Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 02:49 PM EDT

PDB ID	:	3SXT / pdb_00003sxt
Title	:	Crystal Structure of the Quinol Form of Methylamine Dehydrogenase in Complex with the Diferrous Form of MauG
Authors	:	Jensen, L.M.R.; Wilmot, C.M.
Deposited on	:	2011-07-15
Resolution	:	1.81 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:

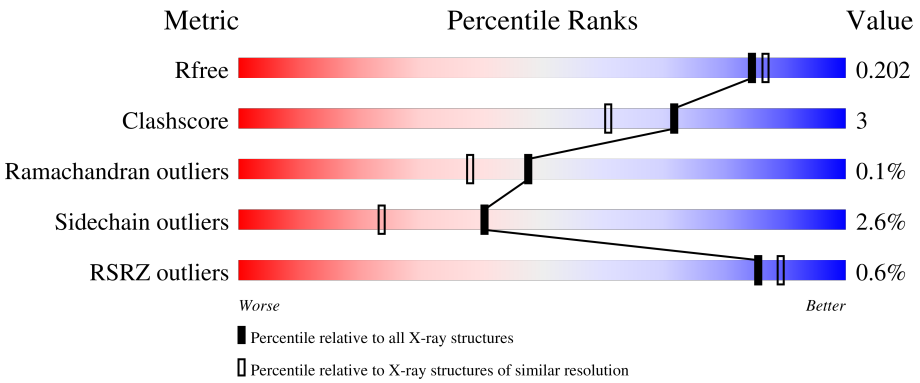
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.81 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}	180053	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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	% 87% 7% 5%
1	B	373	% 86% 9% • •
2	C	137	% 82% 7% • 9%
2	E	137	% 79% 10% • 9%
3	D	386	86% 10% • •

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Mol	Chain	Length	Quality of chain
3	F	386	89% 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	HEC	A	404	X	-	-	-
6	HEC	A	405	X	-	-	-
6	HEC	B	404	X	-	-	-
6	HEC	B	405	X	-	-	-
7	EDO	D	401	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 15339 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	2734	1707	490	526	11	0	0	0
1	B	357	2789	1740	505	532	12	0	4	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	961	594	161	193	13	0	1	0
2	E	125	958	592	161	191	14	0	1	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	375	2943	1868	509	558	8	0	4	0
			Total	C	N	O	S			
3	F	376	2932	1861	502	561	8	0	2	0

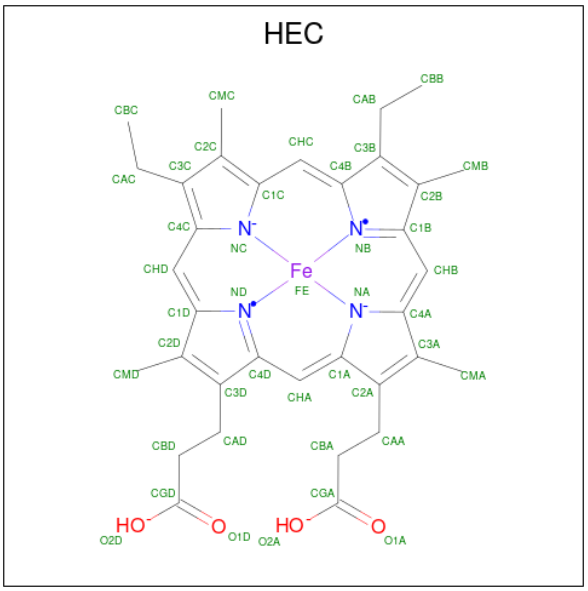
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

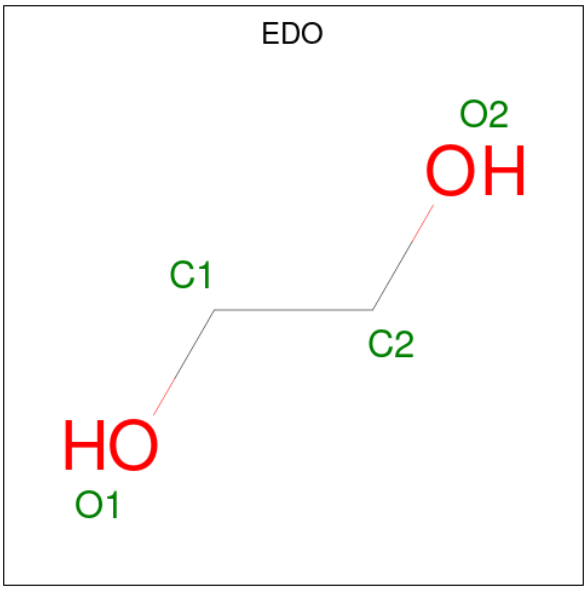
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
5	A	2	2	2	0	0
			Total	Na		
5	B	2	2	2	0	0

- Molecule 6 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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

- Molecule 7 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 8 is water.

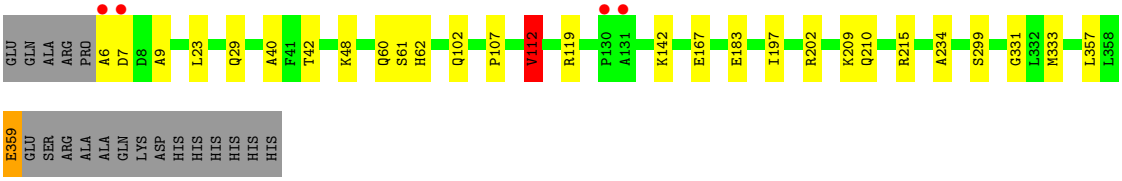
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
8	A	340	340	340	0	0
			Total	O		
8	B	358	358	358	0	0
			Total	O		
8	C	123	123	123	0	0
			Total	O		
8	D	452	452	452	0	0
			Total	O		
8	E	138	138	138	0	0
			Total	O		
8	F	413	413	413	0	0

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.

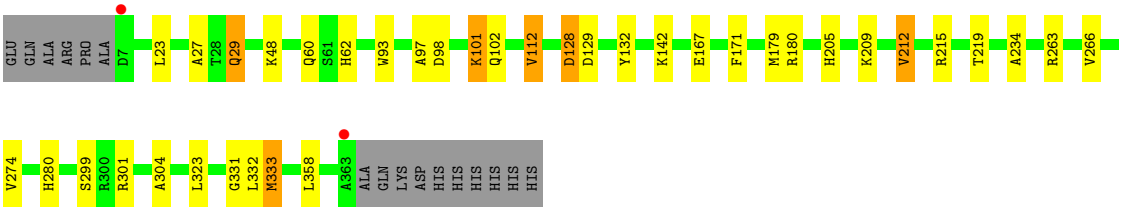
• Molecule 1: Methylamine utilization protein MauG

Chain A:



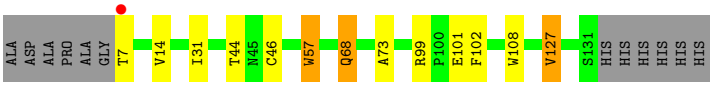
• Molecule 1: Methylamine utilization protein MauG

Chain B:



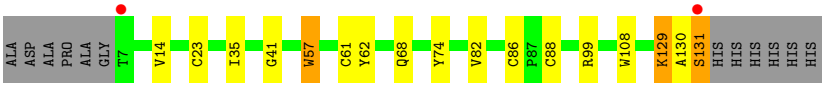
• Molecule 2: Methylamine dehydrogenase light chain

Chain C:



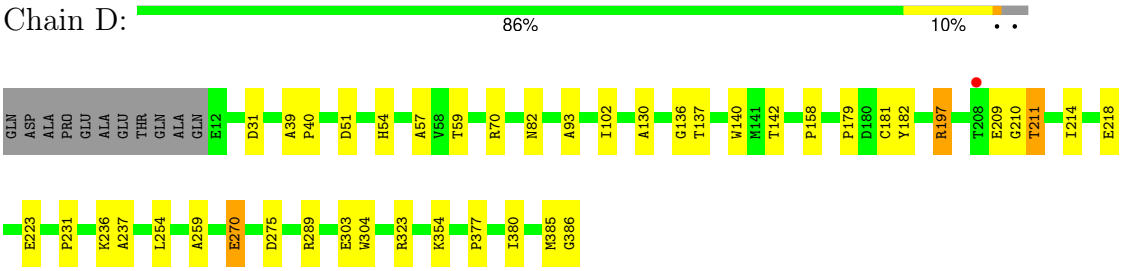
• Molecule 2: Methylamine dehydrogenase light chain

Chain E:



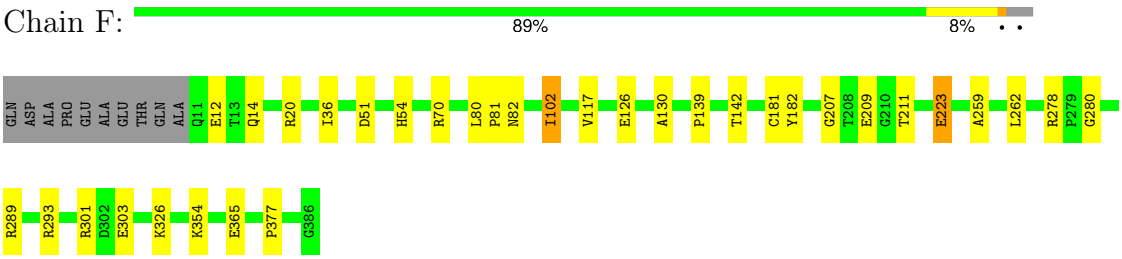
• Molecule 3: Methylamine dehydrogenase heavy chain

