19	51,59,69,70	0
27	UNL	P	308	20/-	0.86	0.20	58,64,72,73	0
24	CHD	P	307	29/29	0.89	0.29	71,80,88,95	0
21	TGL	B	301	63/63	0.90	0.18	33,68,103,114	0
24	CHD	P	301	29/29	0.91	0.12	40,45,52,55	0
30	DMU	M	101	33/33	0.92	0.14	40,46,62,65	0
25	PEK	C	303	53/53	0.93	0.16	34,48,88,97	0
23	EDO	N	614	4/4	0.93	0.16	56,59,63,85	0
31	HEC	2	201	43/43	0.94	0.26	79,101,135,149	0
31	HEC	1	201	43/43	0.95	0.19	57,81,94,99	0
25	PEK	P	303	53/53	0.95	0.13	39,53,94,101	0
16	MG	A	602	1/1	0.95	0.21	36,36,36,36	0
20	PGV	P	304	51/51	0.95	0.13	30,46,73,76	0
16	MG	N	603	1/1	0.96	0.25	42,42,42,42	0
24	CHD	T	103	29/29	0.96	0.08	30,36,42,53	0
24	CHD	C	301	29/29	0.96	0.08	34,40,48,53	0
24	CHD	G	102	29/29	0.96	0.08	35,38,43,52	0
20	PGV	C	304	51/51	0.96	0.12	31,38,95,103	0
23	EDO	F	102	4/4	0.97	0.14	45,47,49,49	0
20	PGV	N	612	51/51	0.97	0.15	33,43,70,80	0
20	PGV	A	608	51/51	0.97	0.15	29,41,68,74	0
23	EDO	C	311	4/4	0.97	0.08	48,51,51,52	0

*Continued on next page...*

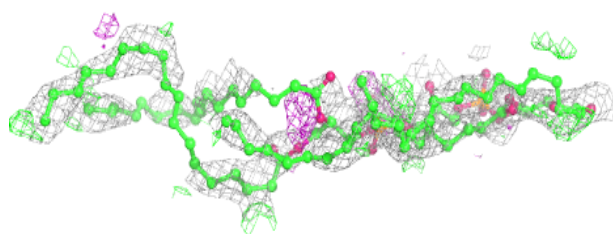
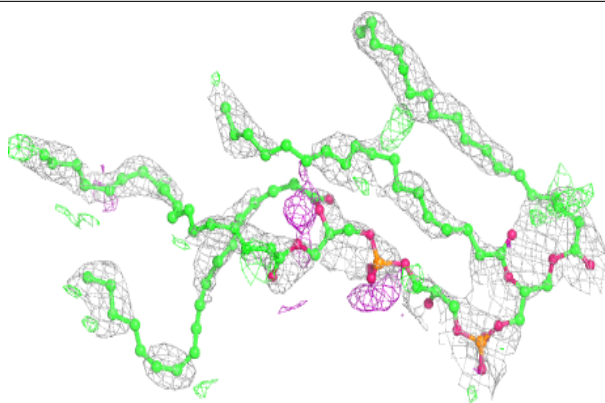
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
23	EDO	G	103	4/4	0.97	0.09	37,39,49,51	0
23	EDO	S	102	4/4	0.97	0.08	44,45,46,53	0
17	NA	N	604	1/1	0.97	0.09	45,45,45,45	0
19	PER	N	607	2/2	0.98	0.10	36,36,36,48	0
23	EDO	B	303	4/4	0.98	0.13	30,31,33,36	0
18	HEA	N	605[B]	60/60	0.98	0.18	32,38,44,47	9
23	EDO	N	613	4/4	0.98	0.16	38,38,39,41	0
18	HEA	N	605[A]	60/60	0.98	0.18	32,38,47,50	9
18	HEA	A	604[A]	60/60	0.99	0.15	23,28,38,40	9
18	HEA	A	604[B]	60/60	0.99	0.15	23,28,35,40	9
18	HEA	N	606	60/60	0.99	0.19	27,33,41,47	0
18	HEA	A	605	60/60	0.99	0.14	22,26,33,39	0
29	ZN	S	101	1/1	0.99	0.05	37,37,37,37	0
19	PER	A	606	2/2	0.99	0.10	40,40,40,54	0
22	CUA	O	301	2/2	0.99	0.09	42,42,42,43	0
15	CU	N	602	1/1	1.00	0.14	35,35,35,35	0
29	ZN	F	101	1/1	1.00	0.10	36,36,36,36	0
22	CUA	B	302	2/2	1.00	0.11	27,27,27,29	0
15	CU	A	601	1/1	1.00	0.13	29,29,29,29	0
17	NA	A	603	1/1	1.00	0.05	31,31,31,31	0

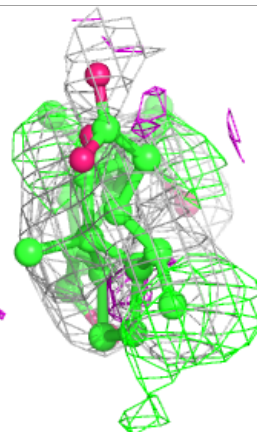
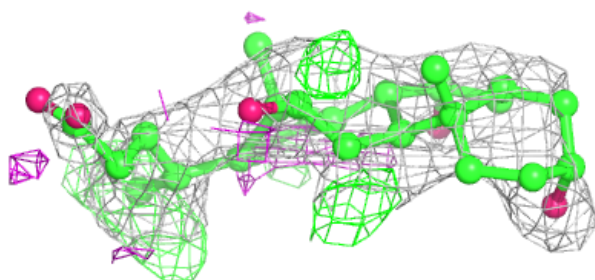
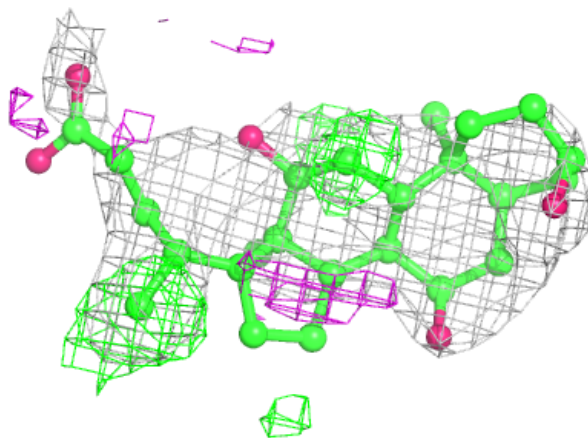
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around CDL G 101:**

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

**Electron density around CHD W 101:**

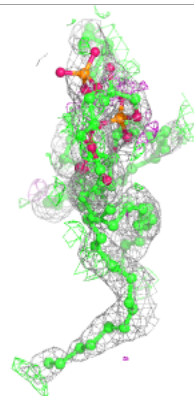
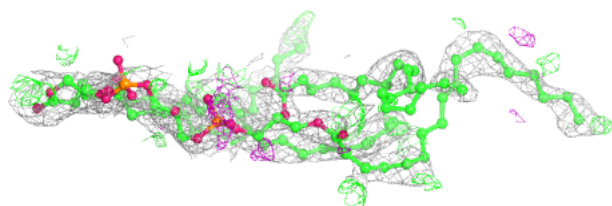
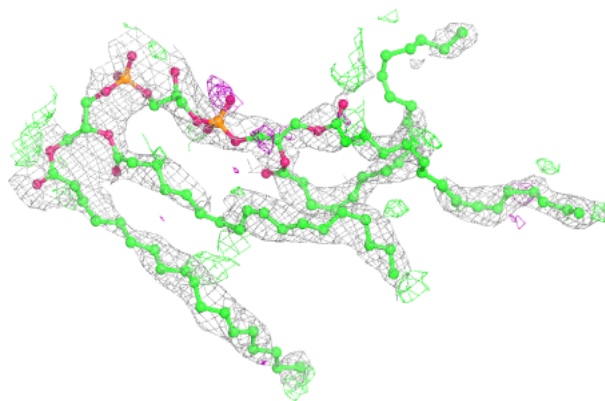
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



