Full wwPDB X-ray Structure Validation Report (i)

Jun 23, 2024 – 02:04 PM EDT

PDB ID	:	5LO9
Title	:	Thiosulfate dehydrogenase (TsdBA) from Marichromatium purpuratum - "as isolated" form
Authors	:	Brito, J.A.; Kurth, J.M.; Reuter, J.; Flegler, A.; Koch, T.; Franke, T.; Klein, E.; Rowe, S.; Butt, J.N.; Denkmann, K.; Pereira, I.A.C.; Dahl, C.; Archer, M.
Deposited on	:	2016-08-08
Resolution	:	2.75 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

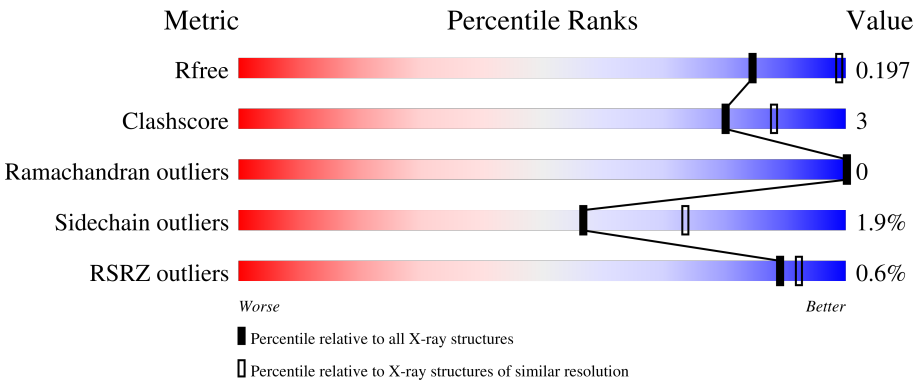
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	526	85% 5% 10%
1	B	526	% 81% 8% 11%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 7584 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.

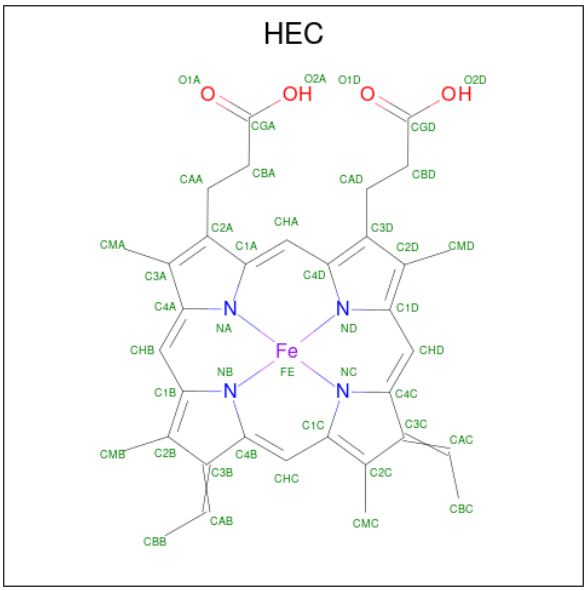
- Molecule 1 is a protein called Cytochrome C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	471	3524	2192	658	655	19	0	0	0
1	B	469	3504	2181	653	651	19	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	519	LEU	-	expression tag	UNP W0DW89
A	520	GLU	-	expression tag	UNP W0DW89
A	521	HIS	-	expression tag	UNP W0DW89
A	522	HIS	-	expression tag	UNP W0DW89
A	523	HIS	-	expression tag	UNP W0DW89
A	524	HIS	-	expression tag	UNP W0DW89
A	525	HIS	-	expression tag	UNP W0DW89
A	526	HIS	-	expression tag	UNP W0DW89
B	519	LEU	-	expression tag	UNP W0DW89
B	520	GLU	-	expression tag	UNP W0DW89
B	521	HIS	-	expression tag	UNP W0DW89
B	522	HIS	-	expression tag	UNP W0DW89
B	523	HIS	-	expression tag	UNP W0DW89
B	524	HIS	-	expression tag	UNP W0DW89
B	525	HIS	-	expression tag	UNP W0DW89
B	526	HIS	-	expression tag	UNP W0DW89

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).

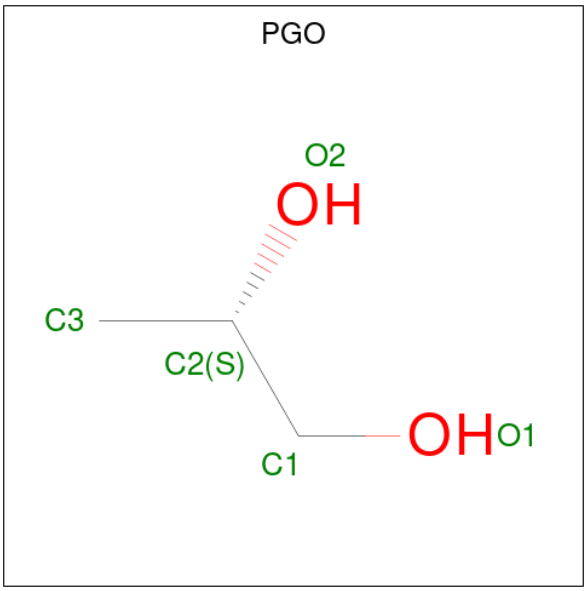


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	B	1	43	34	1	4	4	0	0
			Total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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

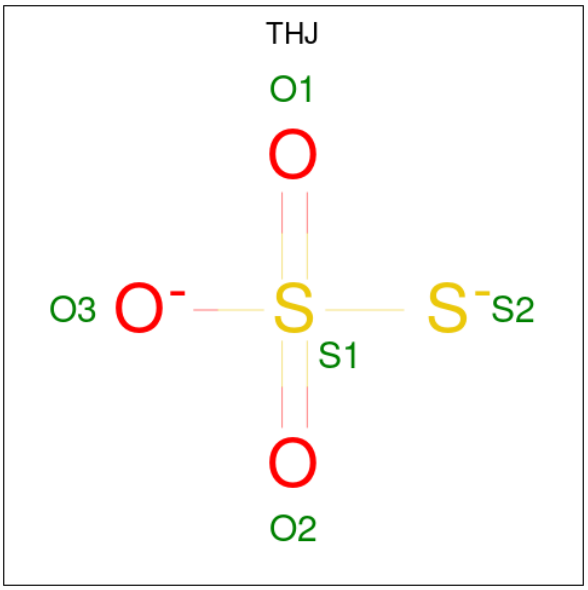
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
3	A	7	7	7	0	0
			Total	Cl		
3	B	4	4	4	0	0

- Molecule 4 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: $C_3H_8O_2$).



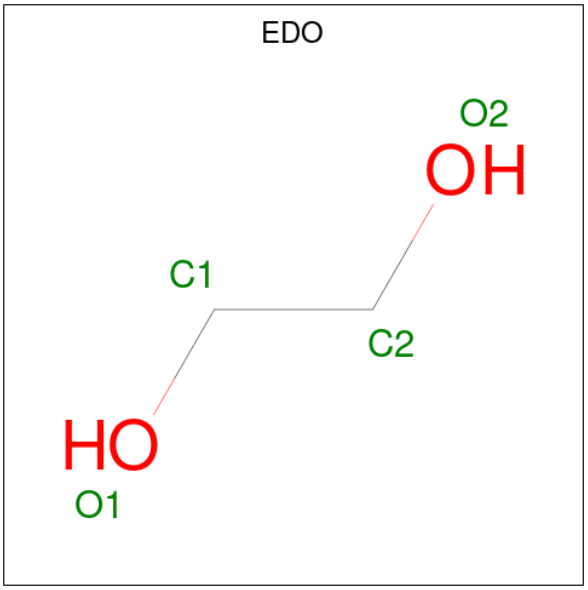
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	5	3	2	0	0
			Total	C	O		
4	A	1	5	3	2	0	0
			Total	C	O		
4	B	1	5	3	2	0	0
			Total	C	O		
4	B	1	5	3	2	0	0

- Molecule 5 is THIOSULFATE (three-letter code: THJ) (formula: O_3S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	A	1	5	3	2	0	0
			Total	O	S		
5	B	1	5	3	2	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



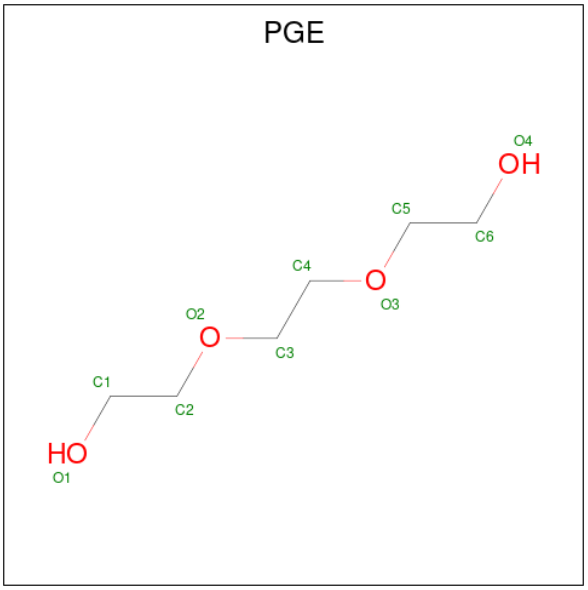
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	4	2	2	0	0
			Total	C	O		
6	A	1	4	2	2	0	0
			Total	C	O		
6	A	1	4	2	2	0	0
			Total	C	O		
6	A	1	4	2	2	0	0
			Total	C	O		
6	A	1	4	2	2	0	0
			Total	C	O		
6	A	1	4	2	2	0	0
			Total	C	O		
6	A	1	4	2	2	0	0
			Total	C	O		
6	A	1	4	2	2	0	0
			Total	C	O		
6	A	1	4	2	2	0	0
			Total	C	O		
6	A	1	4	2	2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	4	2	2	0	0
			Total	C	O		
6	B	1	4	2	2	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
7	A	1	10	6	4	0	0

- Molecule 8 is water.

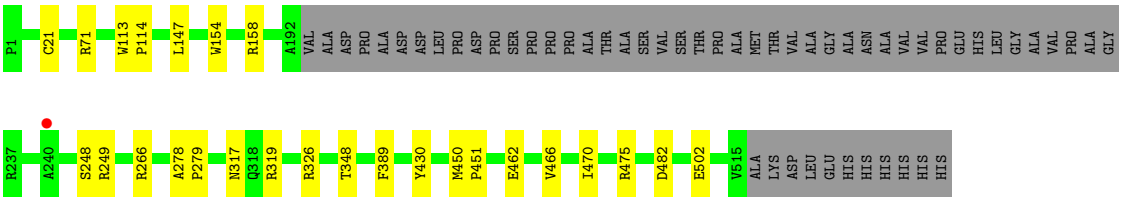
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	69	69	69	0	0
			Total	O		
8	B	44	44	44	0	0

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.

