Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 07:55 PM EDT

PDB ID	:	3PXS
Title	:	Crystal Structure of Diferrous MauG in Complex with Pre-Methylamine Dehydrogenase:
Authors	:	Yukl, E.T.; Goblirsch, B.R.
Deposited on	:	2010-12-10
Resolution	:	2.22 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:

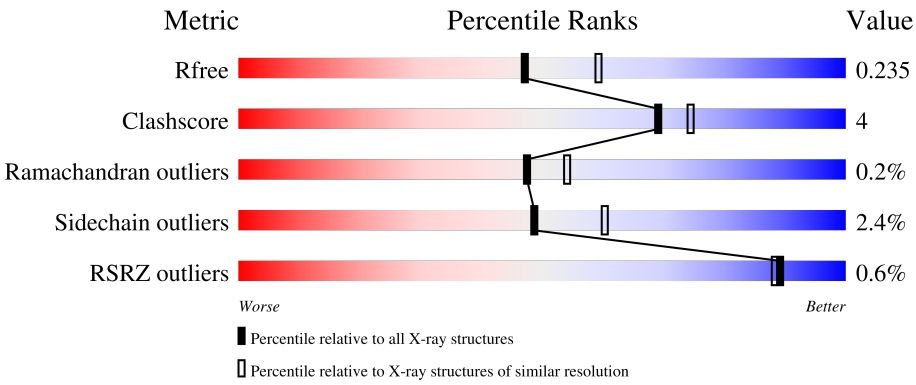
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.22 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	5912 (2.24-2.20)
Clashscore	141614	6646 (2.24-2.20)
Ramachandran outliers	138981	6543 (2.24-2.20)
Sidechain outliers	138945	6544 (2.24-2.20)
RSRZ outliers	127900	5797 (2.24-2.20)

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	373	% 88% 7% 5%
1	B	373	% 86% 9% 5%
2	C	137	% 81% 9% • 9%
2	E	137	76% 14% • 9%
3	D	386	% 87% 11% •

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Mol	Chain	Length	Quality of chain
3	F	386	88% 9% •

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 14569 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 Methylamine utilization protein MauG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	354	2740	1711	491	527	11	0	1	0
1	B	355	2772	1729	499	533	11	0	3	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	368	HIS	-	EXPRESSION TAG	UNP Q51658
A	369	HIS	-	EXPRESSION TAG	UNP Q51658
A	370	HIS	-	EXPRESSION TAG	UNP Q51658
A	371	HIS	-	EXPRESSION TAG	UNP Q51658
A	372	HIS	-	EXPRESSION TAG	UNP Q51658
A	373	HIS	-	EXPRESSION TAG	UNP Q51658
B	368	HIS	-	EXPRESSION TAG	UNP Q51658
B	369	HIS	-	EXPRESSION TAG	UNP Q51658
B	370	HIS	-	EXPRESSION TAG	UNP Q51658
B	371	HIS	-	EXPRESSION TAG	UNP Q51658
B	372	HIS	-	EXPRESSION TAG	UNP Q51658
B	373	HIS	-	EXPRESSION TAG	UNP Q51658

- Molecule 2 is a protein called Methylamine dehydrogenase light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	125	957	592	161	190	14	0	1	0
2	E	125	954	590	161	190	13	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	132	HIS	-	EXPRESSION TAG	UNP P22619
C	133	HIS	-	EXPRESSION TAG	UNP P22619
C	134	HIS	-	EXPRESSION TAG	UNP P22619
C	135	HIS	-	EXPRESSION TAG	UNP P22619
C	136	HIS	-	EXPRESSION TAG	UNP P22619
C	137	HIS	-	EXPRESSION TAG	UNP P22619
E	132	HIS	-	EXPRESSION TAG	UNP P22619
E	133	HIS	-	EXPRESSION TAG	UNP P22619
E	134	HIS	-	EXPRESSION TAG	UNP P22619
E	135	HIS	-	EXPRESSION TAG	UNP P22619
E	136	HIS	-	EXPRESSION TAG	UNP P22619
E	137	HIS	-	EXPRESSION TAG	UNP P22619

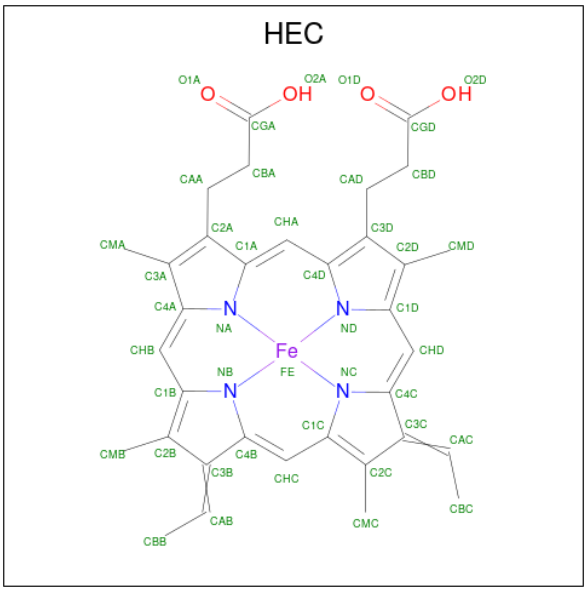
- Molecule 3 is a protein called Methylamine dehydrogenase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	376	2951	1868	508	567	8	0	3	0
			Total	C	N	O	S			
3	F	376	2923	1853	502	560	8	0	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	A	2	2	2	0	0
			Total	Na		
4	B	2	2	2	0	0

- Molecule 5 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).

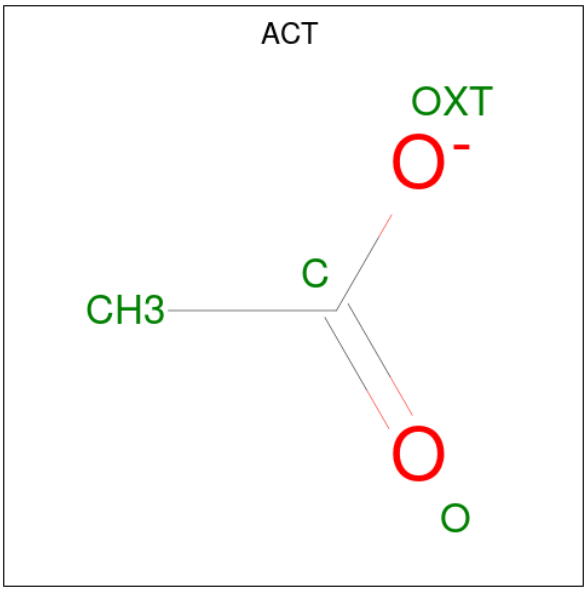


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
5	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	A	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	B	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
5	B	1	43	34	1	4	4	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

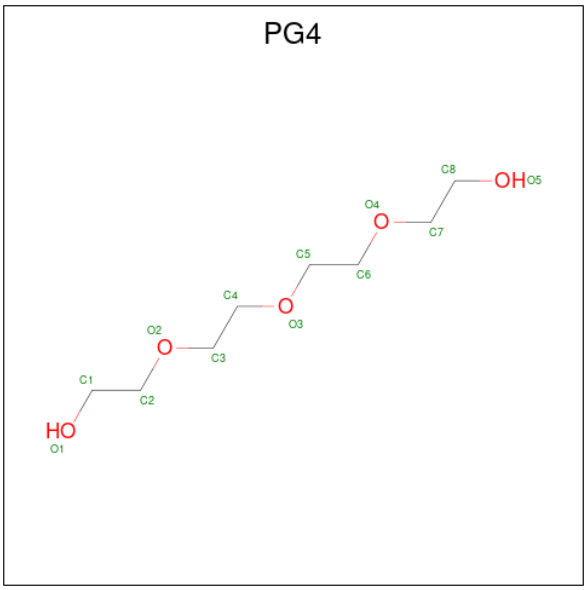
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
6	A	1	1	1	0	0
			Total	Ca		
6	B	1	1	1	0	0

- Molecule 7 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



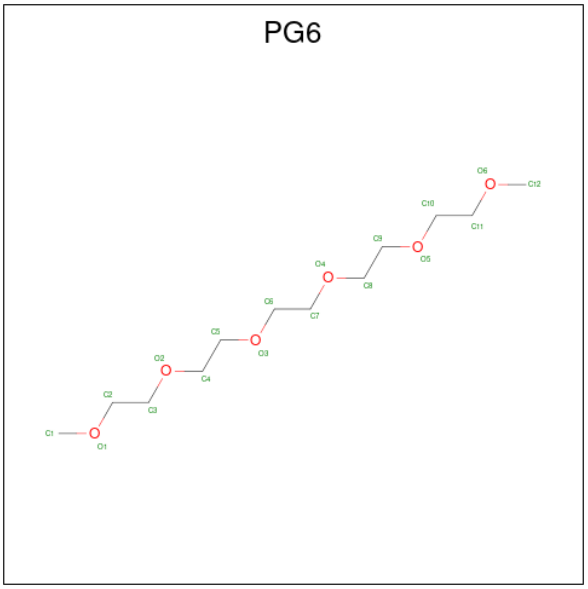
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			4	2	2		
7	D	1	Total	C	O	0	0
			4	2	2		
7	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 8 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	C	O	0	0
			13	8	5		

- Molecule 9 is 1-(2-METHOXY-ETHOXY)-2-{2-[2-(2-METHOXY-ETHOXY]-ETHOXY}-ETHANE (three-letter code: PG6) (formula: $C_{12}H_{26}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
9	F	1	18	12	6	0	0

- Molecule 10 is water.

