



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 04:06 pm BST

PDB ID : 5KLV  
Title : Structure of bos taurus cytochrome bc1 with fenamidone inhibited  
Authors : Xia, D.; Esser, L.; Zhou, F.; Zhou, Y.; Xiao, Y.; Tang, W.K.; Yu, C.A.; Qin, Z.  
Deposited on : 2016-06-25  
Resolution : 2.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

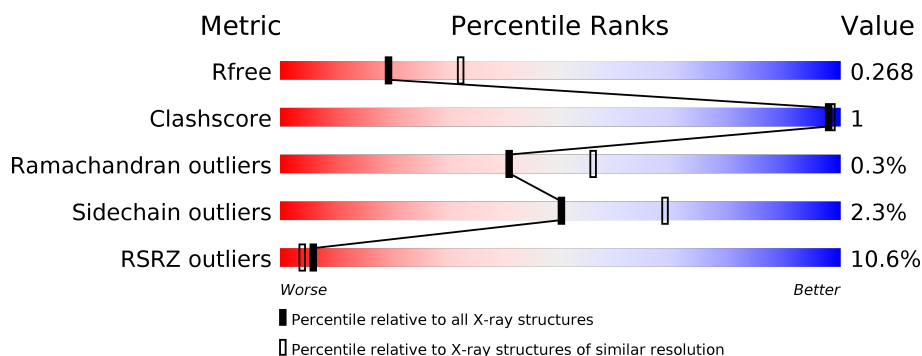
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	446	<div> <div>3%</div> <div>96%</div> <div>.</div> </div>
2	B	439	<div> <div>%</div> <div>95%</div> <div>..</div> </div>
3	C	379	<div> <div>3%</div> <div>96%</div> <div>..</div> </div>
4	D	241	<div> <div>17%</div> <div>95%</div> <div>5%</div> </div>
5	E	196	<div> <div>31%</div> <div>96%</div> <div>.</div> </div>
6	F	110	<div> <div>5%</div> <div>92%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
7	G	80	
8	H	78	
9	I	78	
10	J	63	
11	K	55	

## 2 Entry composition

There are 23 unique types of molecules in this entry. The entry contains 33655 atoms, of which 16742 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 b-c1 complex subunit 1, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	446	Total	C	H	N	O	S	0	0	0
			6799	2161	3341	609	668	20			

- Molecule 2 is a protein called Cytochrome b-c1 complex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	425	Total	C	H	N	O	S	0	0	0
			6328	1998	3147	564	612	7			

- Molecule 3 is a protein called Cytochrome b.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	377	Total	C	H	N	O	S	0	0	0
			6042	2009	3046	470	499	18			

- Molecule 4 is a protein called Cytochrome c1, heme protein, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	241	Total	C	H	N	O	S	0	0	0
			3778	1225	1859	330	349	15			

- Molecule 5 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	E	196	Total	C	H	N	O	S	0	0	0
			3015	957	1497	263	290	8			

- Molecule 6 is a protein called Cytochrome b-c1 complex subunit 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	F	105	Total	C	H	N	O	S	0	0	0
			1816	576	905	166	167	2			

- Molecule 7 is a protein called Cytochrome b-c1 complex subunit 8.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
7	G	75	Total	C	H	N	O	S	0	0	0
			1261	410	633	118	99	1			

- Molecule 8 is a protein called Cytochrome b-c1 complex subunit 6, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
8	H	67	Total	C	H	N	O	S	0	0	0
			1075	332	527	99	112	5			

- Molecule 9 is a protein called Cytochrome b-c1 complex subunit Rieske, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
9	I	34	Total	C	H	N	O	S	0	0	0
			509	149	265	51	43	1			

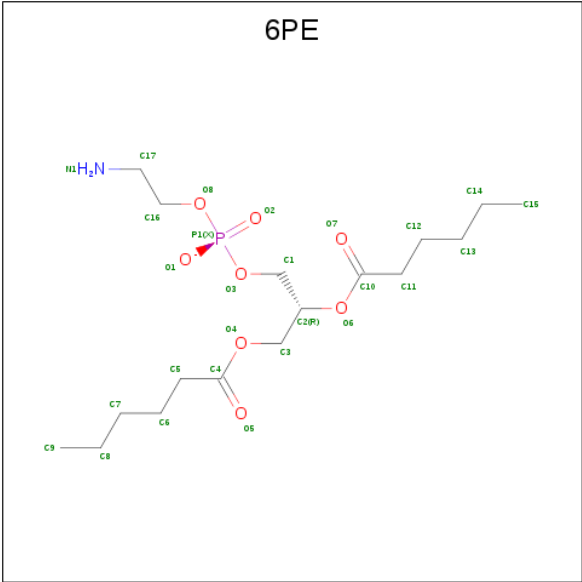
- Molecule 10 is a protein called Cytochrome b-c1 complex subunit 9.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
10	J	61	Total	C	H	N	O	S	0	0	0
			1004	329	502	87	86				

- Molecule 11 is a protein called Cytochrome b-c1 complex subunit 10.

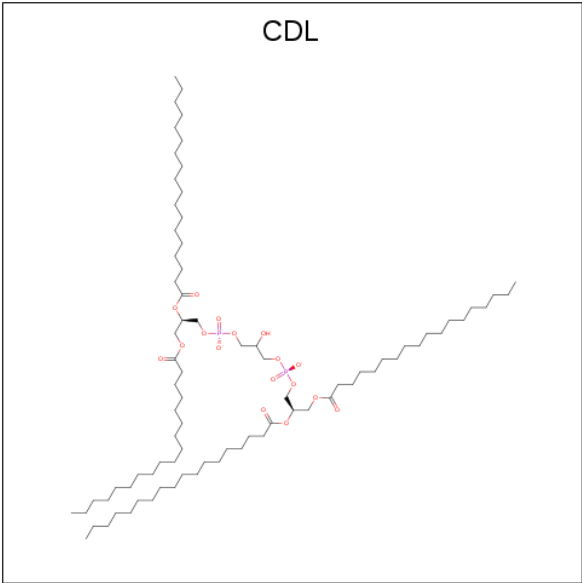
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
11	K	50	Total	C	H	N	O	S	0	0	0
			823	273	413	74	63				

- Molecule 12 is 1,2-DIHEXANOYL-SN-GLYCERO-3-PHOSPHOETHANOLAMINE (three-letter code: 6PE) (formula: C<sub>17</sub>H<sub>33</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
12	A	1	Total 60	C 17	H 33	N 1	O 8	P 1	0	0
12	K	1	Total 60	C 17	H 33	N 1	O 8	P 1	0	0

- Molecule 13 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
13	A	1	Total	C	H	O	P	0	0
			124	41	64	17	2		
13	D	1	Total	C	H	O	P	0	0
			124	41	64	17	2		

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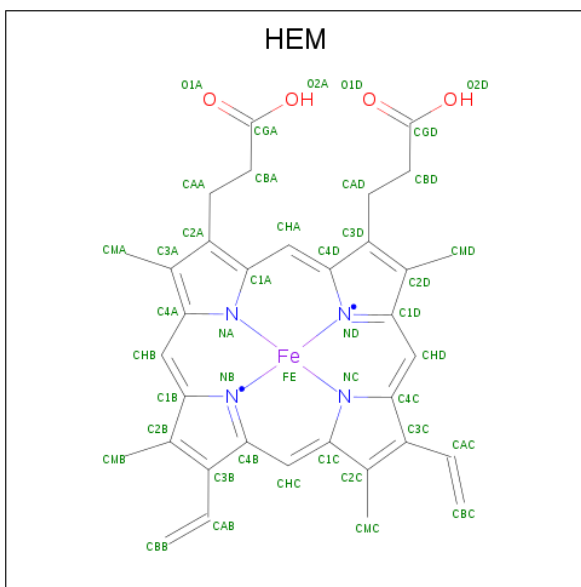
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	G	1	Total	C	H	O	P	0	0
			124	41	64	17	2		

- Molecule 14 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



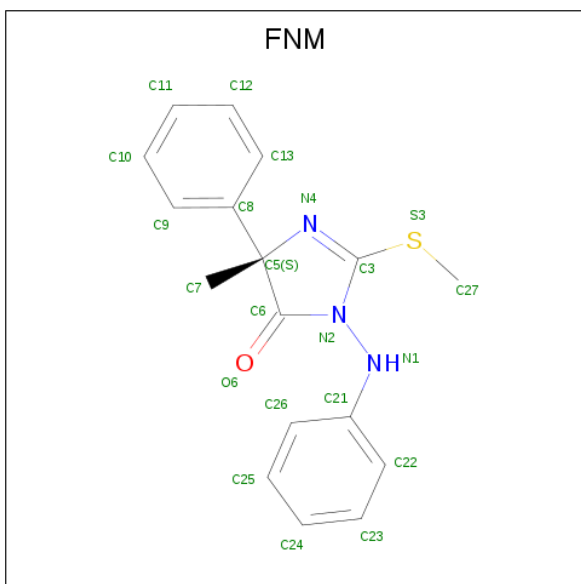
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	B	1	Total	C	H	O	0	0
			14	3	8	3		
14	B	1	Total	C	H	O	0	0
			14	3	8	3		
14	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 15 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
15	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		
15	C	1	Total	C	Fe	H	N	O	0	0
			73	34	1	30	4	4		

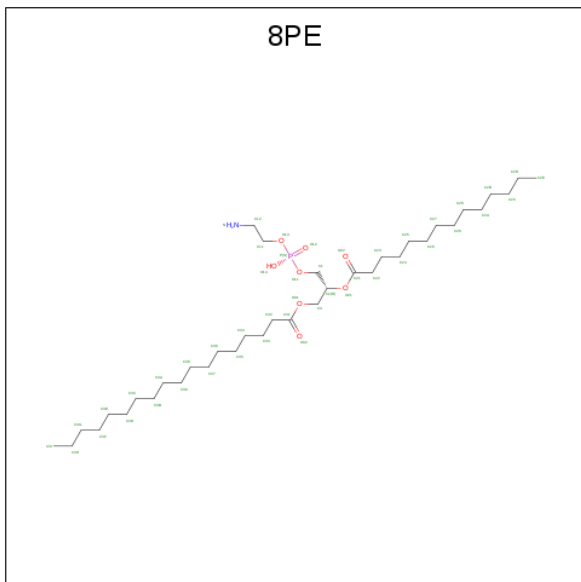
- Molecule 16 is (5S)-5-methyl-2-(methylsulfanyl)-5-phenyl-3-(phenylamino)-3,5-dihydro-4H-imidazol-4-one (three-letter code: FNM) (formula: C<sub>17</sub>H<sub>17</sub>N<sub>3</sub>OS).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
16	C	1	Total	C	H	N	O	S	0	0
			39	17	17	3	1	1		



- Molecule 17 is (2R)-3-{[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-(tetradecanoyloxy)propyl octadecanoate (three-letter code: 8PE) (formula:  $C_{37}H_{74}NO_8P$ ).

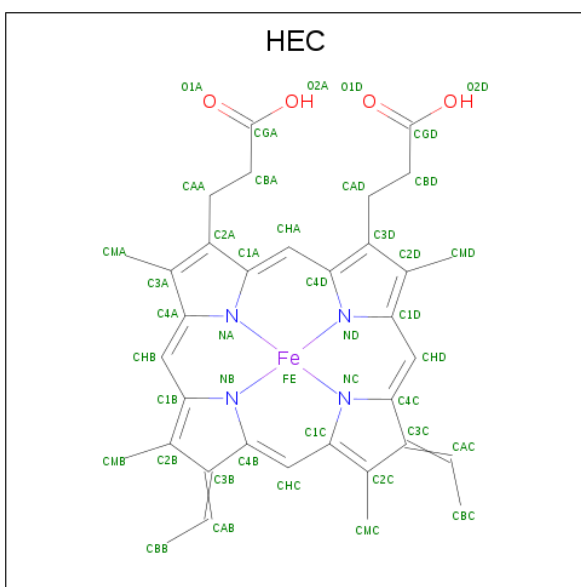


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
17	C	1	Total	C	H	N	O	P	0	0
			120	37	73	1	8	1		

- Molecule 18 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

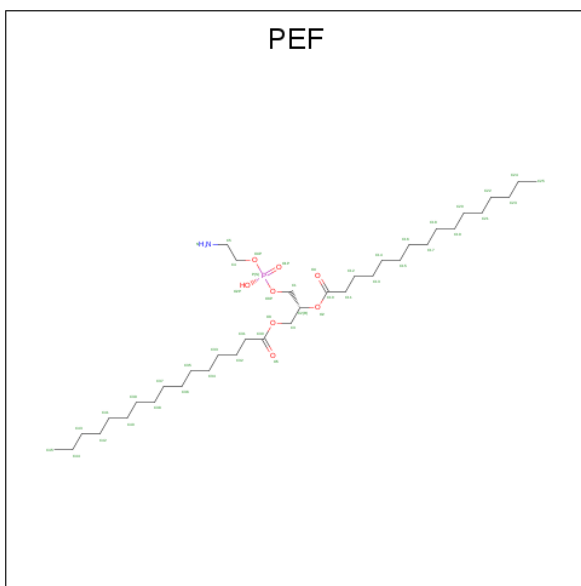
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
18	C	1	Total	Cl	0	0
			1	1		

- Molecule 19 is HEME C (three-letter code: HEC) (formula:  $C_{34}H_{34}FeN_4O_4$ ).



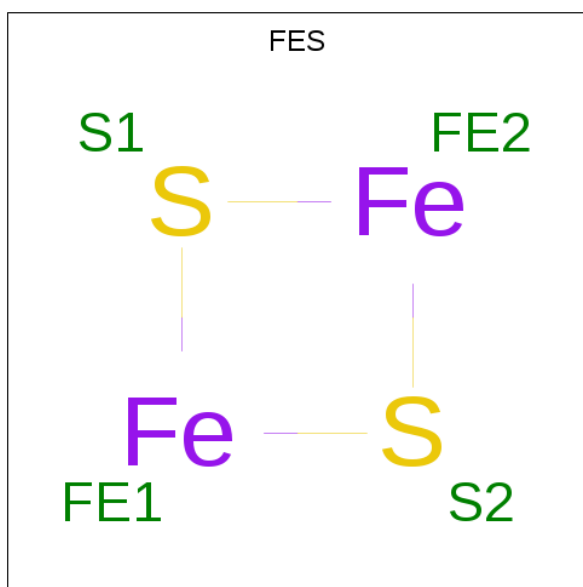
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
19	D	1	Total	C	Fe	H	N	O	0	0
			75	34	1	32	4	4		

- Molecule 20 is DI-PALMITOYL-3-SN-PHOSPHATIDYLETHANOLAMINE (three-letter code: PEF) (formula:  $C_{37}H_{74}NO_8P$ ).