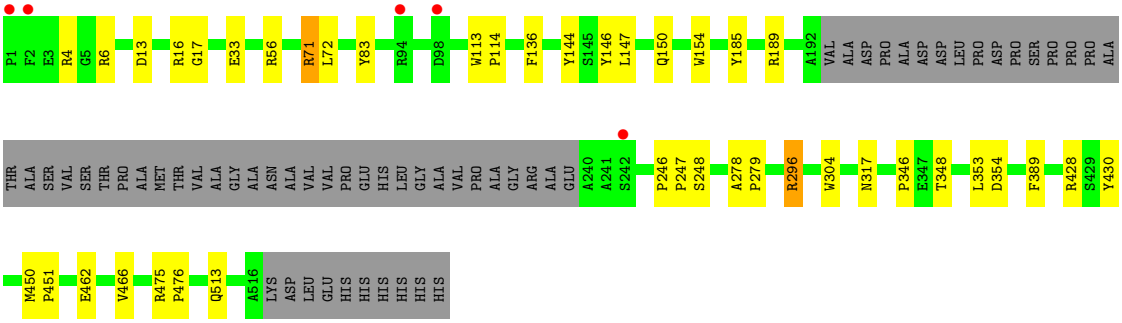
• Molecule 1: Cytochrome C

Chain A:



• Molecule 1: Cytochrome C

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	159.75Å 159.75Å 393.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	113.13 – 2.75 113.13 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.0 (113.13-2.75) 99.0 (113.13-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.73Å)	Xtriage
Refinement program	PHENIX (dev_2276: ???), BUSTER-TNT	Depositor
R, R_{free}	0.157 , 0.198 0.160 , 0.197	Depositor DCC
R_{free} test set	2507 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	51.9	Xtriage
Anisotropy	0.277	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 41.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.006 for -1/3*h+1/3*k+1/3*l,-k,8/3*h+4/3*k+1/3*l 0.020 for -2/3*h-1/3*k-1/3*l,-1/3*h-2/3*k+1/3*l,-4/3*h+4/3*k+1/3*l 0.011 for -h,1/3*h-1/3*k-1/3*l,-4/3*h-8/3*k+1/3*l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7584	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: EDO, CL, HEC, THJ, PGO, PGE

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	0.66	2/3618 (0.1%)	0.76	1/4930 (0.0%)
1	B	0.62	0/3598	0.74	3/4904 (0.1%)
All	All	0.64	2/7216 (0.0%)	0.75	4/9834 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	502	GLU	C-N	7.77	1.49	1.34
1	A	21	CYS	CB-SG	-5.28	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	296	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	A	158	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	B	354	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	B	71	ARG	NE-CZ-NH1	5.08	122.84	120.30

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	3524	0	3355	13	0
1	B	3504	0	3336	23	0
2	A	172	0	121	4	0
2	B	172	0	120	4	0
3	A	7	0	0	0	0
3	B	4	0	0	0	0
4	A	10	0	16	0	0
4	B	10	0	16	1	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	44	0	66	3	0
6	B	4	0	6	0	0
7	A	10	0	14	0	0
8	A	69	0	0	1	0
8	B	44	0	0	2	0
All	All	7584	0	7050	39	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 3.

All (39) 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:B:247:PRO:O	1:B:296:ARG:NH2	2.19	0.76
1:A:462:GLU:O	1:A:466:VAL:HG23	2.08	0.53
1:A:319:ARG:NH2	8:A:1101:HOH:O	2.43	0.51
1:B:462:GLU:O	1:B:466:VAL:HG23	2.11	0.50
1:A:451:PRO:HB3	2:A:1004:HEC:HMC2	1.94	0.49
1:B:296:ARG:NH1	8:B:1101:HOH:O	2.39	0.49
1:B:13:ASP:OD1	1:B:16:ARG:HG3	2.13	0.48
1:A:249:ARG:HG2	6:A:1021:EDO:H22	1.97	0.47
1:B:451:PRO:HB3	2:B:1004:HEC:HMC2	1.96	0.46
1:B:428:ARG:NH1	4:B:1010:PGO:H11	2.31	0.46
1:B:430:TYR:O	1:B:475:ARG:HD3	2.16	0.46
1:A:113:TRP:N	1:A:114:PRO:CD	2.79	0.46
1:A:470:ILE:HD11	2:A:1004:HEC:HMB3	1.97	0.46
1:B:17:GLY:O	1:B:71:ARG:HD3	2.16	0.45
1:A:147:LEU:HD23	2:A:1002:HEC:HMA3	1.98	0.45
1:B:475:ARG:HB2	1:B:476:PRO:CD	2.47	0.45
1:A:249:ARG:NE	6:A:1021:EDO:H21	2.32	0.44
1:B:136:PHE:CE1	2:B:1002:HEC:HMD3	2.52	0.44
1:A:430:TYR:O	1:A:475:ARG:HD3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:ALA:N	1:B:279:PRO:CD	2.81	0.44
2:A:1001:HEC:HMC1	2:A:1001:HEC:HBC3	2.00	0.44
1:B:317:ASN:OD1	1:B:317:ASN:N	2.50	0.44
1:B:6:ARG:HG3	1:B:83:TYR:CE1	2.53	0.43
1:B:346:PRO:HB2	1:B:353:LEU:HD23	2.01	0.43
6:A:1017:EDO:H11	8:B:1131:HOH:O	2.18	0.43
1:B:450:MET:HA	1:B:451:PRO:C	2.40	0.42
1:A:278:ALA:N	1:A:279:PRO:CD	2.82	0.42
1:A:450:MET:HA	1:A:451:PRO:C	2.40	0.42
1:B:33:GLU:OE2	1:B:144:TYR:N	2.51	0.41
1:A:71:ARG:HG2	1:A:71:ARG:HH11	1.86	0.41
2:B:1004:HEC:HMC1	2:B:1004:HEC:HBC3	2.02	0.41
1:A:317:ASN:OD1	1:A:317:ASN:N	2.53	0.41
1:B:185:TYR:CZ	1:B:189:ARG:HD2	2.56	0.41
1:B:13:ASP:CG	1:B:16:ARG:HG3	2.40	0.40
1:B:56:ARG:NH1	1:B:72:LEU:O	2.53	0.40
1:B:147:LEU:HD23	2:B:1002:HEC:HMA3	2.02	0.40
1:B:146:TYR:CE1	1:B:150:GLN:NE2	2.89	0.40
1:B:246:PRO:HG3	1:B:304:TRP:CD1	2.55	0.40
1:B:113:TRP:N	1:B:114:PRO:CD	2.85	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	467/526 (89%)	456 (98%)	11 (2%)	0	100	100
1	B	465/526 (88%)	454 (98%)	11 (2%)	0	100	100
All	All	932/1052 (89%)	910 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	337/378 (89%)	330 (98%)	7 (2%)	53	71
1	B	335/378 (89%)	329 (98%)	6 (2%)	59	75
All	All	672/756 (89%)	659 (98%)	13 (2%)	57	73

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	TRP
1	A	248	SER
1	A	266	ARG
1	A	326	ARG
1	A	348	THR
1	A	389	PHE
1	A	482	ASP
1	B	4	ARG
1	B	154	TRP
1	B	248	SER
1	B	348	THR
1	B	389	PHE
1	B	513	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 38 ligands modelled in this entry, 11 are monoatomic - leaving 27 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	$\#\|Z\| > 2$
5	THJ	A	1008	1	2,4,4	1.71	0	2,6,6	0.58	0
6	EDO	A	1024	-	3,3,3	0.73	0	2,2,2	0.19	0
6	EDO	A	1015	-	3,3,3	0.87	0	2,2,2	0.38	0
6	EDO	A	1021	-	3,3,3	0.61	0	2,2,2	0.95	0
6	EDO	A	1020	-	3,3,3	0.51	0	2,2,2	0.29	0
2	HEC	B	1002	1	32,50,50	2.28	12 (37%)	24,82,82	1.54	4 (16%)
4	PGO	B	1011	-	3,4,4	0.67	0	1,4,4	0.52	0
7	PGE	A	1026	-	9,9,9	0.70	0	8,8,8	0.92	0
2	HEC	A	1002	1	32,50,50	2.23	10 (31%)	24,82,82	1.95	7 (29%)
6	EDO	A	1022	-	3,3,3	0.65	0	2,2,2	0.37	0
2	HEC	A	1004	1	32,50,50	2.10	10 (31%)	24,82,82	1.88	7 (29%)
4	PGO	B	1010	-	3,4,4	0.82	0	1,4,4	2.06	1 (100%)
2	HEC	A	1003	1	32,50,50	2.19	11 (34%)	24,82,82	1.83	8 (33%)
6	EDO	A	1019	-	3,3,3	0.56	0	2,2,2	0.50	0
6	EDO	B	1012	-	3,3,3	0.58	0	2,2,2	0.59	0
2	HEC	B	1003	1	32,50,50	2.29	12 (37%)	24,82,82	2.17	10 (41%)
2	HEC	A	1001	1	32,50,50	2.16	10 (31%)	24,82,82	2.26	8 (33%)
4	PGO	A	1007	-	3,4,4	0.79	0	1,4,4	0.21	0
6	EDO	A	1018	-	3,3,3	0.89	0	2,2,2	0.50	0
2	HEC	B	1001	1	32,50,50	2.42	12 (37%)	24,82,82	2.25	6 (25%)
2	HEC	B	1004	1	32,50,50	2.22	11 (34%)	24,82,82	2.19	9 (37%)
6	EDO	A	1023	-	3,3,3	0.43	0	2,2,2	0.56	0
5	THJ	B	1006	1	2,4,4	1.67	1 (50%)	2,6,6	0.88	0
6	EDO	A	1016	-	3,3,3	0.54	0	2,2,2	0.23	0
4	PGO	A	1014	-	3,4,4	0.66	0	1,4,4	0.95	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
6	EDO	A	1025	-	3,3,3	1.12	0	2,2,2	0.93	0
6	EDO	A	1017	-	3,3,3	1.07	0	2,2,2	0.13	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
6	EDO	A	1024	-	-	1/1/1/1	-
6	EDO	A	1015	-	-	1/1/1/1	-
6	EDO	A	1021	-	-	1/1/1/1	-
6	EDO	A	1020	-	-	0/1/1/1	-
2	HEC	B	1002	1	-	1/10/54/54	-
4	PGO	B	1011	-	-	2/2/2/2	-
7	PGE	A	1026	-	-	5/7/7/7	-
2	HEC	A	1002	1	-	2/10/54/54	-
6	EDO	A	1022	-	-	1/1/1/1	-
2	HEC	A	1004	1	-	4/10/54/54	-
4	PGO	B	1010	-	-	2/2/2/2	-
2	HEC	A	1003	1	-	4/10/54/54	-
6	EDO	A	1019	-	-	1/1/1/1	-
6	EDO	B	1012	-	-	1/1/1/1	-
2	HEC	B	1003	1	-	0/10/54/54	-
2	HEC	A	1001	1	-	0/10/54/54	-
4	PGO	A	1007	-	-	2/2/2/2	-
6	EDO	A	1018	-	-	0/1/1/1	-
2	HEC	B	1001	1	-	1/10/54/54	-
2	HEC	B	1004	1	-	6/10/54/54	-
6	EDO	A	1023	-	-	1/1/1/1	-
6	EDO	A	1016	-	-	1/1/1/1	-
4	PGO	A	1014	-	-	1/2/2/2	-
6	EDO	A	1025	-	-	1/1/1/1	-
6	EDO	A	1017	-	-	0/1/1/1	-