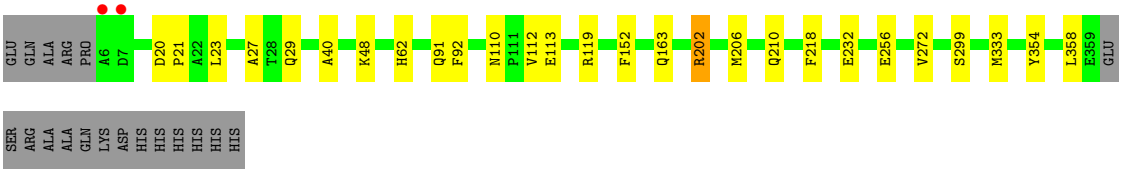
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	202	202	202	0	0
			Total	O		
10	B	221	221	221	0	0
			Total	O		
10	C	66	66	66	0	0
			Total	O		
10	D	214	214	214	0	0
			Total	O		
10	E	75	75	75	0	0
			Total	O		
10	F	273	273	273	0	0

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.

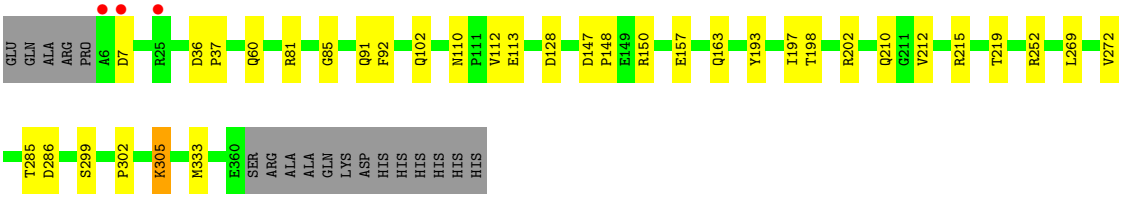
• Molecule 1: Methylamine utilization protein MauG

Chain A:



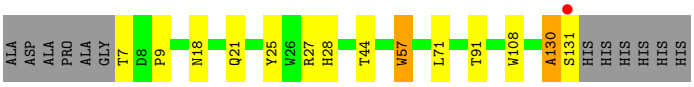
• Molecule 1: Methylamine utilization protein MauG

Chain B:



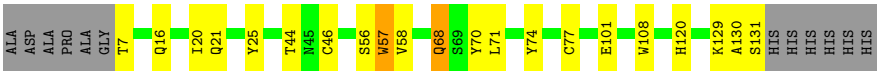
• Molecule 2: Methylamine dehydrogenase light chain

Chain C:



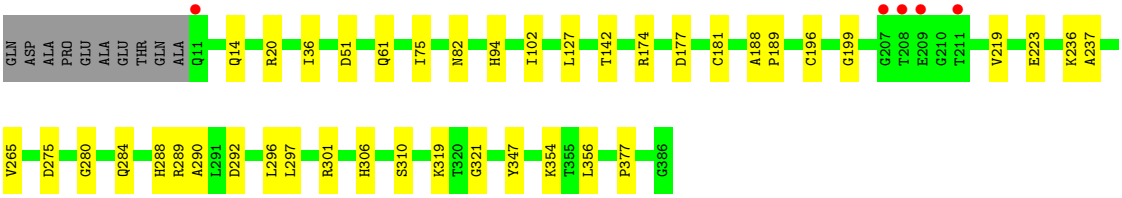
• Molecule 2: Methylamine dehydrogenase light chain

Chain E:



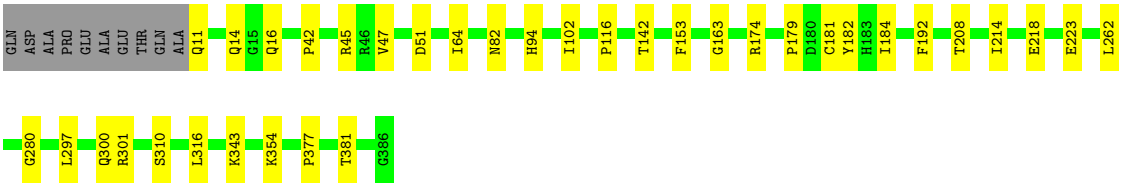
• Molecule 3: Methylamine dehydrogenase heavy chain

Chain D:



• Molecule 3: Methylamine dehydrogenase heavy chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.53Å 83.52Å 107.78Å 109.94° 91.54° 105.78°	Depositor
Resolution (Å)	44.49 – 2.22 44.49 – 2.22	Depositor EDS
% Data completeness (in resolution range)	96.5 (44.49-2.22) 96.5 (44.49-2.22)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.22Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.177 , 0.229 0.180 , 0.235	Depositor DCC
R_{free} test set	4161 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	25.1	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 31.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14569	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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: CA, NA, ACT, HEC, PG4, PG6, 0AF

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	0.40	0/2807	0.54	0/3809
1	B	0.41	0/2836	0.53	0/3846
2	C	0.40	0/969	0.57	0/1323
2	E	0.42	0/963	0.56	0/1315
3	D	0.40	0/3028	0.53	0/4125
3	F	0.43	0/3000	0.55	0/4088
All	All	0.41	0/13603	0.54	0/18506

There are no bond length outliers.

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	2740	0	2616	17	0
1	B	2772	0	2645	25	0
2	C	957	0	864	14	0
2	E	954	0	859	15	0
3	D	2951	0	2828	22	0
3	F	2923	0	2808	14	0
4	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	2	0	0	0	0
5	A	86	0	60	4	0
5	B	86	0	60	3	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	C	4	0	3	0	0
7	D	4	0	3	0	0
7	F	4	0	3	0	0
8	F	13	0	18	0	0
9	F	18	0	26	0	0
10	A	202	0	0	1	0
10	B	221	0	0	2	0
10	C	66	0	0	0	0
10	D	214	0	0	1	0
10	E	75	0	0	1	0
10	F	273	0	0	0	0
All	All	14569	0	12793	97	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 4.