Chain D:



- Molecule 3: Methylamine dehydrogenase heavy chain

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.64Å 135.66Å 111.56Å 90.00° 97.37° 90.00°	Depositor
Resolution (Å)	35.01 – 1.81 35.01 – 1.81	Depositor EDS
% Data completeness (in resolution range)	97.9 (35.01-1.81) 97.9 (35.01-1.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.145 , 0.187 0.162 , 0.202	Depositor DCC
R_{free} test set	8245 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	21.0	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 34.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	15339	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: TOQ, HEC, EDO, NA, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.31	4/2798 (0.1%)	1.11	2/3797 (0.1%)
1	B	1.41	7/2865 (0.2%)	1.16	8/3883 (0.2%)
2	C	1.48	4/972 (0.4%)	1.10	0/1327
2	E	1.65	8/969 (0.8%)	1.23	0/1323
3	D	1.48	9/3032 (0.3%)	1.21	9/4129 (0.2%)
3	F	1.38	3/3015 (0.1%)	1.12	3/4109 (0.1%)
All	All	1.42	35/13651 (0.3%)	1.15	22/18568 (0.1%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	130	ALA	C-O	10.69	1.28	1.23
2	E	82	VAL	CA-CB	9.84	1.64	1.54
2	E	86	CYS	CA-C	9.62	1.59	1.53
3	D	130	ALA	N-CA	8.78	1.52	1.46
1	B	112	VAL	CA-CB	7.79	1.64	1.54
1	B	263	ARG	N-CA	6.90	1.55	1.46
3	D	70	ARG	N-CA	6.71	1.54	1.46
2	E	61	CYS	N-CA	6.66	1.54	1.46
3	F	130	ALA	C-O	6.66	1.27	1.23
1	A	40	ALA	CA-CB	6.44	1.63	1.53
3	D	380	ILE	CA-CB	6.24	1.61	1.54
2	E	35	ILE	C-O	6.14	1.30	1.24
2	E	14	VAL	CA-CB	6.00	1.61	1.54
3	D	93	ALA	CA-CB	5.93	1.63	1.53
3	F	259	ALA	CA-CB	5.87	1.62	1.53
2	C	73	ALA	N-CA	5.85	1.53	1.46
3	D	270	GLU	N-CA	-5.78	1.39	1.46
1	B	266	VAL	CA-CB	5.77	1.61	1.54
2	E	74	TYR	C-O	5.72	1.31	1.23
2	E	62	TYR	CA-C	5.62	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	332	LEU	C-O	-5.49	1.17	1.24
3	D	231	PRO	C-O	5.41	1.30	1.23
3	F	102	ILE	C-O	-5.30	1.17	1.24
2	C	14	VAL	CA-CB	5.30	1.61	1.54
1	A	234	ALA	CA-CB	5.26	1.61	1.53
2	C	31	ILE	CA-CB	5.23	1.60	1.54
3	D	136	GLY	N-CA	5.20	1.51	1.45
1	A	112	VAL	CA-CB	5.19	1.61	1.54
1	B	97	ALA	N-CA	5.18	1.52	1.46
1	B	234	ALA	CA-CB	5.10	1.61	1.53
2	E	41	GLY	C-O	5.06	1.29	1.24
3	D	59	THR	C-O	5.03	1.30	1.23
1	B	205	HIS	N-CA	5.02	1.52	1.46
2	C	127	VAL	N-CA	5.01	1.50	1.46
1	A	197	ILE	CA-CB	5.01	1.60	1.54

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	211	THR	CA-C-N	-7.51	112.59	120.03
3	D	211	THR	C-N-CA	-7.51	112.59	120.03
3	F	303	GLU	N-CA-C	6.63	120.47	112.38
3	D	140	TRP	N-CA-C	-6.44	105.37	112.72
1	B	128	ASP	N-CA-C	6.43	118.37	111.36
1	B	212	VAL	N-CA-CB	-6.27	101.16	111.45
3	D	136	GLY	N-CA-C	-5.89	104.47	111.36
1	A	29	GLN	N-CA-C	5.86	118.31	109.23
3	F	278	ARG	CG-CD-NE	-5.85	99.13	112.00
3	D	210	GLY	N-CA-C	-5.79	104.14	111.72
3	D	31	ASP	N-CA-C	-5.76	100.79	109.95
1	B	274	VAL	N-CA-C	5.60	117.49	112.17
1	B	331	GLY	N-CA-C	-5.47	108.08	115.36
3	F	207	GLY	N-CA-C	-5.39	104.89	112.60
1	B	27	ALA	N-CA-C	5.36	119.10	112.24
1	A	167	GLU	N-CA-C	5.26	117.70	111.33
1	B	29	GLN	N-CA-C	5.24	117.35	109.23
1	B	180	ARG	NE-CZ-NH2	5.14	123.83	119.20
3	D	57	ALA	N-CA-C	-5.07	106.61	112.89
1	B	101	LYS	N-CA-C	-5.04	105.87	111.36
3	D	137	THR	N-CA-C	5.02	116.98	109.59
3	D	385	MET	N-CA-C	-5.02	106.74	112.92