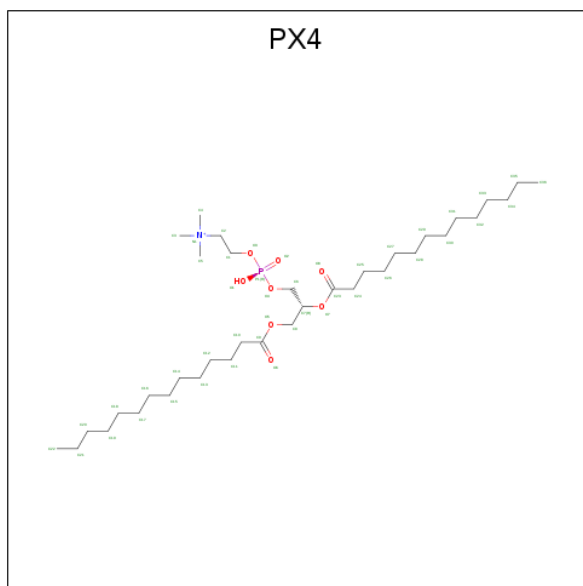
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
20	D	1	Total	C	H	N	O	P	0	0
			118	37	71	1	8	1		

- Molecule 21 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula:  $\text{Fe}_2\text{S}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
21	E	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 22 is 1,2-DIMYRISTOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PX4) (formula:  $C_{36}H_{73}NO_8P$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
22	J	1	Total	C	H	N	O	P	0	0
			118	36	72	1	8	1		

- Molecule 23 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
23	A	8	Total 8	O 8	0	0
23	B	28	Total 28	O 28	0	0
23	C	4	Total 4	O 4	0	0
23	D	4	Total 4	O 4	0	0
23	F	5	Total 5	O 5	0	0
23	I	1	Total 1	O 1	0	0

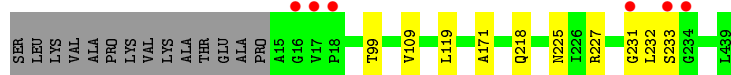
### 3 Residue-property plots [i](#)

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

- Molecule 1: Cytochrome b-c1 complex subunit 1, mitochondrial



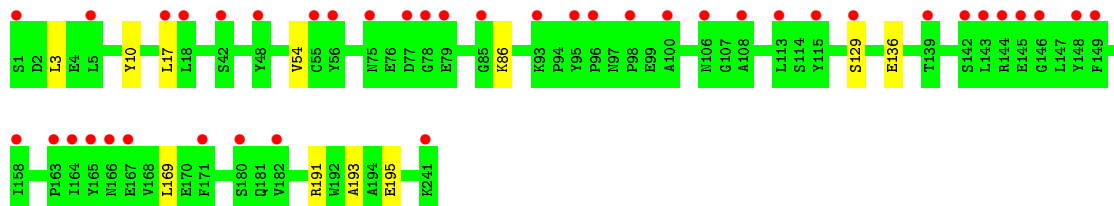
- Molecule 2: Cytochrome b-c1 complex subunit 2, mitochondrial



- Molecule 3: Cytochrome b

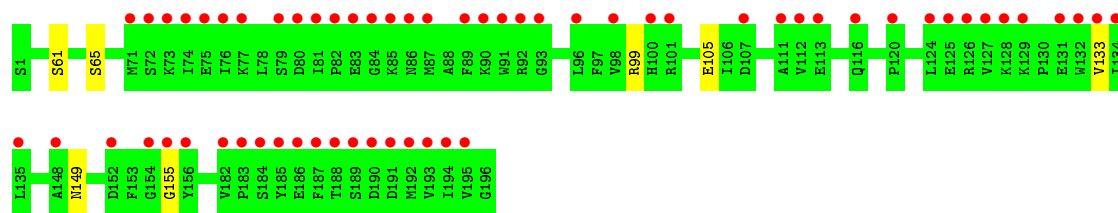


- Molecule 4: Cytochrome c1, heme protein, mitochondrial

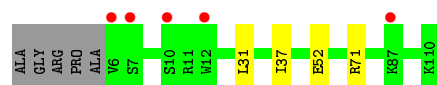


- Molecule 5: Cytochrome b-c1 complex subunit Rieske, mitochondrial

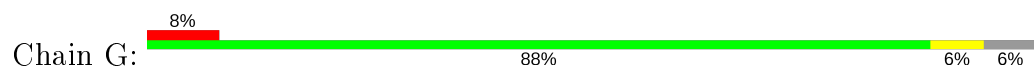




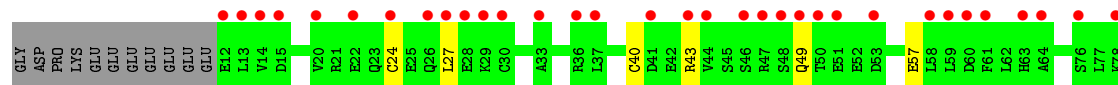
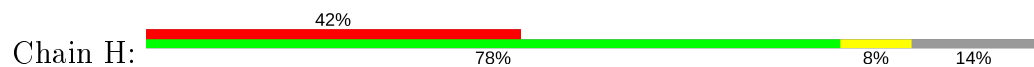
• Molecule 6: Cytochrome b-c1 complex subunit 7



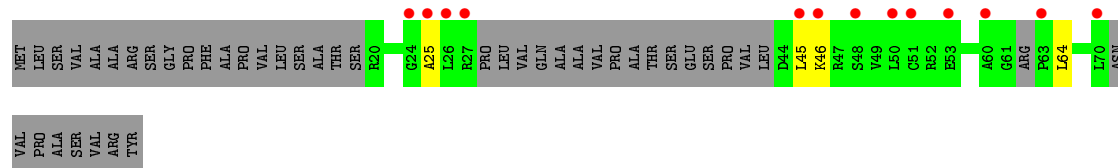
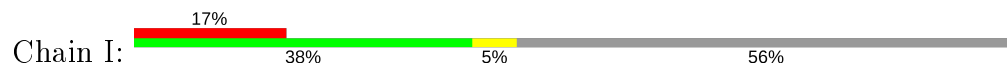
• Molecule 7: Cytochrome b-c1 complex subunit 8



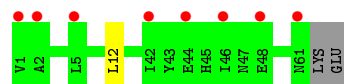
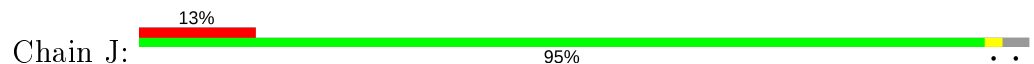
• Molecule 8: Cytochrome b-c1 complex subunit 6, mitochondrial



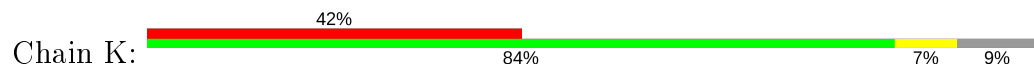
• Molecule 9: Cytochrome b-c1 complex subunit Rieske, mitochondrial

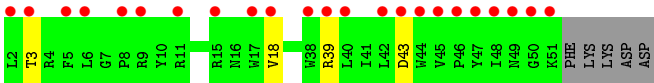


• Molecule 10: Cytochrome b-c1 complex subunit 9



• Molecule 11: Cytochrome b-c1 complex subunit 10





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.99Å 153.99Å 592.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.68 – 2.65 40.69 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.2 (34.68-2.65) 89.2 (40.69-2.65)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.11 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.11rc1_2513: ???)	Depositor
R, $R_{free}$	0.228 , 0.269 0.229 , 0.268	Depositor DCC
$R_{free}$ test set	1692 reflections (1.64%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.8	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	33655	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.13% 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 [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CL, CDL, 8PE, PX4, 6PE, FES, HEC, HEM, FNM, PEF

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.30	0/3531	0.49	0/4792
2	B	0.30	0/3241	0.51	0/4398
3	C	0.29	0/3093	0.46	0/4232
4	D	0.40	1/1978 (0.1%)	0.59	0/2684
5	E	0.28	0/1552	0.47	0/2100
6	F	0.31	0/930	0.48	0/1246
7	G	0.32	0/649	0.48	0/878
8	H	0.27	0/553	0.50	0/741
9	I	0.31	0/242	0.68	0/319
10	J	0.28	0/515	0.47	0/696
11	K	0.29	0/425	0.51	0/584
All	All	0.31	1/16709 (0.0%)	0.50	0/22670

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	10	TYR	C-N	9.74	1.52	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3458	3341	3356	6	0
2	B	3181	3147	3160	2	0
3	C	2996	3046	3058	4	0
4	D	1919	1859	1868	2	0
5	E	1518	1497	1503	2	0
6	F	911	905	906	1	0
7	G	628	633	636	3	0
8	H	548	527	530	2	0
9	I	244	265	265	0	0
10	J	502	502	505	0	0
11	K	410	413	413	1	0
12	A	27	33	33	0	0
12	K	27	33	33	0	0
13	A	60	64	64	0	0
13	D	60	64	64	0	0
13	G	60	64	64	0	0
14	B	18	24	24	0	0
15	C	86	60	60	1	0
16	C	22	17	17	0	0
17	C	47	73	73	0	0
18	C	1	0	0	0	0
19	D	43	32	30	1	0
20	D	47	71	73	0	0
21	E	4	0	0	0	0
22	J	46	72	72	0	0
23	A	8	0	0	1	0
23	B	28	0	0	0	0
23	C	4	0	0	0	0
23	D	4	0	0	0	0
23	F	5	0	0	0	0
23	I	1	0	0	0	0
All	All	16913	16742	16807	22	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (22) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:ASP:O	1:A:194:ARG:NH2	2.22	0.72
1:A:213:GLN:O	1:A:217:SER:OG	2.09	0.70
5:E:99:ARG:NH2	5:E:105:GLU:OE2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:191:ARG:NH1	4:D:195:GLU:OE2	2.28	0.67
11:K:39:ARG:NH1	11:K:43:ASP:OD1	2.31	0.63
7:G:43:ALA:O	7:G:47:ARG:NH1	2.31	0.61
3:C:260:ASN:ND2	3:C:263:ASN:OD1	2.34	0.61
1:A:146:ARG:NH1	1:A:308:GLN:OE1	2.37	0.58
19:D:1001:HEC:HBC3	19:D:1001:HEC:HMC1	1.87	0.57
2:B:225:ASN:OD1	2:B:227:ARG:NH1	2.40	0.55
1:A:261:GLY:O	1:A:267:ASN:ND2	2.41	0.51
6:F:52:GLU:OE2	7:G:11:ARG:NH1	2.44	0.51
8:H:40:CYS:SG	8:H:43:ARG:NH2	2.84	0.50
2:B:231:GLY:O	2:B:233:SER:N	2.46	0.49
3:C:344:GLU:OE2	7:G:70:LYS:NZ	2.38	0.48
3:C:5:ARG:NH1	3:C:20:ASP:OD2	2.47	0.48
1:A:131:ARG:NH1	1:A:174:VAL:O	2.47	0.46
5:E:149:ASN:N	5:E:155:GLY:O	2.48	0.43
1:A:358:LYS:NZ	23:A:601:HOH:O	2.49	0.42
15:C:1002:HEM:HMC2	15:C:1002:HEM:HBC2	2.02	0.41
3:C:71:ARG:NH2	4:D:193:ALA:O	2.51	0.40
8:H:57:GLU:N	8:H:57:GLU:OE2	2.50	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	444/446 (100%)	430 (97%)	13 (3%)	1 (0%)	47 64
2	B	423/439 (96%)	407 (96%)	14 (3%)	2 (0%)	29 43
3	C	375/379 (99%)	365 (97%)	9 (2%)	1 (0%)	41 56
4	D	239/241 (99%)	236 (99%)	3 (1%)	0	100 100
5	E	194/196 (99%)	176 (91%)	18 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	103/110 (94%)	101 (98%)	2 (2%)	0	100	100
7	G	73/80 (91%)	71 (97%)	2 (3%)	0	100	100
8	H	65/78 (83%)	60 (92%)	4 (6%)	1 (2%)	10	15
9	I	28/78 (36%)	25 (89%)	1 (4%)	2 (7%)	1	0
10	J	59/63 (94%)	56 (95%)	3 (5%)	0	100	100
11	K	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
All	All	2051/2165 (95%)	1973 (96%)	71 (4%)	7 (0%)	41	56

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	232	LEU
3	C	343	VAL
9	I	46	LYS
8	H	49	GLN
9	I	25	ALA
2	B	171	ALA
1	A	260	PRO

### 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	370/370 (100%)	363 (98%)	7 (2%)	57	74
2	B	332/343 (97%)	328 (99%)	4 (1%)	71	84
3	C	325/327 (99%)	317 (98%)	8 (2%)	47	66
4	D	206/206 (100%)	199 (97%)	7 (3%)	37	53
5	E	168/168 (100%)	165 (98%)	3 (2%)	59	75
6	F	96/98 (98%)	93 (97%)	3 (3%)	40	57
7	G	66/70 (94%)	65 (98%)	1 (2%)	65	80
8	H	64/74 (86%)	62 (97%)	2 (3%)	40	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	I	25/60 (42%)	23 (92%)	2 (8%)	12	18
10	J	51/53 (96%)	50 (98%)	1 (2%)	55	73
11	K	40/45 (89%)	38 (95%)	2 (5%)	24	38
All	All	1743/1814 (96%)	1703 (98%)	40 (2%)	50	68

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASP
1	A	58	PHE
1	A	120	CYS
1	A	224	ASP
1	A	245	GLU
1	A	279	HIS
1	A	308	GLN
2	B	99	THR
2	B	109	VAL
2	B	119	LEU
2	B	218	GLN
3	C	46	LEU
3	C	88	SER
3	C	90	PHE
3	C	150	LEU
3	C	183	PHE
3	C	303	LEU
3	C	377	LEU
3	C	379	TRP
4	D	3	LEU
4	D	17	LEU
4	D	54	VAL
4	D	86	LYS
4	D	129	SER
4	D	136	GLU
4	D	169	LEU
5	E	61	SER
5	E	65	SER
5	E	133	VAL
6	F	31	LEU
6	F	37	ILE
6	F	71	ARG
7	G	31	SER