All (97) 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)
2:C:57:0AF:HE3	2:C:108:TRP:CD1	1.78	1.19
1:B:215[B]:ARG:HG2	1:B:215[B]:ARG:HH11	0.93	1.07
2:C:57:0AF:CE3	2:C:108:TRP:CD1	2.39	1.05
1:B:215[B]:ARG:HH11	1:B:215[B]:ARG:CG	1.76	0.99
1:B:215[B]:ARG:HG2	1:B:215[B]:ARG:NH1	1.75	0.95
1:B:299:SER:HB2	1:B:333:MET:HG3	1.50	0.93
2:E:57:0AF:HE3	2:E:108:TRP:CD1	2.05	0.91
2:E:57:0AF:CE3	2:E:108:TRP:CD1	2.57	0.88
2:C:57:0AF:CE3	2:C:108:TRP:HD1	1.81	0.88
1:A:299:SER:HB2	1:A:333:MET:HG3	1.61	0.80
3:D:265:VAL:HG21	3:D:321:GLY:HA3	1.64	0.78
2:E:57:0AF:CE3	2:E:108:TRP:HD1	2.01	0.72
3:D:237:ALA:HB2	3:D:289:ARG:HG3	1.72	0.72
2:C:21:GLN:HE22	3:F:14:GLN:HE21	1.35	0.71
3:D:14:GLN:HE21	2:E:21:GLN:HE22	1.39	0.70
1:B:302:PRO:HA	1:B:305[A]:LYS:HE2	1.75	0.68
1:B:212:VAL:HG11	2:E:129:LYS:HE2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:265:VAL:CG2	3:D:321:GLY:HA3	2.27	0.64
3:D:265:VAL:HG21	3:D:321:GLY:CA	2.29	0.63
2:C:57:0AF:CZ3	2:C:108:TRP:HD1	2.14	0.60
2:E:130:ALA:O	2:E:131:SER:HB2	2.02	0.59
3:F:179:PRO:HD3	3:F:214:ILE:HD13	1.85	0.58
1:A:163:GLN:HE22	5:A:500:HEC:HMA1	1.69	0.57
1:A:91:GLN:O	1:A:92:PHE:HB2	2.05	0.56
1:A:40:ALA:HA	1:A:354:TYR:CZ	2.41	0.56
1:B:198:THR:HG22	2:E:58:VAL:HG13	1.87	0.54
1:B:128:ASP:HB3	10:B:606:HOH:O	2.07	0.53
3:F:51:ASP:HA	3:F:377:PRO:HA	1.91	0.53
1:B:193:TYR:O	1:B:197:ILE:HG12	2.08	0.53
1:B:285:THR:HG22	1:B:286:ASP:OD1	2.08	0.53
1:B:91:GLN:O	1:B:92:PHE:HB2	2.08	0.52
1:B:113:GLU:HG2	5:B:500:HEC:HBC2	1.91	0.52
2:E:101:GLU:HA	10:E:948:HOH:O	2.10	0.51
1:A:210:GLN:HE22	2:C:44:THR:HG21	1.76	0.51
1:B:215[B]:ARG:CG	1:B:215[B]:ARG:NH1	2.46	0.51
1:B:210:GLN:HE22	2:E:44:THR:HG21	1.75	0.51
3:D:284:GLN:O	3:D:296:LEU:HD12	2.11	0.51
1:A:29:GLN:HE22	5:A:500:HEC:HBC3	1.77	0.50
3:D:280:GLY:HA3	3:D:301:ARG:CZ	2.42	0.49
1:B:163:GLN:HE22	5:B:500:HEC:HMA1	1.78	0.49
2:E:68:GLN:HB2	2:E:70:TYR:CE1	2.48	0.48
1:A:272:VAL:HG21	5:A:600:HEC:HMA3	1.96	0.48
1:A:48:LYS:H	1:A:62:HIS:CE1	2.32	0.47
2:C:91:THR:HB	3:D:306:HIS:CE1	2.49	0.47
1:A:110:ASN:HB3	1:A:113:GLU:HB2	1.96	0.47
3:D:297:LEU:HD22	3:D:310:SER:HB2	1.97	0.46
3:F:297:LEU:HD22	3:F:310:SER:HB2	1.98	0.46
1:A:202:ARG:NE	10:A:946:HOH:O	2.48	0.45
1:A:202:ARG:HB2	1:A:206:MET:HG3	1.98	0.45
1:A:48:LYS:H	1:A:62:HIS:HE1	1.63	0.45
3:F:280:GLY:HA3	3:F:301:ARG:CZ	2.46	0.45
1:B:272:VAL:HG21	5:B:600:HEC:HMA3	1.98	0.45
1:A:113:GLU:HG2	5:A:500:HEC:HBC2	1.98	0.45
3:F:184:ILE:HG23	3:F:192:PHE:CD2	2.52	0.45
3:D:188:ALA:HB1	3:D:189:PRO:HD2	1.97	0.45
3:F:42:PRO:HG3	3:F:116:PRO:HB2	1.98	0.45
1:A:21:PRO:O	1:A:27:ALA:HA	2.18	0.44
2:E:20:ILE:HG22	2:E:25:TYR:CZ	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:236:LYS:HD3	3:D:289:ARG:NH1	2.32	0.44
1:A:206:MET:CE	1:A:218:PHE:CD2	3.01	0.44
3:D:288:HIS:HE1	3:D:290:ALA:HB3	1.81	0.44
3:F:153:PHE:CE1	3:F:163:GLY:HA3	2.53	0.44
3:F:181:CYS:C	3:F:182:TYR:CD1	2.92	0.44
1:A:119:ARG:HG2	1:A:152:PHE:CG	2.53	0.43
1:B:197:ILE:O	1:B:202:ARG:HD2	2.17	0.43
3:D:292:ASP:OD2	3:D:319:LYS:HE2	2.18	0.43
3:F:47:VAL:HG13	3:F:64:ILE:HB	2.00	0.43
2:C:18:ASN:O	3:F:16:GLN:HA	2.18	0.43
2:C:57:0AF:HBC1	2:C:108:TRP:NE1	2.33	0.43
3:F:82:ASN:HB3	3:F:142:THR:HB	2.00	0.43
3:D:82:ASN:HB3	3:D:142:THR:HB	2.01	0.43
3:D:199:GLY:HA3	3:D:219:VAL:HG13	2.00	0.43
3:D:188:ALA:HB1	3:D:189:PRO:CD	2.49	0.42
1:B:36:ASP:HA	1:B:37:PRO:HD2	1.84	0.42
3:D:347:TYR:HB3	3:D:356:LEU:HD11	2.01	0.42
2:C:7:THR:O	2:C:9:PRO:HD3	2.19	0.42
2:C:25:TYR:HB3	2:C:28:HIS:CD2	2.55	0.42
2:C:130:ALA:O	2:C:131:SER:CB	2.67	0.42
1:B:252:ARG:HD3	10:B:1001:HOH:O	2.18	0.42
1:A:20:ASP:HB3	1:A:23:LEU:HD13	2.01	0.42
3:F:45:ARG:NH2	3:F:343:LYS:O	2.53	0.42
3:F:174:ARG:HD2	3:F:208:THR:O	2.20	0.42
2:E:77:CYS:O	2:E:120:HIS:HB3	2.20	0.42
3:D:51:ASP:HA	3:D:377:PRO:HA	2.01	0.41
2:E:56:SER:HB2	2:E:74:TYR:O	2.20	0.41
1:B:147:ASP:HA	1:B:148:PRO:HD2	1.94	0.41
1:B:305[A]:LYS:H	1:B:305[A]:LYS:HG3	1.68	0.41
2:C:25:TYR:CE2	2:C:27:ARG:HG3	2.56	0.41
3:D:61:GLN:HB3	3:D:75:ILE:HB	2.03	0.41
1:B:81:ARG:HH11	1:B:85:GLY:HA2	1.85	0.41
3:D:20[B]:ARG:HG3	10:D:523:HOH:O	2.20	0.41
1:B:147:ASP:HB3	1:B:150:ARG:HB2	2.02	0.41
1:B:110:ASN:OD1	1:B:112:VAL:HG22	2.21	0.41
3:D:36:ILE:HD13	2:E:46:CYS:HB2	2.03	0.41
1:B:198:THR:CG2	2:E:58:VAL:HG13	2.51	0.40
2:C:130:ALA:O	2:C:131:SER:HB3	2.21	0.40
3:D:181:CYS:HA	3:D:196:CYS:HA	2.02	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	353/373 (95%)	343 (97%)	10 (3%)	0	100	100
1	B	356/373 (95%)	347 (98%)	9 (2%)	0	100	100
2	C	123/137 (90%)	121 (98%)	1 (1%)	1 (1%)	19	18
2	E	122/137 (89%)	119 (98%)	3 (2%)	0	100	100
3	D	377/386 (98%)	366 (97%)	10 (3%)	1 (0%)	41	45
3	F	374/386 (97%)	365 (98%)	8 (2%)	1 (0%)	41	45
All	All	1705/1792 (95%)	1661 (97%)	41 (2%)	3 (0%)	47	54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	130	ALA
3	D	102	ILE
3	F	102	ILE

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	277/292 (95%)	272 (98%)	5 (2%)	59	71
1	B	280/292 (96%)	271 (97%)	9 (3%)	39	49
2	C	105/112 (94%)	104 (99%)	1 (1%)	76	85
2	E	104/112 (93%)	100 (96%)	4 (4%)	33	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	307/311 (99%)	299 (97%)	8 (3%)	46	57
3	F	304/311 (98%)	295 (97%)	9 (3%)	41	51
All	All	1377/1430 (96%)	1341 (97%)	36 (3%)	49	57