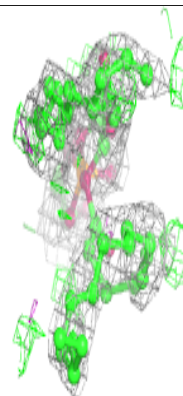
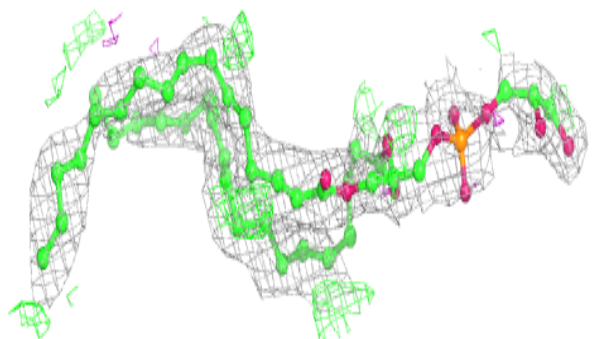
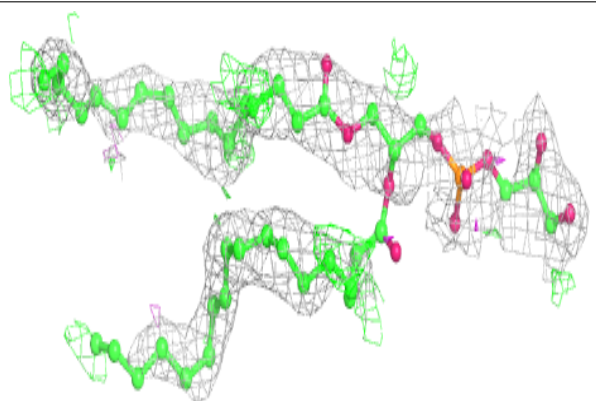


**Electron density around CDL T 101:**

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

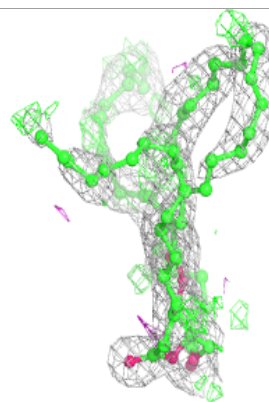
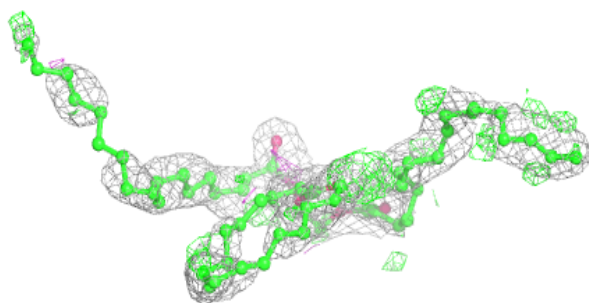
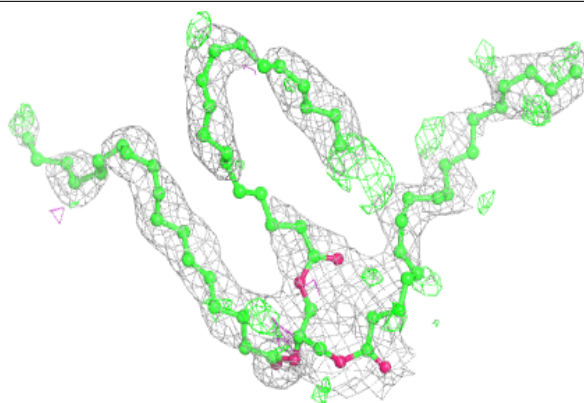
**Electron density around PGV P 305:**

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

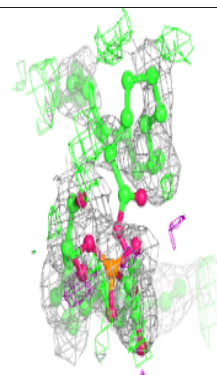
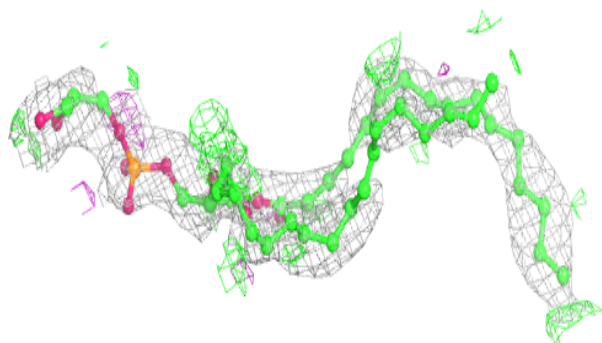
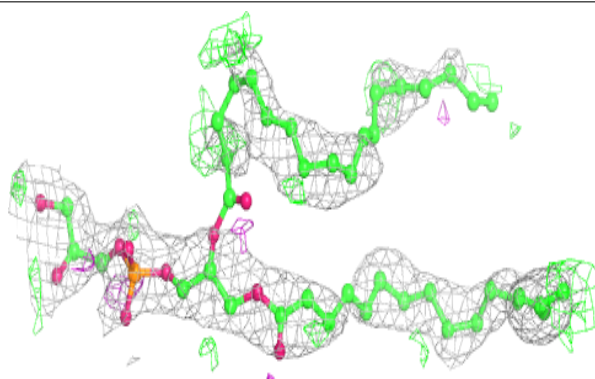


**Electron density around TGL Q 201:**

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

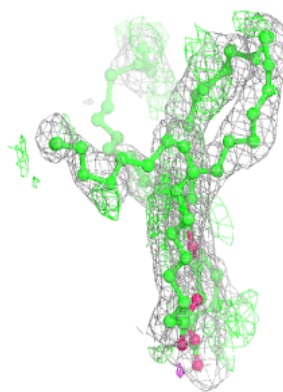
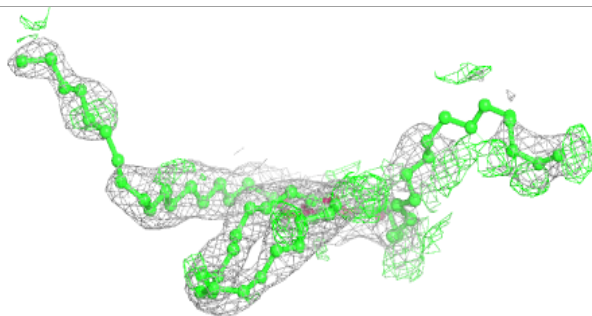
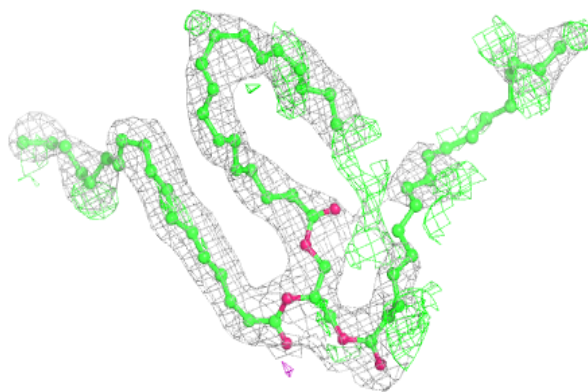
**Electron density around PGV C 305:**

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

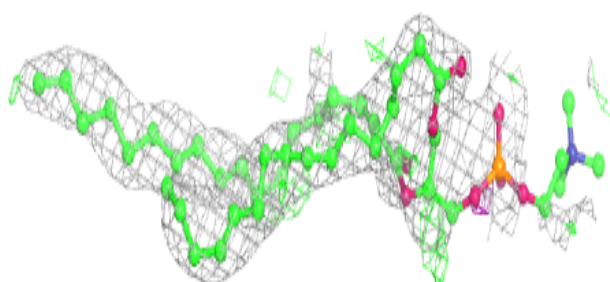
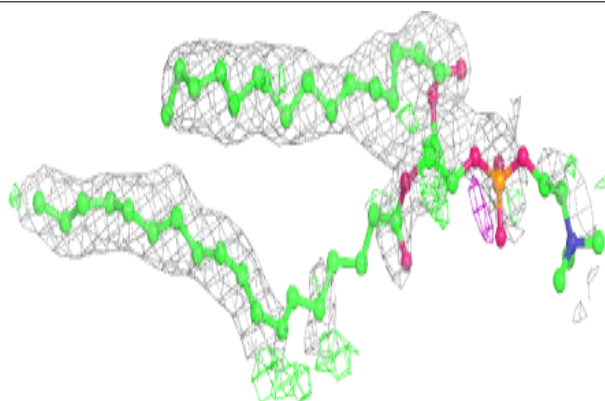