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	2734	0	2607	20	0
1	B	2789	0	2679	14	0
2	C	961	0	864	10	0
2	E	958	0	864	11	0
3	D	2943	0	2850	17	0
3	F	2932	0	2826	20	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	86	0	60	0	0
6	B	86	0	60	1	0
7	A	8	0	12	2	0
7	B	4	0	6	0	0
7	D	4	0	6	4	0
7	F	4	0	6	3	0
8	A	340	0	0	5	0
8	B	358	0	0	2	0
8	C	123	0	0	1	0
8	D	452	0	0	8	0
8	E	138	0	0	0	0
8	F	413	0	0	6	0
All	All	15339	0	12840	88	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 (88) 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:215:ARG:HH12	7:A:406:EDO:H12	1.09	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:401:EDO:H22	8:D:555:HOH:O	1.50	1.12
2:E:130:ALA:O	2:E:131:SER:HB2	1.48	1.06
3:F:126:GLU:H	7:F:401:EDO:H21	1.29	0.97
1:B:48:LYS:H	1:B:62:HIS:HE1	1.15	0.94
1:A:215:ARG:NH1	7:A:406:EDO:H12	1.81	0.94
2:E:99:ARG:NH1	3:F:223:GLU:HG3	1.93	0.83
8:C:295:HOH:O	3:F:36[A]:ILE:HD11	1.79	0.83
1:B:98:ASP:H	1:B:102:GLN:HE21	1.29	0.80
2:E:68:GLN:HB3	2:E:129:LYS:HE3	1.63	0.79
1:A:48:LYS:H	1:A:62:HIS:HE1	1.31	0.79
3:F:126:GLU:H	7:F:401:EDO:C2	2.00	0.74
3:F:326:LYS:HE3	8:F:864:HOH:O	1.88	0.73
1:B:48:LYS:H	1:B:62:HIS:CE1	2.03	0.73
3:D:54:HIS:HD2	8:D:858:HOH:O	1.73	0.70
1:A:359:GLU:OE1	1:A:359:GLU:N	2.23	0.70
3:F:126:GLU:N	7:F:401:EDO:H21	2.06	0.69
3:F:12:GLU:CD	3:F:20:ARG:HH12	2.02	0.68
3:F:12:GLU:OE1	3:F:20:ARG:NH1	2.29	0.64
1:B:98:ASP:H	1:B:102:GLN:NE2	1.95	0.64
1:B:171:PHE:CE1	1:B:215[B]:ARG:HD2	2.33	0.63
1:A:202:ARG:NE	2:C:127:VAL:HB	2.16	0.61
2:C:68:GLN:HE21	2:C:68:GLN:HA	1.64	0.60
1:B:60:GLN:O	1:B:62:HIS:HD2	1.84	0.60
1:A:202:ARG:HE	2:C:127:VAL:HB	1.65	0.60
1:A:119:ARG:NE	8:A:656:HOH:O	2.34	0.59
3:F:14:GLN:HE21	3:F:70:ARG:HH11	1.50	0.59
1:B:179:MET:HE1	2:E:131:SER:C	2.28	0.59
1:A:48:LYS:H	1:A:62:HIS:CE1	2.19	0.58
2:E:57:TOQ:HB	2:E:108:TRP:NE1	2.18	0.57
3:F:293:ARG:HG3	8:F:769:HOH:O	2.03	0.57
1:A:119:ARG:CZ	8:A:656:HOH:O	2.53	0.56
6:B:404:HEC:HMC3	6:B:404:HEC:HBC3	1.87	0.56
2:E:23:CYS:SG	2:E:88[B]:CYS:HB2	2.46	0.55
2:C:101[B]:GLU:OE2	3:D:197:ARG:NH2	2.38	0.54
1:A:6:ALA:HA	1:A:9:ALA:HB3	1.91	0.53
2:C:57:TOQ:HB	2:C:108:TRP:NE1	2.23	0.53
2:E:130:ALA:O	2:E:131:SER:CB	2.34	0.53
3:D:218:GLU:HG2	8:D:785:HOH:O	2.07	0.53
1:A:210:GLN:HE22	2:C:44:THR:HG21	1.74	0.53
3:F:54:HIS:HE1	8:F:663:HOH:O	1.91	0.53
3:F:51:ASP:HA	3:F:377:PRO:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:23:CYS:SG	2:E:88[B]:CYS:SG	3.07	0.52
3:F:280:GLY:HA3	3:F:301:ARG:CZ	2.40	0.52
3:F:326:LYS:CE	8:F:864:HOH:O	2.54	0.51
7:D:401:EDO:H21	8:D:722:HOH:O	2.11	0.50
3:D:237:ALA:HB2	3:D:289:ARG:HG3	1.93	0.50
3:F:181:CYS:C	3:F:182:TYR:CD1	2.89	0.50
2:C:101[B]:GLU:H	2:C:101[B]:GLU:CD	2.20	0.49
1:A:183:GLU:HB2	8:A:783:HOH:O	2.13	0.48
1:A:359:GLU:H	1:A:359:GLU:CD	2.18	0.48
2:E:23:CYS:SG	2:E:88[B]:CYS:CB	3.01	0.48
1:A:61:SER:HB3	1:A:112:VAL:HB	1.95	0.48
1:B:301:ARG:NH1	1:B:333:MET:HE1	2.28	0.47
1:A:107:PRO:HG3	8:A:834:HOH:O	2.14	0.47
3:D:82:ASN:HB3	3:D:142:THR:HB	1.96	0.47
3:D:181:CYS:C	3:D:182:TYR:CD1	2.93	0.47
2:C:101[B]:GLU:HG2	2:C:102:PHE:CD2	2.50	0.46
1:A:60:GLN:O	1:A:62:HIS:HD2	1.97	0.46
1:A:331:GLY:O	3:D:158:PRO:HA	2.16	0.46
1:A:299:SER:HB2	1:A:333:MET:HG3	1.97	0.46
3:D:54:HIS:CD2	8:D:858:HOH:O	2.57	0.46
2:E:57:TOQ:HB	2:E:108:TRP:HE1	1.79	0.46
1:B:101:LYS:HD2	1:B:101:LYS:C	2.41	0.46
1:B:29:GLN:HB3	8:B:640:HOH:O	2.16	0.46
3:F:293:ARG:CG	8:F:769:HOH:O	2.63	0.45
3:D:303:GLU:HG3	3:D:304:TRP:CD1	2.52	0.45
3:D:51:ASP:HA	3:D:377:PRO:HA	1.98	0.45
3:D:179:PRO:HD3	3:D:214:ILE:HD13	1.99	0.44
3:D:197:ARG:O	3:D:197:ARG:HG2	2.17	0.44
2:C:99:ARG:NH1	3:D:223:GLU:O	2.48	0.44
3:F:80:LEU:N	3:F:81:PRO:HD3	2.33	0.44
3:D:236:LYS:NZ	3:D:386:GLY:O	2.45	0.43
3:F:82:ASN:HB3	3:F:142:THR:HB	2.00	0.43
2:C:46:CYS:HB2	3:F:36[B]:ILE:HD13	1.99	0.43
2:E:129:LYS:HD2	2:E:129:LYS:HA	1.82	0.43
7:D:401:EDO:O2	8:D:873:HOH:O	2.21	0.43
1:A:359:GLU:N	1:A:359:GLU:CD	2.77	0.42
1:B:299:SER:HB3	1:B:304:ALA:CB	2.49	0.42
1:B:209:LYS:HG3	8:B:820:HOH:O	2.19	0.42
3:F:289:ARG:NH2	8:F:893:HOH:O	2.53	0.42
1:A:42:THR:HB	8:A:526:HOH:O	2.20	0.42
1:B:129:ASP:HB3	1:B:132:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:254:LEU:HD23	3:D:259:ALA:HA	2.02	0.41
3:D:39:ALA:HB1	3:D:40:PRO:HD2	2.03	0.41
1:B:93:TRP:CE2	1:B:280:HIS:HA	2.56	0.41
3:D:211:THR:HB	8:D:740:HOH:O	2.22	0.40
7:D:401:EDO:C2	8:D:722:HOH:O	2.69	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	352/373 (94%)	345 (98%)	7 (2%)	0	100	100
1	B	359/373 (96%)	349 (97%)	10 (3%)	0	100	100
2	C	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
2	E	123/137 (90%)	121 (98%)	2 (2%)	0	100	100
3	D	377/386 (98%)	367 (97%)	8 (2%)	2 (0%)	24	14
3	F	376/386 (97%)	363 (96%)	12 (3%)	1 (0%)	36	26
All	All	1710/1792 (95%)	1666 (97%)	41 (2%)	3 (0%)	48	33

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	102[A]	ILE
3	D	102[B]	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	276/292 (94%)	268 (97%)	8 (3%)	37	19
1	B	283/292 (97%)	273 (96%)	10 (4%)	32	13
2	C	105/112 (94%)	103 (98%)	2 (2%)	50	37
2	E	105/112 (94%)	103 (98%)	2 (2%)	50	37
3	D	307/311 (99%)	300 (98%)	7 (2%)	44	28
3	F	306/311 (98%)	298 (97%)	8 (3%)	40	23
All	All	1382/1430 (97%)	1345 (97%)	37 (3%)	40	22

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	23	LEU
1	A	102	GLN
1	A	112	VAL
1	A	142	LYS
1	A	209	LYS
1	A	357	LEU
1	A	359	GLU
1	B	23	LEU
1	B	112	VAL
1	B	128	ASP
1	B	142	LYS
1	B	167	GLU
1	B	212	VAL
1	B	219	THR
1	B	323	LEU
1	B	333	MET
1	B	358	LEU
2	C	7	THR
2	C	68	GLN
3	D	197	ARG
3	D	209	GLU

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Mol	Chain	Res	Type
3	D	270	GLU
3	D	275	ASP
3	D	323[A]	ARG
3	D	323[B]	ARG
3	D	354	LYS
2	E	129	LYS
2	E	131	SER
3	F	117	VAL
3	F	139	PRO
3	F	209	GLU
3	F	211	THR
3	F	223	GLU
3	F	262	LEU
3	F	354	LYS
3	F	365	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	62	HIS
1	A	210	GLN
1	B	29	GLN
1	B	60	GLN
1	B	62	HIS
1	B	102	GLN
3	D	30	GLN
3	D	50	ASN
3	D	61	GLN
3	D	331	HIS
3	D	378	GLN
2	E	21	GLN
3	F	14	GLN
3	F	30	GLN
3	F	54	HIS
3	F	61	GLN
3	F	331	HIS

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	TOQ	E	57	2	16,17,18	1.93	3 (18%)	17,24,26	1.85	5 (29%)
2	TOQ	C	57	2	16,17,18	0.96	0	17,24,26	1.18	2 (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	TOQ	E	57	2	-	0/5/6/8	0/2/2/2
2	TOQ	C	57	2	-	0/5/6/8	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57	TOQ	CD1-CG	4.17	1.43	1.36
2	E	57	TOQ	CD1-NE1	-3.81	1.31	1.37
2	E	57	TOQ	CE3-CD2	3.27	1.44	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	57	TOQ	CB-CG-CD1	-3.65	119.85	126.97
2	E	57	TOQ	CB-CG-CD2	3.61	133.63	126.70
2	C	57	TOQ	CB-CG-CD2	3.14	132.74	126.70
2	E	57	TOQ	CE3-CZ3-CH2	-2.85	117.65	120.50
2	E	57	TOQ	CE2-NE1-CD1	2.47	111.06	108.93
2	C	57	TOQ	CB-CG-CD1	-2.42	122.24	126.97
2	E	57	TOQ	CE2-CZ2-CH2	2.07	120.34	117.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	57	TOQ	2	0
2	C	57	TOQ	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides 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	$\#\|Z\| > 2$
7	EDO	D	401	-	3,3,3	0.69	0	2,2,2	0.41	0
7	EDO	A	406	-	3,3,3	0.29	0	2,2,2	0.63	0
7	EDO	A	407	-	3,3,3	0.37	0	2,2,2	0.92	0
7	EDO	B	406	-	3,3,3	0.55	0	2,2,2	0.42	0
7	EDO	F	401	-	3,3,3	0.55	0	2,2,2	0.40	0
6	HEC	A	405	1	50,50,50	2.29	22 (44%)	68,82,82	1.92	21 (30%)
6	HEC	A	404	8,1	50,50,50	2.40	24 (48%)	68,82,82	2.10	28 (41%)
6	HEC	B	404	1	50,50,50	2.45	21 (42%)	68,82,82	2.11	23 (33%)
6	HEC	B	405	1	50,50,50	1.99	17 (34%)	68,82,82	2.33	25 (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
7	EDO	D	401	-	-	1/1/1/1	-
7	EDO	A	406	-	-	1/1/1/1	-
7	EDO	A	407	-	-	0/1/1/1	-
7	EDO	B	406	-	-	0/1/1/1	-
7	EDO	F	401	-	-	1/1/1/1	-
6	HEC	A	405	1	1/1/3/7	4/14/54/54	-
6	HEC	A	404	8,1	1/1/3/7	6/14/54/54	-
6	HEC	B	404	1	1/1/3/7	6/14/54/54	-
6	HEC	B	405	1	1/1/3/7	6/14/54/54	-