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	VAL
1	A	202	ARG
1	A	232	GLU
1	A	256	GLU
1	A	358	LEU
1	B	7	ASP
1	B	60[A]	GLN
1	B	60[B]	GLN
1	B	102	GLN
1	B	157	GLU
1	B	219	THR
1	B	269	LEU
1	B	305[A]	LYS
1	B	305[B]	LYS
2	C	71	LEU
3	D	94	HIS
3	D	127	LEU
3	D	174	ARG
3	D	177[A]	ASP
3	D	177[B]	ASP
3	D	223	GLU
3	D	275	ASP
3	D	354	LYS
2	E	7	THR
2	E	16	GLN
2	E	68	GLN
2	E	71	LEU
3	F	11	GLN
3	F	94	HIS
3	F	218	GLU
3	F	223	GLU
3	F	262	LEU
3	F	300	GLN
3	F	316	LEU

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Mol	Chain	Res	Type
3	F	354	LYS
3	F	381	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	29	GLN
1	A	62	HIS
1	A	91	GLN
1	A	163	GLN
1	A	210	GLN
1	B	29	GLN
1	B	91	GLN
1	B	163	GLN
1	B	210	GLN
3	D	14	GLN
3	F	14	GLN
3	F	30	GLN
3	F	300	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	0AF	E	57	2	13,16,17	2.01	4 (30%)	9,22,24	1.66	2 (22%)
2	0AF	C	57	2	13,16,17	1.75	4 (30%)	9,22,24	1.19	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	0AF	E	57	2	-	1/4/6/8	0/2/2/2
2	0AF	C	57	2	-	0/4/6/8	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57	0AF	CZ2-CE2	-4.96	1.35	1.42
2	C	57	0AF	CZ2-CE2	-4.35	1.36	1.42
2	E	57	0AF	CD1-NE1	-2.81	1.30	1.36
2	E	57	0AF	CE3-CD2	-2.70	1.36	1.42
2	C	57	0AF	CE3-CD2	-2.64	1.37	1.42
2	E	57	0AF	CE2-NE1	-2.33	1.31	1.39
2	C	57	0AF	CE2-NE1	-2.32	1.31	1.39
2	C	57	0AF	CD1-NE1	-2.24	1.32	1.36

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	57	0AF	CH2-CZ2-CE2	3.06	123.53	120.11
2	E	57	0AF	CZ3-CH2-CZ2	-2.96	116.77	120.37
2	C	57	0AF	CE3-CD2-CG	-2.92	129.06	134.42

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	57	0AF	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	57	0AF	3	0
2	C	57	0AF	5	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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	HEC	A	500	1	32,50,50	1.64	8 (25%)	30,82,82	2.55	9 (30%)
5	HEC	B	600	1	32,50,50	1.58	8 (25%)	30,82,82	2.89	10 (33%)
7	ACT	D	387	-	3,3,3	0.84	0	3,3,3	1.42	0
7	ACT	C	138	-	3,3,3	0.83	0	3,3,3	1.21	0
7	ACT	F	389	-	3,3,3	0.81	0	3,3,3	1.34	0
5	HEC	B	500	1	32,50,50	1.58	8 (25%)	30,82,82	2.58	11 (36%)
8	PG4	F	387	-	12,12,12	0.51	0	11,11,11	0.23	0
9	PG6	F	388	-	17,17,17	0.56	0	16,16,16	0.25	0
5	HEC	A	600	1	32,50,50	1.62	8 (25%)	30,82,82	2.89	11 (36%)

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
5	HEC	A	500	1	-	4/10/54/54	-
5	HEC	B	600	1	-	2/10/54/54	-
5	HEC	B	500	1	-	1/10/54/54	-
8	PG4	F	387	-	-	6/10/10/10	-
9	PG6	F	388	-	-	9/15/15/15	-
5	HEC	A	600	1	-	2/10/54/54	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	500	HEC	C3C-C4C	3.74	1.49	1.43
5	A	600	HEC	C4B-C3B	3.44	1.49	1.43
5	B	500	HEC	C4B-C3B	3.33	1.49	1.43
5	A	600	HEC	C2A-C1A	3.32	1.49	1.42
5	A	500	HEC	C4B-C3B	3.30	1.49	1.43
5	B	500	HEC	C3C-C4C	3.29	1.49	1.43
5	B	600	HEC	C3C-C4C	3.28	1.49	1.43
5	B	600	HEC	C4B-C3B	3.19	1.48	1.43
5	A	500	HEC	C2A-C1A	3.05	1.49	1.42
5	A	500	HEC	C3A-C4A	3.03	1.49	1.42
5	B	600	HEC	C3A-C4A	2.99	1.49	1.42
5	A	600	HEC	C3C-C4C	2.97	1.48	1.43
5	A	600	HEC	C4D-CHA	2.93	1.49	1.41
5	B	500	HEC	C3A-C4A	2.92	1.49	1.42
5	A	500	HEC	C1D-CHD	2.89	1.49	1.41
5	B	500	HEC	C2A-C1A	2.87	1.48	1.42
5	B	600	HEC	C2A-C1A	2.81	1.48	1.42
5	A	600	HEC	C1C-CHC	2.69	1.48	1.41
5	B	600	HEC	C4D-CHA	2.65	1.48	1.41
5	B	500	HEC	C1B-CHB	2.64	1.48	1.41
5	A	500	HEC	C4D-CHA	2.62	1.48	1.41
5	B	500	HEC	C1C-CHC	2.62	1.48	1.41
5	A	600	HEC	C3A-C4A	2.61	1.48	1.42
5	B	500	HEC	C1D-CHD	2.58	1.48	1.41
5	B	600	HEC	C1C-CHC	2.56	1.48	1.41
5	A	500	HEC	C1C-CHC	2.54	1.48	1.41
5	B	500	HEC	C4D-CHA	2.52	1.48	1.41
5	A	500	HEC	C1B-CHB	2.52	1.48	1.41
5	A	600	HEC	C1B-CHB	2.38	1.47	1.41
5	B	600	HEC	C1B-CHB	2.37	1.47	1.41
5	A	600	HEC	C1D-CHD	2.37	1.47	1.41
5	B	600	HEC	C1D-CHD	2.29	1.47	1.41

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	600	HEC	CBB-CAB-C3B	-8.21	108.27	127.49
5	A	500	HEC	CBB-CAB-C3B	-7.76	109.33	127.49
5	B	600	HEC	CBC-CAC-C3C	-7.48	109.99	127.49
5	A	600	HEC	CBC-CAC-C3C	-7.29	110.43	127.49
5	A	600	HEC	CBB-CAB-C3B	-7.14	110.79	127.49
5	B	500	HEC	CBB-CAB-C3B	-7.08	110.91	127.49
5	B	500	HEC	CBC-CAC-C3C	-6.38	112.56	127.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	500	HEC	CBC-CAC-C3C	-5.99	113.47	127.49
5	B	600	HEC	CBD-CAD-C3D	-5.63	103.08	112.54
5	A	600	HEC	CBD-CAD-C3D	-5.48	103.32	112.54
5	A	600	HEC	C1D-C2D-C3D	-5.39	103.25	107.00
5	B	600	HEC	C1D-C2D-C3D	-5.30	103.31	107.00
5	A	500	HEC	C1D-C2D-C3D	-4.71	103.72	107.00
5	B	500	HEC	C1D-C2D-C3D	-3.93	104.26	107.00
5	B	500	HEC	CBA-CAA-C2A	-3.86	106.19	112.55
5	A	600	HEC	CBA-CAA-C2A	-3.82	106.26	112.55
5	A	600	HEC	CMB-C2B-C3B	3.57	130.02	125.82
5	B	500	HEC	CMB-C2B-C3B	3.52	129.96	125.82
5	A	600	HEC	CMC-C2C-C3C	3.35	129.76	125.82
5	A	500	HEC	CMC-C2C-C3C	3.28	129.68	125.82
5	B	600	HEC	CBA-CAA-C2A	-2.93	107.73	112.55
5	B	600	HEC	CMB-C2B-C3B	2.92	129.25	125.82
5	B	600	HEC	CMC-C2C-C3C	2.82	129.14	125.82
5	B	500	HEC	O2D-CGD-CBD	2.68	122.47	114.00
5	B	600	HEC	C4C-C3C-C2C	-2.65	103.49	106.35
5	B	500	HEC	C4C-C3C-C2C	-2.65	103.49	106.35
5	A	500	HEC	C4C-C3C-C2C	-2.63	103.52	106.35
5	A	600	HEC	CMD-C2D-C3D	2.63	129.90	124.94
5	A	600	HEC	C4C-C3C-C2C	-2.59	103.55	106.35
5	B	500	HEC	CBD-CAD-C3D	-2.52	108.30	112.54
5	A	500	HEC	C2B-C3B-C4B	-2.48	103.68	106.35
5	A	500	HEC	CMB-C2B-C3B	2.47	128.73	125.82
5	B	500	HEC	CMC-C2C-C3C	2.45	128.70	125.82
5	A	500	HEC	CBD-CAD-C3D	-2.44	108.44	112.54
5	A	600	HEC	C2B-C3B-C4B	-2.37	103.79	106.35
5	A	600	HEC	CMA-C3A-C2A	2.31	129.30	124.94
5	B	600	HEC	CMA-C3A-C2A	2.30	129.27	124.94
5	B	500	HEC	O1D-CGD-CBD	-2.28	115.86	123.09
5	B	600	HEC	CMD-C2D-C3D	2.10	128.91	124.94
5	B	500	HEC	CMA-C3A-C2A	2.04	128.79	124.94
5	A	500	HEC	C3B-C4B-NB	2.02	114.75	110.94