**Electron density around TGL D 201:**

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

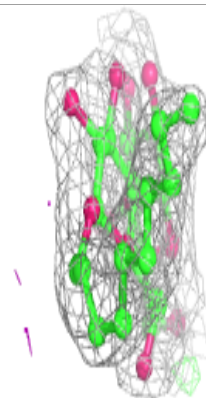
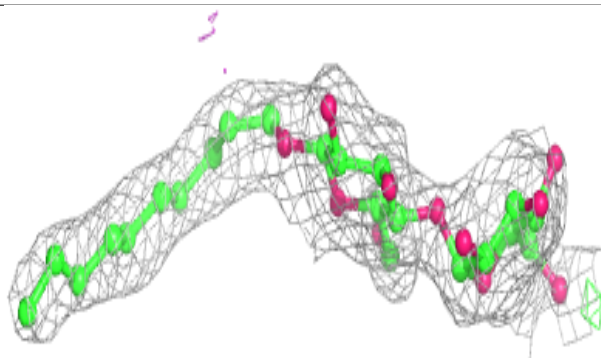
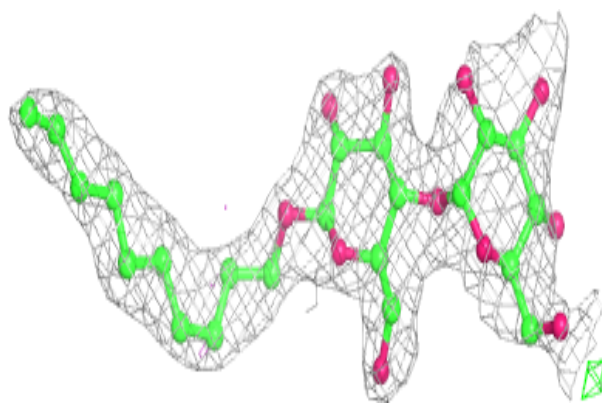
**Electron density around PSC E 201:**

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

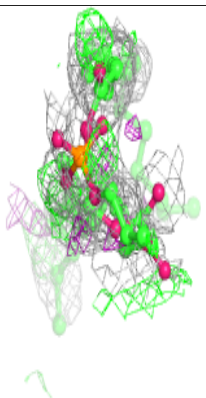
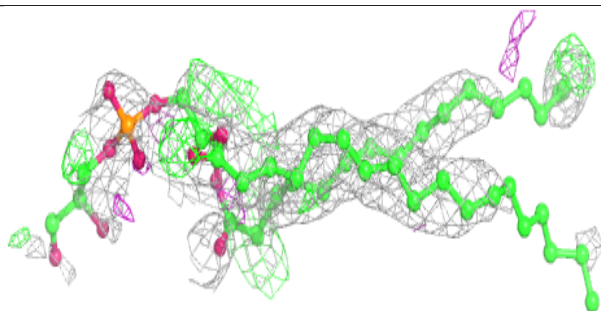
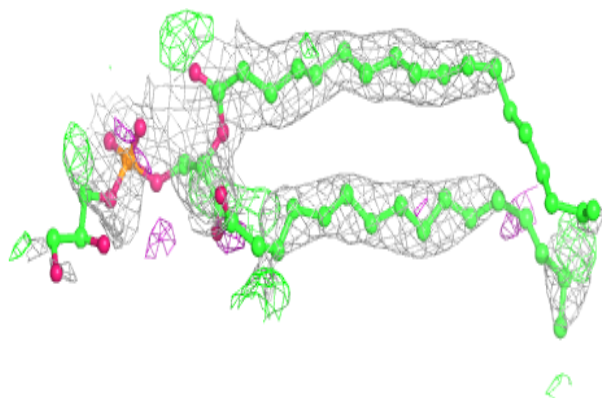


**Electron density around DMU Z 101:**

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

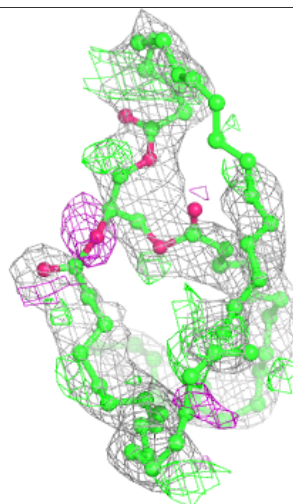
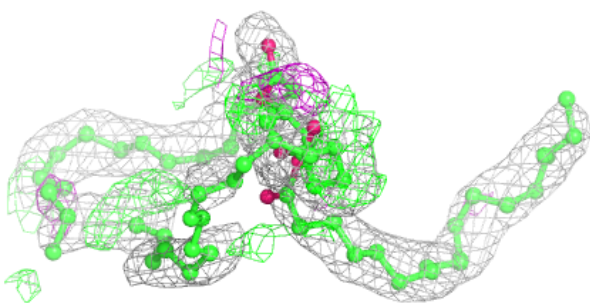
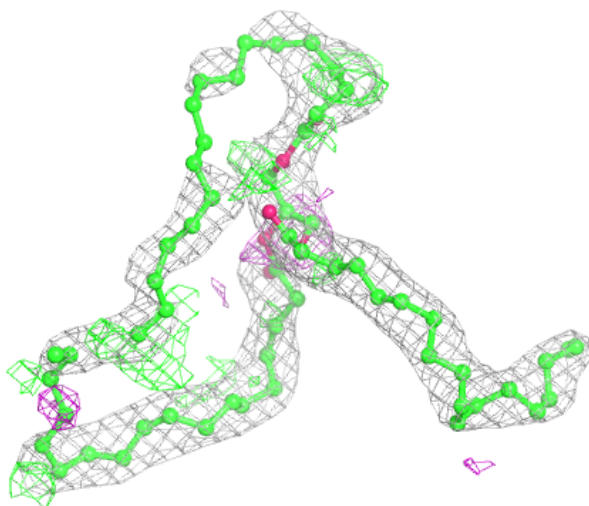
**Electron density around PGV A 607:**

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



**Electron density around TGL L 101:**

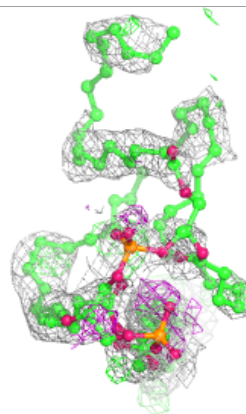
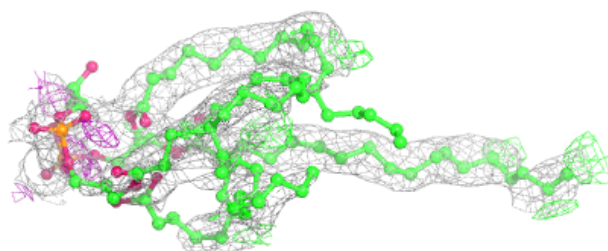
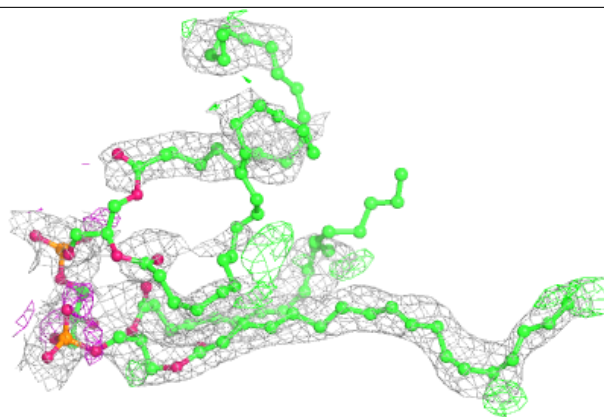
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



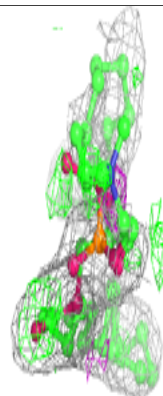
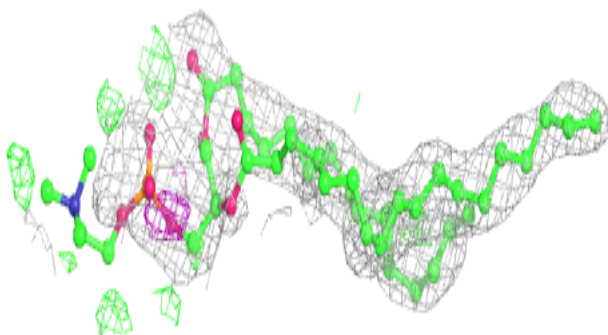
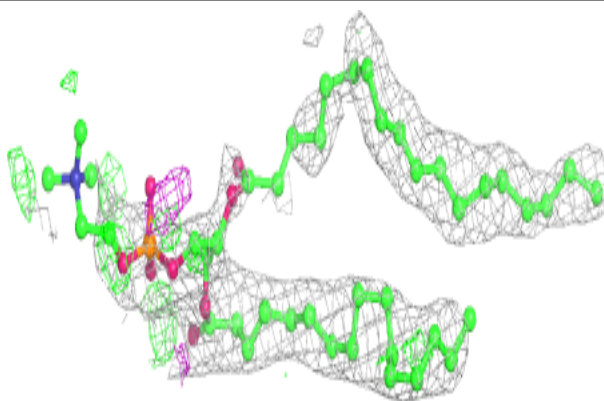