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	HEC	C3C-C2C	6.99	1.48	1.40
2	B	1002	HEC	C2B-C3B	6.78	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1003	HEC	C3C-C2C	6.65	1.47	1.40
2	B	1003	HEC	C3C-C2C	6.65	1.47	1.40
2	B	1001	HEC	C2B-C3B	6.64	1.47	1.40
2	B	1004	HEC	C2B-C3B	6.37	1.47	1.40
2	A	1002	HEC	C3C-C2C	6.33	1.47	1.40
2	A	1002	HEC	C2B-C3B	6.13	1.47	1.40
2	A	1001	HEC	C2B-C3B	5.96	1.47	1.40
2	B	1004	HEC	C3C-C2C	5.77	1.46	1.40
2	A	1004	HEC	C2B-C3B	5.38	1.46	1.40
2	A	1001	HEC	C3C-C2C	5.25	1.46	1.40
2	B	1002	HEC	C3C-C2C	5.12	1.46	1.40
2	A	1003	HEC	C2B-C3B	5.11	1.46	1.40
2	B	1003	HEC	C2B-C3B	5.07	1.46	1.40
2	A	1004	HEC	C3C-C2C	4.50	1.45	1.40
2	B	1003	HEC	C2A-C3A	3.58	1.48	1.37
2	B	1001	HEC	C2A-C3A	3.56	1.48	1.37
2	B	1002	HEC	C3C-C4C	3.48	1.49	1.43
2	B	1001	HEC	C3C-C4C	3.44	1.49	1.43
2	B	1002	HEC	C3D-C2D	3.43	1.47	1.37
2	A	1003	HEC	C3D-C2D	3.43	1.47	1.37
2	B	1003	HEC	C3D-C2D	3.37	1.47	1.37
2	A	1002	HEC	C3C-C4C	3.34	1.49	1.43
2	A	1004	HEC	C3C-C4C	3.34	1.49	1.43
2	B	1001	HEC	C3D-C2D	3.23	1.47	1.37
2	B	1003	HEC	C4B-C3B	3.18	1.48	1.43
2	A	1002	HEC	C2A-C3A	3.15	1.47	1.37
2	B	1002	HEC	C4B-C3B	3.13	1.48	1.43
2	A	1001	HEC	C2A-C1A	3.13	1.49	1.42
2	B	1002	HEC	C2A-C3A	3.12	1.46	1.37
2	A	1004	HEC	C4B-C3B	3.05	1.48	1.43
2	A	1003	HEC	C3C-C4C	3.04	1.48	1.43
2	A	1001	HEC	C2A-C3A	3.03	1.46	1.37
2	B	1003	HEC	C1D-CHD	3.02	1.49	1.41
2	B	1004	HEC	C4B-C3B	3.02	1.48	1.43
2	B	1002	HEC	C3A-C4A	3.02	1.49	1.42
2	A	1004	HEC	C2A-C1A	2.98	1.49	1.42
2	A	1002	HEC	C3A-C4A	2.96	1.49	1.42
2	B	1004	HEC	C2A-C3A	2.94	1.46	1.37
2	A	1004	HEC	C3A-C4A	2.92	1.49	1.42
2	B	1001	HEC	C2A-C1A	2.91	1.49	1.42
2	B	1001	HEC	C4B-C3B	2.89	1.48	1.43
2	B	1003	HEC	C2A-C1A	2.87	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1003	HEC	C3A-C4A	2.77	1.48	1.42
2	B	1002	HEC	C1D-CHD	2.76	1.48	1.41
2	A	1001	HEC	C3D-C2D	2.75	1.45	1.37
2	B	1003	HEC	CBD-CGD	2.75	1.57	1.50
2	B	1002	HEC	C2A-C1A	2.74	1.48	1.42
2	A	1003	HEC	C2A-C3A	2.72	1.45	1.37
2	B	1004	HEC	C1D-CHD	2.72	1.48	1.41
2	A	1004	HEC	C3D-C2D	2.71	1.45	1.37
2	B	1001	HEC	C1C-CHC	2.71	1.48	1.41
2	A	1003	HEC	C4B-C3B	2.68	1.47	1.43
2	A	1001	HEC	C3C-C4C	2.67	1.47	1.43
2	B	1004	HEC	C3D-C2D	2.67	1.45	1.37
2	A	1004	HEC	C2A-C3A	2.66	1.45	1.37
2	B	1001	HEC	C3A-C4A	2.61	1.48	1.42
2	A	1001	HEC	C4D-CHA	2.60	1.48	1.41
2	B	1004	HEC	C1B-CHB	2.57	1.48	1.41
2	A	1001	HEC	C3A-C4A	2.57	1.48	1.42
2	A	1003	HEC	C2A-C1A	2.56	1.48	1.42
2	A	1001	HEC	C1C-CHC	2.56	1.48	1.41
2	A	1004	HEC	C1D-CHD	2.54	1.48	1.41
2	B	1004	HEC	C3A-C4A	2.51	1.48	1.42
2	B	1001	HEC	C4D-CHA	2.51	1.48	1.41
2	A	1002	HEC	C4B-C3B	2.51	1.47	1.43
2	B	1001	HEC	C1D-CHD	2.48	1.47	1.41
2	A	1001	HEC	C4B-C3B	2.48	1.47	1.43
2	A	1002	HEC	C3D-C2D	2.44	1.44	1.37
2	B	1004	HEC	C1C-CHC	2.42	1.47	1.41
2	B	1004	HEC	C2A-C1A	2.41	1.48	1.42
2	B	1004	HEC	C3C-C4C	2.33	1.47	1.43
2	A	1002	HEC	C2A-C1A	2.33	1.47	1.42
2	B	1002	HEC	C1B-CHB	2.27	1.47	1.41
2	B	1003	HEC	C1C-CHC	2.25	1.47	1.41
2	B	1001	HEC	C1B-CHB	2.23	1.47	1.41
2	A	1003	HEC	C1B-CHB	2.21	1.47	1.41
5	B	1006	THJ	O2-S1	2.16	1.52	1.45
2	A	1003	HEC	C1C-CHC	2.16	1.47	1.41
2	B	1003	HEC	C3C-C4C	2.15	1.47	1.43
2	B	1002	HEC	C1C-CHC	2.13	1.46	1.41
2	A	1002	HEC	C4D-CHA	2.12	1.46	1.41
2	B	1003	HEC	C4D-CHA	2.11	1.46	1.41
2	B	1002	HEC	C4D-CHA	2.07	1.46	1.41
2	B	1003	HEC	C3A-C4A	2.07	1.47	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1004	HEC	O2D-CGD	-2.03	1.23	1.30
2	A	1003	HEC	C1D-CHD	2.01	1.46	1.41
2	A	1002	HEC	C1D-CHD	2.01	1.46	1.41

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1001	HEC	CBA-CAA-C2A	-5.96	102.56	112.60
2	A	1001	HEC	CBD-CAD-C3D	-5.34	103.51	112.62
2	A	1001	HEC	C1D-C2D-C3D	-4.68	103.74	107.00
2	B	1002	HEC	C1D-C2D-C3D	-4.64	103.77	107.00
2	B	1003	HEC	C4C-C3C-C2C	-4.51	101.48	106.35
2	B	1003	HEC	CMC-C2C-C3C	4.31	130.89	125.82
2	B	1001	HEC	C1D-C2D-C3D	-4.25	104.04	107.00
2	A	1003	HEC	CMC-C2C-C3C	4.01	130.53	125.82
2	B	1004	HEC	CBA-CAA-C2A	-3.91	106.01	112.60
2	A	1002	HEC	C4C-C3C-C2C	-3.91	102.13	106.35
2	A	1002	HEC	CMC-C2C-C3C	3.87	130.37	125.82
2	A	1001	HEC	CBA-CAA-C2A	-3.81	106.18	112.60
2	B	1004	HEC	C2B-C3B-C4B	-3.78	102.27	106.35
2	B	1001	HEC	CBD-CAD-C3D	-3.73	106.26	112.62
2	B	1001	HEC	C4C-C3C-C2C	-3.69	102.37	106.35
2	A	1004	HEC	CBD-CAD-C3D	-3.68	106.33	112.62
2	B	1004	HEC	C1D-C2D-C3D	-3.57	104.51	107.00
2	A	1004	HEC	C4C-C3C-C2C	-3.56	102.51	106.35
2	B	1004	HEC	C4C-C3C-C2C	-3.49	102.58	106.35
2	B	1004	HEC	CMC-C2C-C3C	3.44	129.87	125.82
2	B	1003	HEC	CMB-C2B-C3B	3.43	129.86	125.82
2	B	1001	HEC	CMB-C2B-C3B	3.41	129.83	125.82
2	A	1004	HEC	C1D-C2D-C3D	-3.38	104.64	107.00
2	A	1002	HEC	C1D-C2D-C3D	-3.37	104.65	107.00
2	A	1004	HEC	C2B-C3B-C4B	-3.36	102.73	106.35
2	A	1001	HEC	C4C-C3C-C2C	-3.29	102.81	106.35
2	A	1001	HEC	CMB-C2B-C3B	3.22	129.60	125.82
2	A	1002	HEC	CMB-C2B-C3B	3.07	129.44	125.82
2	A	1002	HEC	C2B-C3B-C4B	-3.06	103.05	106.35
2	B	1004	HEC	CMD-C2D-C1D	2.97	133.03	128.46
2	A	1004	HEC	CMC-C2C-C3C	2.92	129.25	125.82
2	A	1001	HEC	CMC-C2C-C3C	2.87	129.19	125.82
2	A	1004	HEC	CBA-CAA-C2A	-2.85	107.80	112.60
2	B	1003	HEC	CMC-C2C-C1C	-2.84	124.09	128.46
2	B	1004	HEC	CBD-CAD-C3D	-2.83	107.79	112.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1004	HEC	O2D-CGD-CBD	2.81	123.07	114.03
2	B	1002	HEC	C4C-C3C-C2C	-2.80	103.33	106.35
2	B	1003	HEC	CBA-CAA-C2A	-2.79	107.90	112.60
2	B	1003	HEC	O2D-CGD-CBD	2.76	122.91	114.03
2	A	1003	HEC	CMD-C2D-C3D	2.73	130.09	124.94
2	B	1001	HEC	CMC-C2C-C3C	2.68	128.97	125.82
2	A	1001	HEC	C2B-C3B-C4B	-2.63	103.52	106.35
2	A	1003	HEC	CMD-C2D-C1D	-2.55	124.55	128.46
2	B	1003	HEC	CMD-C2D-C1D	-2.49	124.64	128.46
2	B	1003	HEC	CMD-C2D-C3D	2.45	129.56	124.94
2	A	1003	HEC	C4C-C3C-C2C	-2.44	103.72	106.35
2	B	1002	HEC	C2B-C3B-C4B	-2.39	103.77	106.35
2	B	1002	HEC	CMB-C2B-C3B	2.39	128.63	125.82
2	A	1003	HEC	C1D-C2D-C3D	-2.37	105.35	107.00
2	A	1003	HEC	CMB-C2B-C3B	2.34	128.58	125.82
2	A	1004	HEC	CMB-C2B-C3B	2.33	128.56	125.82
2	A	1002	HEC	O1D-CGD-CBD	-2.32	115.64	123.08
2	A	1001	HEC	O2A-CGA-CBA	2.30	121.41	114.03
2	B	1003	HEC	C2B-C3B-C4B	-2.26	103.91	106.35
2	A	1003	HEC	C2B-C3B-C4B	-2.24	103.93	106.35
2	A	1003	HEC	CBA-CAA-C2A	-2.20	108.89	112.60
2	B	1003	HEC	CMA-C3A-C2A	2.20	129.09	124.94
2	B	1004	HEC	CMB-C2B-C3B	2.17	128.37	125.82
2	A	1002	HEC	O2D-CGD-CBD	2.07	120.69	114.03
4	B	1010	PGO	O2-C2-C3	2.06	118.30	109.38

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1004	HEC	C1A-C2A-CAA-CBA
2	B	1004	HEC	C3A-C2A-CAA-CBA
2	B	1004	HEC	C2A-CAA-CBA-CGA
4	A	1007	PGO	O1-C1-C2-C3
4	A	1007	PGO	O1-C1-C2-O2
4	B	1010	PGO	O1-C1-C2-C3
4	B	1010	PGO	O1-C1-C2-O2
4	B	1011	PGO	O1-C1-C2-O2
2	A	1004	HEC	C2A-CAA-CBA-CGA
2	A	1004	HEC	C3D-CAD-CBD-CGD
7	A	1026	PGE	O2-C3-C4-O3
6	A	1021	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	A	1016	EDO	O1-C1-C2-O2
6	A	1019	EDO	O1-C1-C2-O2
6	B	1012	EDO	O1-C1-C2-O2
2	B	1004	HEC	C3D-CAD-CBD-CGD
7	A	1026	PGE	O1-C1-C2-O2
4	A	1014	PGO	O1-C1-C2-O2
6	A	1022	EDO	O1-C1-C2-O2
6	A	1023	EDO	O1-C1-C2-O2
7	A	1026	PGE	C6-C5-O3-C4
7	A	1026	PGE	C3-C4-O3-C5
4	B	1011	PGO	O1-C1-C2-C3
7	A	1026	PGE	O3-C5-C6-O4
2	A	1003	HEC	C2D-C3D-CAD-CBD
2	A	1003	HEC	C4D-C3D-CAD-CBD
2	A	1004	HEC	C1A-C2A-CAA-CBA
2	A	1004	HEC	C3A-C2A-CAA-CBA
6	A	1025	EDO	O1-C1-C2-O2
2	B	1004	HEC	CAD-CBD-CGD-O2D
6	A	1024	EDO	O1-C1-C2-O2
2	B	1004	HEC	CAD-CBD-CGD-O1D
2	A	1002	HEC	CAD-CBD-CGD-O1D
2	A	1003	HEC	CAD-CBD-CGD-O2D
2	A	1003	HEC	CAD-CBD-CGD-O1D
2	A	1002	HEC	CAD-CBD-CGD-O2D
6	A	1015	EDO	O1-C1-C2-O2
2	B	1001	HEC	CAD-CBD-CGD-O2D
2	B	1002	HEC	CAD-CBD-CGD-O2D

There are no ring outliers.