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	387	PG4	O2-C3-C4-O3
9	F	388	PG6	O3-C6-C7-O4
9	F	388	PG6	O4-C8-C9-O5

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Mol	Chain	Res	Type	Atoms
9	F	388	PG6	C10-C11-O6-C12
8	F	387	PG4	C5-C6-O4-C7
9	F	388	PG6	C8-C9-O5-C10
9	F	388	PG6	C2-C3-O2-C4
8	F	387	PG4	O3-C5-C6-O4
8	F	387	PG4	C3-C4-O3-C5
9	F	388	PG6	C4-C5-O3-C6
9	F	388	PG6	O5-C10-C11-O6
5	B	500	HEC	C3D-CAD-CBD-CGD
5	B	600	HEC	CAD-CBD-CGD-O2D
5	A	600	HEC	CAD-CBD-CGD-O2D
8	F	387	PG4	C8-C7-O4-C6
5	B	600	HEC	CAD-CBD-CGD-O1D
9	F	388	PG6	C5-C4-O2-C3
5	A	600	HEC	CAD-CBD-CGD-O1D
5	A	500	HEC	CAD-CBD-CGD-O2D
9	F	388	PG6	C3-C2-O1-C1
8	F	387	PG4	O4-C7-C8-O5
5	A	500	HEC	CAA-CBA-CGA-O2A
5	A	500	HEC	CAD-CBD-CGD-O1D
5	A	500	HEC	CAA-CBA-CGA-O1A

There are no ring outliers.

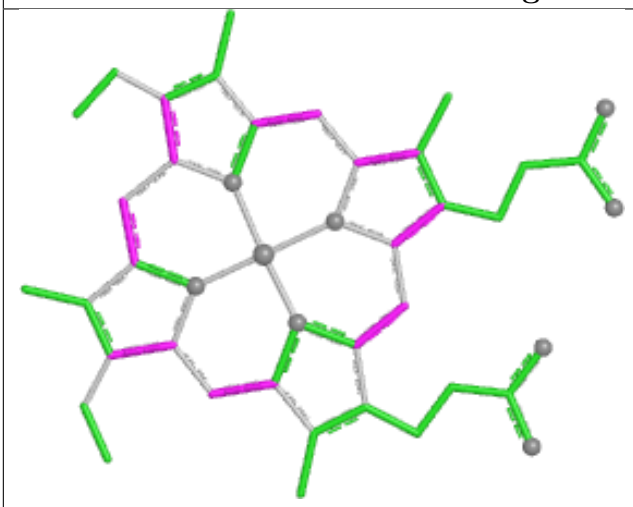
4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	500	HEC	3	0
5	B	600	HEC	1	0
5	B	500	HEC	2	0
5	A	600	HEC	1	0

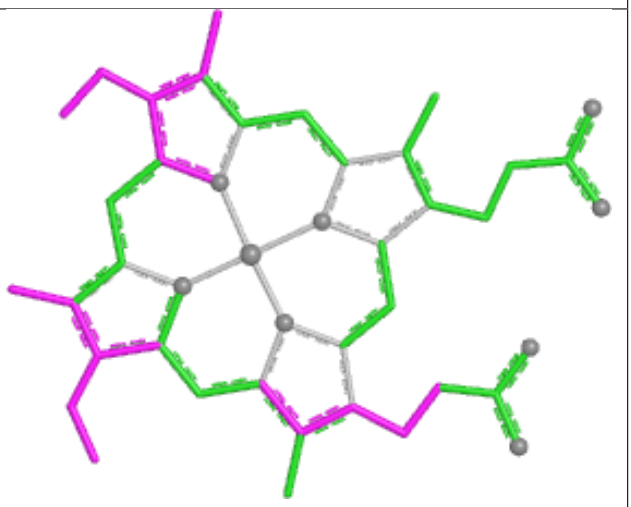
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