**Electron density around CDL P 306:**

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

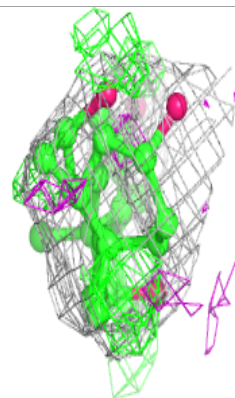
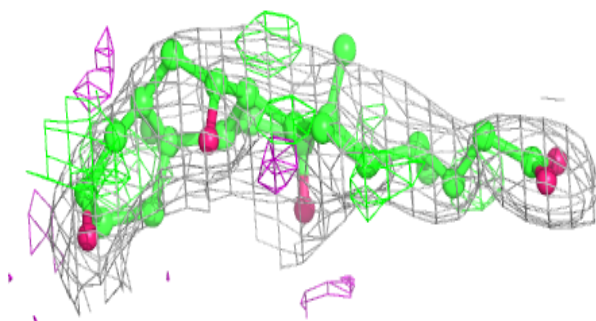
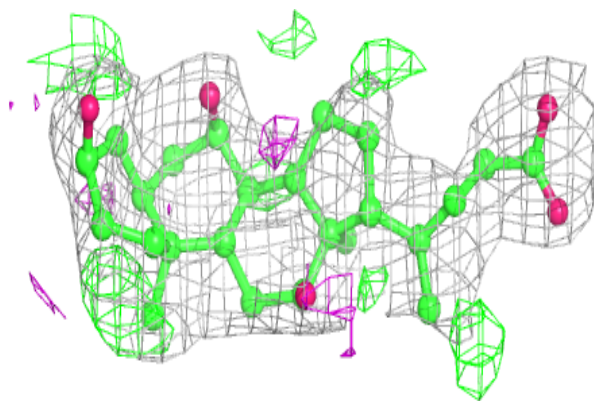
**Electron density around PSC V 101:**

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

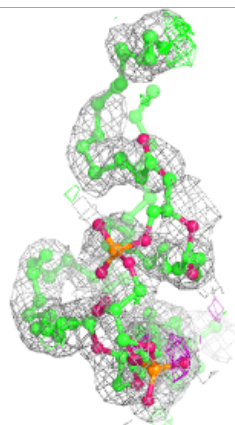
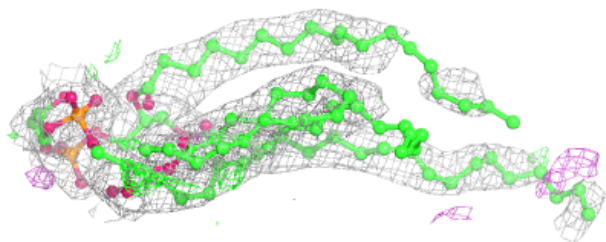
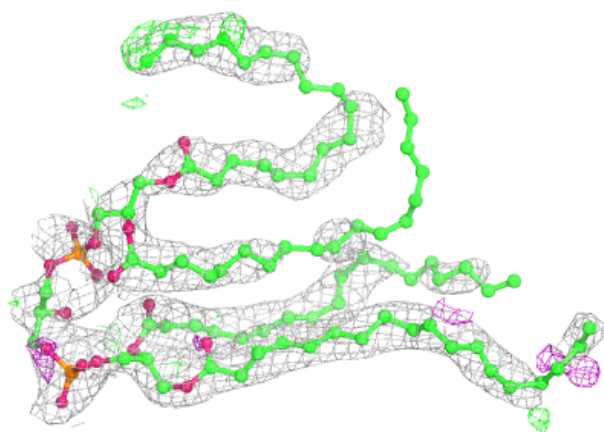


**Electron density around CHD C 307:**

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

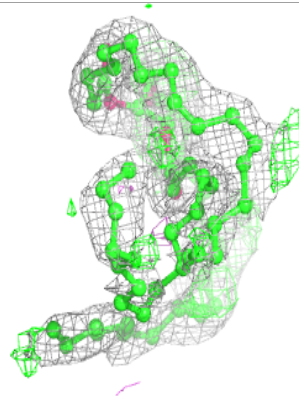
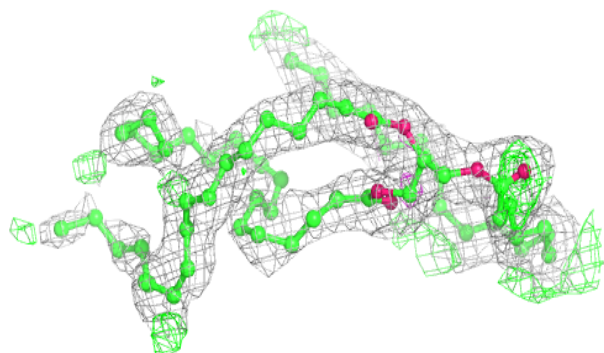
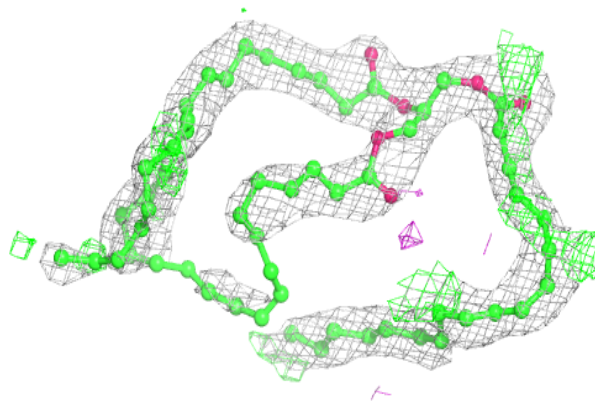
**Electron density around CDL C 306:**

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

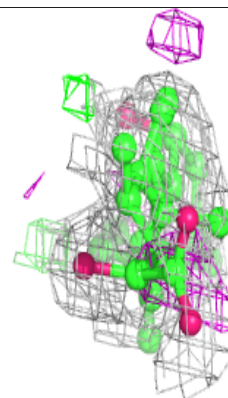
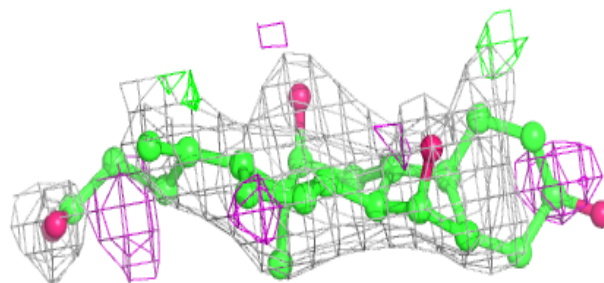
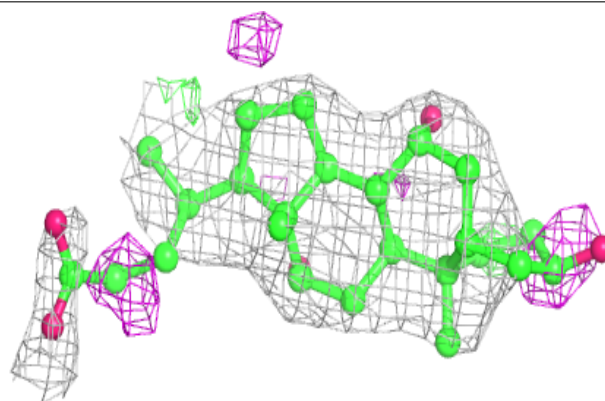


**Electron density around TGL N 608:**

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

**Electron density around CHD J 101:**

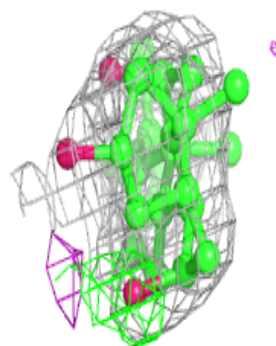
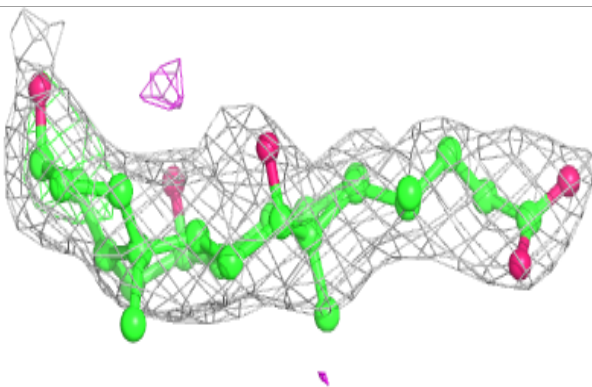
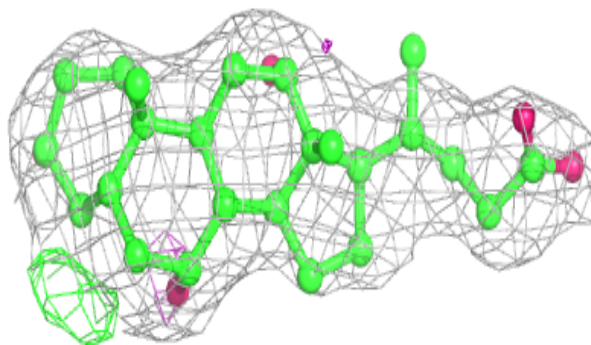
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