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	404	HEC	CHD-C1D	5.29	1.49	1.38
6	A	404	HEC	CHA-C1A	4.97	1.48	1.38
6	A	405	HEC	CHC-C4B	4.97	1.48	1.38
6	B	404	HEC	CHB-C1B	4.94	1.50	1.39
6	A	404	HEC	CHD-C1D	4.87	1.48	1.38
6	A	405	HEC	CHB-C4A	4.72	1.47	1.38
6	A	404	HEC	CHB-C4A	4.69	1.47	1.38
6	A	404	HEC	CHB-C1B	4.61	1.49	1.39
6	B	404	HEC	CHA-C1A	4.45	1.47	1.38
6	A	405	HEC	FE-NB	4.37	2.08	1.94
6	B	405	HEC	CHC-C4B	4.19	1.46	1.38
6	A	404	HEC	FE-NB	4.13	2.07	1.94
6	B	405	HEC	C4A-NA	-4.11	1.31	1.39
6	B	404	HEC	CHC-C4B	4.04	1.46	1.38
6	B	404	HEC	FE-NC	3.99	2.08	1.95
6	B	404	HEC	C1C-NC	-3.94	1.32	1.39
6	A	404	HEC	C1D-ND	-3.85	1.33	1.40
6	A	404	HEC	C1B-NB	-3.72	1.31	1.38
6	A	405	HEC	CHB-C1B	3.70	1.47	1.39
6	A	404	HEC	FE-ND	3.70	2.06	1.94
6	B	405	HEC	C1A-NA	-3.67	1.32	1.39
6	B	404	HEC	CHB-C4A	3.66	1.45	1.38
6	A	405	HEC	C4C-NC	-3.63	1.32	1.39
6	B	404	HEC	CHC-C1C	3.62	1.47	1.39
6	A	404	HEC	FE-NA	3.61	2.07	1.95
6	B	404	HEC	FE-ND	3.52	2.05	1.94
6	A	405	HEC	CHA-C1A	3.49	1.45	1.38
6	B	404	HEC	C4C-NC	-3.49	1.33	1.39
6	A	405	HEC	FE-NA	3.48	2.06	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	404	HEC	C1D-ND	-3.48	1.34	1.40
6	B	404	HEC	FE-NA	3.48	2.06	1.95
6	A	404	HEC	CHD-C4C	3.43	1.47	1.39
6	A	405	HEC	FE-ND	3.42	2.05	1.94
6	A	405	HEC	C1A-NA	-3.42	1.33	1.39
6	B	405	HEC	CHA-C4D	3.39	1.46	1.39
6	B	404	HEC	FE-NB	3.37	2.05	1.94
6	B	404	HEC	CHA-C4D	3.29	1.46	1.39
6	A	404	HEC	FE-NC	3.21	2.05	1.95
6	B	404	HEC	C1A-NA	-3.16	1.33	1.39
6	B	405	HEC	CHA-C1A	3.09	1.44	1.38
6	B	405	HEC	CHB-C4A	3.09	1.44	1.38
6	B	405	HEC	FE-NA	3.04	2.05	1.95
6	A	405	HEC	CBD-CAD	3.01	1.62	1.51
6	A	405	HEC	CHD-C4C	2.99	1.46	1.39
6	B	405	HEC	CHB-C1B	2.98	1.46	1.39
6	A	405	HEC	CHD-C1D	2.94	1.44	1.38
6	A	405	HEC	FE-NC	2.92	2.04	1.95
6	B	405	HEC	CHD-C4C	2.88	1.45	1.39
6	A	404	HEC	C1C-NC	-2.85	1.34	1.39
6	A	405	HEC	C1D-ND	-2.85	1.35	1.40
6	B	405	HEC	CHD-C1D	2.85	1.44	1.38
6	B	405	HEC	FE-ND	2.83	2.03	1.94
6	A	405	HEC	C1B-NB	-2.83	1.33	1.38
6	B	404	HEC	C4B-NB	-2.83	1.35	1.40
6	A	405	HEC	C4A-NA	-2.80	1.34	1.39
6	B	404	HEC	O2D-CGD	-2.79	1.21	1.30
6	A	405	HEC	CHA-C4D	2.78	1.45	1.39
6	B	405	HEC	C4C-NC	-2.74	1.34	1.39
6	A	404	HEC	C4A-NA	-2.71	1.34	1.39
6	A	404	HEC	CHC-C4B	2.70	1.43	1.38
6	B	405	HEC	C1C-NC	-2.70	1.34	1.39
6	A	404	HEC	C1A-NA	-2.67	1.34	1.39
6	B	404	HEC	CHD-C4C	2.63	1.45	1.39
6	A	405	HEC	C4B-NB	-2.61	1.35	1.40
6	B	405	HEC	C1D-ND	-2.60	1.35	1.40
6	A	404	HEC	CHC-C1C	2.51	1.45	1.39
6	B	405	HEC	C4D-ND	-2.49	1.34	1.38
6	A	404	HEC	C4B-NB	-2.44	1.36	1.40
6	A	404	HEC	C3B-C2B	2.38	1.41	1.36
6	B	404	HEC	C4A-NA	-2.36	1.35	1.39
6	A	404	HEC	C4C-NC	-2.33	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	404	HEC	O2A-CGA	-2.33	1.23	1.30
6	A	404	HEC	C1C-C2C	2.30	1.48	1.43
6	A	404	HEC	CMC-C2C	2.30	1.55	1.50
6	B	404	HEC	CBD-CAD	2.25	1.59	1.51
6	B	405	HEC	FE-NB	2.23	2.01	1.94
6	A	405	HEC	C1C-NC	-2.19	1.35	1.39
6	A	405	HEC	C1C-C2C	2.16	1.48	1.43
6	A	404	HEC	CHA-C4D	2.10	1.44	1.39
6	A	405	HEC	O2D-CGD	-2.04	1.24	1.30
6	B	404	HEC	O2A-CGA	-2.02	1.24	1.30
6	B	405	HEC	FE-NC	2.01	2.01	1.95
6	A	404	HEC	C1B-C2B	2.01	1.48	1.44
6	A	405	HEC	CHC-C1C	2.01	1.43	1.39