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Mol	Chain	Res	Type
8	H	24	CYS
8	H	27	LEU
9	I	45	LEU
9	I	64	LEU
10	J	12	LEU
11	K	3	THR
11	K	18	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	A	119	ASN
1	A	189	HIS
1	A	240	GLN
1	A	339	GLN
2	B	154	ASN
2	B	198	HIS
2	B	218	GLN
2	B	313	ASN
2	B	401	GLN
3	C	15	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 1 is monoatomic - leaving 16 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	$\# Z  > 2$
13	CDL	D	1003	-	59,59,99	1.31	6 (10%)	65,71,111	1.17	5 (7%)
15	HEM	C	1002	3	27,50,50	1.80	5 (18%)	17,82,82	1.73	3 (17%)
12	6PE	A	501	-	26,26,26	1.65	6 (23%)	29,31,31	1.15	3 (10%)
19	HEC	D	1001	4	26,50,50	2.31	4 (15%)	18,82,82	1.52	4 (22%)
21	FES	E	1001	5	0,4,4	0.00	-	-		
13	CDL	A	502	-	59,59,99	1.29	7 (11%)	65,71,111	1.07	4 (6%)
22	PX4	J	101	-	45,45,45	1.27	3 (6%)	51,53,53	0.97	4 (7%)
16	FNM	C	1003	-	23,24,24	1.14	3 (13%)	25,34,34	1.39	4 (16%)
13	CDL	G	101	-	59,59,99	1.27	6 (10%)	65,71,111	1.02	4 (6%)
14	GOL	B	501	-	5,5,5	0.35	0	5,5,5	0.17	0
14	GOL	B	502	-	5,5,5	0.35	0	5,5,5	0.22	0
12	6PE	K	101	-	26,26,26	1.63	6 (23%)	29,31,31	1.19	2 (6%)
17	8PE	C	1004	-	46,46,46	1.65	7 (15%)	49,51,51	1.10	4 (8%)
15	HEM	C	1001	3	27,50,50	1.83	5 (18%)	17,82,82	1.77	4 (23%)
20	PEF	D	1002	-	46,46,46	1.08	3 (6%)	49,51,51	0.82	2 (4%)
14	GOL	B	503	-	5,5,5	0.36	0	5,5,5	0.20	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CDL	D	1003	-	-	35/70/70/110	-
15	HEM	C	1002	3	-	0/6/54/54	-
12	6PE	A	501	-	-	9/30/30/30	-
19	HEC	D	1001	4	-	0/6/54/54	-
21	FES	E	1001	5	-	-	0/1/1/1
13	CDL	A	502	-	-	26/70/70/110	-
22	PX4	J	101	-	-	20/49/49/49	-
16	FNM	C	1003	-	-	3/12/31/31	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CDL	G	101	-	-	24/70/70/110	-
14	GOL	B	501	-	-	3/4/4/4	-
14	GOL	B	502	-	-	2/4/4/4	-
12	6PE	K	101	-	-	10/30/30/30	-
17	8PE	C	1004	-	-	25/50/50/50	-
15	HEM	C	1001	3	-	1/6/54/54	-
20	PEF	D	1002	-	-	21/50/50/50	-
14	GOL	B	503	-	-	2/4/4/4	-

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	D	1001	HEC	C3B-C2B	-5.92	1.34	1.40
19	D	1001	HEC	C3C-C2C	-5.62	1.34	1.40
19	D	1001	HEC	C3D-C2D	5.49	1.53	1.37
17	C	1004	8PE	P-O11	4.82	1.78	1.59
22	J	101	PX4	P1-O3	4.64	1.78	1.59
13	D	1003	CDL	OA8-CA7	4.30	1.45	1.33
15	C	1001	HEM	C3C-CAC	4.14	1.56	1.47
15	C	1002	HEM	C3B-CAB	4.13	1.56	1.47
13	D	1003	CDL	OA6-CA5	4.11	1.45	1.34
15	C	1001	HEM	C3B-CAB	4.06	1.56	1.47
13	A	502	CDL	OA6-CA5	4.04	1.45	1.34
13	G	101	CDL	OA8-CA7	3.99	1.45	1.33
13	G	101	CDL	OA6-CA5	3.99	1.45	1.34
13	A	502	CDL	OA8-CA7	3.98	1.45	1.33
12	K	101	6PE	C3-C2	3.84	1.62	1.50
17	C	1004	8PE	C3-C2	3.73	1.62	1.50
15	C	1002	HEM	C3C-CAC	3.67	1.55	1.47
12	A	501	6PE	C3-C2	3.60	1.61	1.50
13	G	101	CDL	OB8-CB7	3.54	1.43	1.33
13	D	1003	CDL	OB8-CB7	3.51	1.43	1.33
15	C	1002	HEM	C3C-C2C	-3.50	1.35	1.40
13	A	502	CDL	OB8-CB7	3.46	1.43	1.33
17	C	1004	8PE	P-O13	3.29	1.72	1.59
13	G	101	CDL	OB6-CB5	3.27	1.43	1.34
13	D	1003	CDL	OB6-CB5	3.27	1.43	1.34
13	A	502	CDL	OB6-CB5	3.26	1.43	1.34
15	C	1002	HEM	C3B-C2B	-3.19	1.35	1.40
15	C	1001	HEM	C3C-C2C	-3.18	1.36	1.40
20	D	1002	PEF	P-O4P	3.16	1.72	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	A	501	6PE	C5-C4	3.05	1.59	1.50
15	C	1001	HEM	C3B-C2B	-3.04	1.36	1.40
16	C	1003	FNM	C3-S3	3.03	1.79	1.74
12	A	501	6PE	C1-C2	3.02	1.60	1.50
17	C	1004	8PE	C32-C31	2.96	1.59	1.50
12	K	101	6PE	C5-C4	2.96	1.59	1.50
20	D	1002	PEF	P-O3P	2.82	1.70	1.59
12	K	101	6PE	C11-C10	2.82	1.58	1.50
12	A	501	6PE	C11-C10	2.78	1.58	1.50
12	K	101	6PE	C1-C2	2.78	1.59	1.50
16	C	1003	FNM	C21-N1	2.67	1.45	1.41
22	J	101	PX4	C6-C7	2.66	1.58	1.50
12	K	101	6PE	O6-C10	2.62	1.41	1.34
12	K	101	6PE	O4-C4	2.61	1.41	1.33
17	C	1004	8PE	C1-C2	2.55	1.58	1.50
12	A	501	6PE	O4-C4	2.50	1.40	1.33
17	C	1004	8PE	C33-C32	2.50	1.61	1.52
12	A	501	6PE	O6-C10	2.48	1.41	1.34
13	D	1003	CDL	C31-CA7	2.28	1.57	1.50
13	G	101	CDL	OA6-CA4	-2.21	1.41	1.46
22	J	101	PX4	O3-C1	-2.21	1.35	1.44
13	A	502	CDL	C11-CA5	2.20	1.57	1.50
13	A	502	CDL	OA6-CA4	-2.18	1.41	1.46
13	D	1003	CDL	C11-CA5	2.16	1.57	1.50
17	C	1004	8PE	O31-C31	2.15	1.39	1.33
15	C	1002	HEM	CAA-C2A	2.14	1.55	1.52
13	G	101	CDL	C11-CA5	2.12	1.56	1.50
13	A	502	CDL	C31-CA7	2.09	1.56	1.50
15	C	1001	HEM	CAA-C2A	2.03	1.55	1.52
16	C	1003	FNM	C27-S3	2.03	1.88	1.78
19	D	1001	HEC	C3B-C4B	2.01	1.46	1.43
20	D	1002	PEF	C3-C2	2.01	1.56	1.50

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	502	CDL	OB6-CB5-C51	4.45	121.09	111.50
13	D	1003	CDL	OA6-CA5-C11	4.26	120.68	111.50
15	C	1001	HEM	CMB-C2B-C3B	4.14	132.42	124.68
13	G	101	CDL	OB6-CB5-C51	3.89	119.89	111.50
17	C	1004	8PE	O21-C21-C22	3.77	119.63	111.50
13	G	101	CDL	OA6-CA5-C11	3.63	119.32	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	C	1003	FNM	C5-C6-N2	-3.59	104.51	107.77
13	A	502	CDL	OA6-CA5-C11	3.58	119.22	111.50
12	K	101	6PE	O6-C10-C11	3.58	119.22	111.50
13	D	1003	CDL	OB6-CB5-C51	3.58	119.21	111.50
15	C	1002	HEM	CMB-C2B-C3B	3.53	131.29	124.68
15	C	1002	HEM	CMC-C2C-C3C	3.49	131.21	124.68
17	C	1004	8PE	O31-C31-C32	3.28	122.20	111.91
16	C	1003	FNM	O6-C6-C5	3.28	129.32	126.03
22	J	101	PX4	O1-P1-O2	3.25	128.32	112.24
13	D	1003	CDL	OA8-CA7-C31	3.19	121.92	111.91
15	C	1001	HEM	CMC-C2C-C3C	3.16	130.60	124.68
16	C	1003	FNM	C27-S3-C3	-3.15	96.18	100.40
17	C	1004	8PE	O31-C31-O32	-3.09	115.79	123.59
15	C	1002	HEM	CBD-CAD-C3D	-2.99	106.96	112.48
12	A	501	6PE	O6-C10-C11	2.99	117.95	111.50
20	D	1002	PEF	O2P-P-O1P	2.98	126.99	112.24
19	D	1001	HEC	CMB-C2B-C1B	-2.61	124.44	128.46
16	C	1003	FNM	C21-N1-N2	2.55	121.14	116.23
15	C	1001	HEM	CBA-CAA-C2A	-2.50	107.88	112.49
12	K	101	6PE	O4-C3-C2	2.46	115.59	108.43
13	D	1003	CDL	OB8-CB7-C71	2.43	119.55	111.91
13	A	502	CDL	OA8-CA7-C31	2.37	119.36	111.91
13	G	101	CDL	OB8-CB7-C71	2.36	119.30	111.91
12	A	501	6PE	O4-C3-C2	2.33	115.21	108.43
22	J	101	PX4	O3-P1-O2	-2.30	100.06	109.07
13	G	101	CDL	OA8-CA7-C31	2.29	119.11	111.91
15	C	1001	HEM	CMD-C2D-C1D	-2.29	124.94	128.46
22	J	101	PX4	O5-C9-O6	-2.29	117.81	123.59
17	C	1004	8PE	O21-C21-O22	-2.28	118.19	123.70
22	J	101	PX4	O7-C23-O8	-2.26	118.25	123.70
19	D	1001	HEC	CMC-C2C-C1C	-2.24	125.03	128.46
13	A	502	CDL	OB8-CB7-C71	2.20	118.82	111.91
19	D	1001	HEC	C1D-C2D-C3D	-2.16	105.49	107.00
12	A	501	6PE	O4-C4-C5	2.15	118.65	111.91
19	D	1001	HEC	CAA-CBA-CGA	-2.14	109.07	112.67
13	D	1003	CDL	OA6-CA4-CA6	2.11	116.05	108.40
20	D	1002	PEF	O2-C10-C11	2.05	115.93	111.50

There are no chirality outliers.

All (181) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	D	1003	CDL	O1-C1-CA2-OA2
13	D	1003	CDL	O1-C1-CB2-OB2
13	D	1003	CDL	CA3-OA5-PA1-OA3
13	D	1003	CDL	CA3-OA5-PA1-OA4
13	D	1003	CDL	OA7-CA5-OA6-CA4
13	D	1003	CDL	CB3-OB5-PB2-OB2
12	A	501	6PE	C1-O3-P1-O2
12	A	501	6PE	O6-C2-C3-O4
12	A	501	6PE	C11-C10-O6-C2
13	A	502	CDL	CB2-OB2-PB2-OB3
13	G	101	CDL	CB3-OB5-PB2-OB3
14	B	501	GOL	O2-C2-C3-O3
12	K	101	6PE	C16-O8-P1-O1
17	C	1004	8PE	C11-O13-P-O12
17	C	1004	8PE	O32-C31-O31-C3
20	D	1002	PEF	C11-C10-O2-C2
20	D	1002	PEF	C1-O3P-P-O1P
14	B	503	GOL	O1-C1-C2-O2
14	B	503	GOL	O1-C1-C2-C3
17	C	1004	8PE	C32-C31-O31-C3
13	D	1003	CDL	OA9-CA7-OA8-CA6
13	D	1003	CDL	OB9-CB7-OB8-CB6
12	K	101	6PE	O5-C4-O4-C3
12	A	501	6PE	O7-C10-O6-C2
13	A	502	CDL	OB7-CB5-OB6-CB4
20	D	1002	PEF	O4-C10-O2-C2
13	D	1003	CDL	C31-CA7-OA8-CA6
13	D	1003	CDL	C71-CB7-OB8-CB6
13	D	1003	CDL	C11-CA5-OA6-CA4
13	A	502	CDL	C51-CB5-OB6-CB4
22	J	101	PX4	C10-C9-O5-C8
12	K	101	6PE	C5-C4-O4-C3
13	A	502	CDL	O1-C1-CB2-OB2
22	J	101	PX4	C24-C23-O7-C7
22	J	101	PX4	O6-C9-O5-C8
17	C	1004	8PE	C28-C29-C2A-C2B
13	A	502	CDL	CA2-C1-CB2-OB2
13	D	1003	CDL	CB7-C71-C72-C73
13	A	502	CDL	CB7-C71-C72-C73
22	J	101	PX4	C23-C24-C25-C26
13	D	1003	CDL	CA3-OA5-PA1-OA2
17	C	1004	8PE	C1-O11-P-O13
17	C	1004	8PE	C11-O13-P-O11

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Mol	Chain	Res	Type	Atoms
13	D	1003	CDL	CA2-C1-CB2-OB2
13	D	1003	CDL	C51-CB5-OB6-CB4
13	A	502	CDL	C31-CA7-OA8-CA6
20	D	1002	PEF	C3-C2-O2-C10
13	D	1003	CDL	OB7-CB5-OB6-CB4
20	D	1002	PEF	C10-C11-C12-C13
17	C	1004	8PE	C3B-C3C-C3D-C3E
17	C	1004	8PE	C26-C27-C28-C29
13	D	1003	CDL	C12-C13-C14-C15
22	J	101	PX4	C28-C29-C30-C31
17	C	1004	8PE	C25-C26-C27-C28
13	A	502	CDL	CA5-C11-C12-C13
13	G	101	CDL	CB5-C51-C52-C53
22	J	101	PX4	C11-C12-C13-C14
14	B	501	GOL	C1-C2-C3-O3
17	C	1004	8PE	C38-C39-C3A-C3B
22	J	101	PX4	C26-C27-C28-C29
17	C	1004	8PE	C3D-C3E-C3F-C3G
13	D	1003	CDL	C31-C32-C33-C34
20	D	1002	PEF	C13-C14-C15-C16
13	D	1003	CDL	C51-C52-C53-C54
13	A	502	CDL	OA9-CA7-OA8-CA6
20	D	1002	PEF	C30-C31-C32-C33
13	G	101	CDL	C32-C33-C34-C35
20	D	1002	PEF	C37-C38-C39-C40
13	G	101	CDL	C51-CB5-OB6-CB4
20	D	1002	PEF	C32-C33-C34-C35
20	D	1002	PEF	C33-C34-C35-C36
13	A	502	CDL	OA7-CA5-OA6-CA4
22	J	101	PX4	O8-C23-O7-C7
12	A	501	6PE	C10-C11-C12-C13
22	J	101	PX4	C33-C34-C35-C36
17	C	1004	8PE	C3A-C3B-C3C-C3D
13	A	502	CDL	C11-CA5-OA6-CA4
13	G	101	CDL	C11-CA5-OA6-CA4
13	G	101	CDL	OA6-CA4-CA6-OA8
13	G	101	CDL	OA7-CA5-OA6-CA4
13	G	101	CDL	OB7-CB5-OB6-CB4
17	C	1004	8PE	C22-C21-O21-C2
13	G	101	CDL	C71-C72-C73-C74
17	C	1004	8PE	C35-C36-C37-C38
12	A	501	6PE	C1-O3-P1-O8