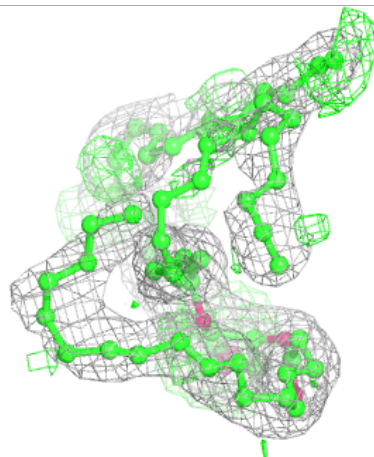
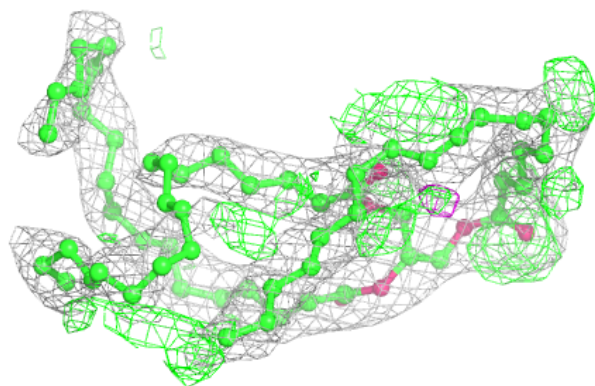
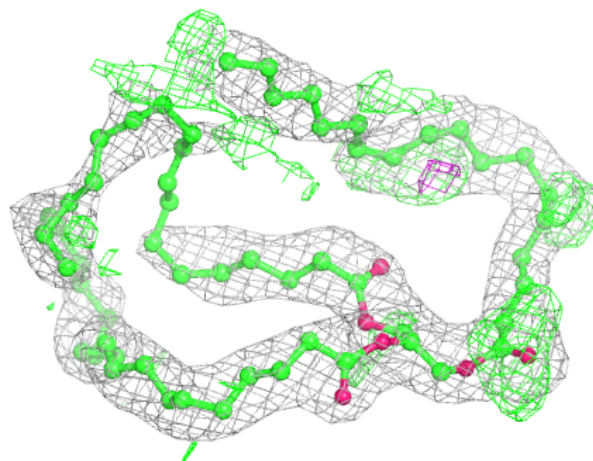
**Electron density around CHD P 307:**

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



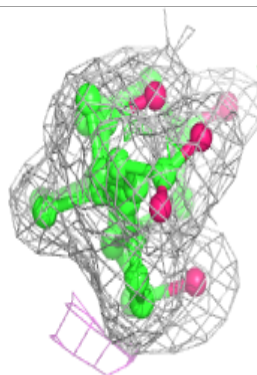
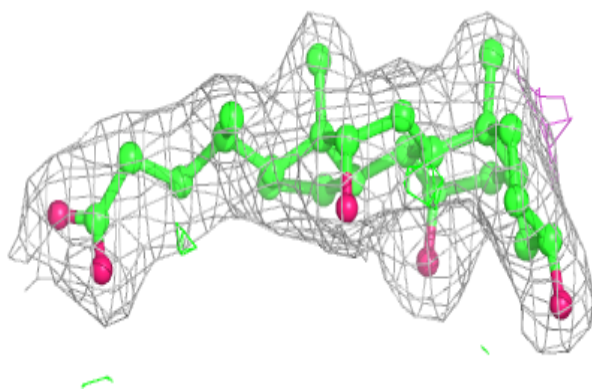
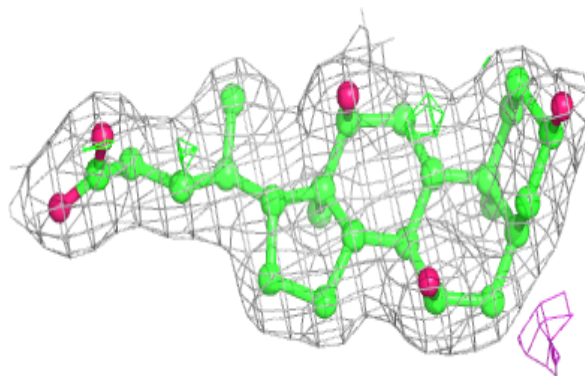
**Electron density around TGL B 301:**

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

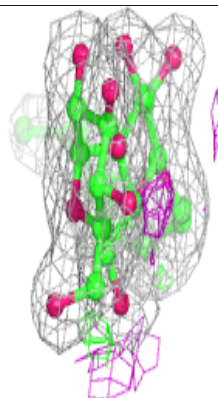
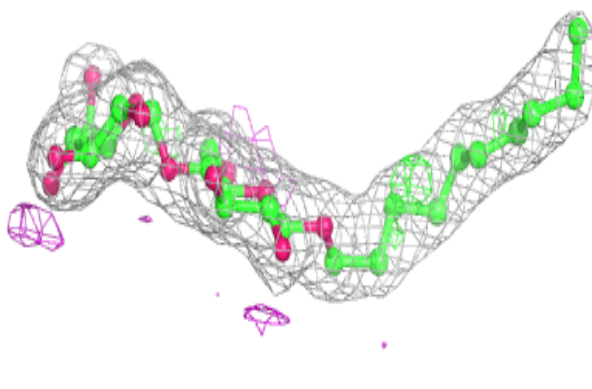
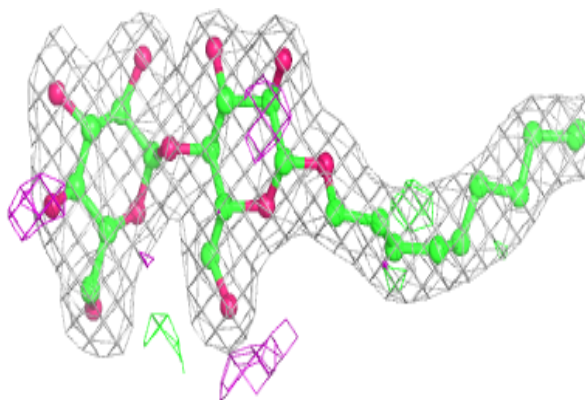


**Electron density around CHD P 301:**

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

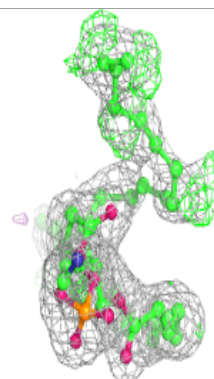
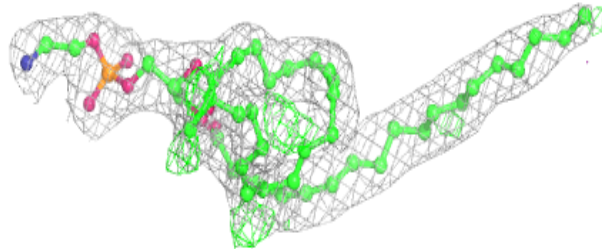
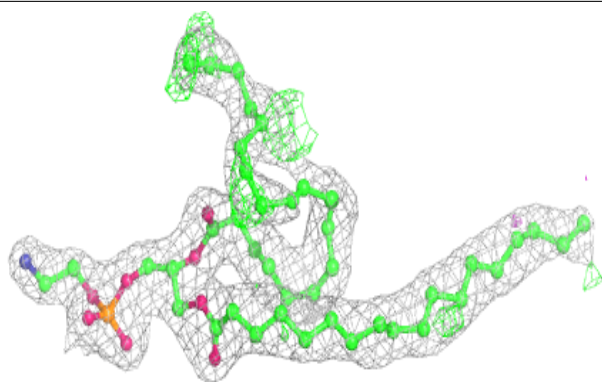
**Electron density around DMU M 101:**