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	405	HEC	CBD-CAD-C3D	-6.34	94.99	112.53
6	B	405	HEC	C2D-C1D-ND	6.05	116.79	109.84
6	B	405	HEC	CBD-CAD-C3D	-5.77	96.57	112.53
6	B	404	HEC	CHD-C1D-ND	-5.06	118.10	124.37
6	B	405	HEC	C1D-C2D-C3D	-5.02	101.70	106.98
6	B	405	HEC	C2B-C1B-NB	4.91	115.58	109.90
6	B	404	HEC	C3D-C4D-ND	4.77	114.96	110.35
6	B	405	HEC	C3D-C4D-ND	4.70	114.89	110.35
6	B	404	HEC	C2D-C1D-ND	4.67	115.21	109.84
6	A	404	HEC	C3B-C4B-NB	4.48	115.08	110.17
6	A	404	HEC	CBD-CAD-C3D	-4.47	100.18	112.53
6	B	404	HEC	C3B-C4B-NB	4.39	114.98	110.17
6	B	405	HEC	C3B-C4B-NB	4.29	114.87	110.17
6	A	404	HEC	C1C-C2C-C3C	-4.20	102.01	106.82
6	A	404	HEC	C3D-C4D-ND	4.09	114.30	110.35
6	A	405	HEC	C2B-C1B-NB	3.98	114.50	109.90
6	A	405	HEC	C3B-C4B-NB	3.80	114.33	110.17
6	B	404	HEC	C1D-ND-C4D	-3.72	100.80	105.21
6	B	405	HEC	C4B-NB-C1B	-3.72	100.81	105.21
6	B	405	HEC	CHB-C4A-NA	3.70	128.48	124.45
6	B	404	HEC	CBD-CAD-C3D	-3.68	102.37	112.53
6	B	404	HEC	C2B-C1B-NB	3.60	114.06	109.90
6	A	404	HEC	C4B-C3B-C2B	-3.54	101.75	106.89
6	B	405	HEC	CAC-C3C-C2C	3.48	132.39	126.89
6	B	405	HEC	CHD-C1D-ND	-3.47	120.08	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	404	HEC	CAC-C3C-C2C	3.46	132.37	126.89
6	A	405	HEC	C1C-C2C-C3C	-3.46	102.86	106.82
6	A	405	HEC	C3C-C4C-NC	3.42	113.95	110.15
6	A	404	HEC	CHD-C1D-ND	-3.32	120.26	124.37
6	B	404	HEC	CHA-C4D-C3D	-3.32	119.94	124.77
6	B	405	HEC	C1D-ND-C4D	-3.29	101.31	105.21
6	A	404	HEC	C3C-C4C-NC	3.24	113.74	110.15
6	A	404	HEC	C2D-C1D-ND	3.23	113.55	109.84
6	B	404	HEC	C1D-C2D-C3D	-3.17	103.64	106.98
6	B	405	HEC	CHB-C1B-NB	-3.15	121.04	124.42
6	B	404	HEC	CHC-C4B-C3B	-3.14	119.43	125.23
6	B	404	HEC	CMD-C2D-C1D	3.12	129.92	125.03
6	B	404	HEC	CAC-C3C-C2C	3.04	131.69	126.89
6	A	404	HEC	C2C-C1C-NC	3.03	114.99	110.14
6	B	405	HEC	C1C-C2C-C3C	-3.02	103.36	106.82
6	A	405	HEC	CMC-C2C-C3C	3.01	132.02	125.62
6	A	404	HEC	CAB-C3B-C2B	2.99	133.06	127.56
6	A	404	HEC	CHC-C4B-C3B	-2.99	119.71	125.23
6	A	404	HEC	CBB-CAB-C3B	-2.97	104.36	112.42
6	A	404	HEC	CHA-C4D-C3D	-2.93	120.50	124.77
6	B	404	HEC	C1B-C2B-C3B	-2.91	103.92	106.98
6	B	404	HEC	O2D-CGD-O1D	-2.87	115.94	123.33
6	A	405	HEC	C4B-C3B-C2B	-2.80	102.82	106.89
6	B	405	HEC	CHA-C4D-ND	-2.79	121.42	124.42
6	A	405	HEC	CBA-CAA-C2A	-2.74	104.94	112.53
6	A	405	HEC	C2D-C1D-ND	2.74	112.99	109.84
6	B	405	HEC	CHB-C4A-C3A	-2.74	119.79	125.49
6	A	405	HEC	C3D-C4D-ND	2.72	112.98	110.35
6	B	405	HEC	CMA-C3A-C2A	2.69	133.42	126.15
6	A	405	HEC	C1D-C2D-C3D	-2.67	104.18	106.98
6	A	404	HEC	C2B-C1B-NB	2.63	112.94	109.90
6	A	405	HEC	C2C-C1C-NC	2.62	114.34	110.14
6	A	405	HEC	O1D-CGD-CBD	-2.62	114.80	123.09
6	B	404	HEC	CAB-C3B-C4B	2.60	128.17	124.79
6	B	404	HEC	CHB-C1B-NB	-2.59	121.64	124.42
6	A	404	HEC	CAC-C3C-C4C	-2.53	121.43	124.91
6	A	404	HEC	O2A-CGA-CBA	2.51	121.92	114.00
6	A	405	HEC	C4A-C3A-C2A	-2.50	103.26	106.97
6	A	404	HEC	CMA-C3A-C2A	2.47	132.84	126.15
6	B	405	HEC	CMC-C2C-C3C	2.46	130.85	125.62
6	B	405	HEC	CMD-C2D-C1D	2.42	128.81	125.03
6	B	405	HEC	O2A-CGA-CBA	2.41	121.63	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	405	HEC	CAC-C3C-C2C	2.39	130.68	126.89
6	A	404	HEC	CMD-C2D-C1D	2.37	128.74	125.03
6	B	405	HEC	C2C-C1C-NC	2.36	113.92	110.14
6	A	404	HEC	C2A-C1A-NA	2.33	112.58	110.32
6	A	404	HEC	C3A-C4A-NA	2.31	113.90	109.64
6	B	405	HEC	C4B-C3B-C2B	-2.29	103.55	106.89
6	A	405	HEC	CBB-CAB-C3B	-2.29	106.20	112.42
6	A	404	HEC	O2D-CGD-CBD	2.28	121.22	114.00
6	B	404	HEC	CAD-C3D-C4D	2.28	128.67	124.70
6	A	404	HEC	C1D-C2D-C3D	-2.27	104.59	106.98
6	B	404	HEC	C4B-NB-C1B	-2.23	102.57	105.21
6	B	405	HEC	CHC-C1C-C2C	-2.15	121.19	127.43
6	B	404	HEC	C4B-C3B-C2B	-2.15	103.77	106.89
6	B	404	HEC	C4D-C3D-C2D	-2.13	103.79	106.89
6	A	404	HEC	C4D-C3D-C2D	-2.12	103.80	106.89
6	A	405	HEC	CHC-C4B-NB	-2.11	121.75	124.37
6	B	404	HEC	C3C-C4C-NC	2.11	112.50	110.15
6	B	405	HEC	C1A-C2A-C3A	-2.11	104.33	107.11
6	B	404	HEC	CBA-CAA-C2A	-2.11	106.70	112.53
6	B	404	HEC	CHB-C4A-C3A	-2.10	121.11	125.49
6	A	404	HEC	CAD-C3D-C4D	2.06	128.28	124.70
6	A	404	HEC	C4A-C3A-C2A	-2.06	103.92	106.97
6	B	405	HEC	CAC-C3C-C4C	-2.04	122.11	124.91
6	A	405	HEC	CHA-C4D-ND	-2.04	122.23	124.42
6	A	404	HEC	CMC-C2C-C1C	2.03	128.51	125.42
6	A	405	HEC	C3A-C4A-NA	2.03	113.38	109.64
6	B	405	HEC	CAB-C3B-C2B	2.02	131.27	127.56
6	A	405	HEC	CHB-C1B-C2B	-2.01	121.85	125.03
6	A	404	HEC	CHB-C4A-C3A	-2.01	121.30	125.49
6	A	405	HEC	CAB-C3B-C4B	2.00	127.39	124.79

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	404	HEC	NA
6	A	405	HEC	NA
6	B	404	HEC	NA
6	B	405	HEC	NA

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	404	HEC	C4C-C3C-CAC-CBC
6	B	404	HEC	C2C-C3C-CAC-CBC
6	B	405	HEC	C2C-C3C-CAC-CBC
6	B	405	HEC	C4C-C3C-CAC-CBC
6	A	404	HEC	C2C-C3C-CAC-CBC
6	A	405	HEC	C4C-C3C-CAC-CBC
6	A	405	HEC	C2C-C3C-CAC-CBC
6	A	404	HEC	C4C-C3C-CAC-CBC
6	A	404	HEC	C2B-C3B-CAB-CBB
7	A	406	EDO	O1-C1-C2-O2
6	B	405	HEC	C2B-C3B-CAB-CBB
7	D	401	EDO	O1-C1-C2-O2
6	A	404	HEC	C4B-C3B-CAB-CBB
6	B	405	HEC	C4B-C3B-CAB-CBB
7	F	401	EDO	O1-C1-C2-O2
6	B	404	HEC	CAD-CBD-CGD-O2D
6	A	404	HEC	CAA-CBA-CGA-O2A
6	A	404	HEC	CAA-CBA-CGA-O1A
6	B	404	HEC	CAA-CBA-CGA-O2A
6	A	405	HEC	CAD-CBD-CGD-O1D
6	A	405	HEC	CAD-CBD-CGD-O2D
6	B	405	HEC	CAD-CBD-CGD-O2D
6	B	404	HEC	CAD-CBD-CGD-O1D
6	B	404	HEC	CAA-CBA-CGA-O1A
6	B	405	HEC	CAD-CBD-CGD-O1D

There are no ring outliers.

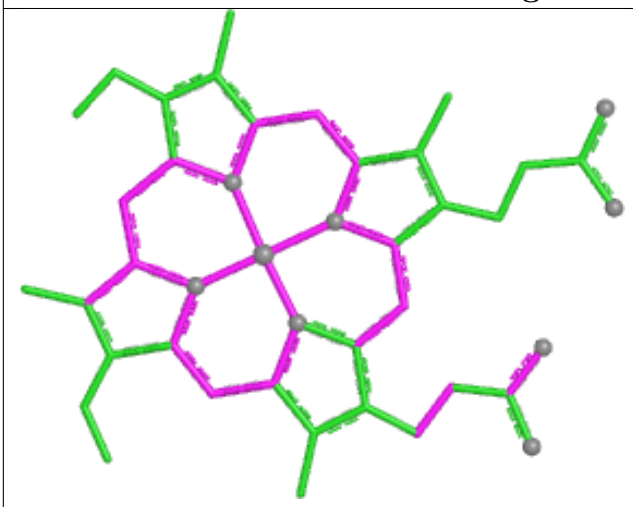
4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	401	EDO	4	0
7	A	406	EDO	2	0
7	F	401	EDO	3	0
6	B	404	HEC	1	0