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Mol	Chain	Res	Type	Atoms
13	A	502	CDL	CB2-OB2-PB2-OB5
13	A	502	CDL	OB5-CB3-CB4-CB6
13	D	1003	CDL	C72-C73-C74-C75
13	D	1003	CDL	CB2-C1-CA2-OA2
13	A	502	CDL	C12-C13-C14-C15
13	A	502	CDL	CA3-CA4-CA6-OA8
12	K	101	6PE	C1-C2-C3-O4
17	C	1004	8PE	C1-C2-C3-O31
17	C	1004	8PE	C24-C25-C26-C27
13	D	1003	CDL	CA5-C11-C12-C13
13	A	502	CDL	C14-C15-C16-C17
13	G	101	CDL	C71-CB7-OB8-CB6
22	J	101	PX4	C29-C30-C31-C32
13	D	1003	CDL	CA6-CA4-OA6-CA5
20	D	1002	PEF	C17-C18-C19-C20
22	J	101	PX4	O4-C6-C7-O7
20	D	1002	PEF	O5-C30-O3-C3
13	A	502	CDL	OA6-CA4-CA6-OA8
12	K	101	6PE	O6-C2-C3-O4
16	C	1003	FNM	N4-C5-C8-C9
16	C	1003	FNM	N4-C5-C8-C13
13	G	101	CDL	C12-C13-C14-C15
22	J	101	PX4	O4-C6-C7-C8
17	C	1004	8PE	O11-C1-C2-C3
12	K	101	6PE	O8-C16-C17-N1
12	K	101	6PE	O7-C10-O6-C2
20	D	1002	PEF	C15-C16-C17-C18
13	D	1003	CDL	CA3-CA4-CA6-OA8
12	A	501	6PE	C1-C2-C3-O4
13	G	101	CDL	CA3-CA4-CA6-OA8
13	D	1003	CDL	CB5-C51-C52-C53
13	G	101	CDL	OB9-CB7-OB8-CB6
14	B	502	GOL	O1-C1-C2-O2
13	D	1003	CDL	OA5-CA3-CA4-OA6
13	G	101	CDL	OA5-CA3-CA4-OA6
13	G	101	CDL	C14-C15-C16-C17
22	J	101	PX4	C27-C28-C29-C30
13	A	502	CDL	OA5-CA3-CA4-CA6
13	G	101	CDL	OA5-CA3-CA4-CA6
22	J	101	PX4	C6-C7-C8-O5
13	A	502	CDL	OA5-CA3-CA4-OA6
16	C	1003	FNM	N4-C3-S3-C27

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Mol	Chain	Res	Type	Atoms
22	J	101	PX4	O7-C7-C8-O5
13	A	502	CDL	C73-C74-C75-C76
20	D	1002	PEF	C19-C20-C21-C22
22	J	101	PX4	C12-C13-C14-C15
12	K	101	6PE	C16-O8-P1-O3
20	D	1002	PEF	C1-O3P-P-O4P
13	A	502	CDL	C11-C12-C13-C14
12	A	501	6PE	C2-C1-O3-P1
20	D	1002	PEF	C18-C19-C20-C21
13	A	502	CDL	CB2-OB2-PB2-OB4
12	K	101	6PE	C16-O8-P1-O2
17	C	1004	8PE	C1-O11-P-O12
17	C	1004	8PE	C11-O13-P-O14
20	D	1002	PEF	C31-C30-O3-C3
22	J	101	PX4	C30-C31-C32-C33
20	D	1002	PEF	C36-C37-C38-C39
13	A	502	CDL	OB5-CB3-CB4-OB6
17	C	1004	8PE	O11-C1-C2-O21
22	J	101	PX4	O3-C1-C2-N1
13	D	1003	CDL	OA6-CA4-CA6-OA8
13	G	101	CDL	C11-C12-C13-C14
13	D	1003	CDL	CB6-CB4-OB6-CB5
17	C	1004	8PE	C3E-C3F-C3G-C3H
17	C	1004	8PE	O21-C2-C3-O31
13	D	1003	CDL	C74-C75-C76-C77
12	K	101	6PE	C2-C1-O3-P1
15	C	1001	HEM	C3D-CAD-CBD-CGD
20	D	1002	PEF	C38-C39-C40-C41
17	C	1004	8PE	C34-C35-C36-C37
20	D	1002	PEF	C31-C32-C33-C34
13	G	101	CDL	CB3-CB4-CB6-OB8
13	A	502	CDL	C74-C75-C76-C77
13	D	1003	CDL	C54-C55-C56-C57
12	A	501	6PE	O3-C1-C2-C3
13	D	1003	CDL	C11-C12-C13-C14
13	D	1003	CDL	C73-C74-C75-C76
17	C	1004	8PE	C2A-C2B-C2C-C2D
22	J	101	PX4	C15-C16-C17-C18
13	G	101	CDL	C32-C31-CA7-OA8
13	D	1003	CDL	C52-C51-CB5-OB6
13	G	101	CDL	C52-C51-CB5-OB6
17	C	1004	8PE	C2-C1-O11-P

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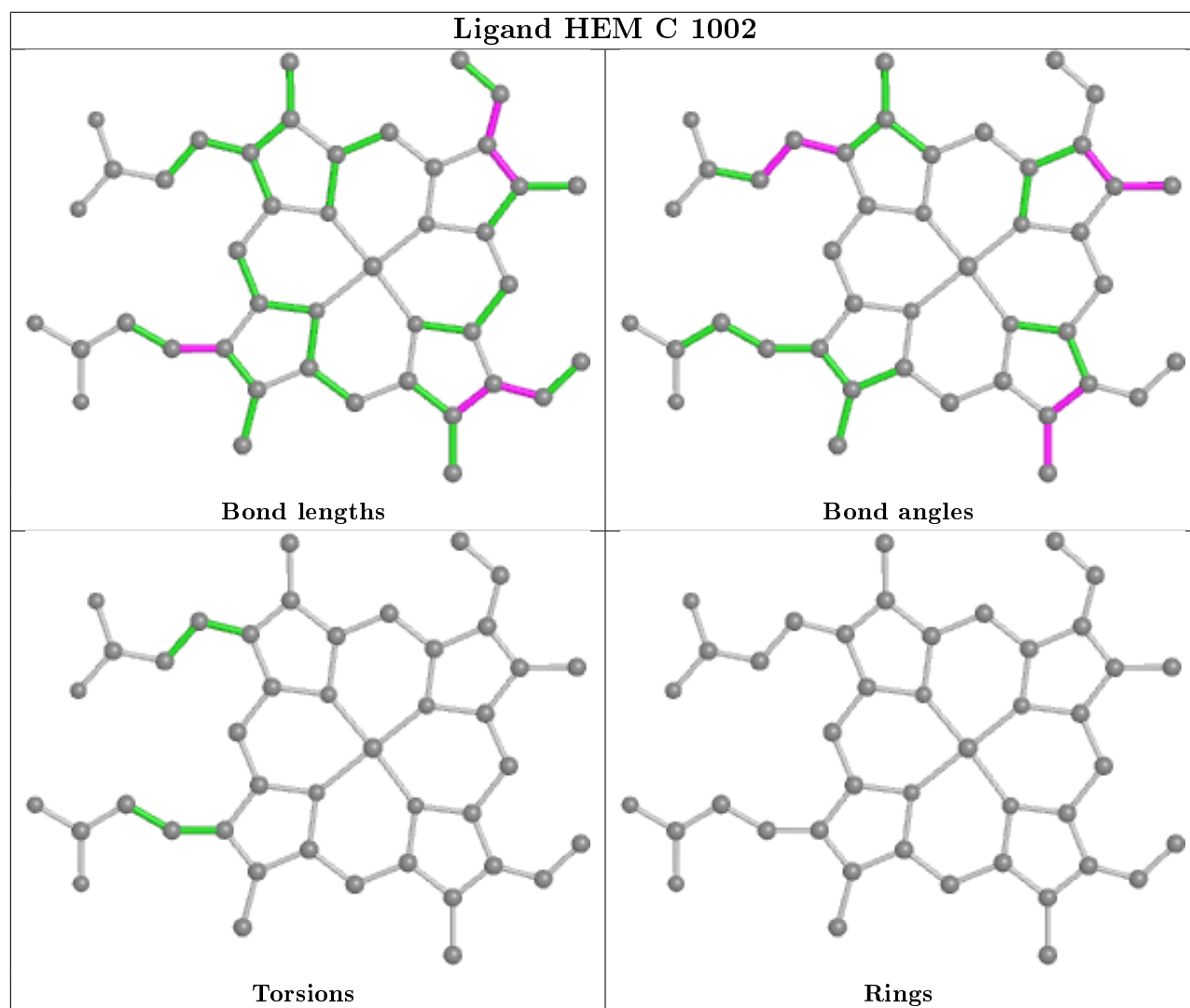
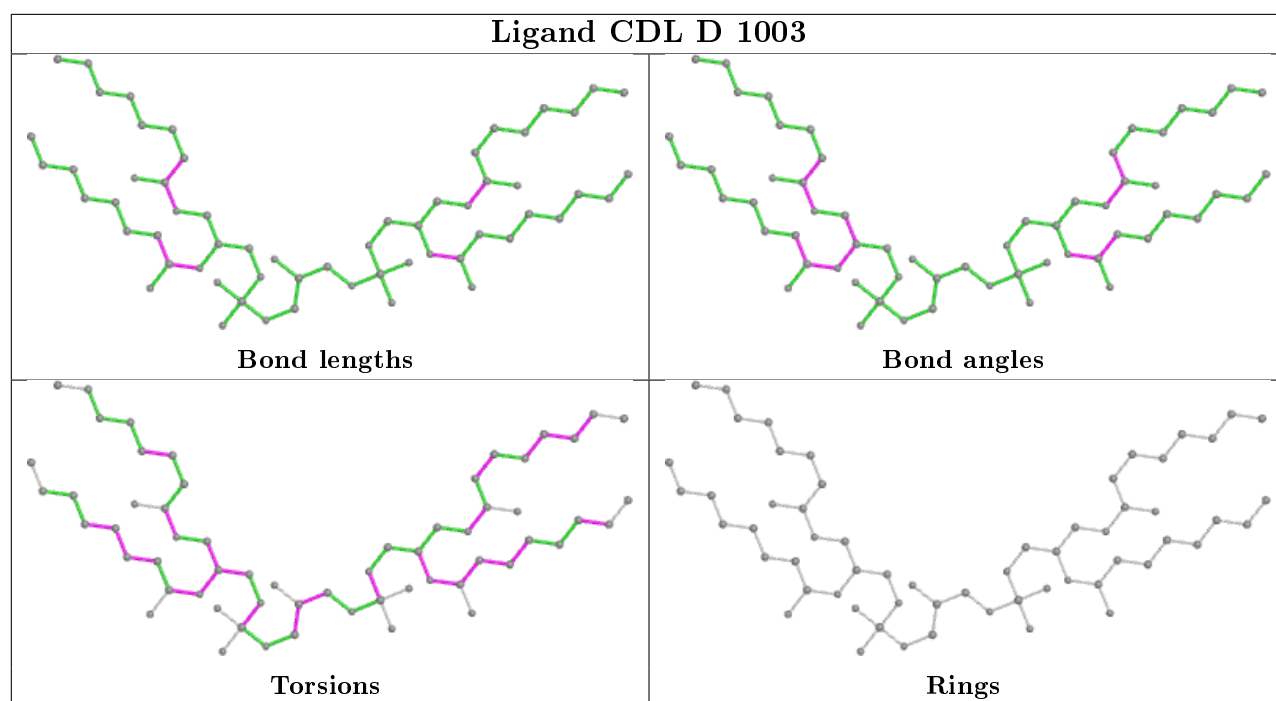
Mol	Chain	Res	Type	Atoms
14	B	501	GOL	O1-C1-C2-C3
14	B	502	GOL	O1-C1-C2-C3
13	D	1003	CDL	CB3-OB5-PB2-OB4
22	J	101	PX4	C6-O4-P1-O2
13	G	101	CDL	CA2-OA2-PA1-OA3
20	D	1002	PEF	C1-O3P-P-O2P
13	D	1003	CDL	C52-C51-CB5-OB7
13	G	101	CDL	C72-C71-CB7-OB8
13	G	101	CDL	C32-C31-CA7-OA9
13	A	502	CDL	C52-C51-CB5-OB6
13	G	101	CDL	C52-C51-CB5-OB7
13	A	502	CDL	C52-C51-CB5-OB7

There are no ring outliers.