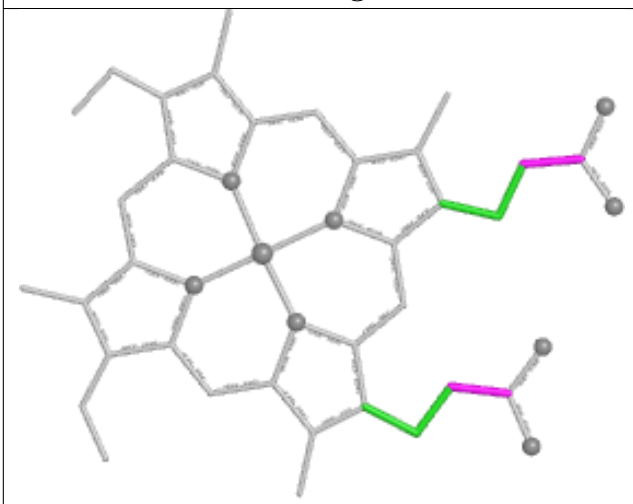
Ligand HEC A 500



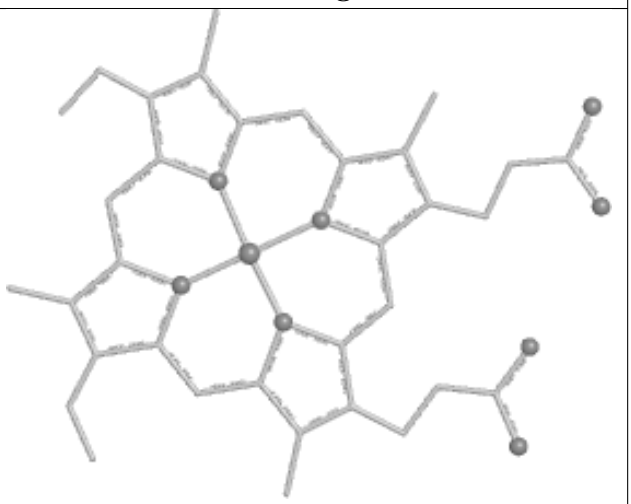
Bond lengths



Bond angles

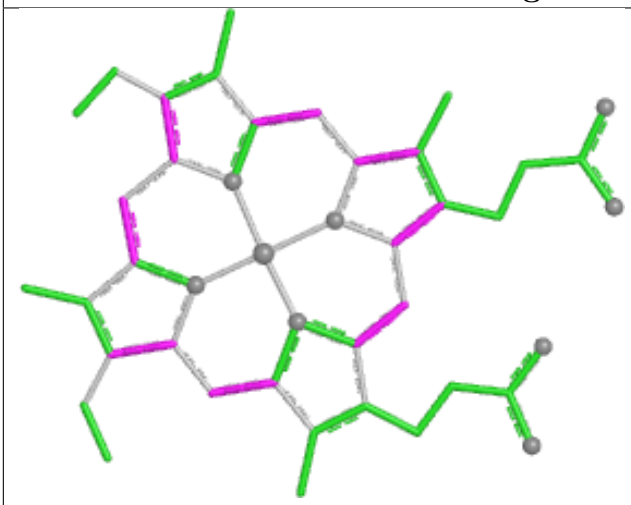


Torsions

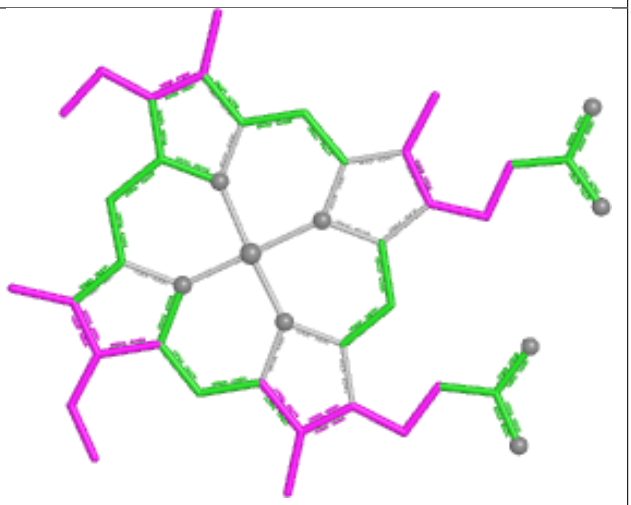


Rings

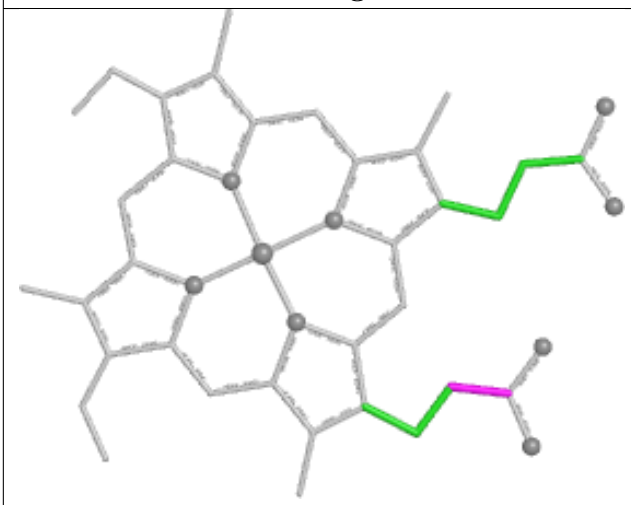
Ligand HEC B 600



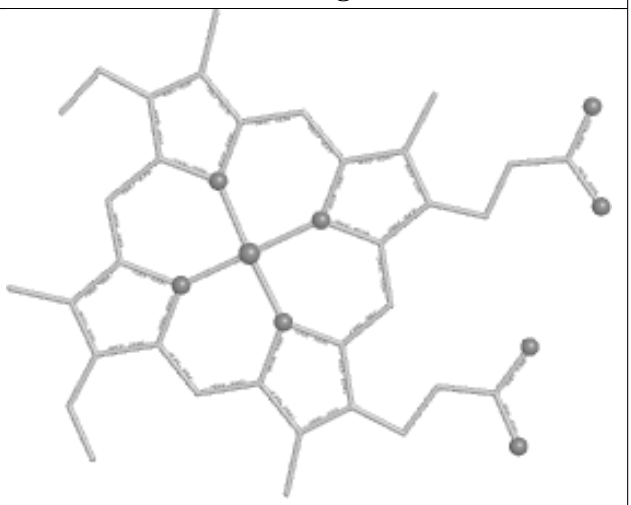
Bond lengths



Bond angles

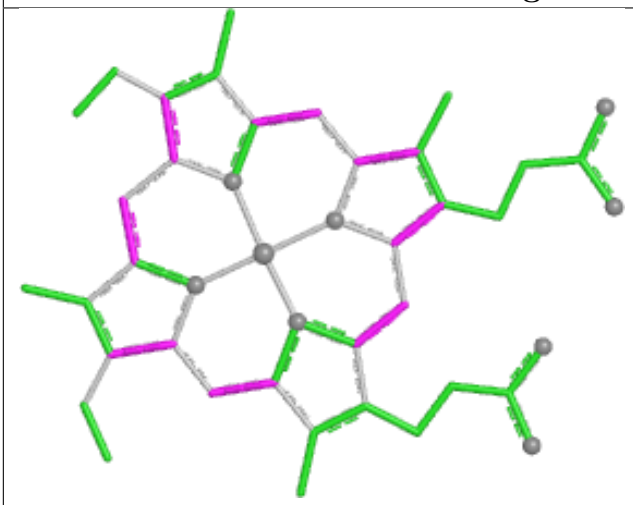


Torsions

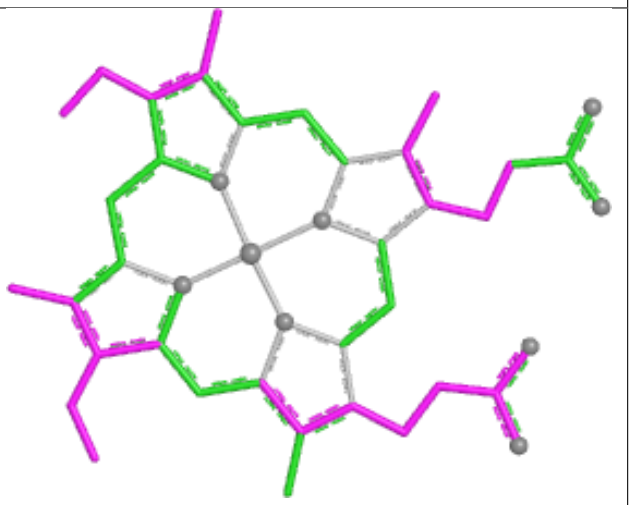


Rings

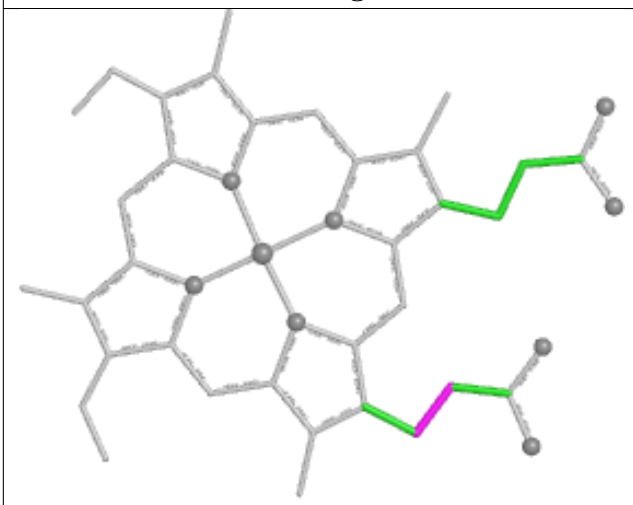
Ligand HEC B 500



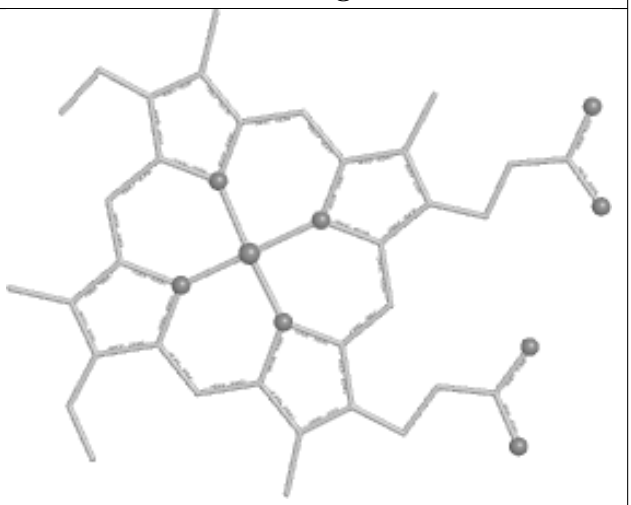
Bond lengths



Bond angles



Torsions



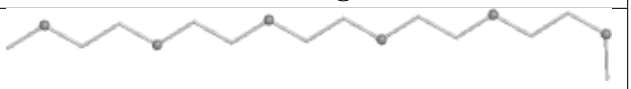
Rings

Ligand PG6 F 388

Bond lengths

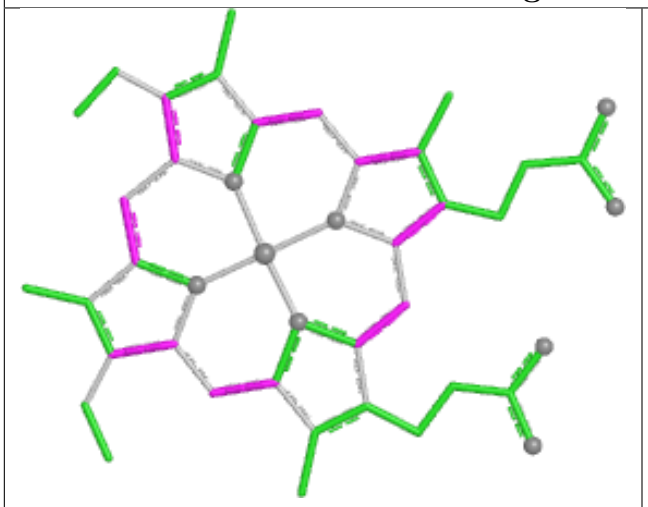
Bond angles

Torsions

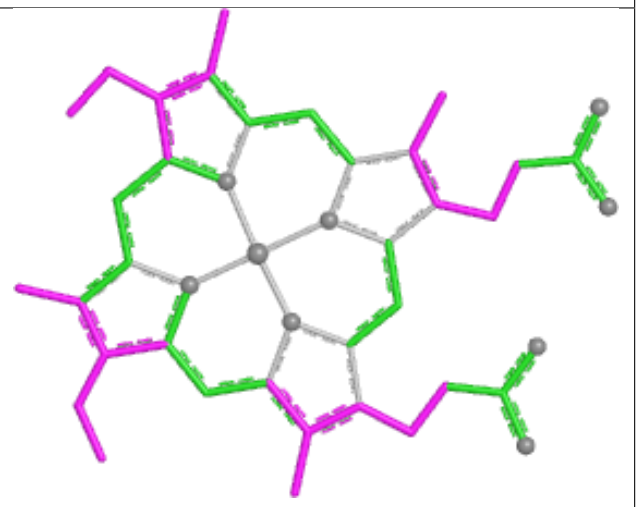


Rings

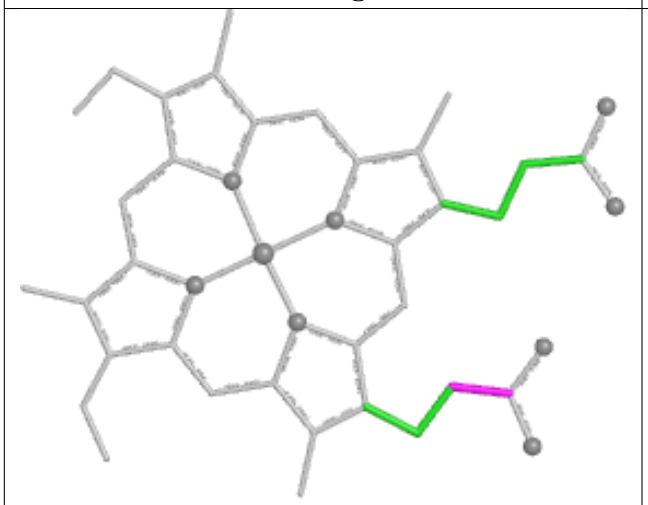
Ligand HEC A 600



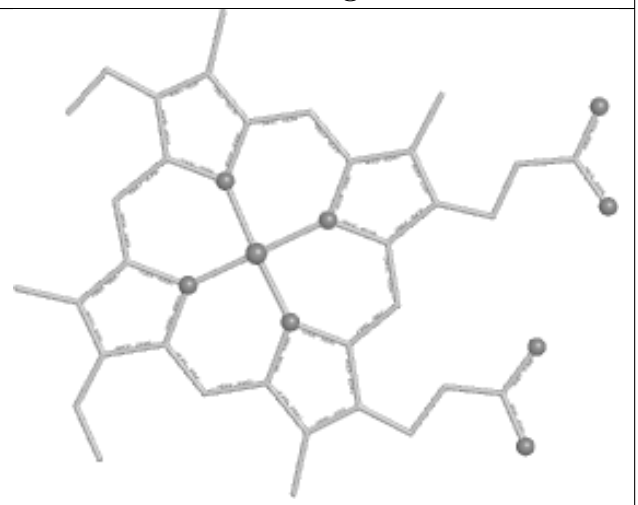
Bond lengths



Bond angles



Torsions



Rings

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	354/373 (94%)	-0.61	2 (0%) 89 88	20, 28, 38, 51	0
1	B	355/373 (95%)	-0.61	3 (0%) 86 85	18, 28, 40, 53	0
2	C	124/137 (90%)	-0.31	1 (0%) 86 85	20, 25, 33, 49	0
2	E	124/137 (90%)	-0.37	0 100 100	18, 22, 31, 46	0
3	D	376/386 (97%)	-0.49	5 (1%) 77 75	18, 28, 42, 56	0