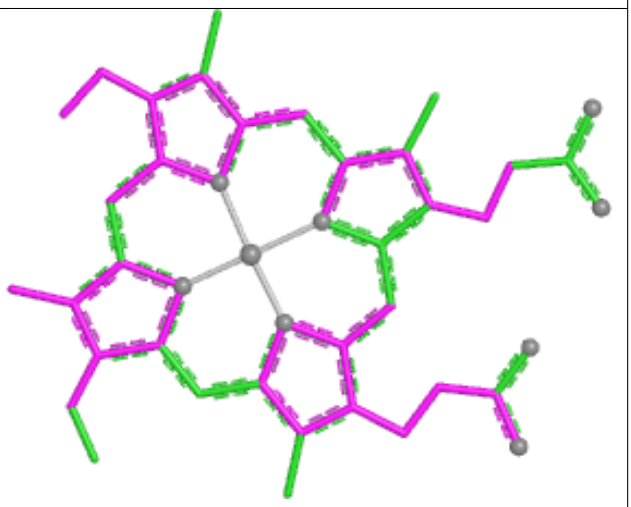
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

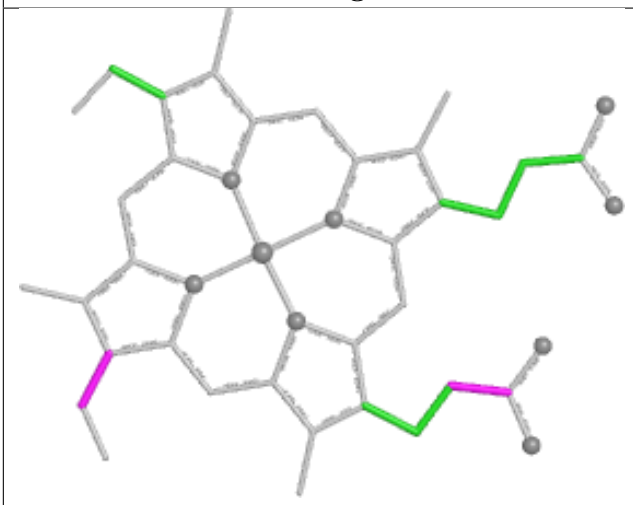
Ligand HEC A 405



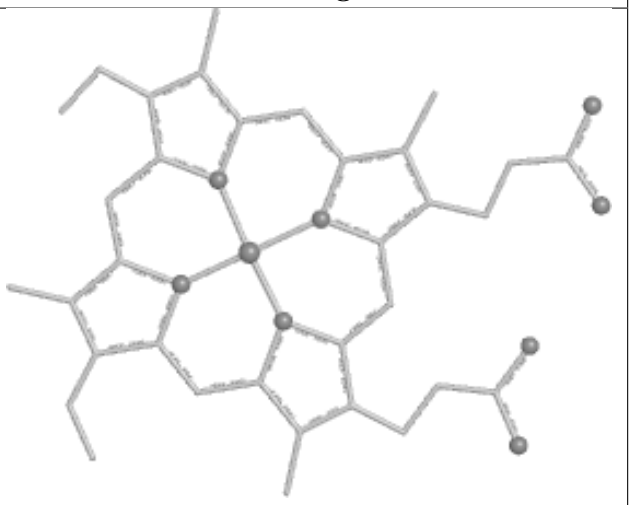
Bond lengths



Bond angles

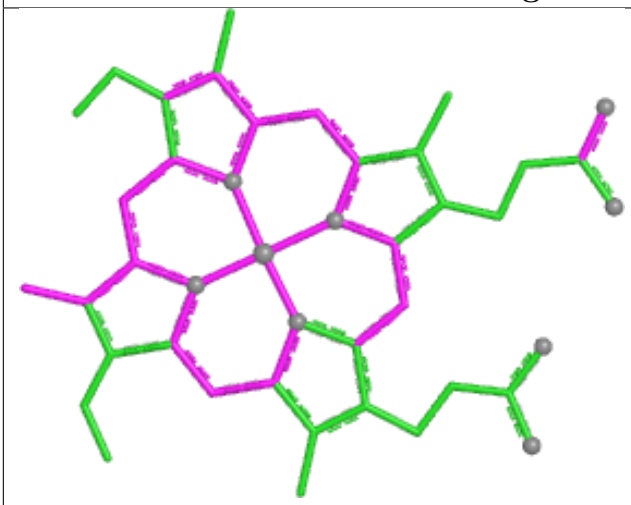


Torsions

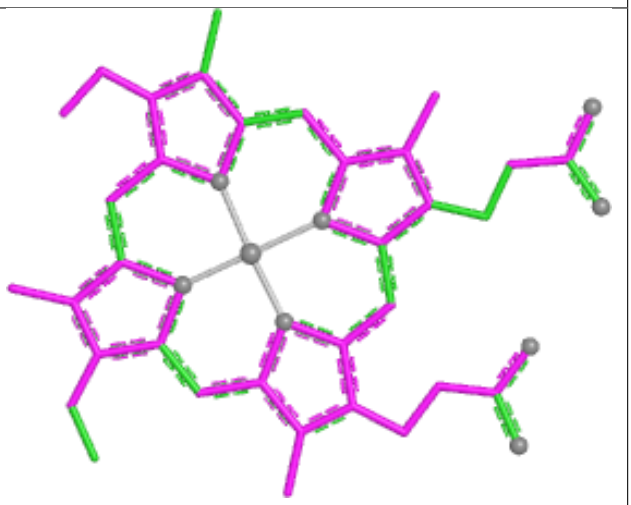


Rings

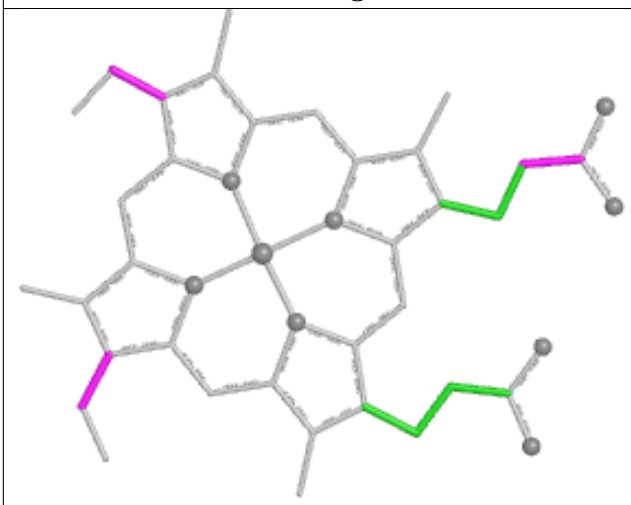
Ligand HEC A 404



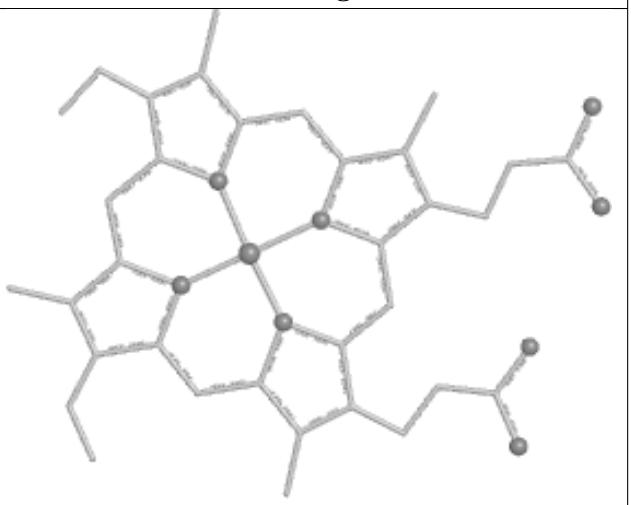
Bond lengths



Bond angles

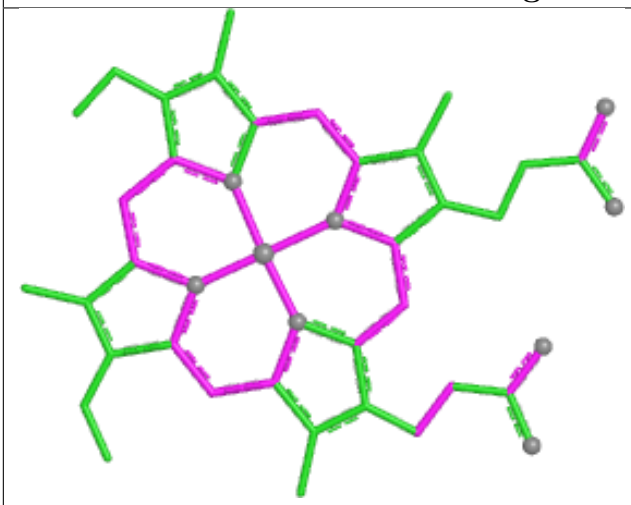


Torsions

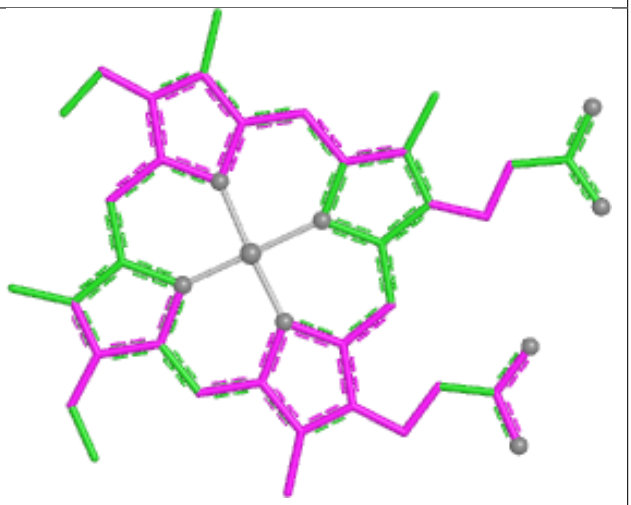


Rings

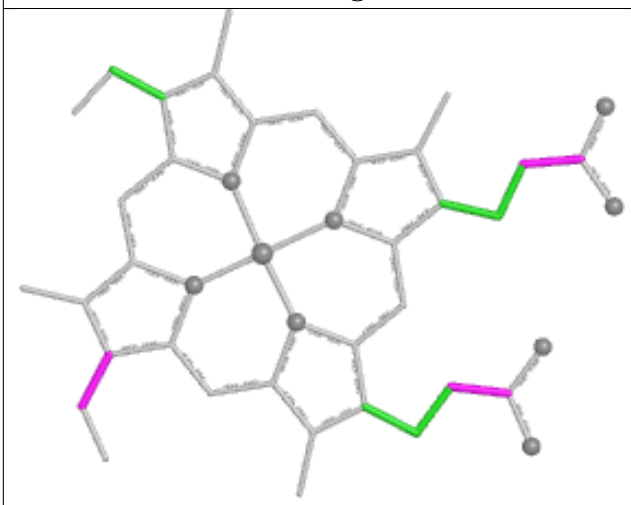
Ligand HEC B 404



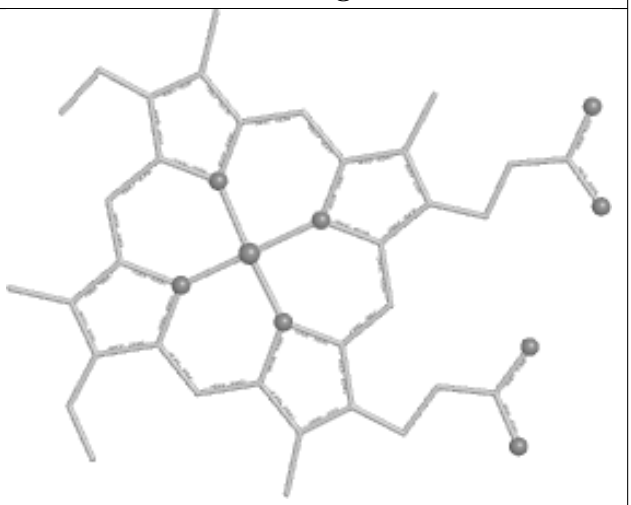
Bond lengths



Bond angles

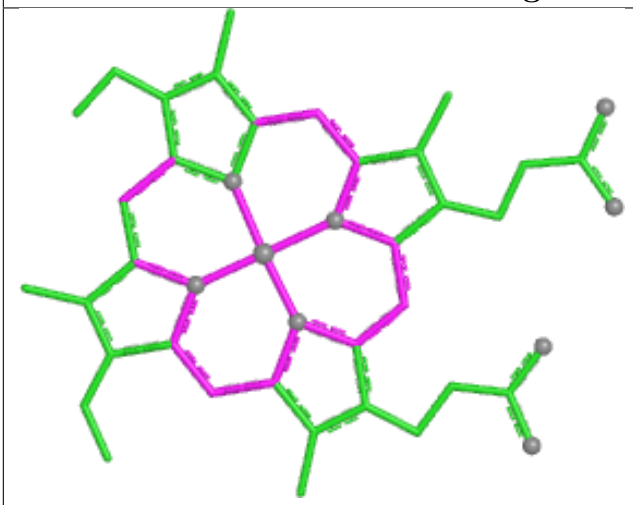


Torsions

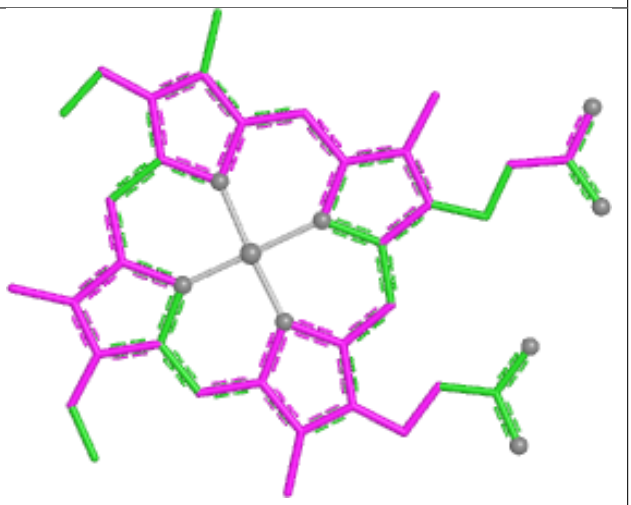


Rings

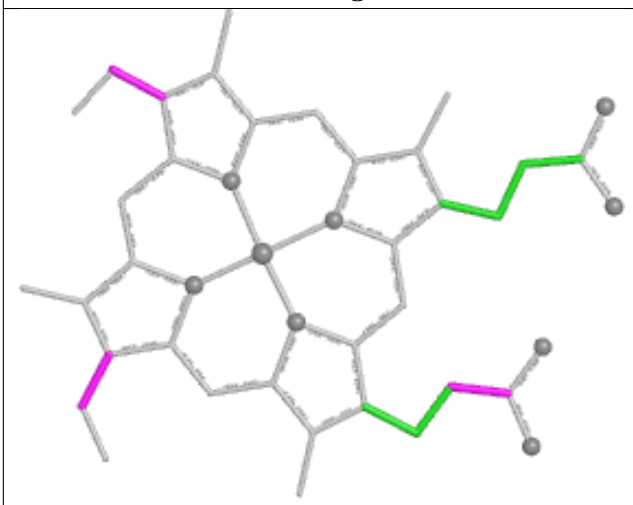
Ligand HEC B 405