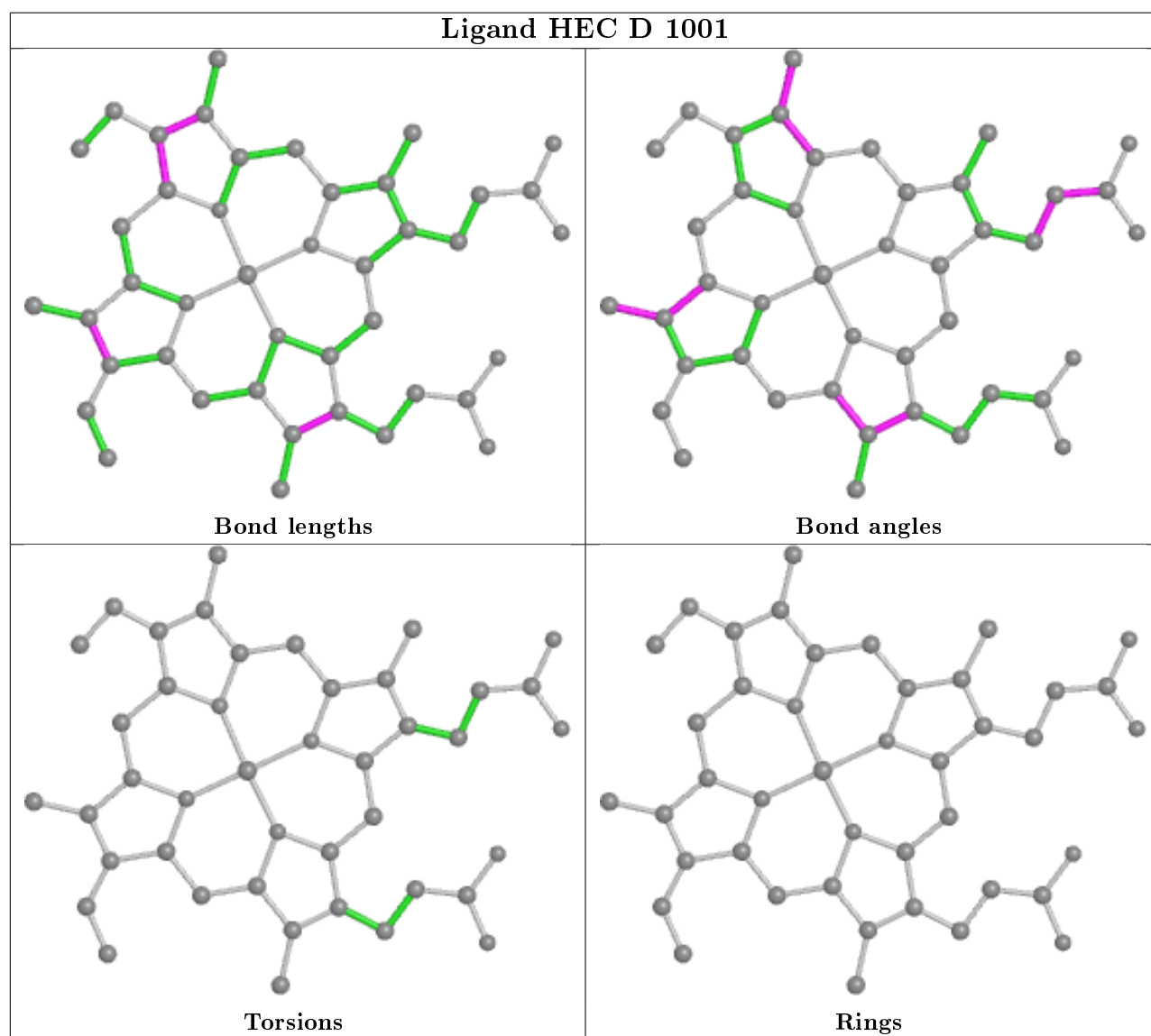
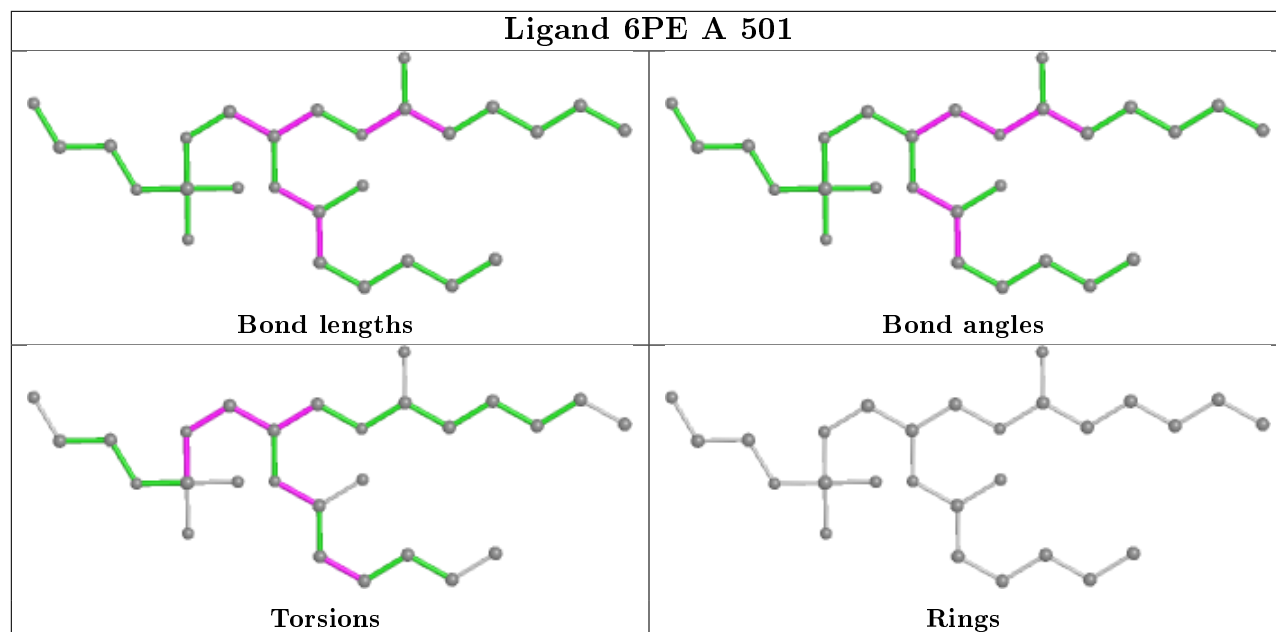
2 monomers are involved in 2 short contacts:

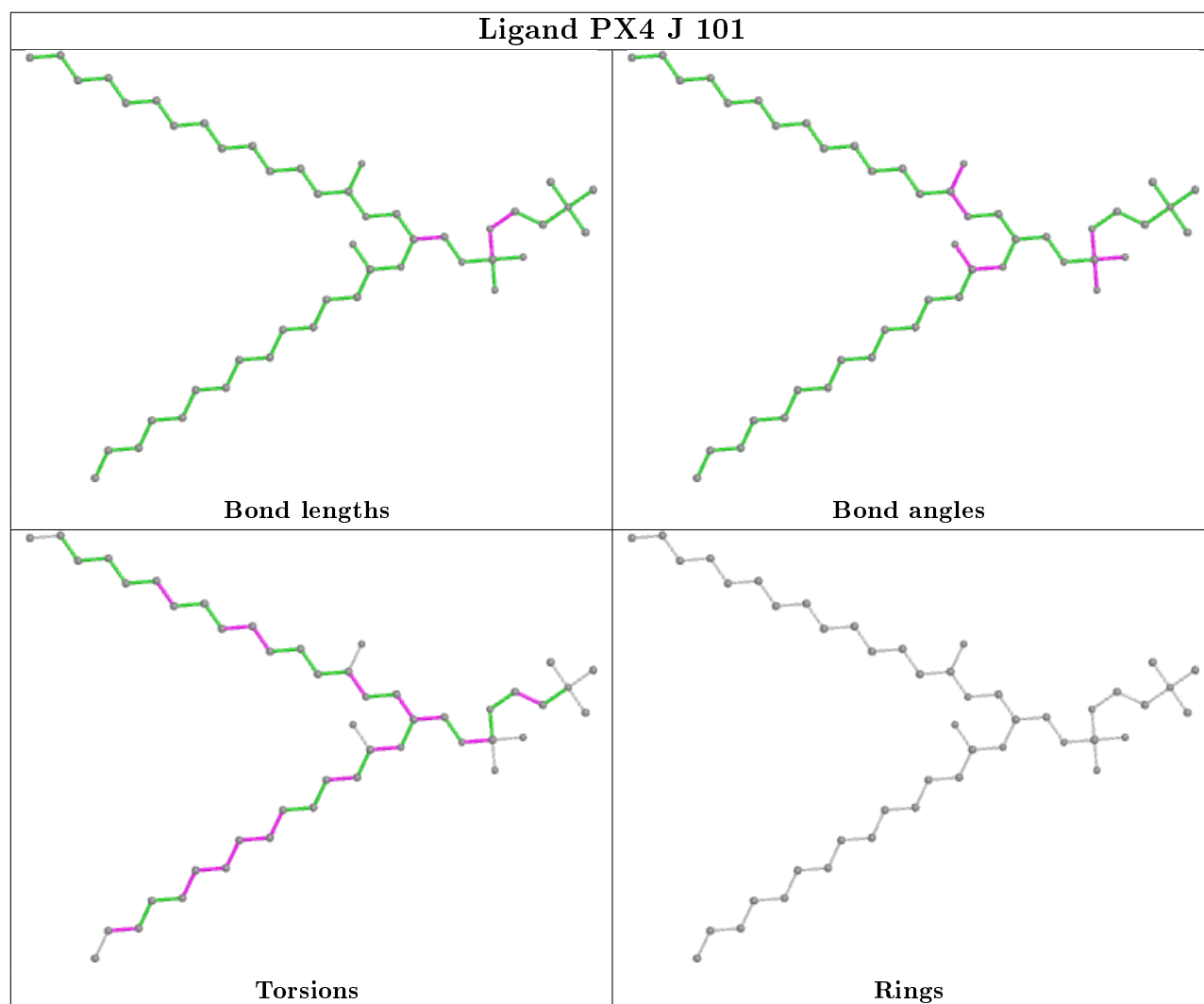
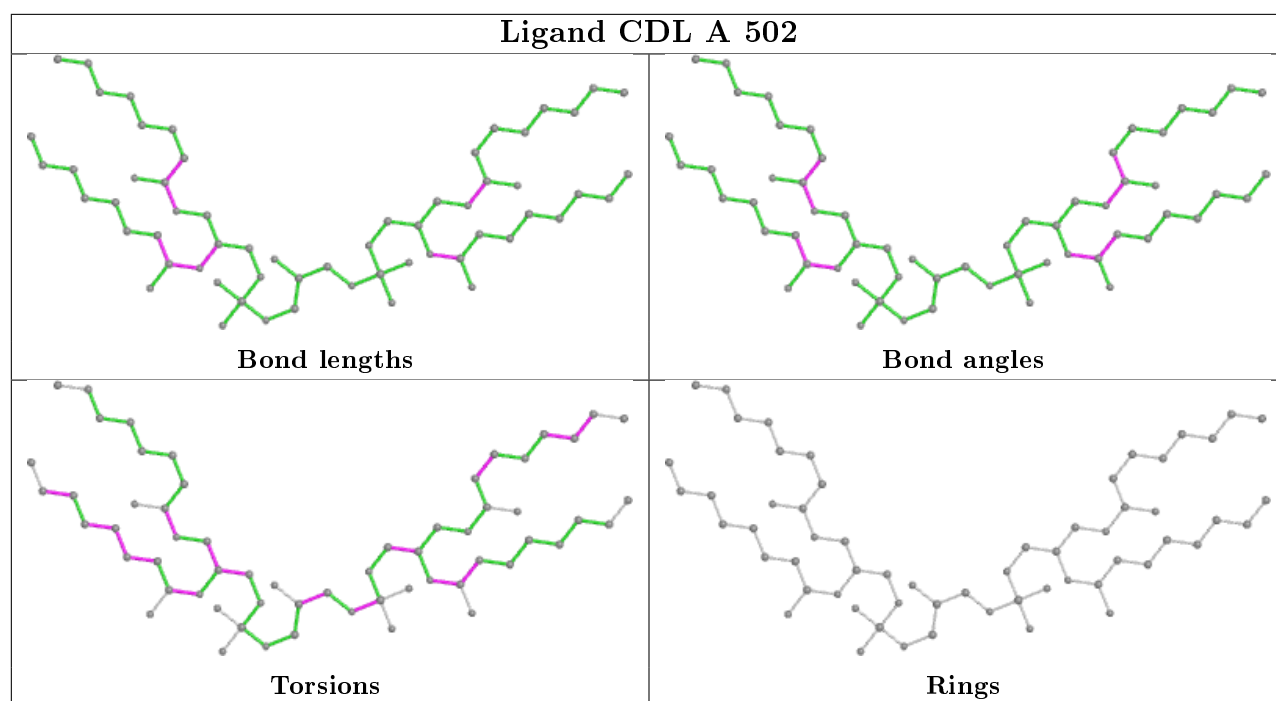
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	C	1002	HEM	1	0
19	D	1001	HEC	1	0

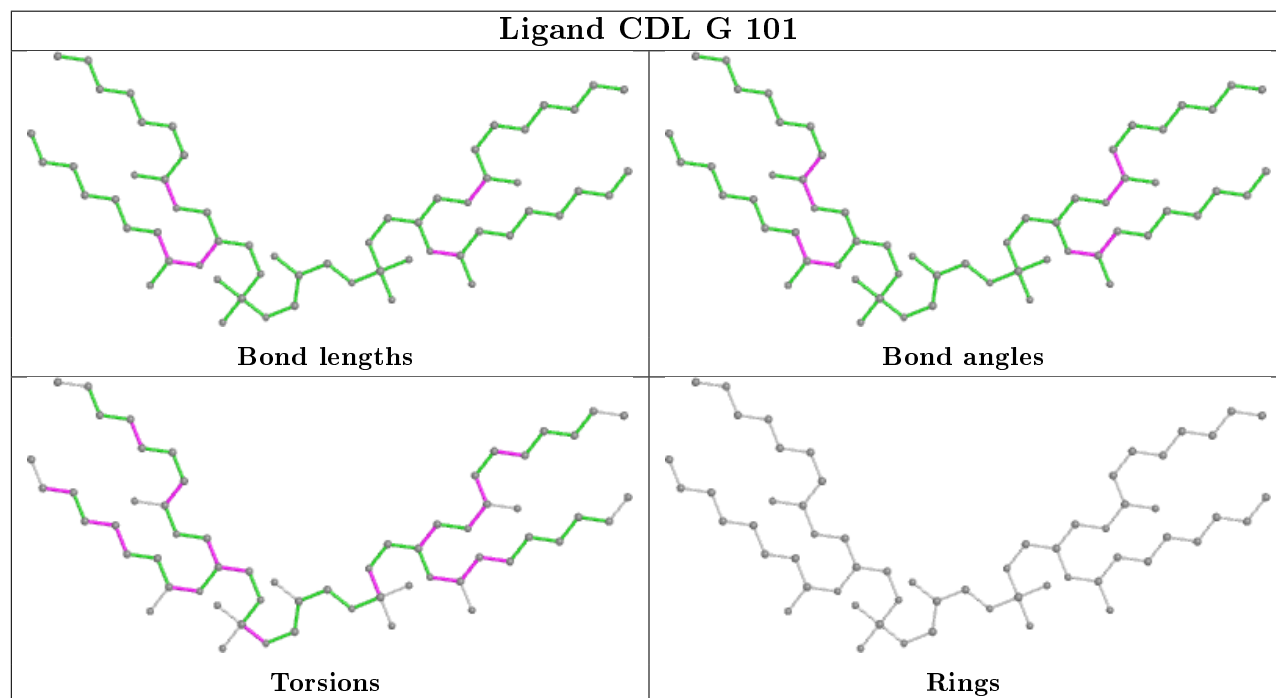
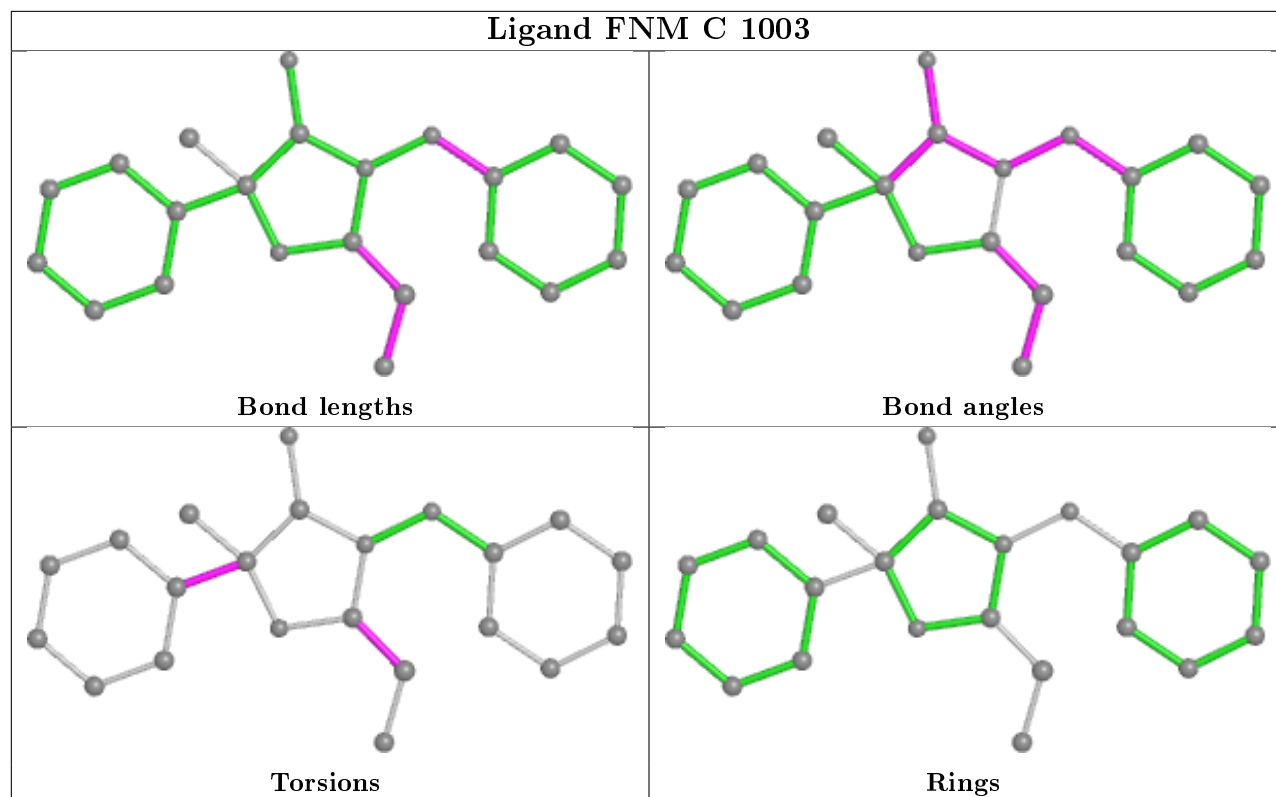
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