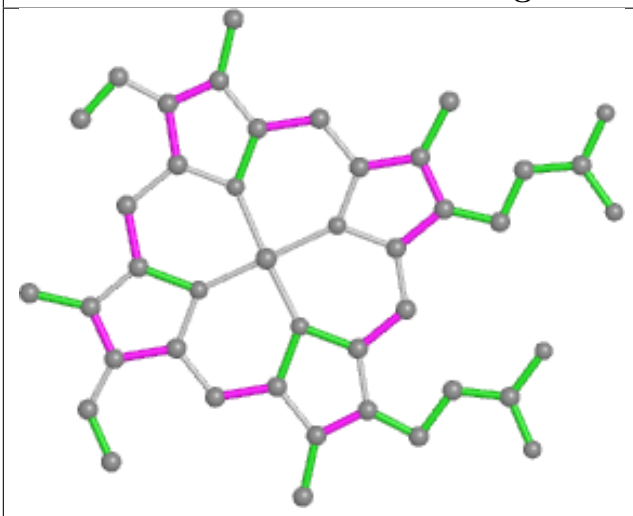
8 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1021	EDO	2	0
2	B	1002	HEC	2	0
2	A	1002	HEC	1	0
2	A	1004	HEC	2	0
4	B	1010	PGO	1	0
2	A	1001	HEC	1	0
2	B	1004	HEC	2	0
6	A	1017	EDO	1	0

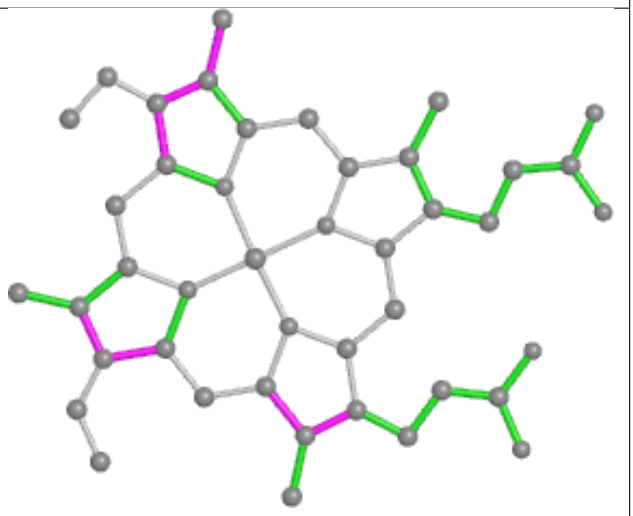
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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 then 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.