3	F	376/386 (97%)	-0.61	0 100 100	16, 23, 35, 47	0
All	All	1709/1792 (95%)	-0.54	11 (0%) 89 88	16, 26, 40, 56	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ALA	5.7
3	D	208	THR	5.3
1	B	6	ALA	5.2
3	D	209	GLU	4.1
1	B	7	ASP	3.7
1	A	7	ASP	3.4
2	C	131	SER	3.1
3	D	207	GLY	3.0
3	D	211	THR	3.0
3	D	11	GLN	2.6
1	B	25	ARG	2.1

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
2	0AF	E	57	15/16	0.91	0.18	29,31,35,36	0
2	0AF	C	57	15/16	0.92	0.15	28,31,34,35	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

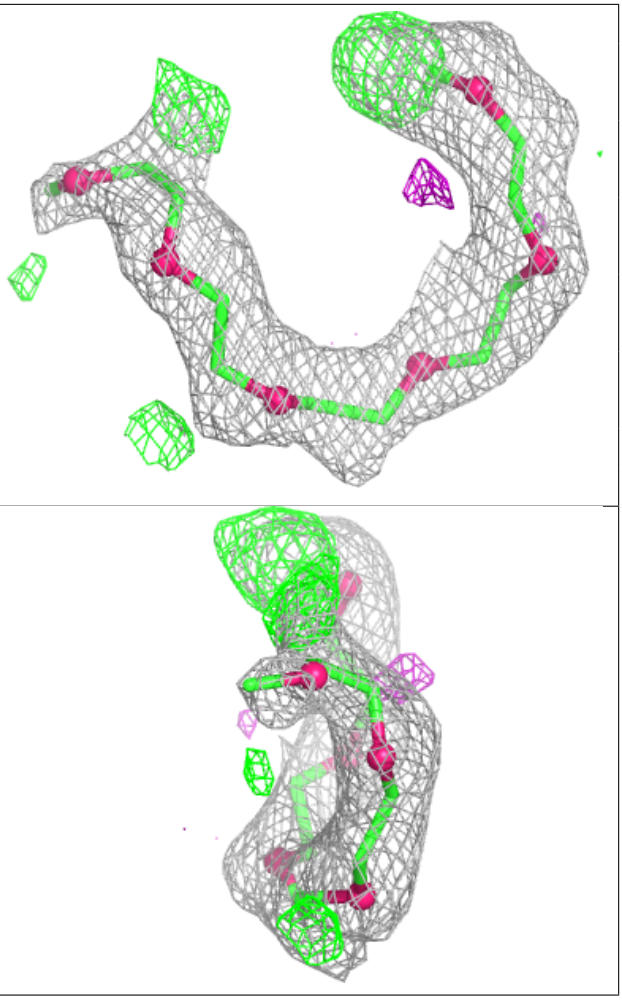
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	PG4	F	387	13/13	0.74	0.21	65,67,69,69	0
9	PG6	F	388	18/18	0.77	0.17	49,55,61,61	0
7	ACT	F	389	4/4	0.93	0.13	41,41,41,42	0
4	NA	A	375	1/1	0.93	0.05	30,30,30,30	0
7	ACT	D	387	4/4	0.93	0.15	41,42,42,42	0
4	NA	B	375	1/1	0.94	0.08	31,31,31,31	0
7	ACT	C	138	4/4	0.94	0.13	32,32,32,32	0
4	NA	B	374	1/1	0.95	0.05	32,32,32,32	0
5	HEC	B	600	43/43	0.97	0.11	14,16,19,21	0
5	HEC	A	500	43/43	0.97	0.09	22,24,26,26	0
4	NA	A	374	1/1	0.98	0.04	25,25,25,25	0
5	HEC	A	600	43/43	0.98	0.11	16,18,21,22	0
5	HEC	B	500	43/43	0.98	0.10	21,23,24,25	0
6	CA	A	400	1/1	0.99	0.06	20,20,20,20	0
6	CA	B	400	1/1	1.00	0.06	17,17,17,17	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.