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



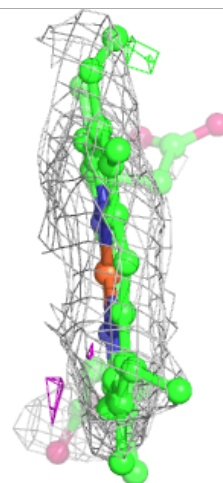
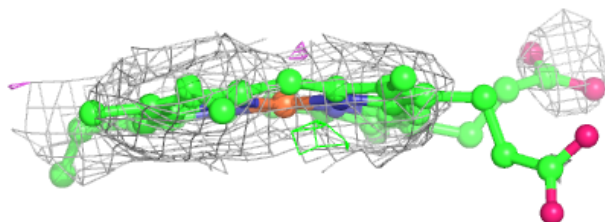
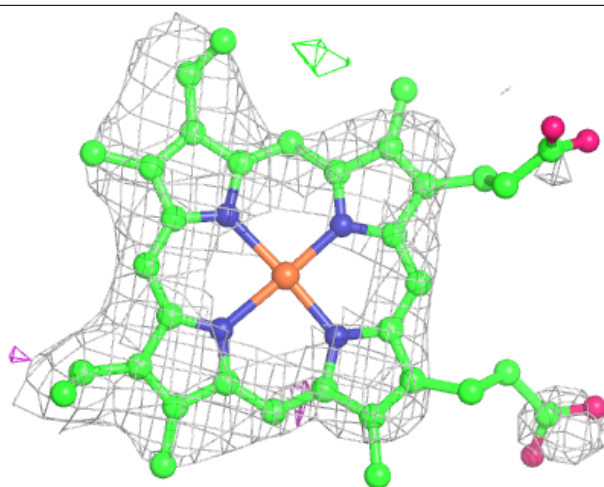
**Electron density around PEK C 303:**

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



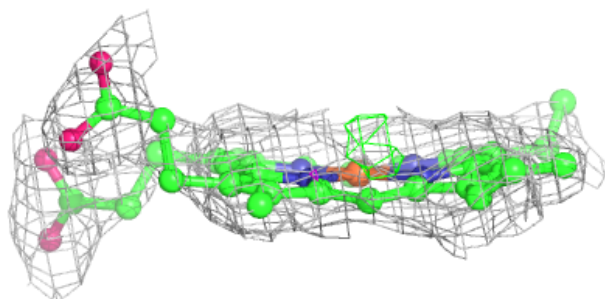
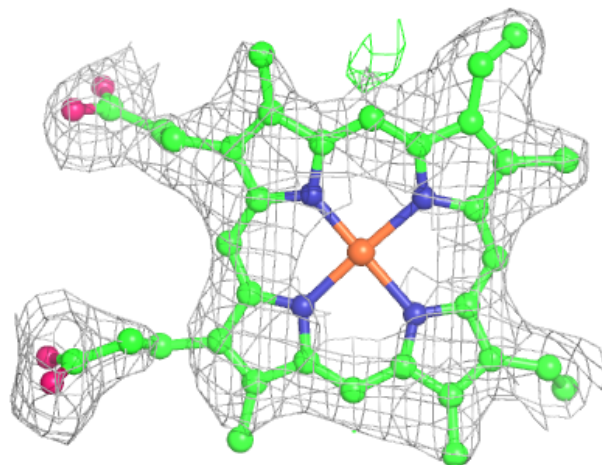
**Electron density around HEC 2 201:**

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



**Electron density around HEC 1 201:**

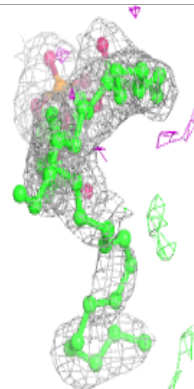
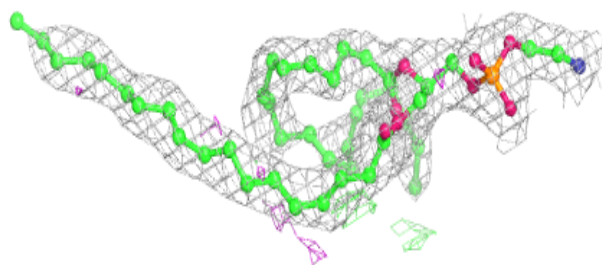
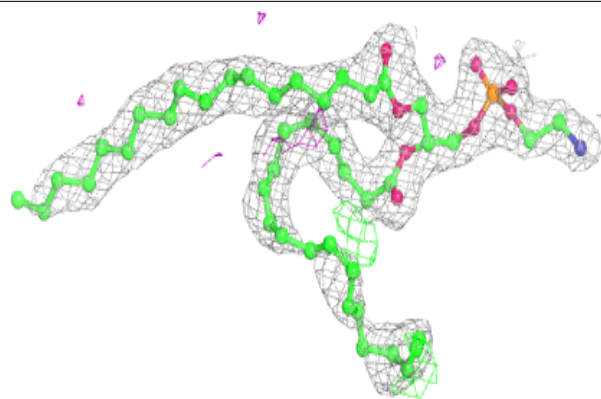
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



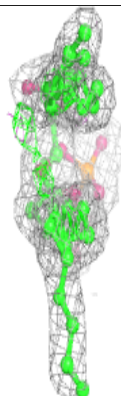
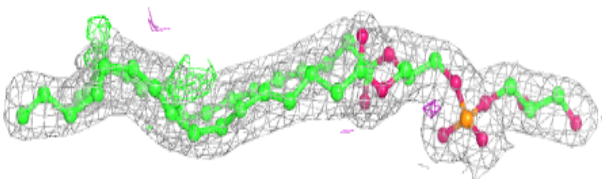
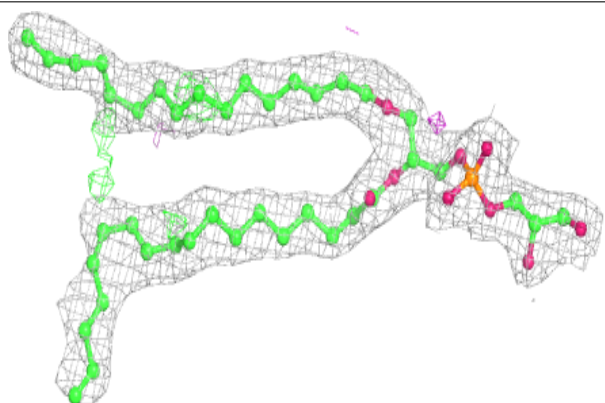


**Electron density around PEK P 303:**

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

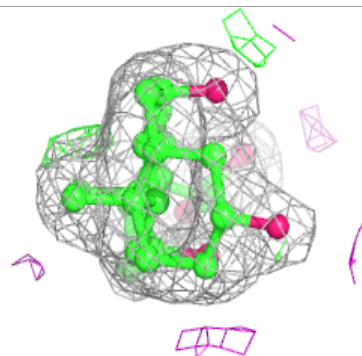
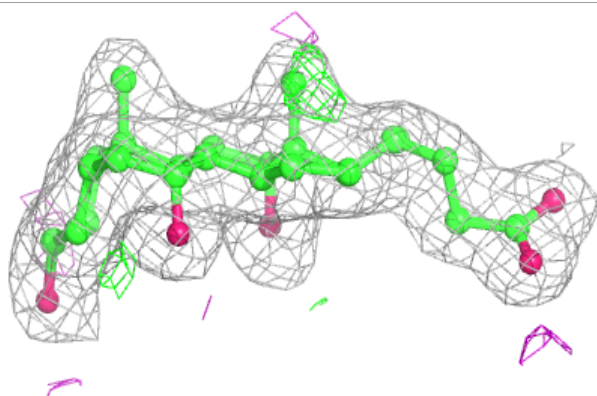
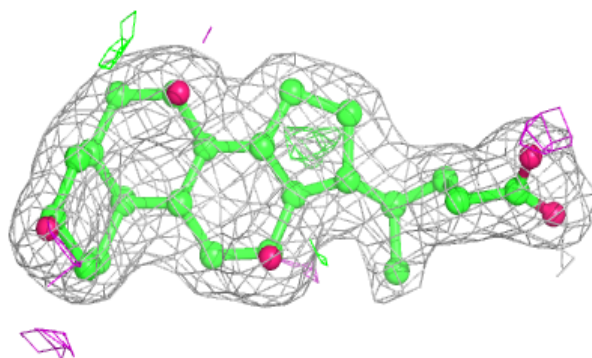
**Electron density around PGV P 304:**