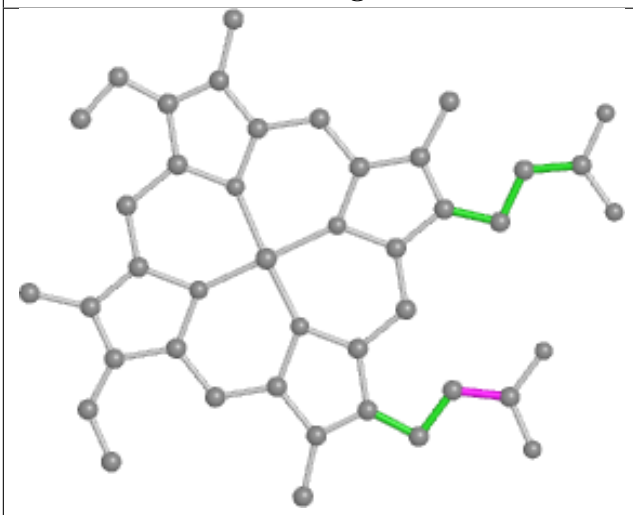
Ligand HEC B 1002



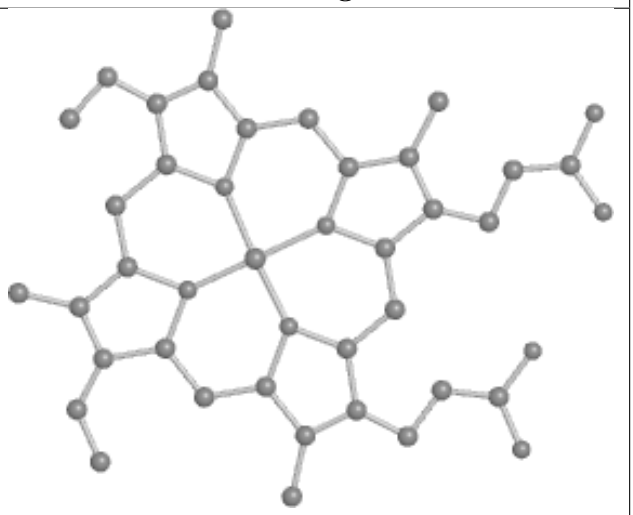
Bond lengths



Bond angles

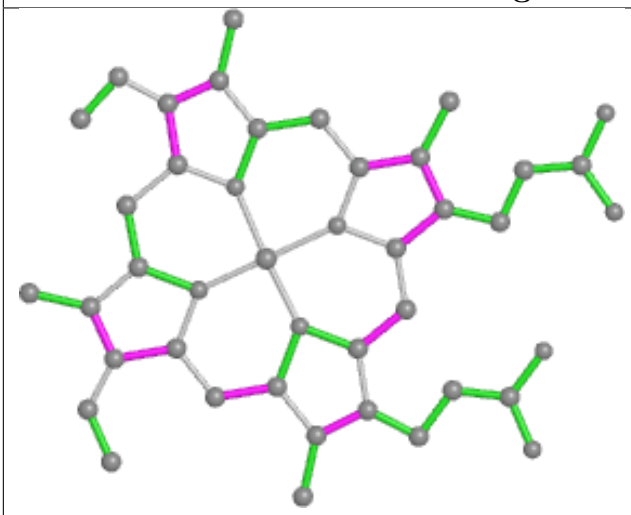


Torsions

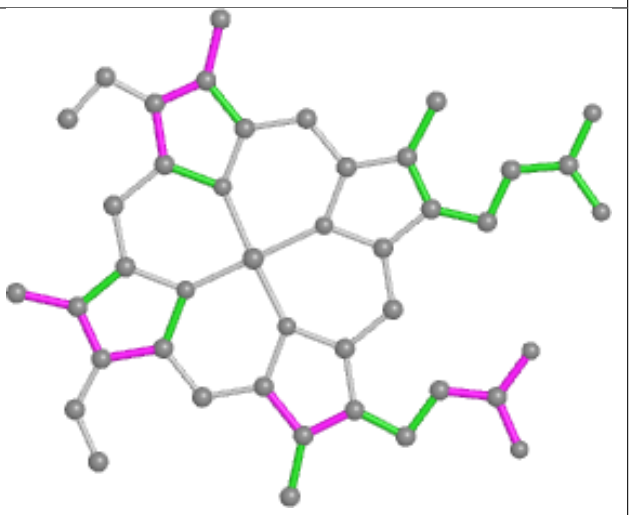


Rings

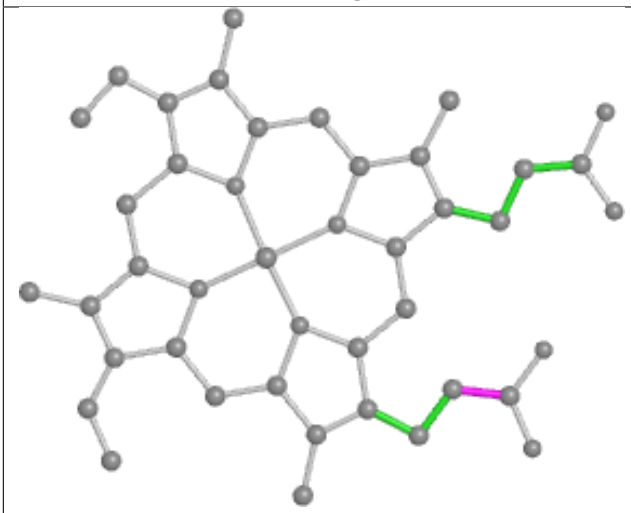
Ligand HEC A 1002



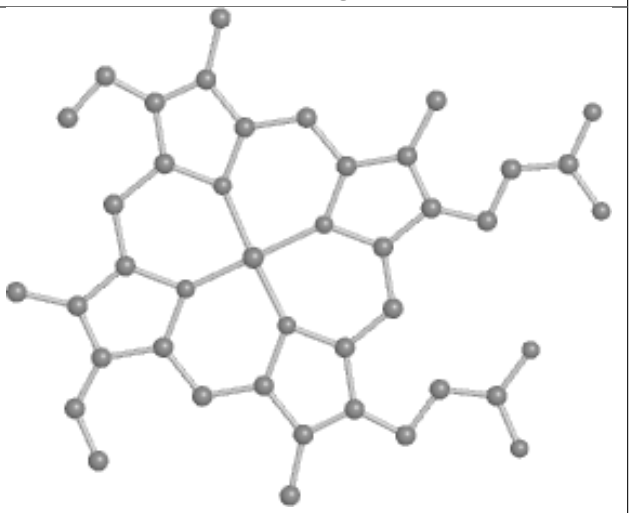
Bond lengths



Bond angles

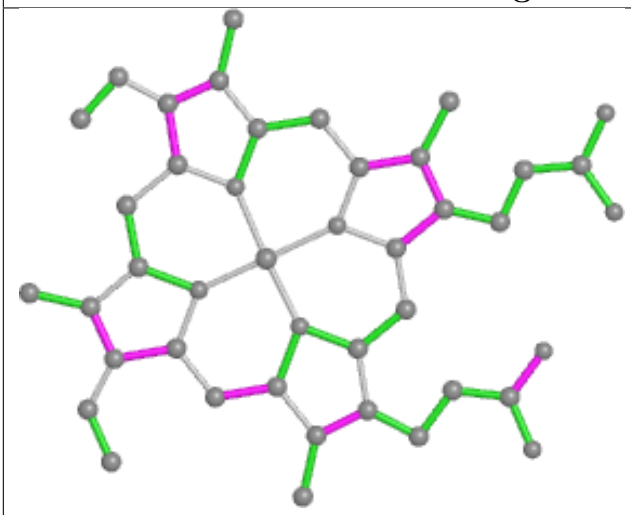


Torsions

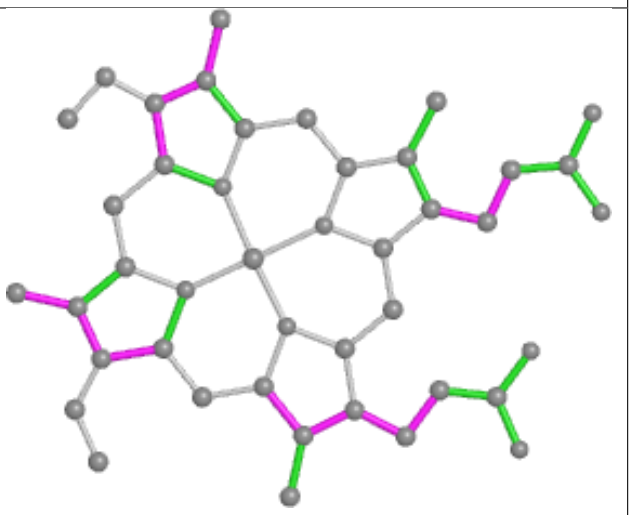


Rings

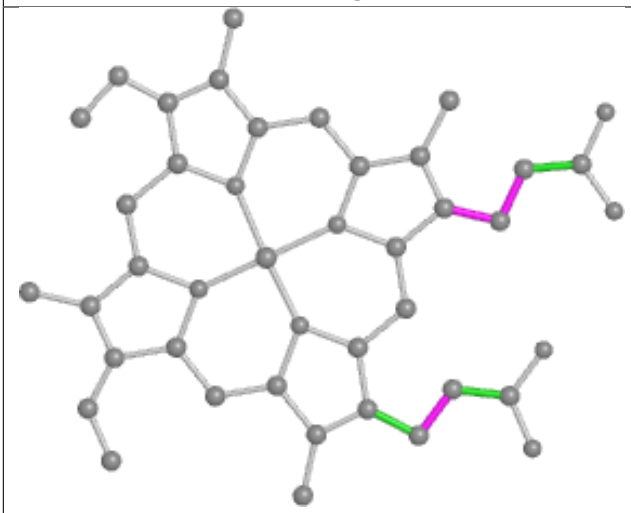
Ligand HEC A 1004



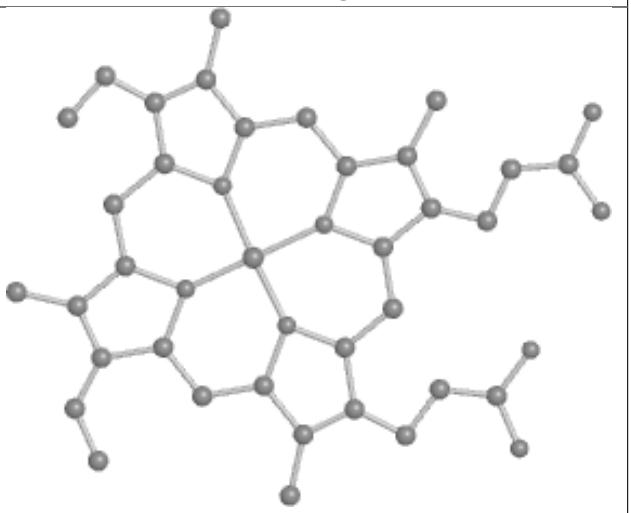
Bond lengths



Bond angles

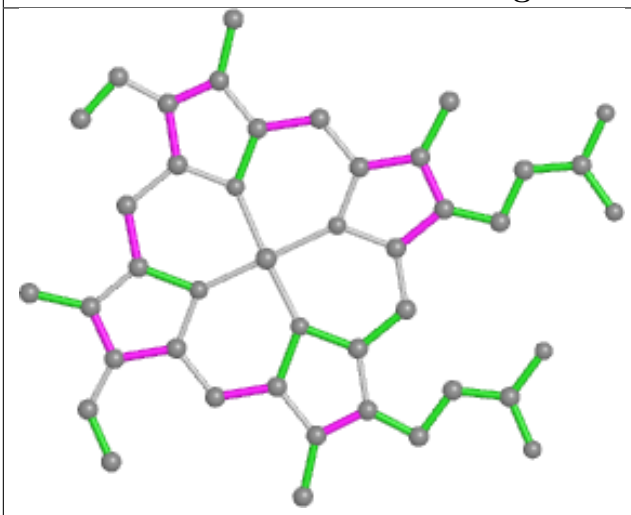


Torsions

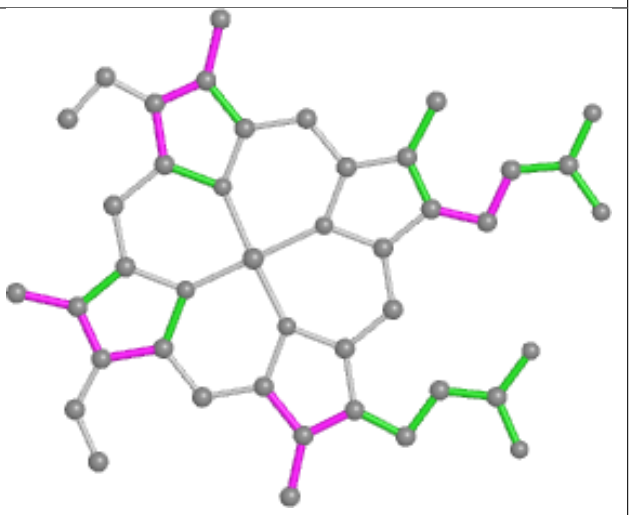


Rings

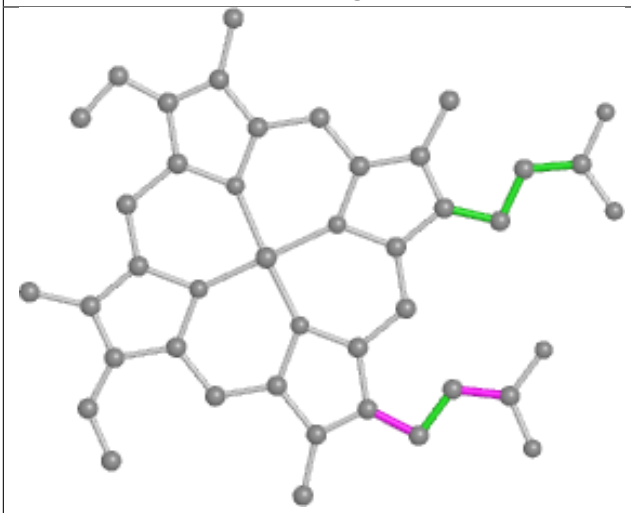
Ligand HEC A 1003



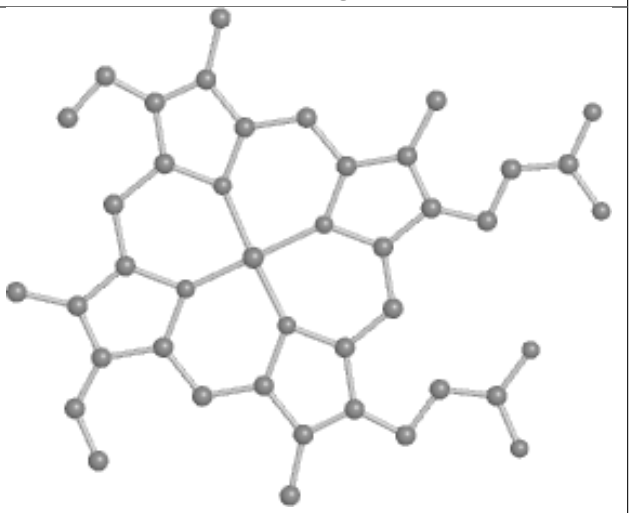
Bond lengths



Bond angles

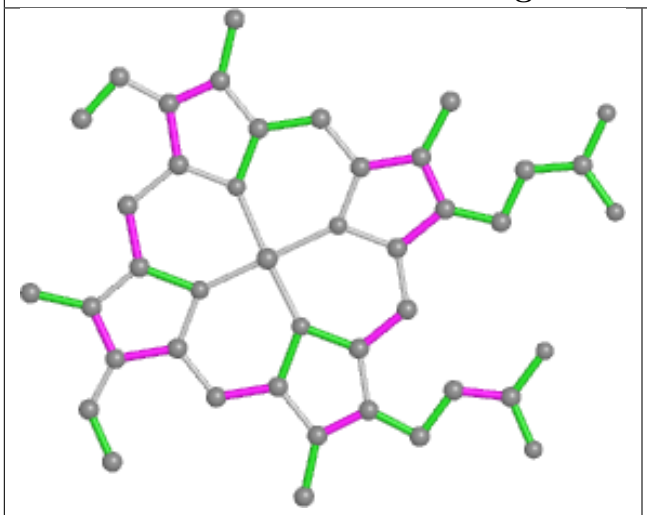


Torsions

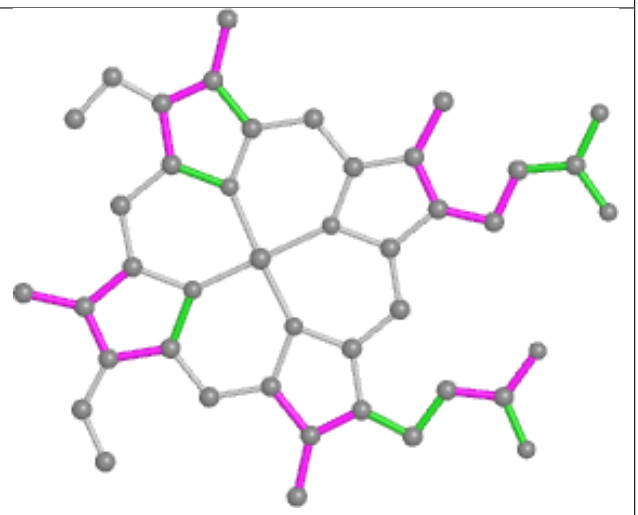


Rings

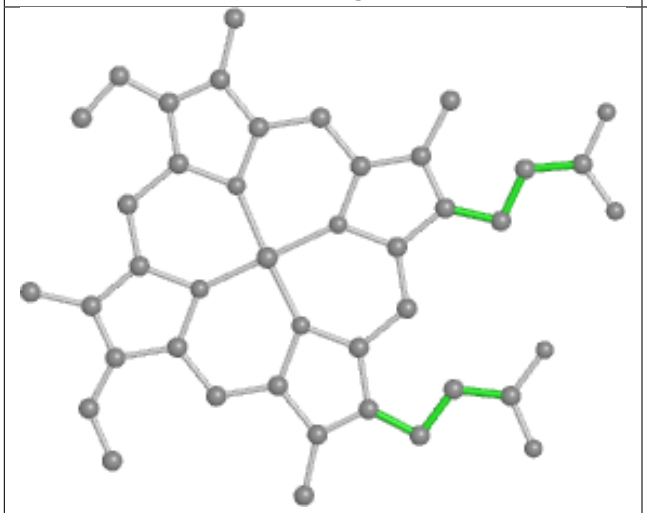
Ligand HEC B 1003



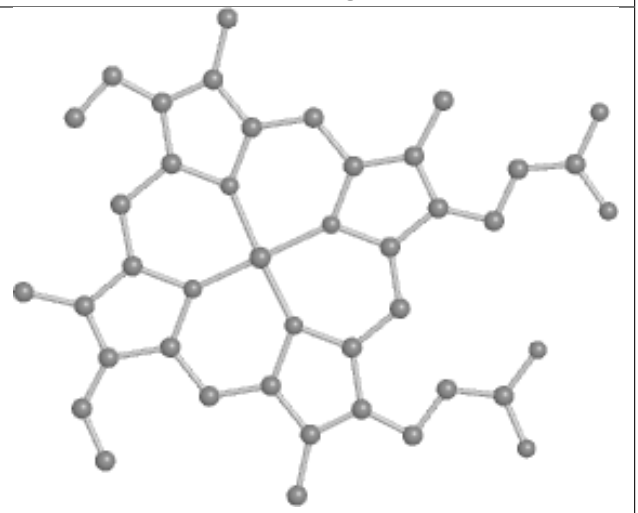
Bond lengths



Bond angles

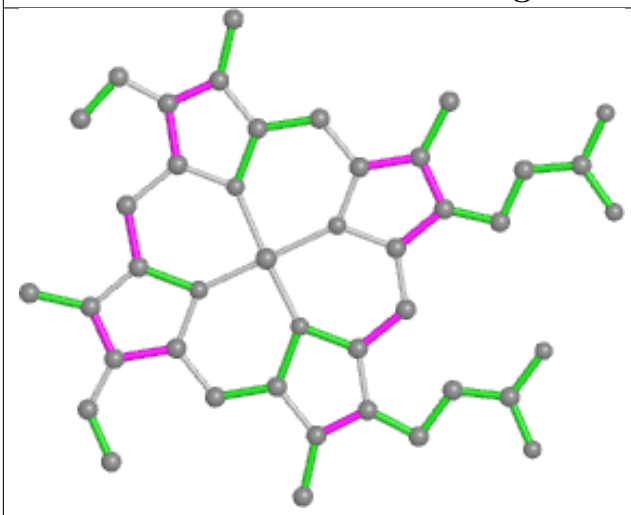


Torsions

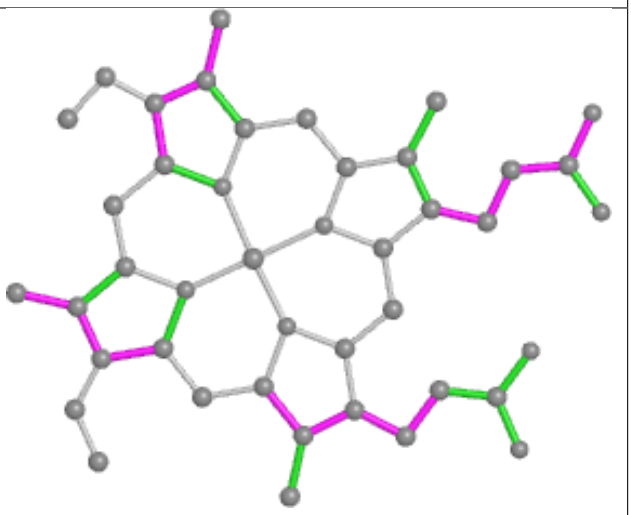


Rings

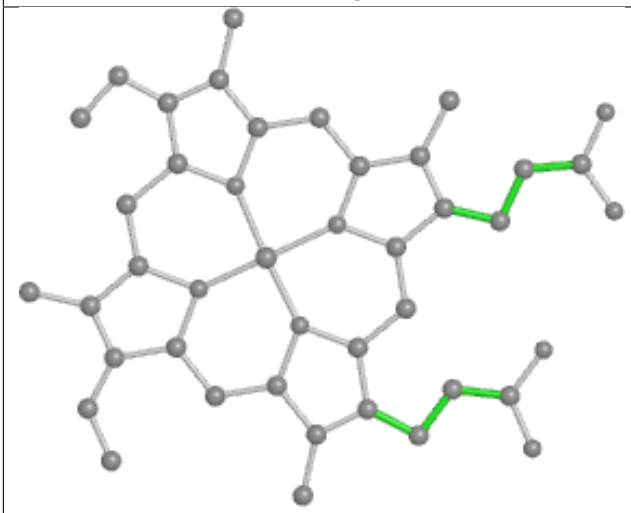
Ligand HEC A 1001



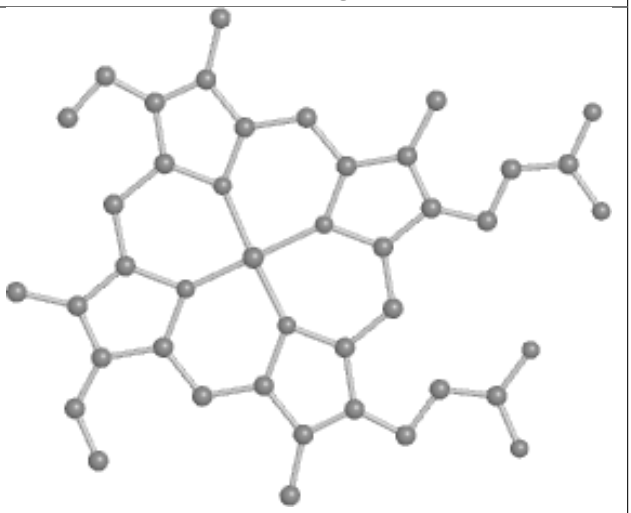
Bond lengths



Bond angles

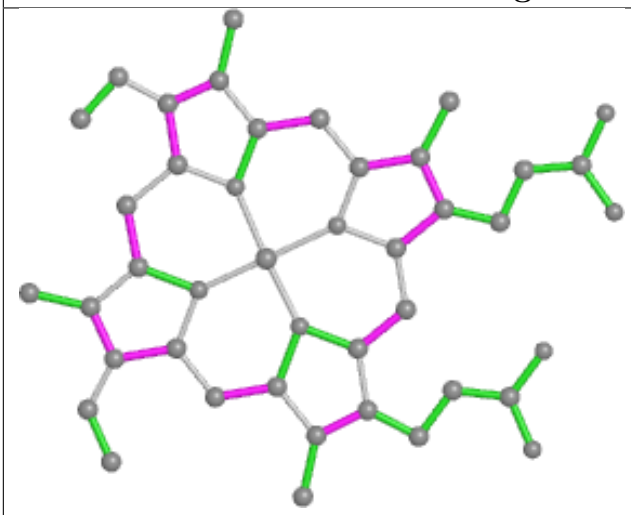


Torsions

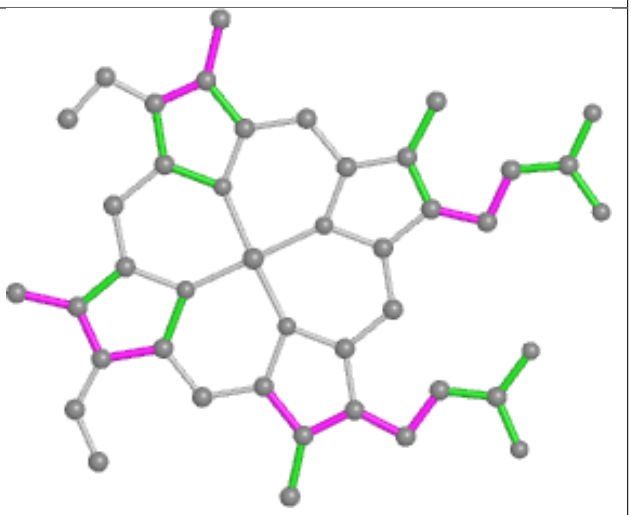


Rings

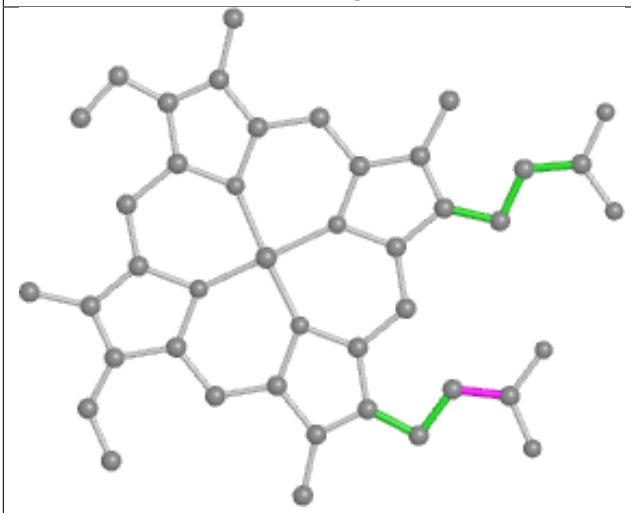
Ligand HEC B 1001