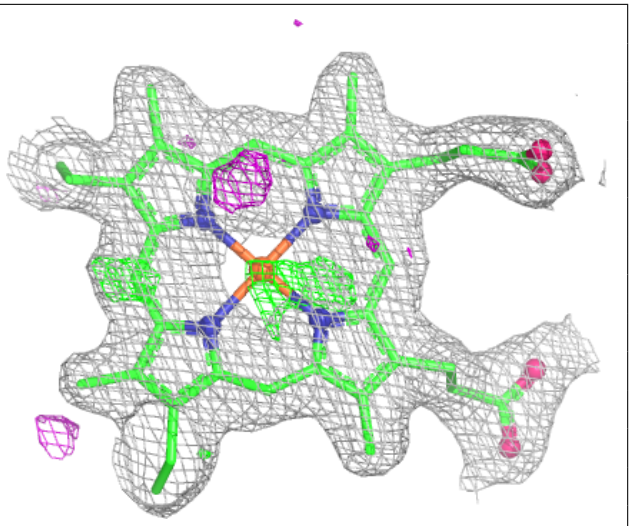
Electron density around PG6 F 388:

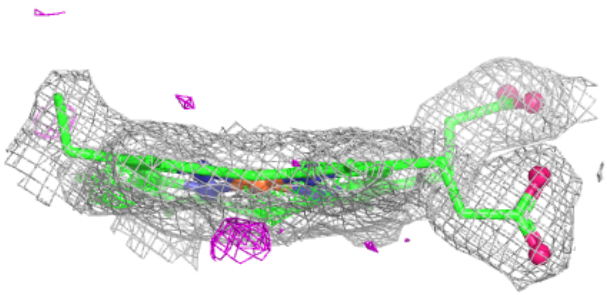
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

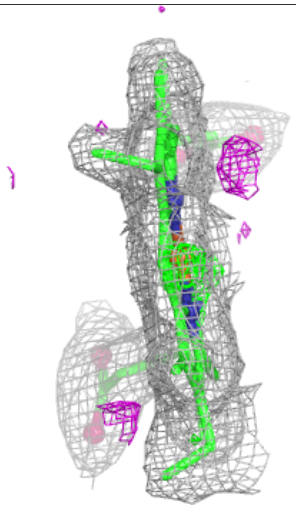


Electron density around HEC B 600:

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

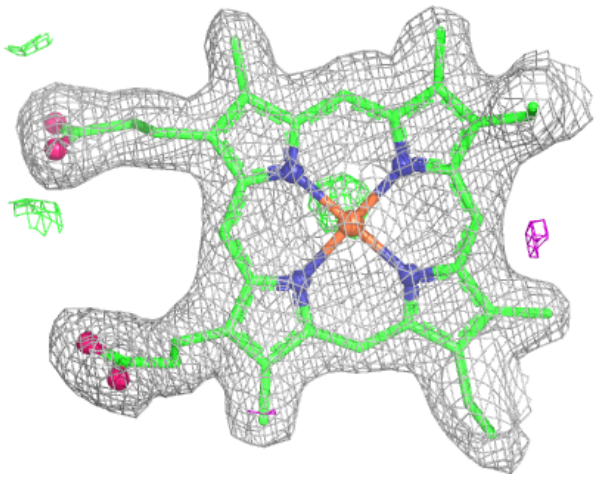


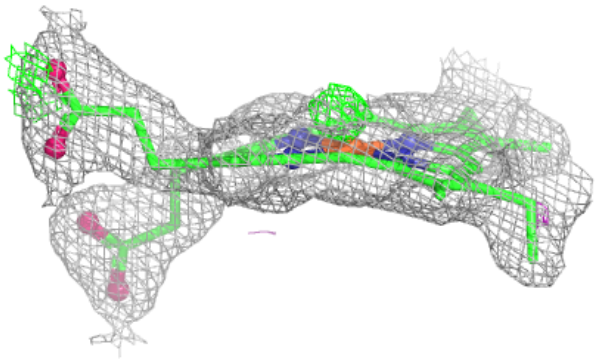


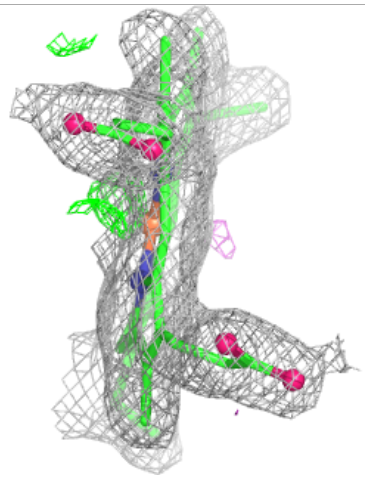


Electron density around HEC A 500:

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

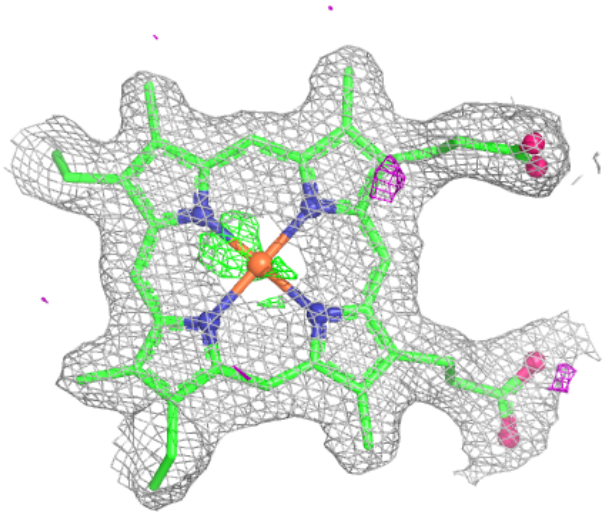


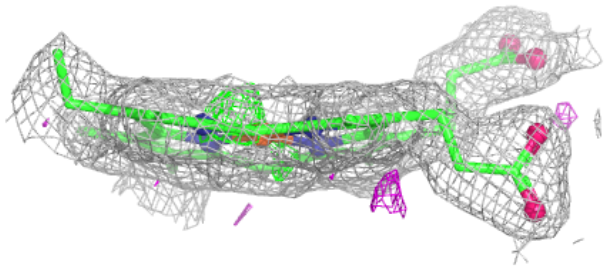




Electron density around HEC A 600:

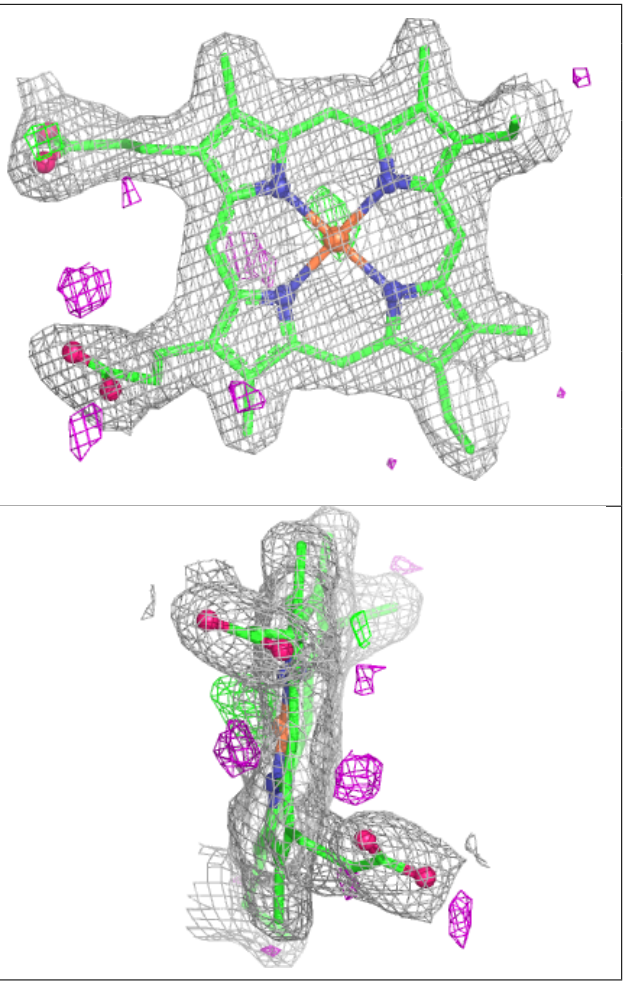
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around HEC B 500:

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.