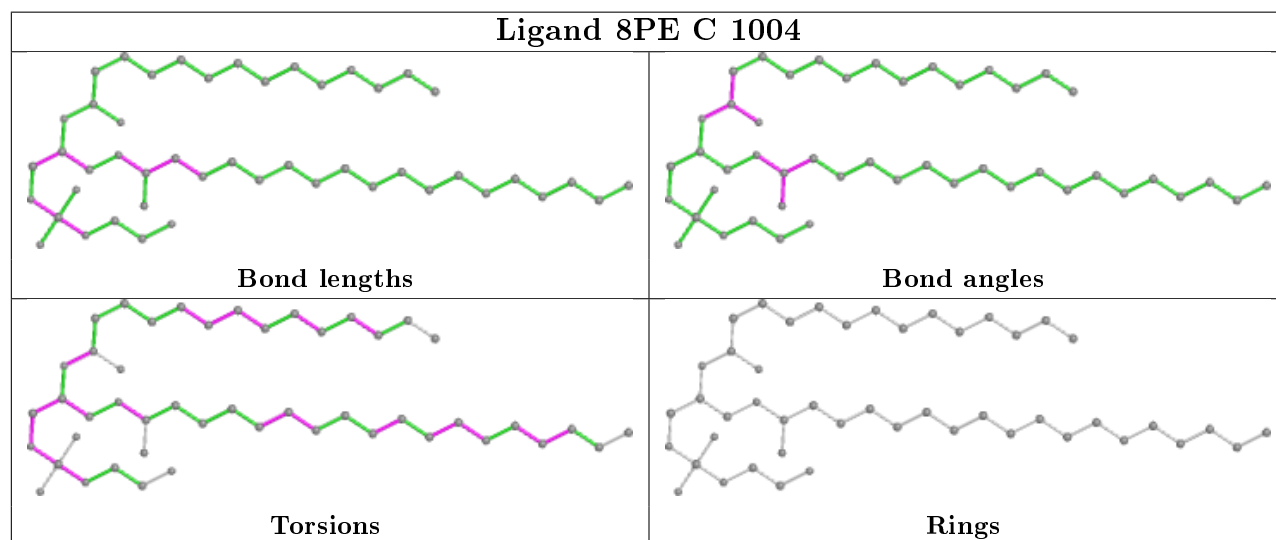
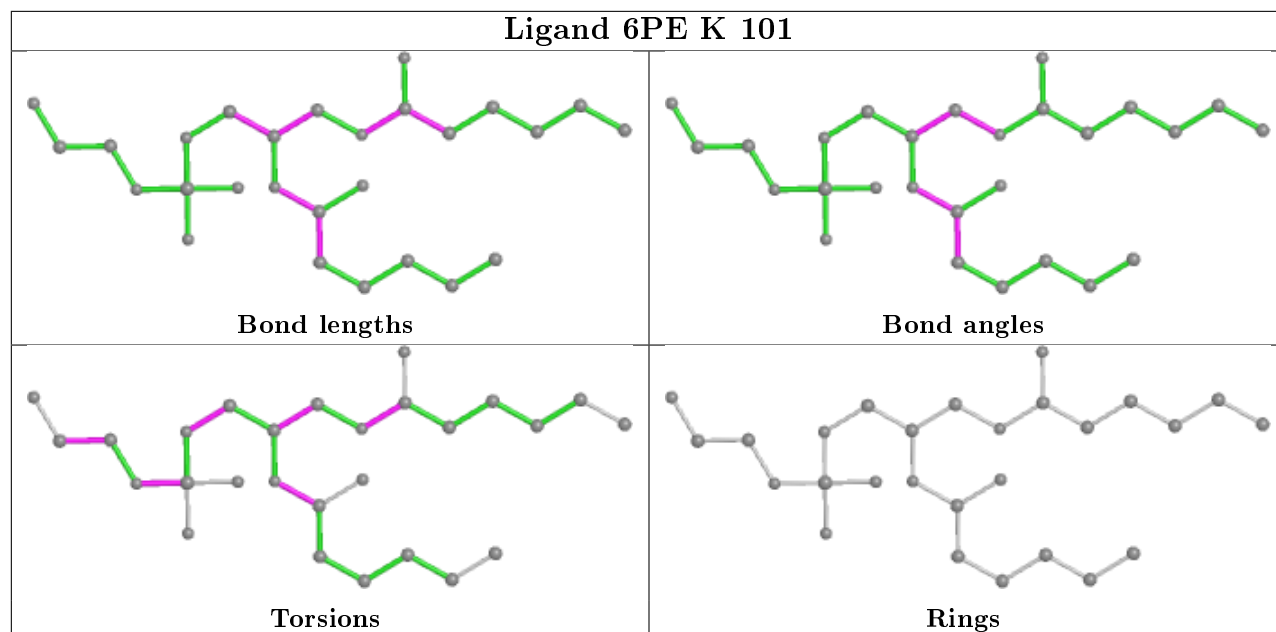


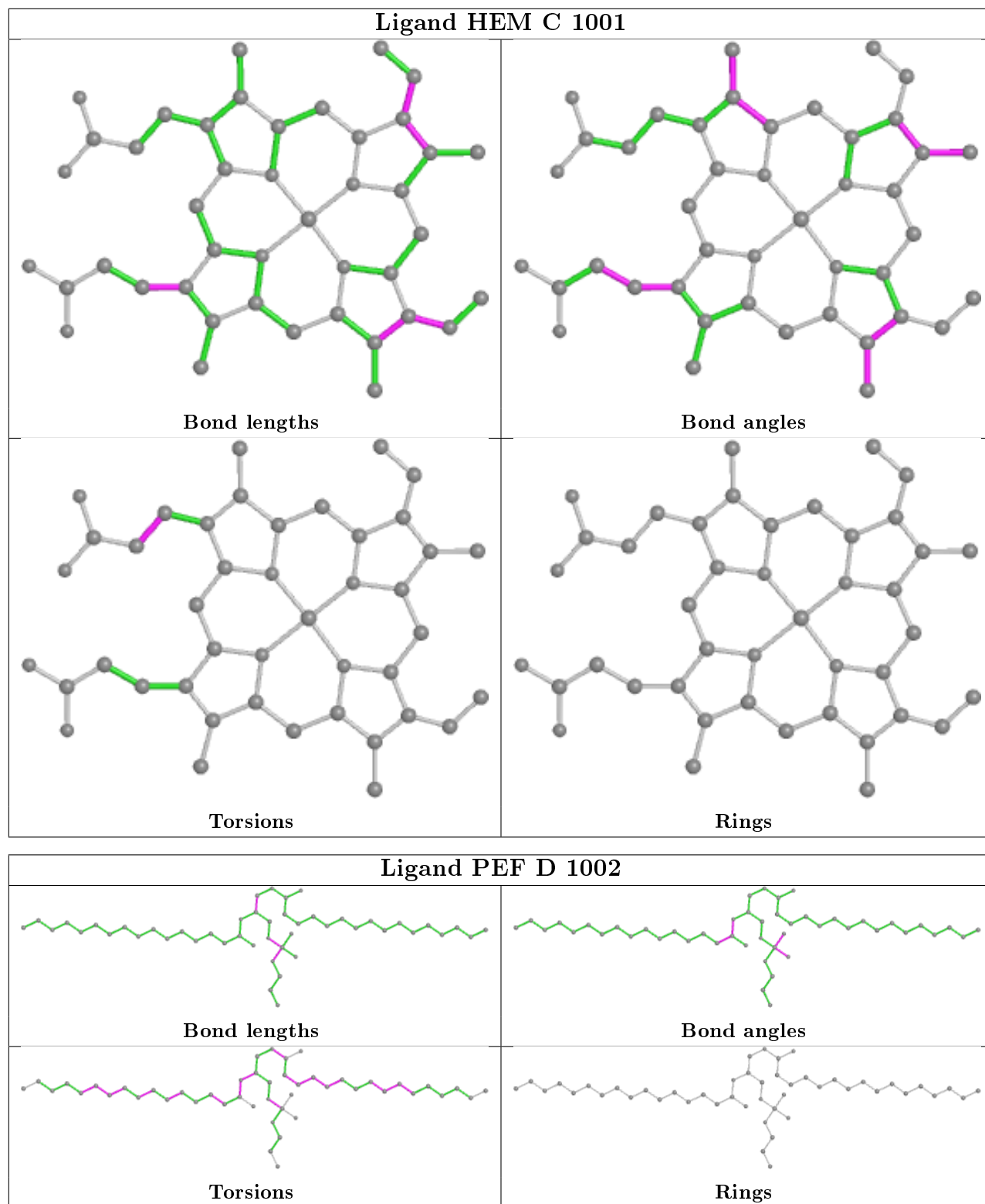












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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	446/446 (100%)	0.37	13 (2%) 51 48	40, 64, 101, 189	0
2	B	425/439 (96%)	0.17	6 (1%) 75 73	31, 47, 82, 180	0
3	C	377/379 (99%)	0.38	11 (2%) 51 48	48, 70, 101, 129	0
4	D	241/241 (100%)	0.97	41 (17%) 1 1	48, 112, 153, 188	0
5	E	196/196 (100%)	1.62	61 (31%) 0 0	66, 119, 197, 246	0
6	F	105/110 (95%)	0.41	5 (4%) 30 27	38, 60, 110, 166	0
7	G	75/80 (93%)	0.37	6 (8%) 12 9	42, 79, 127, 161	0
8	H	67/78 (85%)	2.19	33 (49%) 0 0	108, 140, 175, 211	0
9	I	34/78 (43%)	1.69	13 (38%) 0 0	45, 78, 105, 111	0
10	J	61/63 (96%)	0.93	8 (13%) 3 2	74, 96, 137, 166	0
11	K	50/55 (90%)	1.62	23 (46%) 0 0	72, 92, 146, 167	0
All	All	2077/2165 (95%)	0.65	220 (10%) 6 4	31, 72, 151, 246	0

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
10	J	1	VAL	11.0
5	E	190	ASP	10.0
5	E	187	PHE	9.4
11	K	44	TRP	9.2
5	E	76	ILE	8.7
11	K	51	LYS	8.0
8	H	13	LEU	7.6
5	E	191	ASP	7.4
8	H	14	VAL	7.4
5	E	75	GLU	7.3
5	E	195	VAL	7.1
5	E	74	ILE	7.0