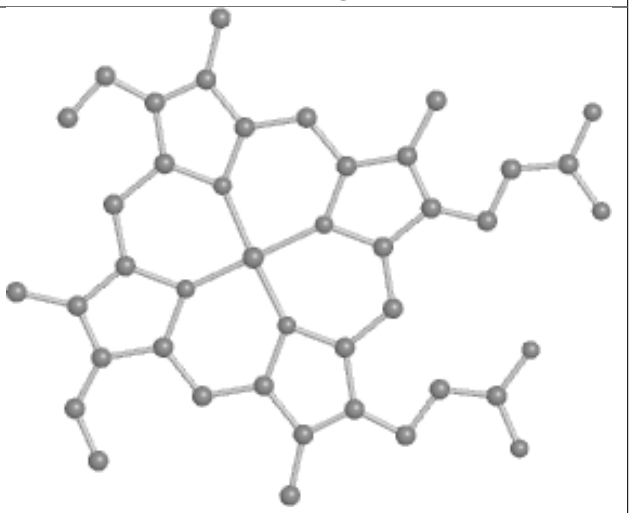
Bond lengths



Bond angles

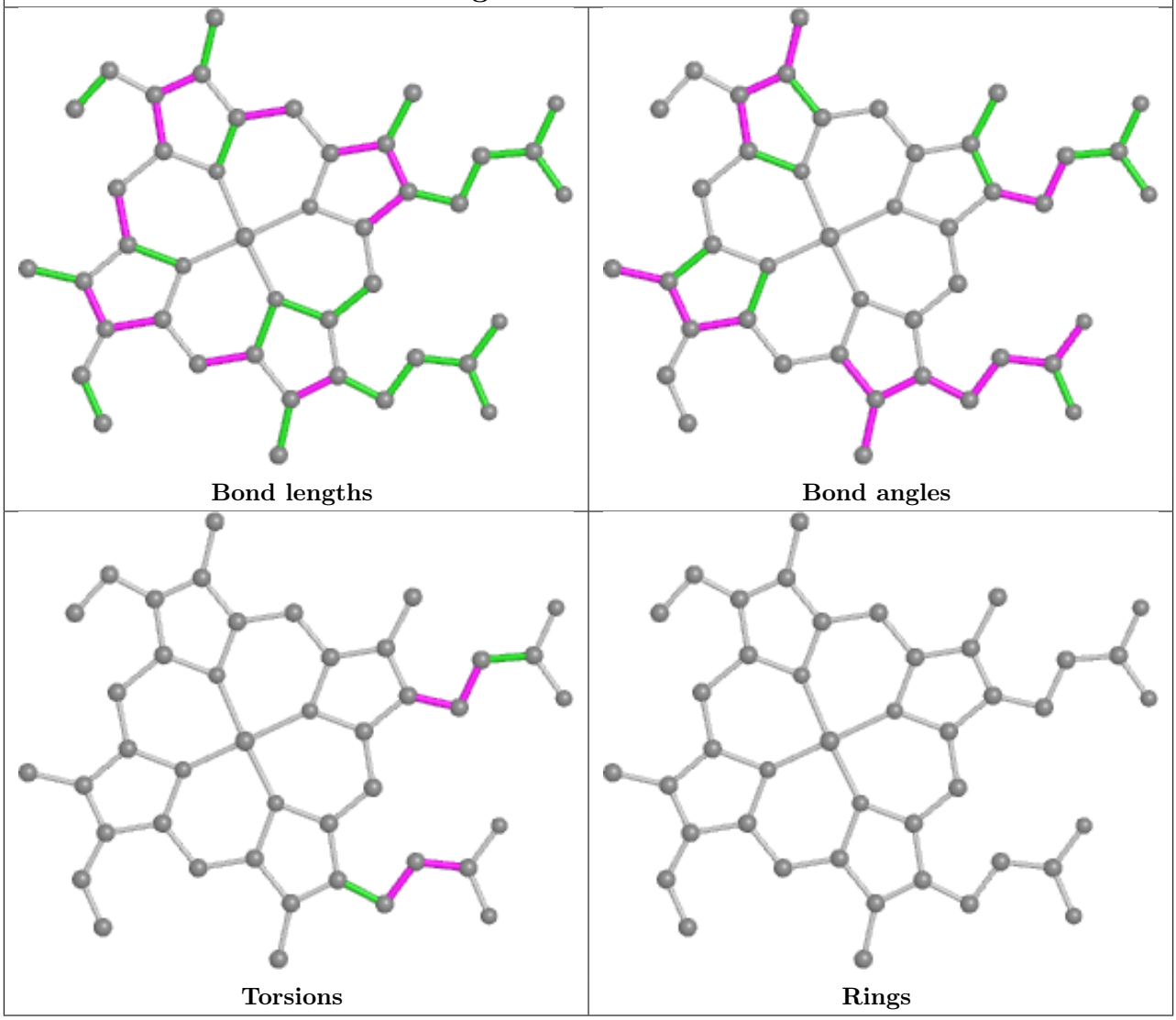


Torsions



Rings

Ligand HEC B 1004



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, 95th 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^2)	Q<0.9
1	A	471/526 (89%)	0.04	1 (0%)	95	97	33, 44, 74, 97	0
1	B	469/526 (89%)	0.19	5 (1%)	80	86	35, 53, 84, 104	0
All	All	940/1052 (89%)	0.11	6 (0%)	89	92	33, 48, 80, 104	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2	PHE	4.1
1	A	240	ALA	3.7
1	B	94	ARG	2.5
1	B	242	SER	2.5
1	B	1	PRO	2.3
1	B	98	ASP	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

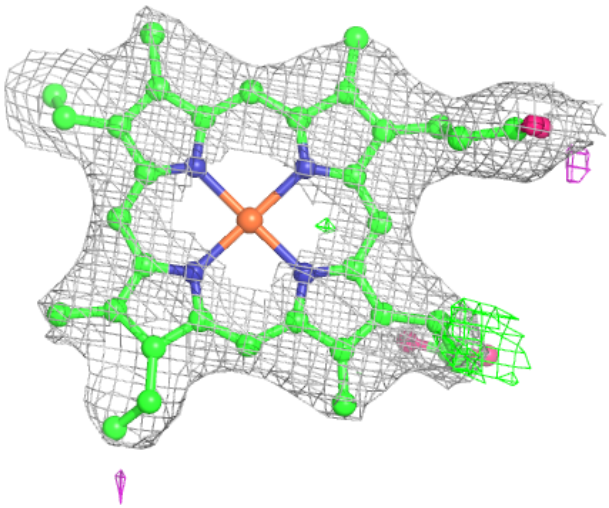
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

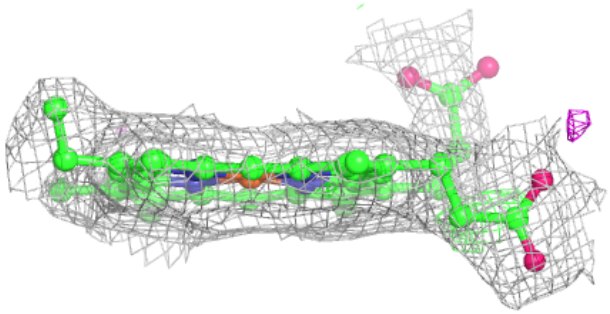
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	EDO	A	1025	4/4	0.75	0.33	52,64,65,65	0
4	PGO	A	1007	5/5	0.78	0.25	54,60,70,74	0
3	CL	B	1009	1/1	0.81	0.12	93,93,93,93	0
6	EDO	A	1017	4/4	0.82	0.32	48,55,64,68	0
3	CL	A	1009	1/1	0.84	0.19	91,91,91,91	0
3	CL	A	1012	1/1	0.84	0.27	93,93,93,93	0
3	CL	A	1006	1/1	0.84	0.36	92,92,92,92	1
7	PGE	A	1026	10/10	0.84	0.29	61,68,80,81	0
6	EDO	B	1012	4/4	0.86	0.27	54,58,65,68	0
6	EDO	A	1024	4/4	0.86	0.17	70,78,78,79	0
6	EDO	A	1018	4/4	0.87	0.20	49,53,58,61	0
4	PGO	B	1011	5/5	0.88	0.37	61,67,68,72	0
3	CL	B	1007	1/1	0.89	0.20	92,92,92,92	0
3	CL	A	1013	1/1	0.90	0.32	99,99,99,99	0
5	THJ	A	1008	5/5	0.91	0.25	58,62,68,106	5
5	THJ	B	1006	5/5	0.91	0.22	52,55,64,112	5