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

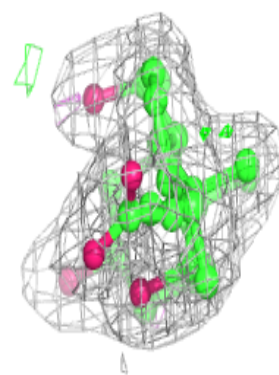
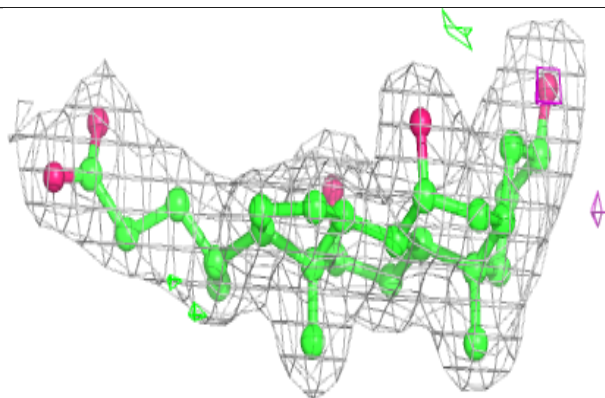
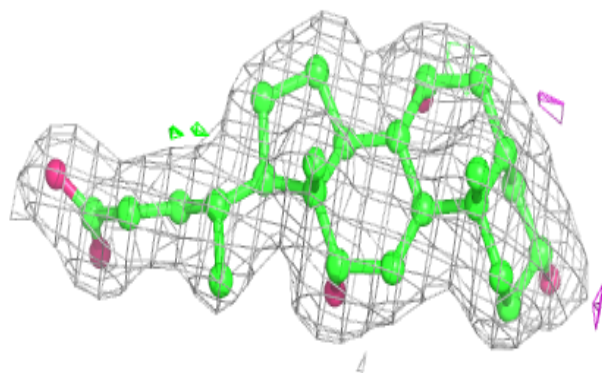


**Electron density around CHD T 103:**

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

**Electron density around CHD C 301:**

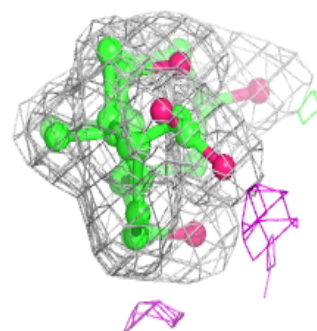
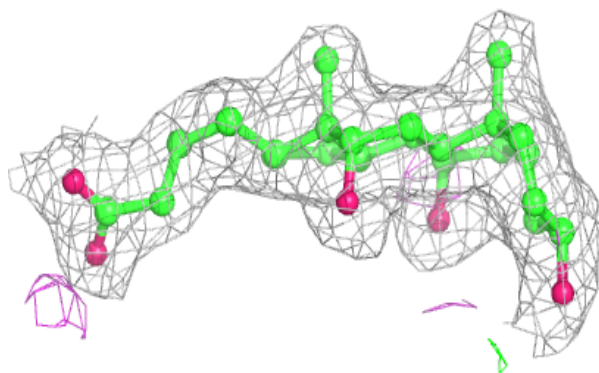
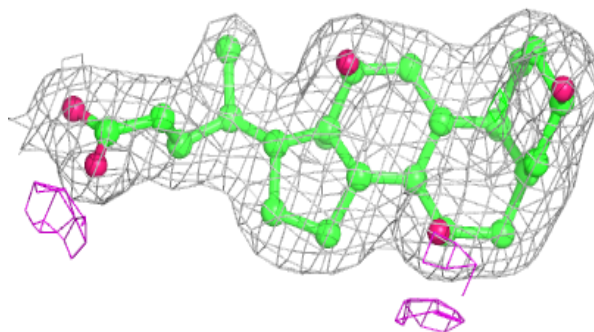
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



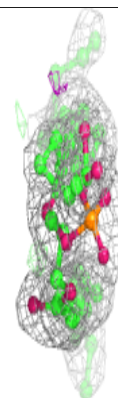
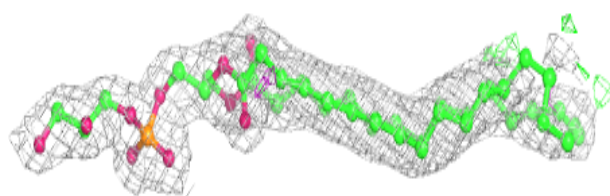
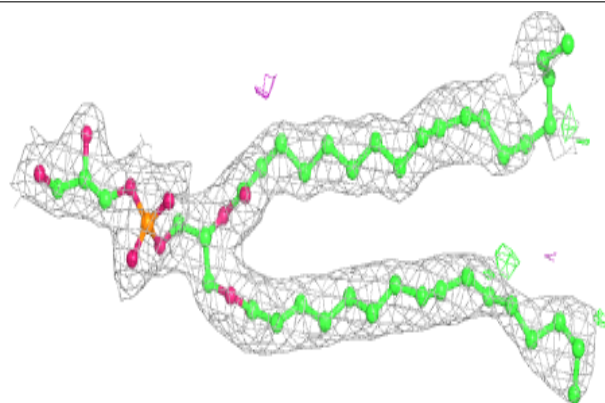


**Electron density around CHD G 102:**

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

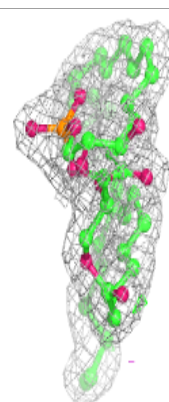
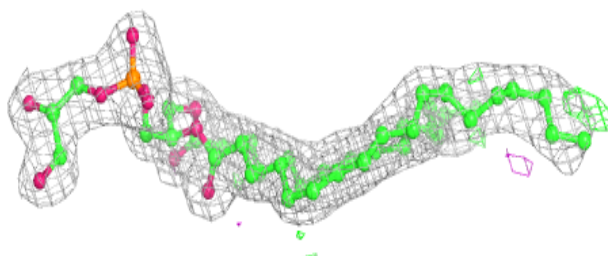
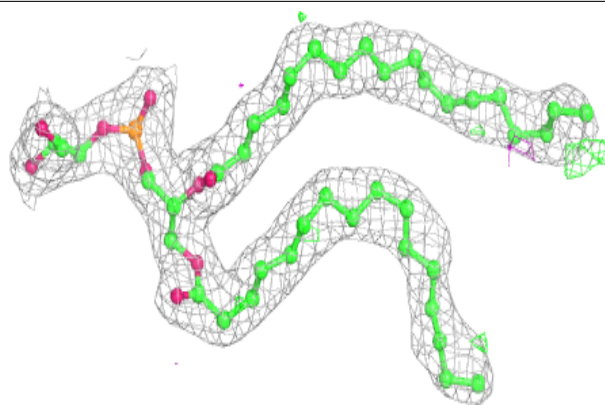
**Electron density around PGV C 304:**

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

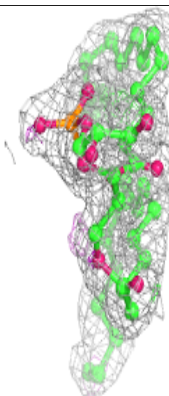
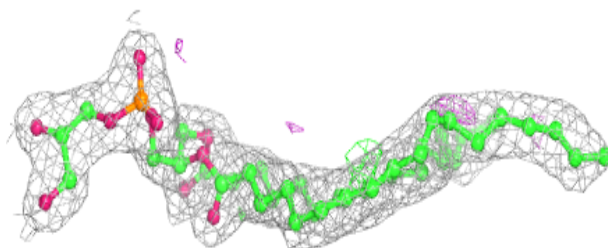
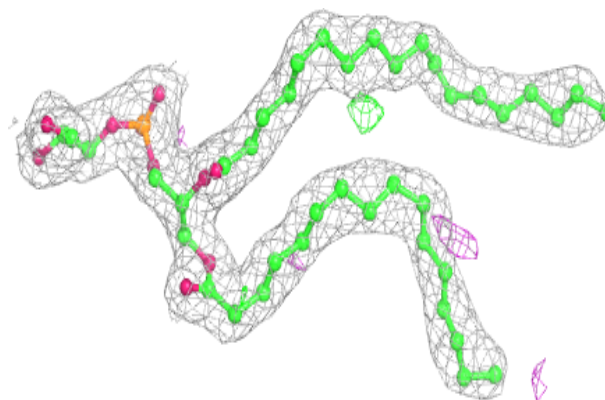