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Mol	Chain	Res	Type	RSRZ
10	J	61	ASN	7.0
5	E	186	GLU	6.7
1	A	222	THR	6.6
8	H	78	LYS	6.4
5	E	124	LEU	6.2
5	E	134	ILE	6.2
5	E	188	THR	6.1
8	H	44	VAL	6.0
8	H	12	GLU	5.9
5	E	193	VAL	5.9
8	H	48	SER	5.8
5	E	194	ILE	5.7
5	E	80	ASP	5.7
1	A	227	ALA	5.5
5	E	192	MET	5.4
5	E	77	LYS	5.3
4	D	55	CYS	5.2
8	H	22	GLU	5.1
10	J	2	ALA	5.1
8	H	36	ARG	5.0
5	E	154	GLY	5.0
5	E	189	SER	4.8
1	A	225	GLU	4.8
5	E	185	TYR	4.8
4	D	143	LEU	4.7
5	E	86	ASN	4.7
5	E	132	TRP	4.7
5	E	85	LYS	4.7
9	I	50	LEU	4.7
5	E	135	LEU	4.6
5	E	127	VAL	4.6
5	E	79	SER	4.6
5	E	89	PHE	4.6
7	G	75	ALA	4.6
4	D	79	GLU	4.4
2	B	17	VAL	4.3
11	K	15	ARG	4.3
5	E	113	GLU	4.3
4	D	142	SER	4.2
1	A	226	ASP	4.1
8	H	47	ARG	4.0
5	E	120	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
6	F	6	VAL	4.0
4	D	56	TYR	3.9
4	D	98	PRO	3.9
5	E	84	GLY	3.9
9	I	46	LYS	3.9
8	H	46	SER	3.9
5	E	128	LYS	3.8
11	K	40	LEU	3.8
9	I	48	SER	3.8
4	D	146	GLY	3.8
8	H	49	GLN	3.8
1	A	223	TYR	3.8
6	F	10	SER	3.8
5	E	96	LEU	3.8
11	K	2	LEU	3.7
7	G	73	ASN	3.7
5	E	71	MET	3.7
5	E	72	SER	3.7
4	D	48	TYR	3.6
4	D	139	THR	3.6
9	I	45	LEU	3.6
5	E	81	ILE	3.6
10	J	5	LEU	3.6
4	D	167	GLU	3.6
10	J	46	ILE	3.5
5	E	148	ALA	3.5
5	E	83	GLU	3.5
7	G	70	LYS	3.5
4	D	1	SER	3.5
7	G	67	GLU	3.5
5	E	82	PRO	3.5
1	A	229	PRO	3.5
1	A	224	ASP	3.5
1	A	206	ARG	3.5
8	H	37	LEU	3.5
11	K	42	LEU	3.4
5	E	87	MET	3.4
11	K	5	PHE	3.4
2	B	233	SER	3.4
4	D	145	GLU	3.4
7	G	74	PRO	3.4
4	D	18	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
9	I	24	GLY	3.3
4	D	96	PRO	3.3
8	H	26	GLN	3.3
6	F	12	TRP	3.3
11	K	43	ASP	3.3
2	B	16	GLY	3.2
8	H	50	THR	3.1
5	E	111	ALA	3.1
5	E	107	ASP	3.1
5	E	112	VAL	3.0
5	E	131	GLU	3.0
5	E	73	LYS	3.0
8	H	28	GLU	3.0
5	E	156	TYR	3.0
11	K	48	ILE	2.9
8	H	63	HIS	2.9
5	E	125	GLU	2.9
4	D	77	ASP	2.9
8	H	64	ALA	2.8
11	K	38	TRP	2.8
11	K	6	LEU	2.8
8	H	59	LEU	2.8
5	E	182	VAL	2.8
6	F	7	SER	2.8
5	E	90	LYS	2.8
3	C	18	PHE	2.8
4	D	100	ALA	2.7
11	K	50	GLY	2.7
5	E	133	VAL	2.7
8	H	29	LYS	2.7
1	A	19	LEU	2.7
4	D	164	ILE	2.7
2	B	18	PRO	2.7
9	I	70	LEU	2.7
8	H	60	ASP	2.7
3	C	102	LEU	2.7
11	K	49	ASN	2.7
9	I	53	GLU	2.7
11	K	39	ARG	2.6
11	K	47	TYR	2.6
9	I	63	PRO	2.6
5	E	98	VAL	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	B	231	GLY	2.6
4	D	163	PRO	2.6
8	H	27	LEU	2.6
11	K	11	ARG	2.6
8	H	41	ASP	2.6
4	D	85	GLY	2.6
4	D	180	SER	2.6
4	D	93	LYS	2.6
8	H	20	VAL	2.6
3	C	103	TYR	2.5
3	C	267	HIS	2.5
4	D	148	TYR	2.5
4	D	5	LEU	2.5
5	E	100	HIS	2.5
9	I	60	ALA	2.5
4	D	182	VAL	2.5
4	D	78	GLY	2.5
8	H	76	SER	2.5
1	A	221	GLY	2.5
4	D	241	LYS	2.5
5	E	93	GLY	2.5
9	I	51	CYS	2.5
4	D	165	TYR	2.5
10	J	42	ILE	2.4
6	F	87	LYS	2.4
5	E	126	ARG	2.4
11	K	17	TRP	2.4
10	J	48	GLU	2.4
5	E	116	GLN	2.4
3	C	28	SER	2.4
4	D	158	ILE	2.4
5	E	183	PRO	2.3
4	D	42	SER	2.3
2	B	234	GLY	2.3
4	D	171	PHE	2.3
7	G	66	PHE	2.3
5	E	129	LYS	2.3
8	H	61	PHE	2.3
8	H	53	ASP	2.3
11	K	3	THR	2.3
8	H	24	CYS	2.3
9	I	27	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	30	TRP	2.3
3	C	155	TYR	2.3
9	I	25	ALA	2.3
4	D	144	ARG	2.3
5	E	101	ARG	2.3
11	K	45	VAL	2.3
5	E	155	GLY	2.2
10	J	44	GLU	2.2
11	K	8	PRO	2.2
4	D	108	ALA	2.2
4	D	17	LEU	2.2
8	H	15	ASP	2.2
8	H	43	ARG	2.2
9	I	26	LEU	2.2
11	K	18	VAL	2.2
4	D	75	ASN	2.1
4	D	129	SER	2.1
3	C	160	LEU	2.1
4	D	149	PHE	2.1
1	A	39	VAL	2.1
1	A	228	VAL	2.1
4	D	113	LEU	2.1
8	H	33	ALA	2.1
3	C	25	SER	2.1
8	H	30	CYS	2.1
8	H	58	LEU	2.1
1	A	1	THR	2.1
4	D	166	ASN	2.1
5	E	91	TRP	2.1
4	D	106	ASN	2.1
3	C	29	SER	2.1
5	E	184	SER	2.1
3	C	372	ILE	2.0
11	K	9	ARG	2.0
4	D	95	TYR	2.0
4	D	115	TYR	2.0
5	E	152	ASP	2.0
8	H	51	GLU	2.0
11	K	46	PRO	2.0
5	E	92	ARG	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

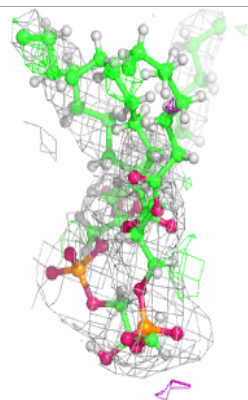
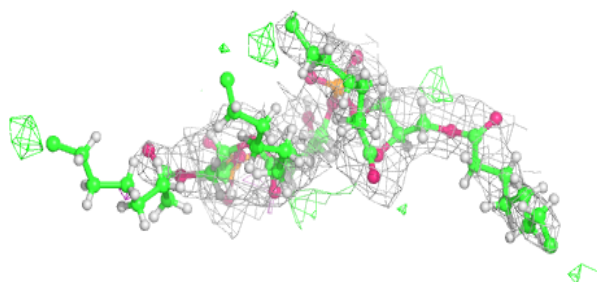
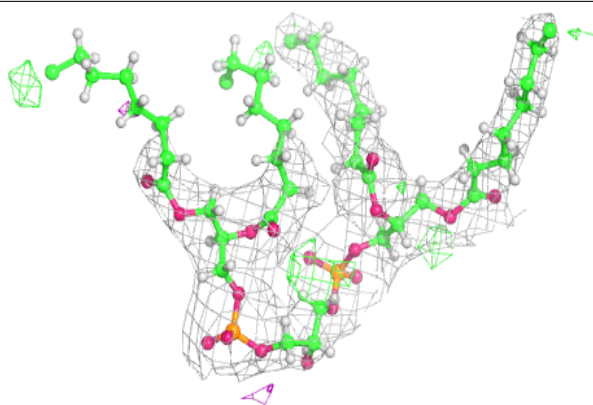
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
14	GOL	B	501	6/6	0.64	0.38	75,91,92,92	0
13	CDL	D	1003	60/100	0.69	0.34	76,101,123,124	0
13	CDL	G	101	60/100	0.74	0.36	77,96,114,115	0
22	PX4	J	101	46/46	0.82	0.34	86,107,120,120	0
12	6PE	K	101	27/27	0.84	0.34	102,123,132,132	0
14	GOL	B	503	6/6	0.85	0.58	82,99,100,100	0
17	8PE	C	1004	47/47	0.88	0.36	50,81,106,109	0
12	6PE	A	501	27/27	0.88	0.33	80,97,116,116	0
20	PEF	D	1002	47/47	0.89	0.27	69,88,106,106	0
13	CDL	A	502	60/100	0.90	0.35	70,100,123,124	0
18	CL	C	1005	1/1	0.92	0.24	62,62,62,62	0
14	GOL	B	502	6/6	0.92	0.20	60,72,74,74	0
16	FNM	C	1003	22/22	0.94	0.19	79,88,107,108	0
19	HEC	D	1001	43/43	0.96	0.23	101,125,151,156	0
15	HEM	C	1002	43/43	0.97	0.23	55,61,75,75	0
15	HEM	C	1001	43/43	0.97	0.24	71,79,96,104	0
21	FES	E	1001	4/4	0.98	0.13	104,105,106,106	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.

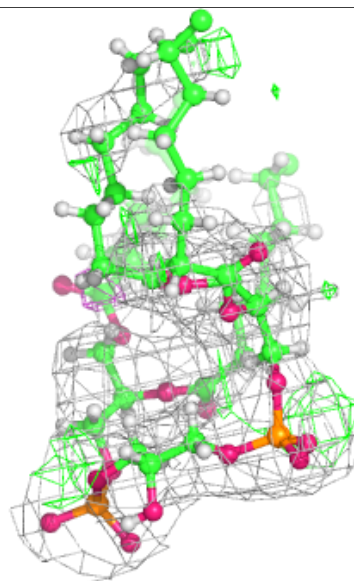
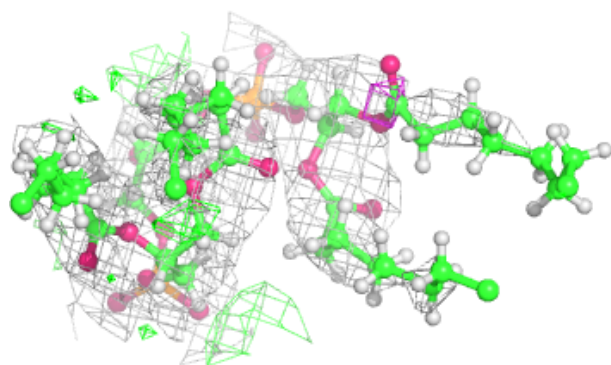
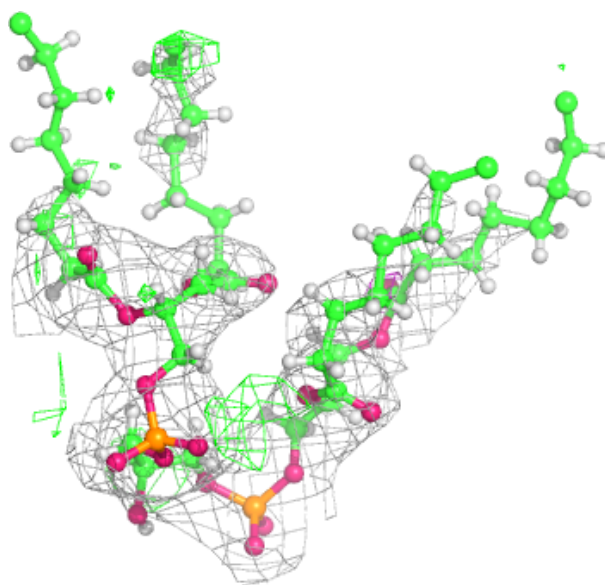
**Electron density around CDL D 1003:**

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



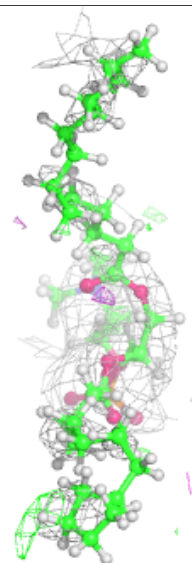
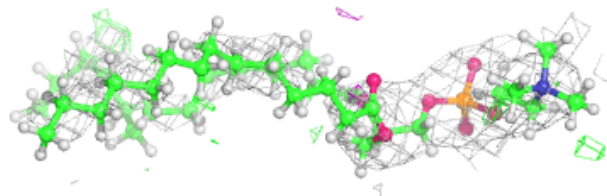
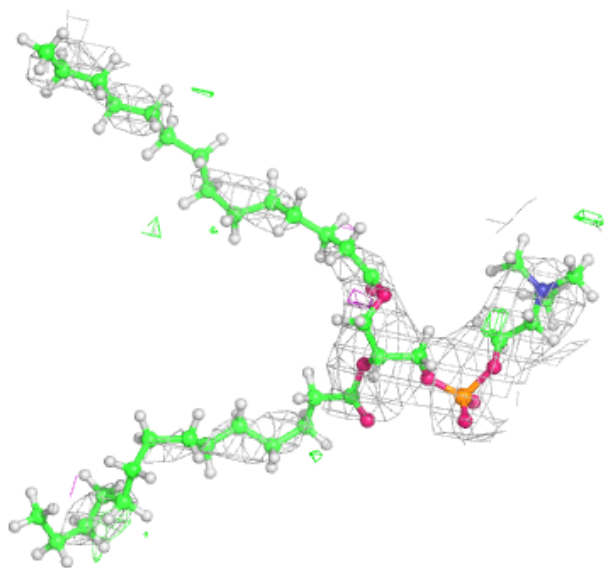
**Electron density around CDL G 101:**

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



**Electron density around PX4 J 101:**

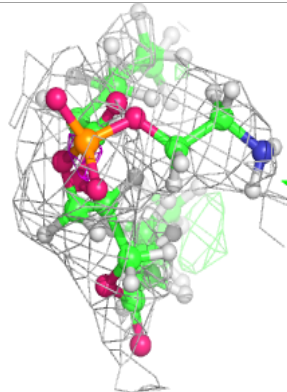
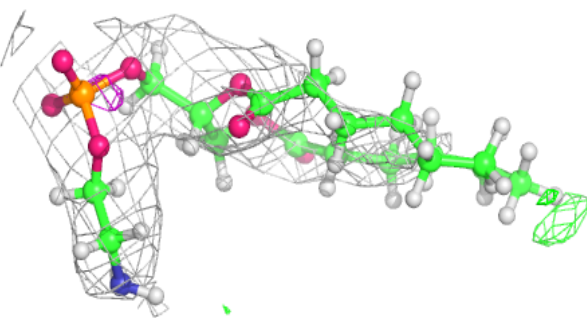
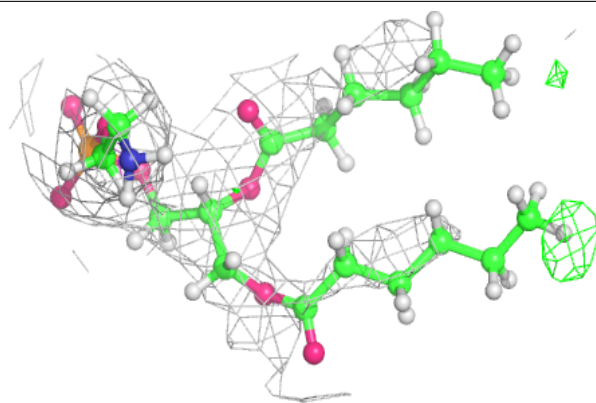
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



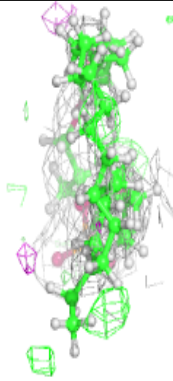
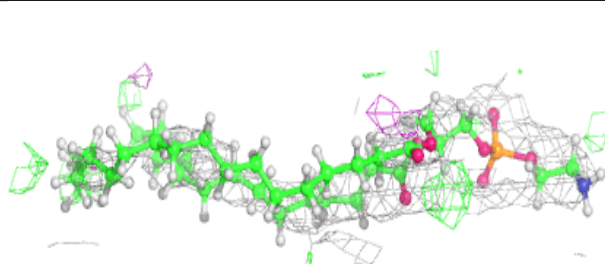
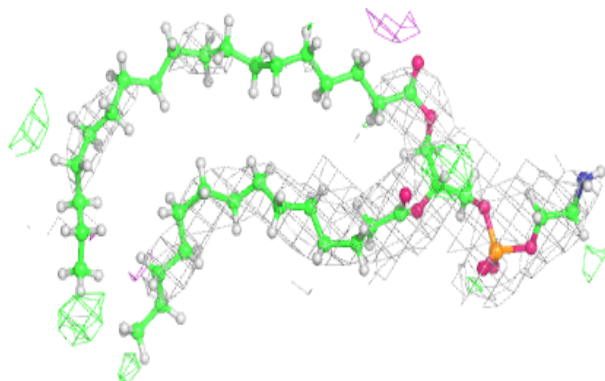