6	EDO	A	1021	4/4	0.91	0.30	32,44,51,56	0
6	EDO	A	1022	4/4	0.91	0.27	51,58,64,66	0
3	CL	B	1008	1/1	0.92	0.13	96,96,96,96	0
6	EDO	A	1019	4/4	0.92	0.36	70,74,84,89	0
6	EDO	A	1015	4/4	0.93	0.20	49,53,54,65	0
3	CL	A	1011	1/1	0.93	0.27	85,85,85,85	0
6	EDO	A	1020	4/4	0.94	0.18	57,64,68,71	0
6	EDO	A	1023	4/4	0.94	0.23	61,66,66,73	0
4	PGO	B	1010	5/5	0.94	0.22	57,59,65,65	0
6	EDO	A	1016	4/4	0.95	0.26	55,55,63,71	0
4	PGO	A	1014	5/5	0.95	0.18	65,75,86,86	5
3	CL	A	1010	1/1	0.95	0.25	83,83,83,83	0
2	HEC	A	1003	43/43	0.98	0.19	28,36,69,93	0
3	CL	B	1005	1/1	0.98	0.17	74,74,74,74	0
2	HEC	B	1001	43/43	0.98	0.20	46,61,73,76	0
2	HEC	B	1002	43/43	0.98	0.16	40,52,59,69	0
2	HEC	B	1003	43/43	0.98	0.19	31,39,56,94	0
2	HEC	B	1004	43/43	0.98	0.17	32,45,52,60	0
2	HEC	A	1004	43/43	0.99	0.20	30,36,44,49	0
2	HEC	A	1002	43/43	0.99	0.18	28,35,43,45	0
3	CL	A	1005	1/1	0.99	0.28	63,63,63,63	0
2	HEC	A	1001	43/43	0.99	0.18	35,43,49,56	0

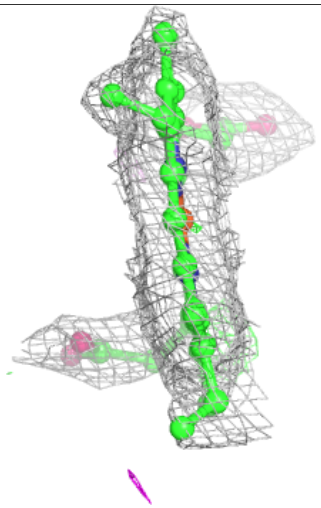
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEC A 1003:

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

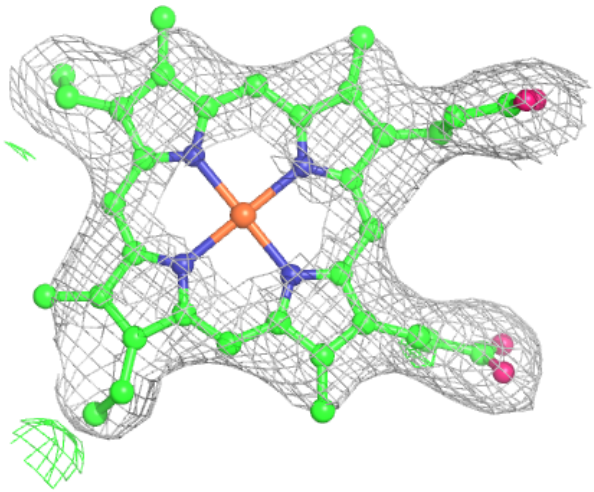


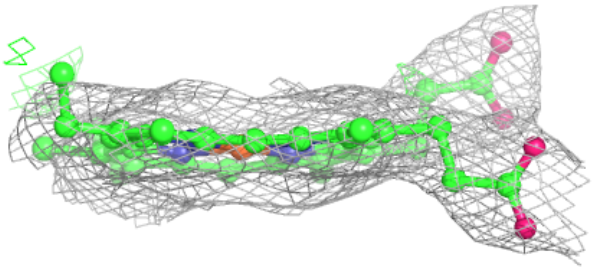


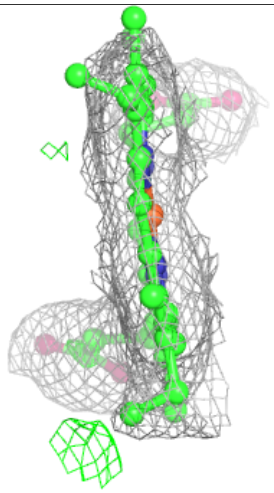


Electron density around HEC B 1001:

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

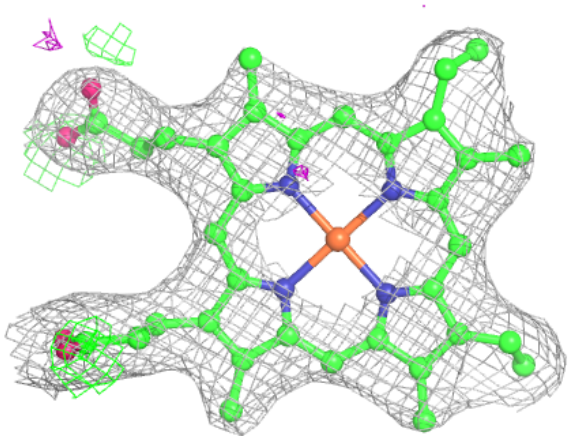


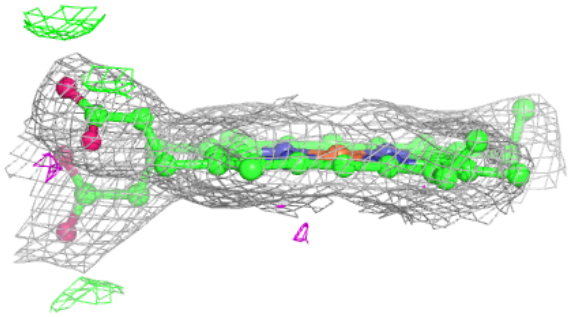


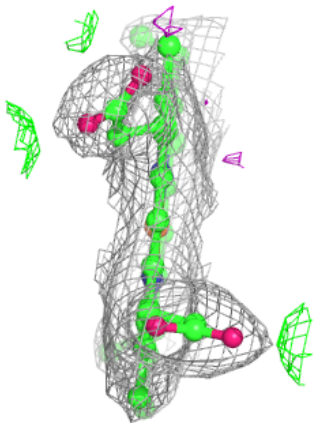


Electron density around HEC B 1002:

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

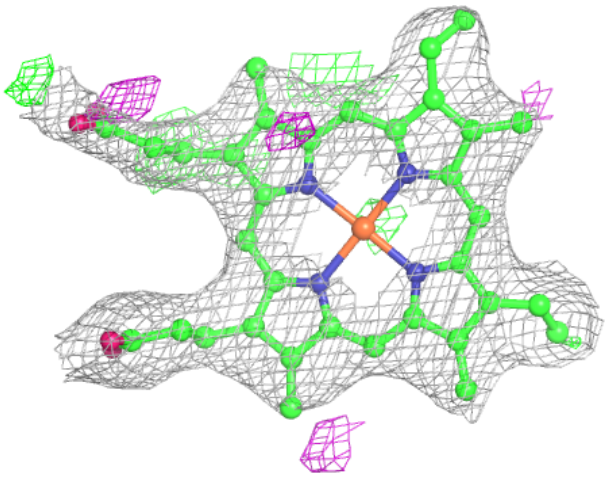


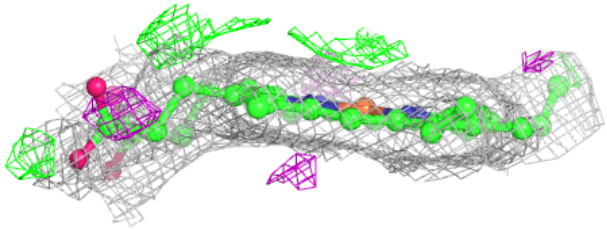


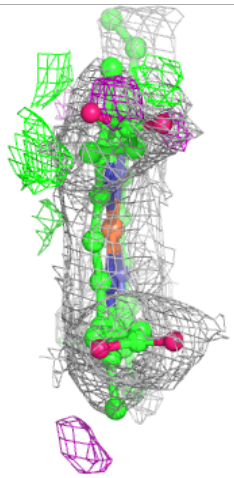


Electron density around HEC B 1003:

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

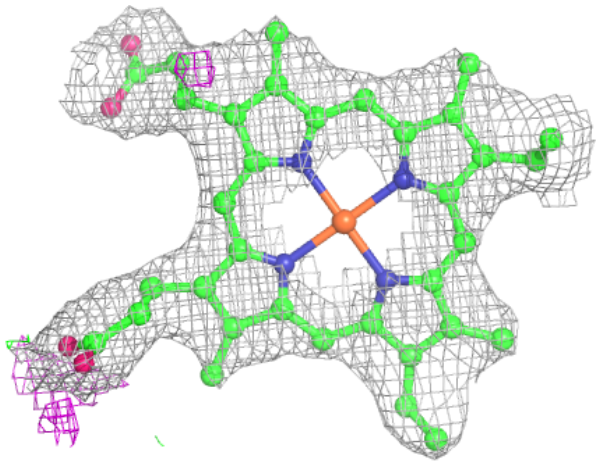


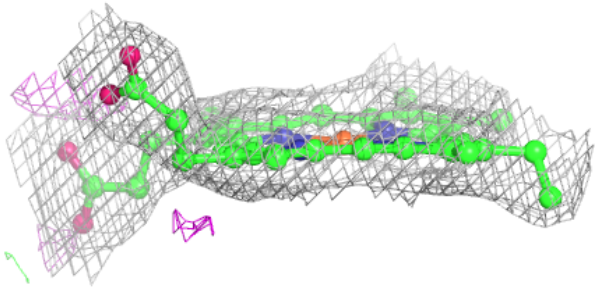


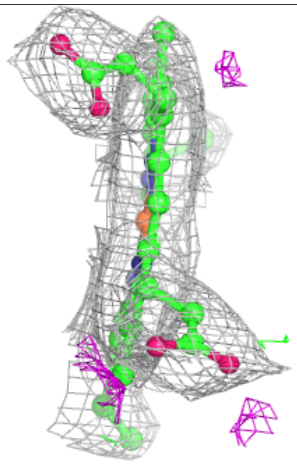


Electron density around HEC B 1004:

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

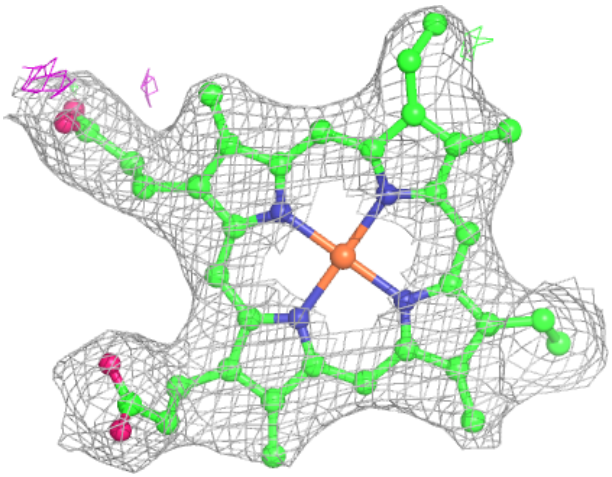


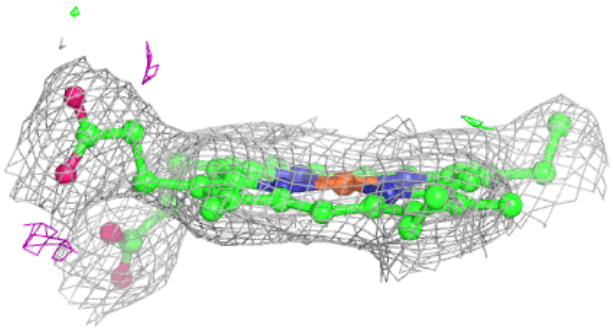


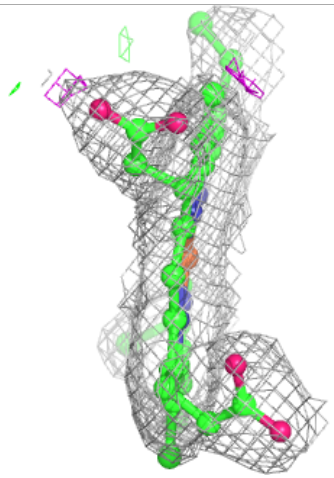


Electron density around HEC A 1004:

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

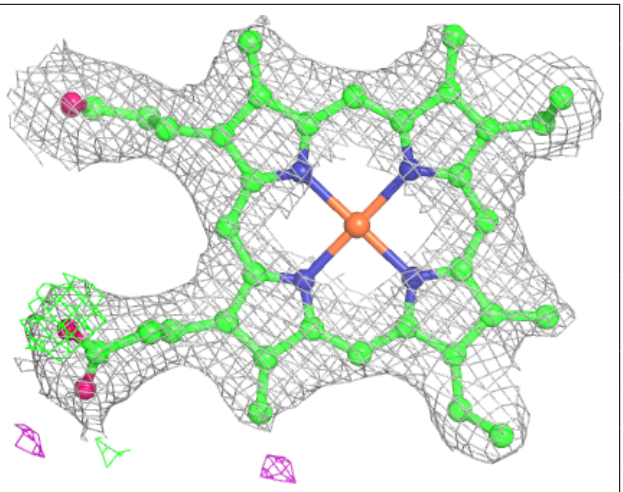


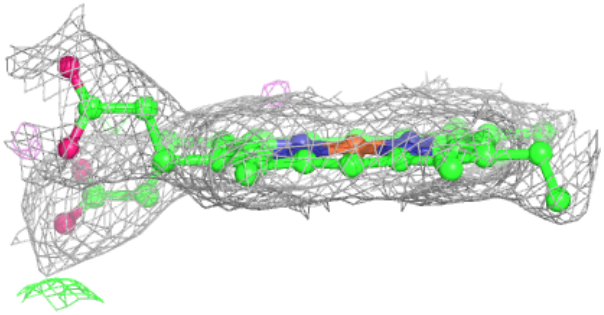


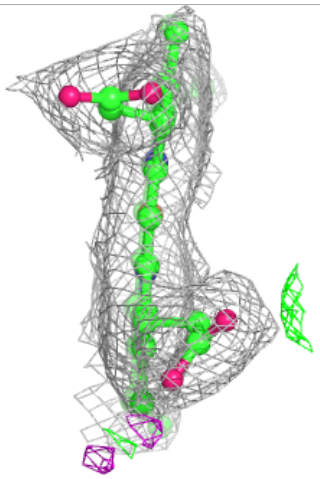


Electron density around HEC A 1002:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

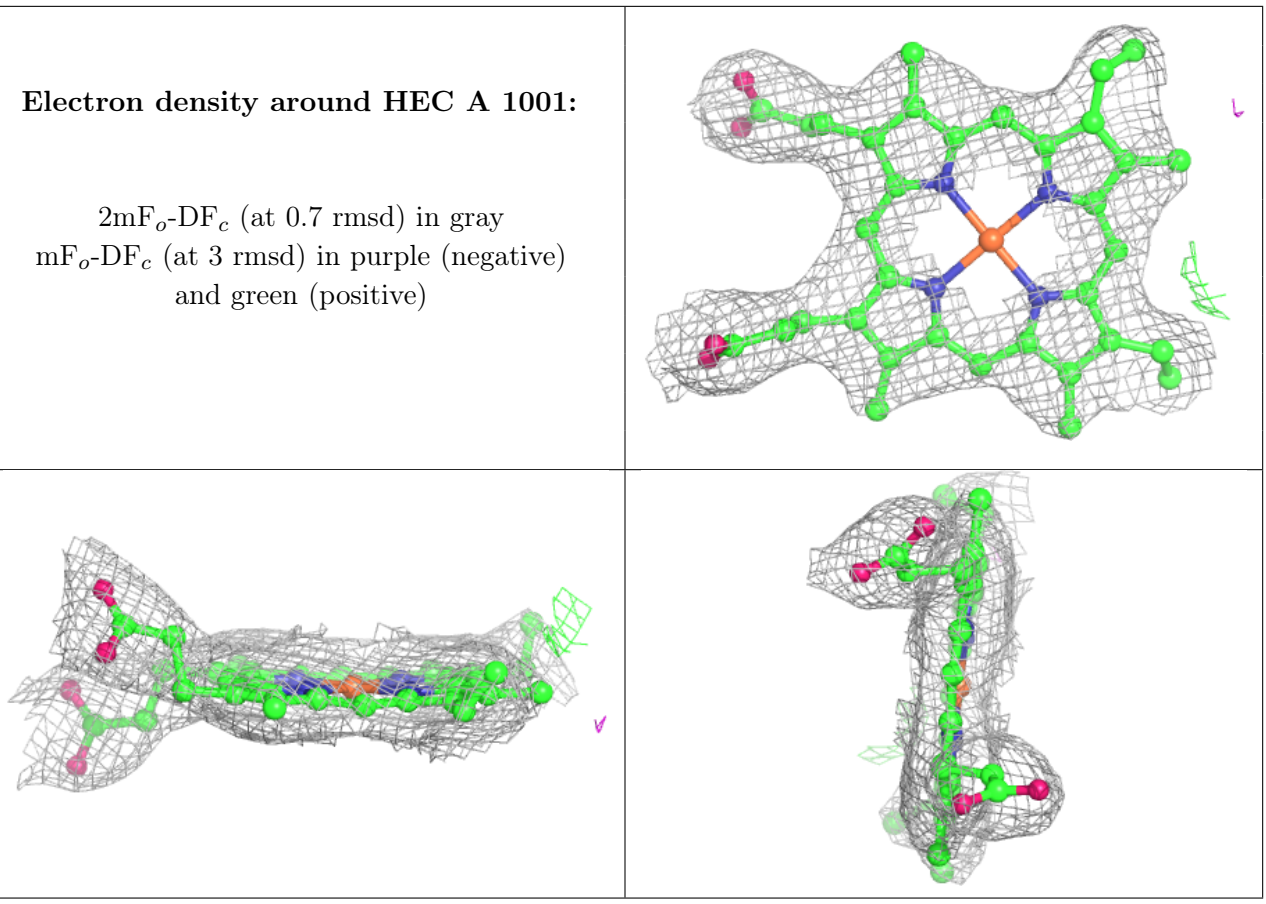






Electron density around HEC A 1001:

$2mF_o$-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.