**Electron density around PGV N 612:**

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

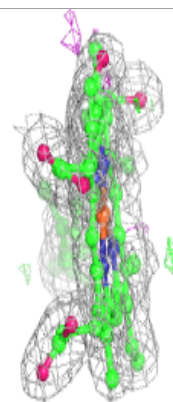
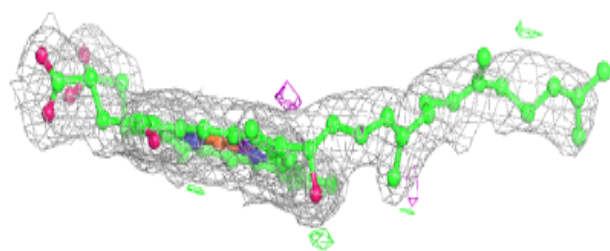
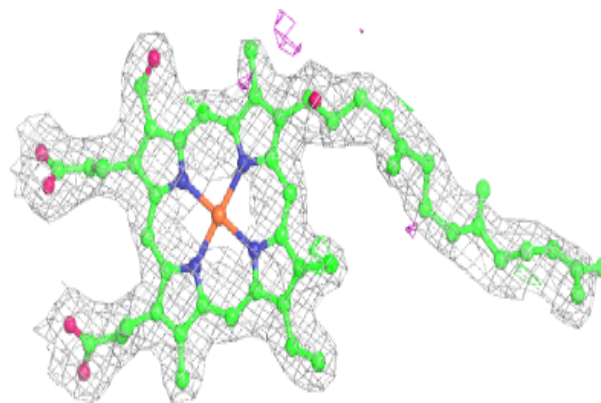
**Electron density around PGV A 608:**

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

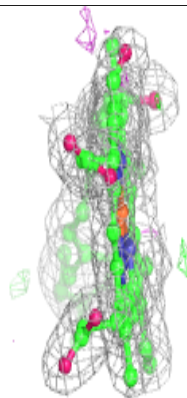
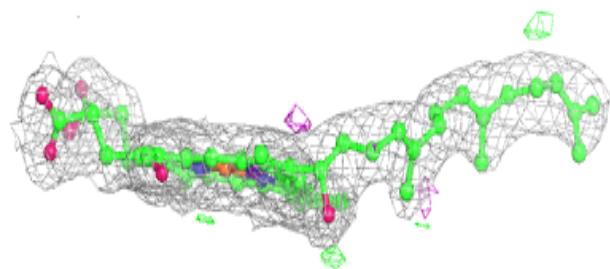
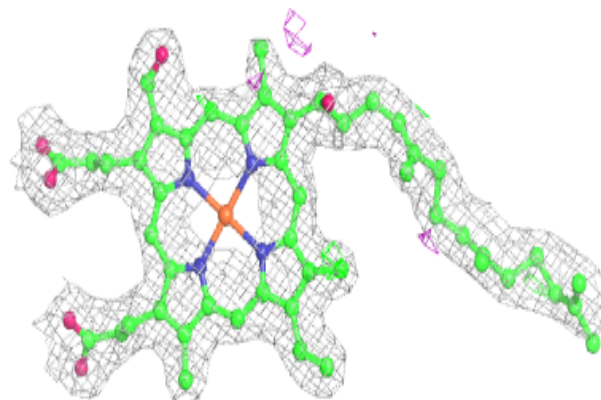


**Electron density around HEA N 605 (B):**

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

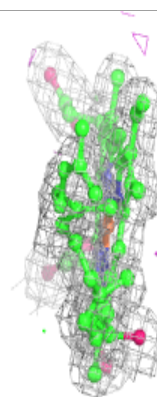
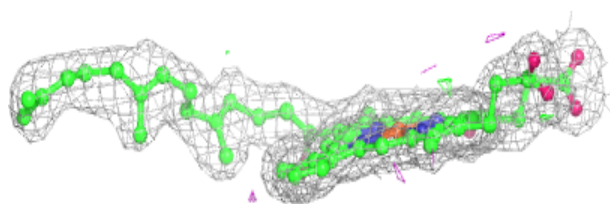
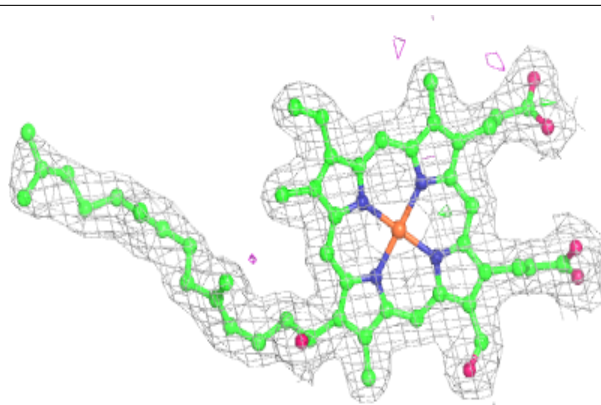
**Electron density around HEA N 605 (A):**

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

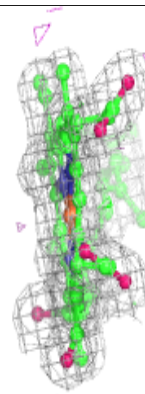
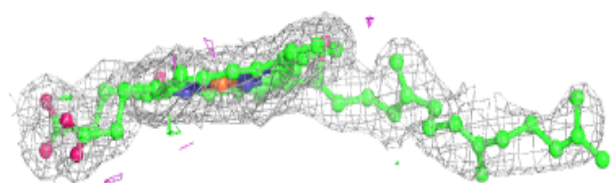
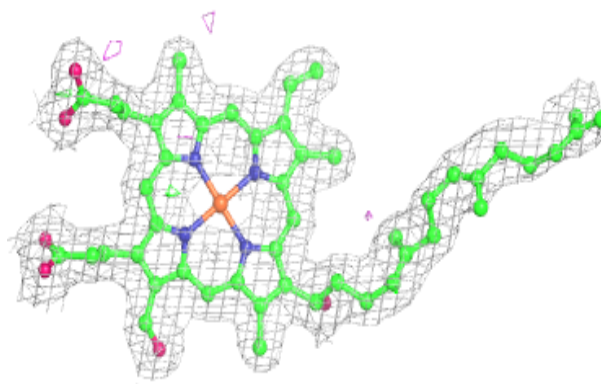


**Electron density around HEA A 604 (A):**

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

**Electron density around HEA A 604 (B):**

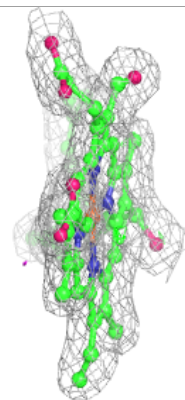
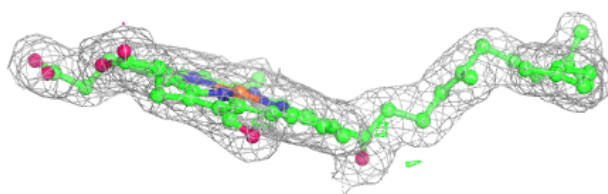
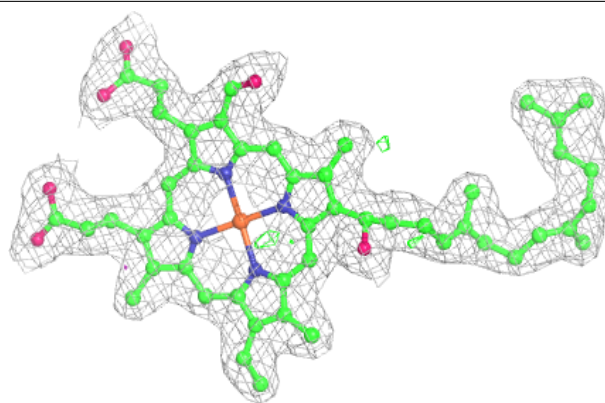
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



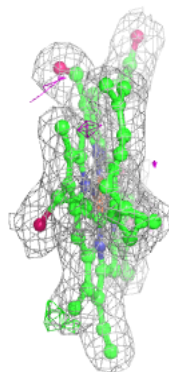
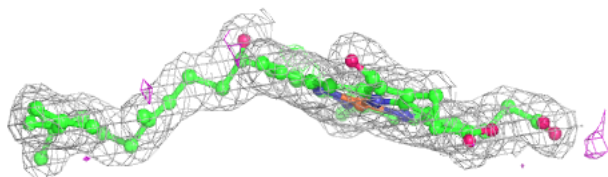
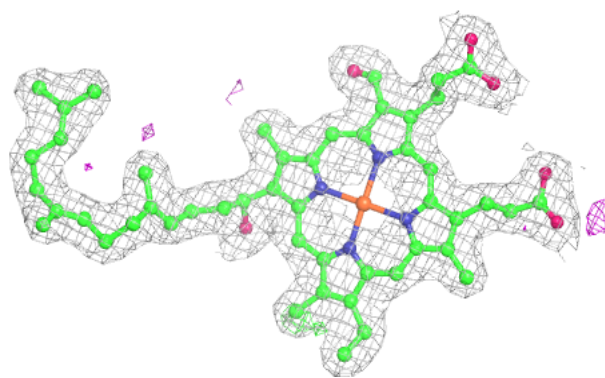


**Electron density around HEA N 606:**

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

**Electron density around HEA A 605:**

$2mF_o-DF_c$  (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.