**Electron density around 6PE K 101:**

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

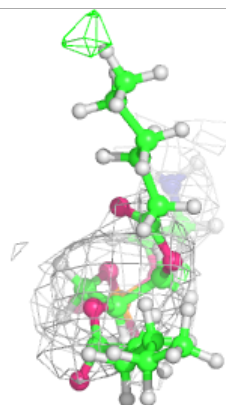
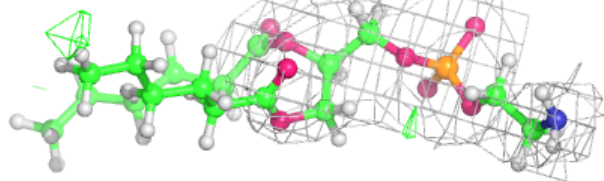
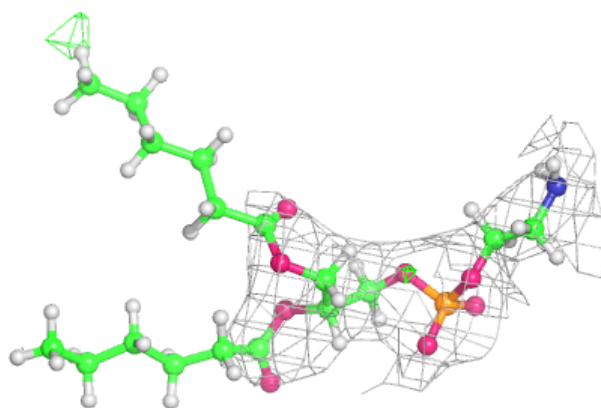
**Electron density around 8PE C 1004:**

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



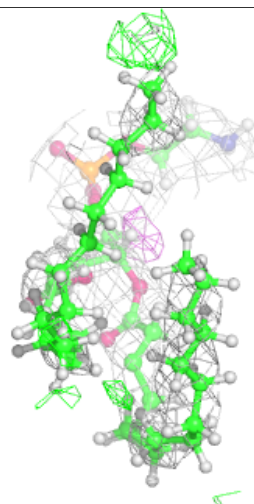
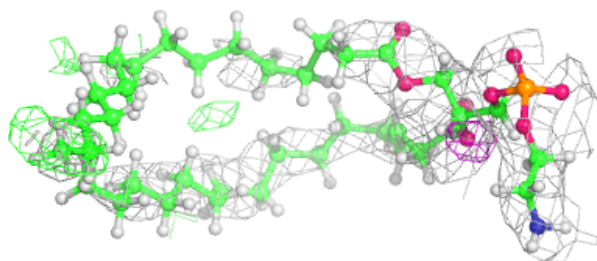
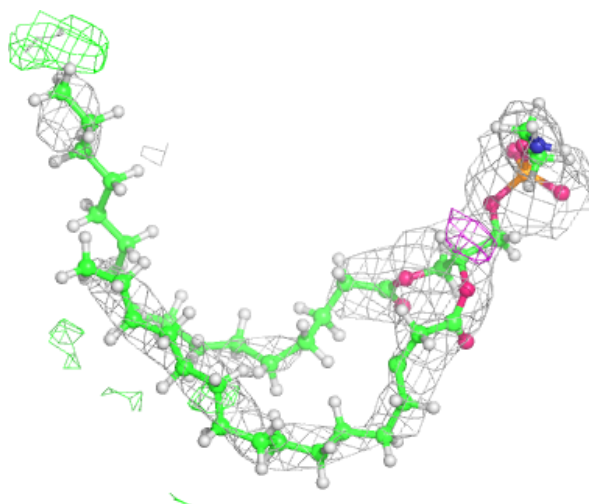
**Electron density around 6PE A 501:**

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



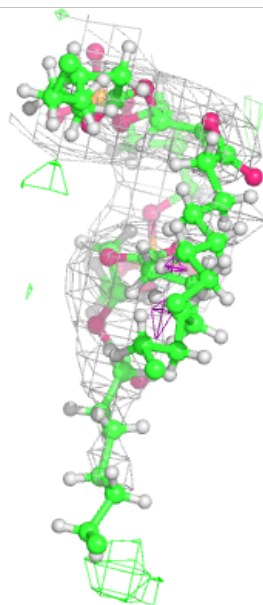
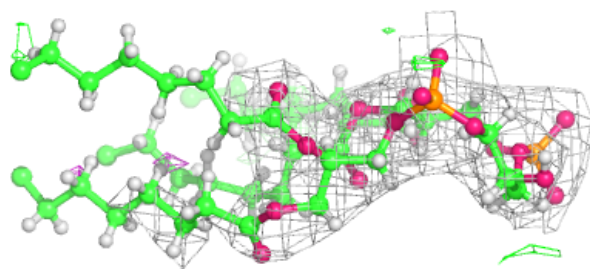
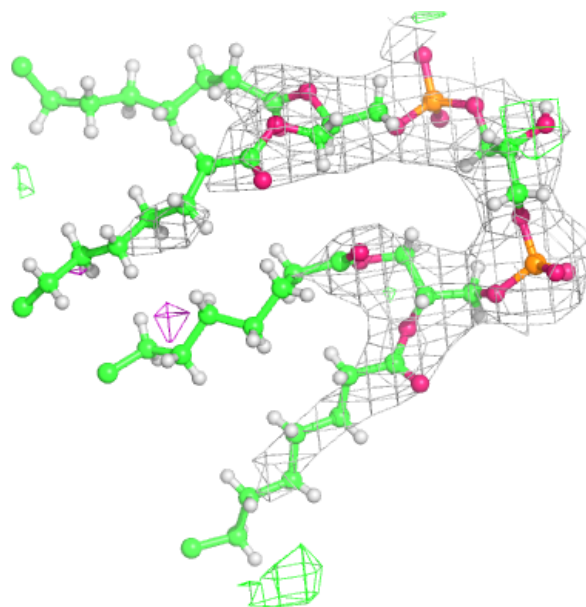
**Electron density around PEF D 1002:**

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



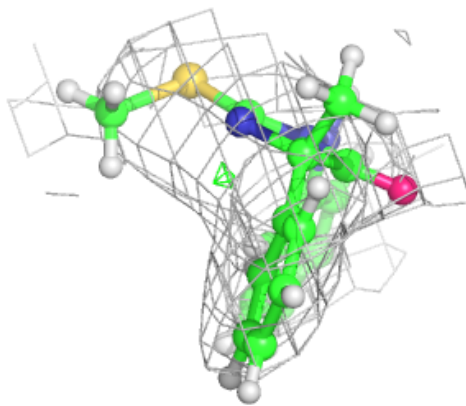
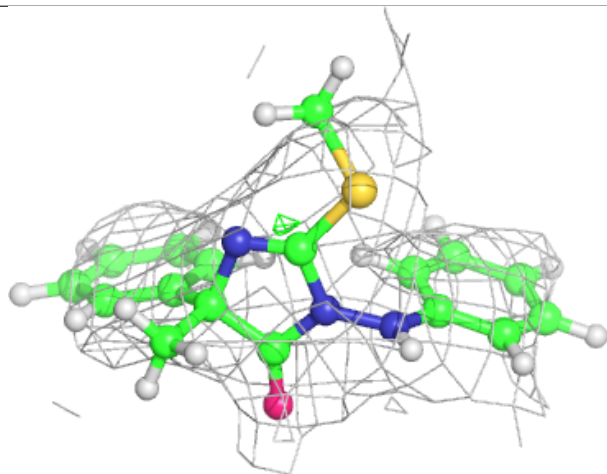
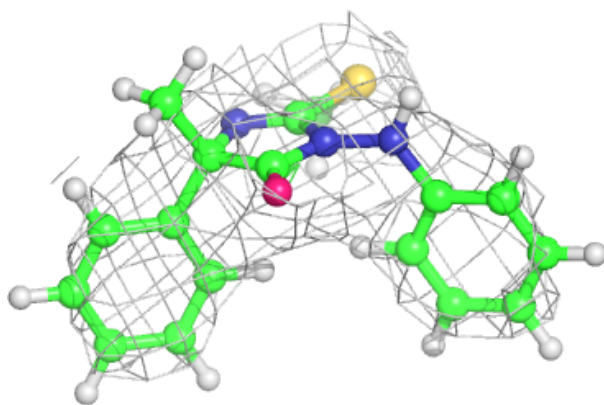
**Electron density around CDL A 502:**

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



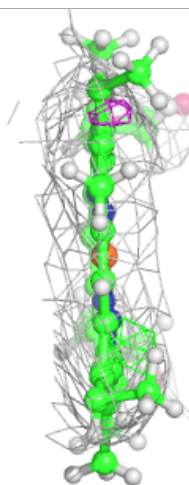
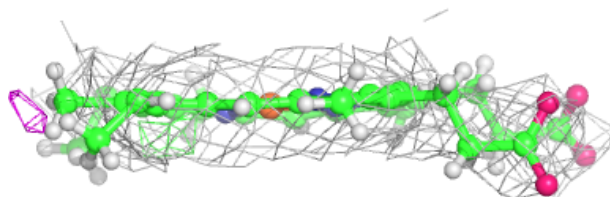
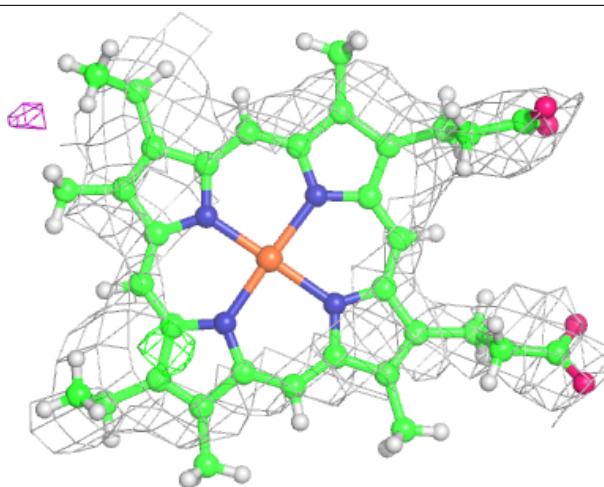
**Electron density around FNM C 1003:**

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



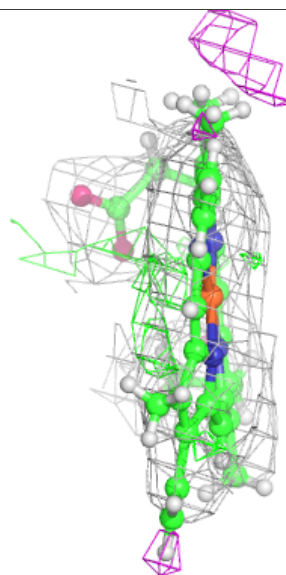
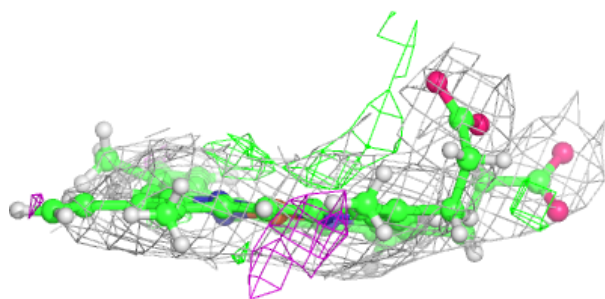
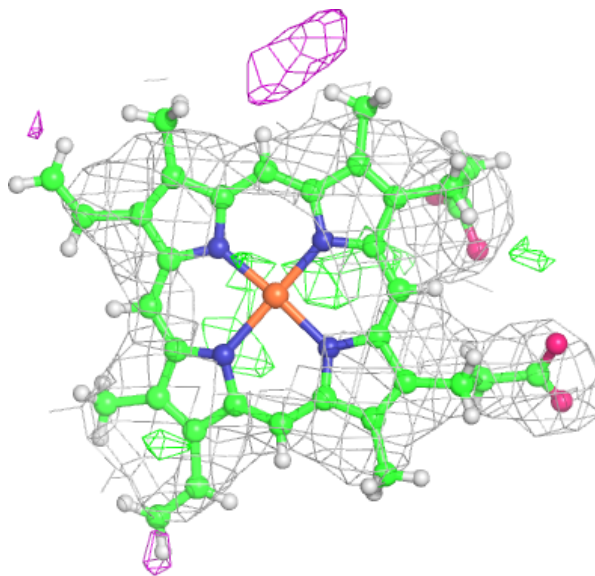
**Electron density around HEC D 1001:**

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



**Electron density around HEM C 1002:**

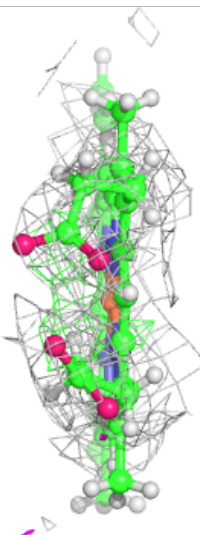
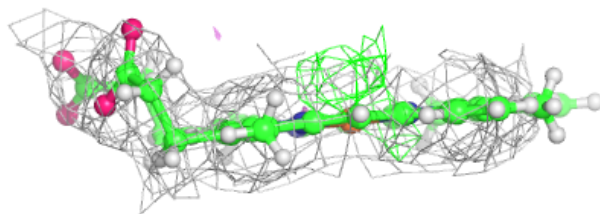
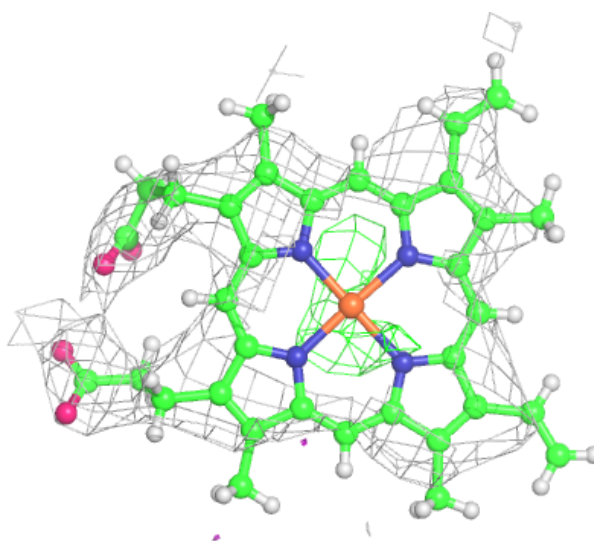
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM C 1001:**

$2mF_o-DF_c$  (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.