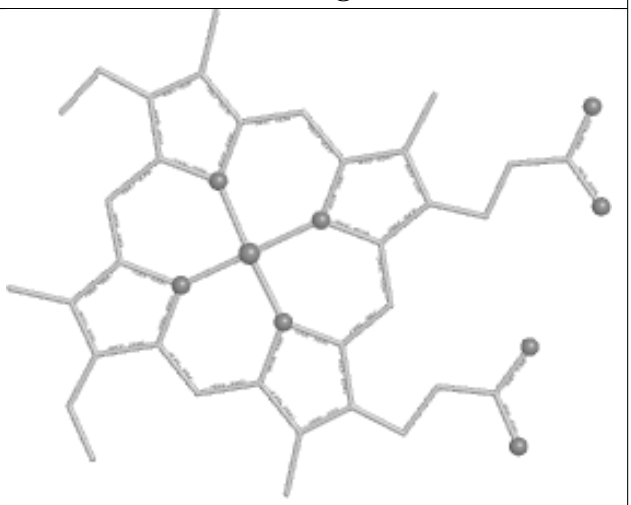
Bond lengths



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%)	-0.16	4 (1%)	78	82	22, 33, 46, 68	0
1	B	357/373 (95%)	-0.14	2 (0%)	85	89	14, 30, 50, 63	4 (1%)
2	C	124/137 (90%)	-0.36	1 (0%)	82	87	15, 26, 36, 52	1 (0%)
2	E	124/137 (90%)	-0.64	2 (1%)	70	77	14, 21, 31, 52	1 (0%)
3	D	375/386 (97%)	-0.47	1 (0%)	90	93	12, 25, 40, 60	4 (1%)
3	F	376/386 (97%)	-0.36	0	100	100	17, 29, 46, 66	2 (0%)
All	All	1710/1792 (95%)	-0.32	10 (0%)	85	89	12, 28, 45, 68	12 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	ALA	5.2
2	E	131	SER	4.6
1	B	363	ALA	3.3
2	E	7	THR	2.5
1	A	131	ALA	2.4
1	B	7	ASP	2.4
1	A	7	ASP	2.4
1	A	130	PRO	2.2
2	C	7	THR	2.1
3	D	208	THR	2.0

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	TOQ	C	57	16/17	0.97	0.06	22,26,29,29	0
2	TOQ	E	57	16/17	0.97	0.06	20,22,28,28	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

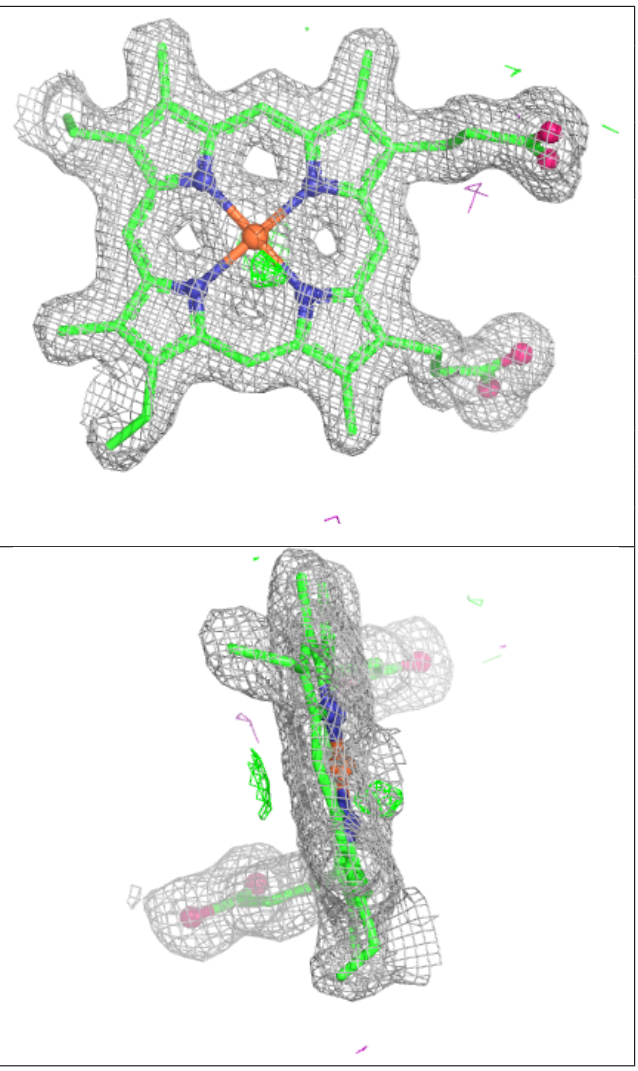
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	EDO	A	407	4/4	0.82	0.14	55,55,55,60	0
7	EDO	D	401	4/4	0.86	0.22	41,46,46,48	0
7	EDO	F	401	4/4	0.88	0.17	42,44,48,49	0
7	EDO	B	406	4/4	0.91	0.15	40,44,44,45	0
7	EDO	A	406	4/4	0.92	0.11	52,53,53,53	0
5	NA	A	402	1/1	0.95	0.07	34,34,34,34	0
5	NA	B	403	1/1	0.96	0.07	39,39,39,39	0
5	NA	A	403	1/1	0.96	0.06	40,40,40,40	0
5	NA	B	402	1/1	0.97	0.08	40,40,40,40	0
6	HEC	B	404	43/43	0.98	0.06	22,27,30,31	0
6	HEC	A	404	43/43	0.98	0.06	24,29,31,34	0
6	HEC	A	405	43/43	0.99	0.05	20,22,25,26	0
4	CA	B	401	1/1	0.99	0.03	25,25,25,25	0
6	HEC	B	405	43/43	0.99	0.05	16,20,24,24	0
4	CA	A	401	1/1	0.99	0.02	25,25,25,25	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.

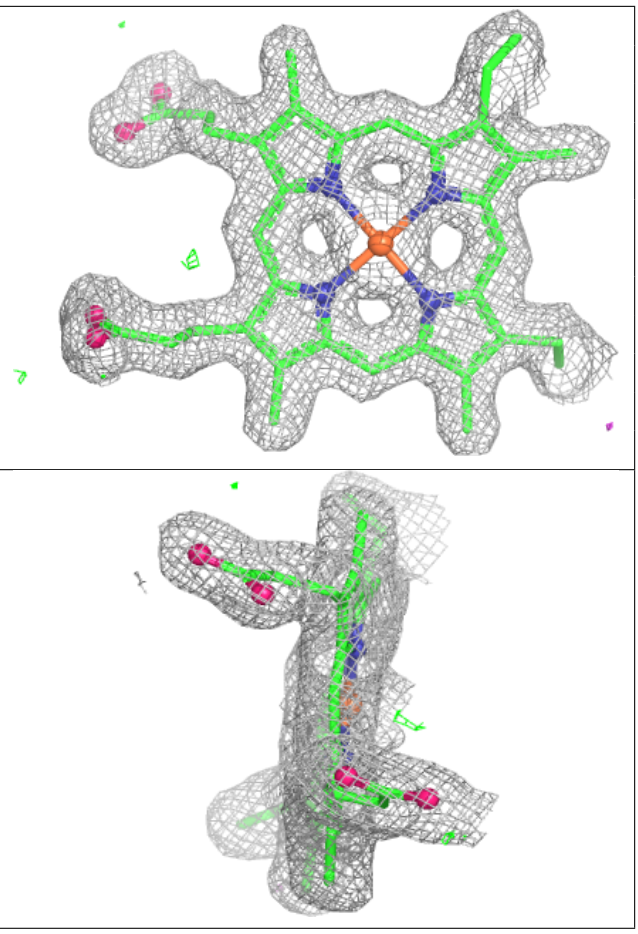
Electron density around HEC B 404:

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



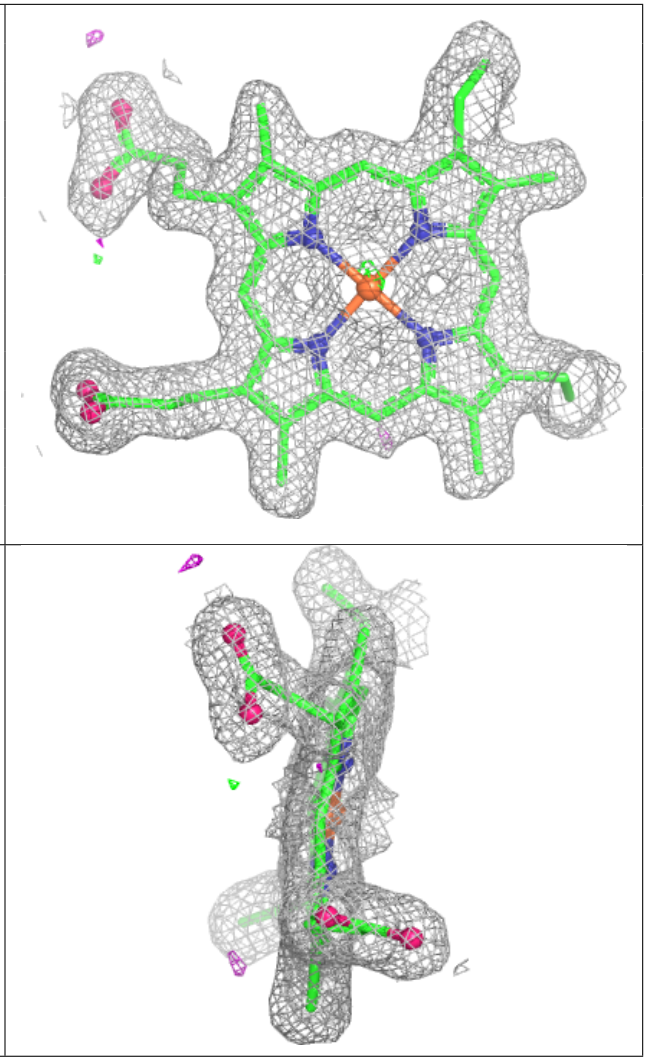
Electron density around HEC A 404:

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



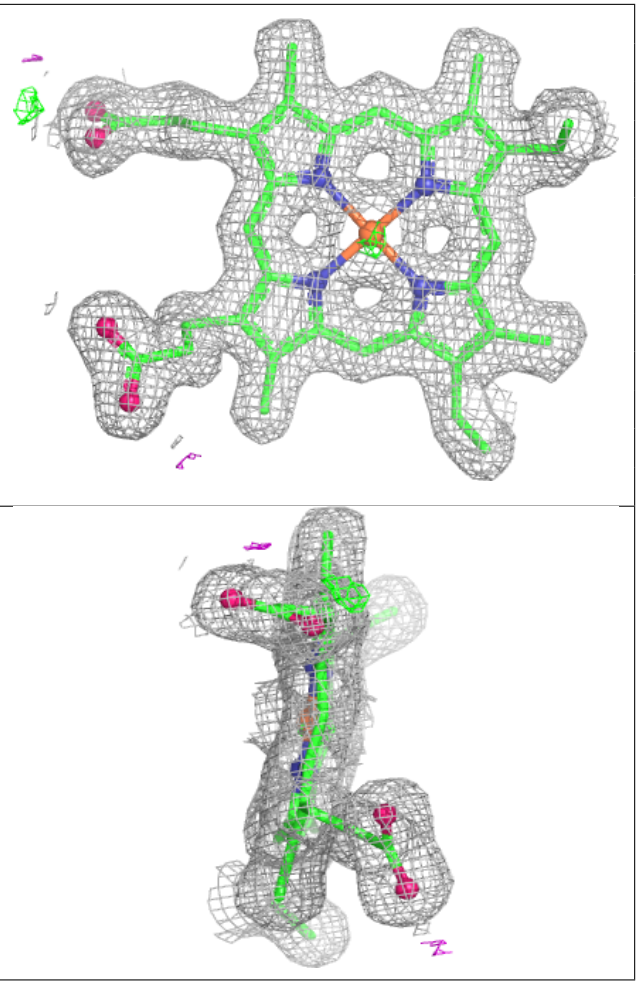
Electron density around HEC A 405:

$2mF_o$-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 405:

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.