Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 10:36 PM EDT

PDB ID	:	4FAN / pdb_00004fan
Title	:	Crystal Structure of WT MauG in Complex with Pre-Methylamine Dehydrogenase Aged 40 Days
Authors	:	Yukl, E.T.; Wilmot, C.M.
Deposited on	:	2012-05-22
Resolution	:	2.08 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:

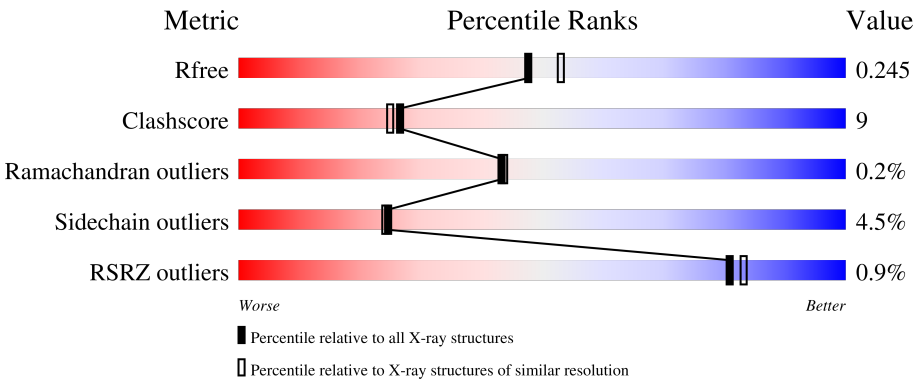
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.08 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	8172 (2.10-2.06)
Clashscore	190562	8714 (2.10-2.06)
Ramachandran outliers	187476	8641 (2.10-2.06)
Sidechain outliers	187428	8642 (2.10-2.06)
RSRZ outliers	180081	8177 (2.10-2.06)

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	69% 24% • 5%
1	B	373	81% 13% • •
2	C	137	2% 64% 26% • 6%
2	E	137	% 62% 26% • 9%
3	D	385	2% 71% 26% • •

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Mol	Chain	Length	Quality of chain
3	F	385	% 80% 17%

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
5	HEC	A	402	X	-	-	-
5	HEC	A	403	X	-	-	-
5	HEC	B	402	X	-	-	-
5	HEC	B	403	X	-	-	-

2 Entry composition (i)

There are 11 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	2777	1731	498	537	11	0	5	0
1	B	357	2768	1726	497	533	12	0	1	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	129	1009	622	175	197	15	0	3	0
2	E	125	972	601	162	193	16	0	4	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

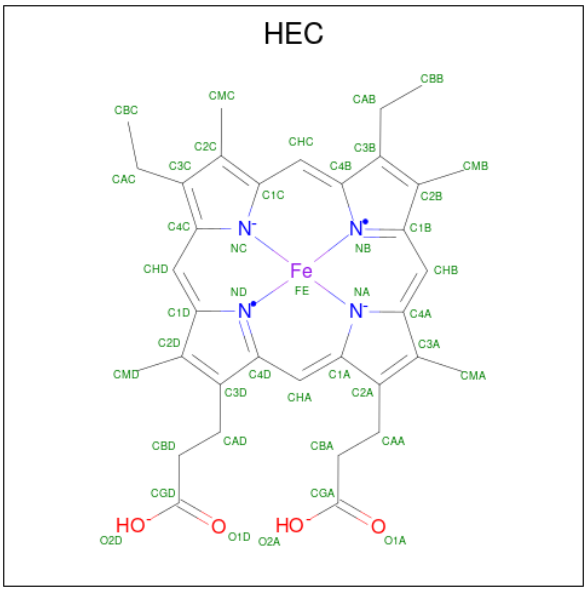
- Molecule 3 is a protein called Methylamine dehydrogenase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	D	376	2934	1859	503	563	9	0	2	0
			Total	C	N	O	S			
3	F	376	2954	1870	509	566	9	0	4	0

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

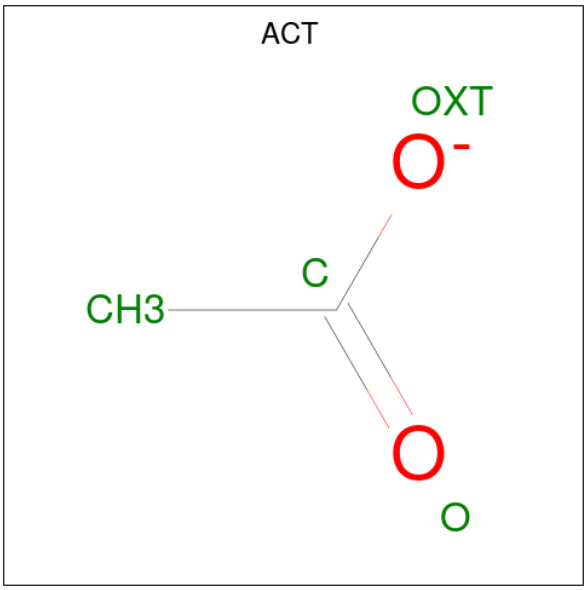
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
4	A	1	1	1	0	0
			Total	Ca		
4	B	1	1	1	0	0

- Molecule 5 is HEME C (CCD ID: HEC) (formula: $C_{34}H_{36}FeN_4O_4$).



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 ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).

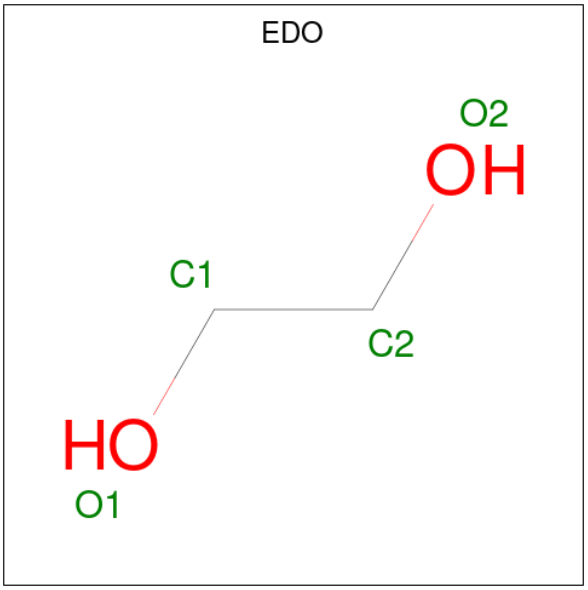


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	4	2	2	0	0

- Molecule 7 is SODIUM ION (CCD ID: NA) (formula: Na).

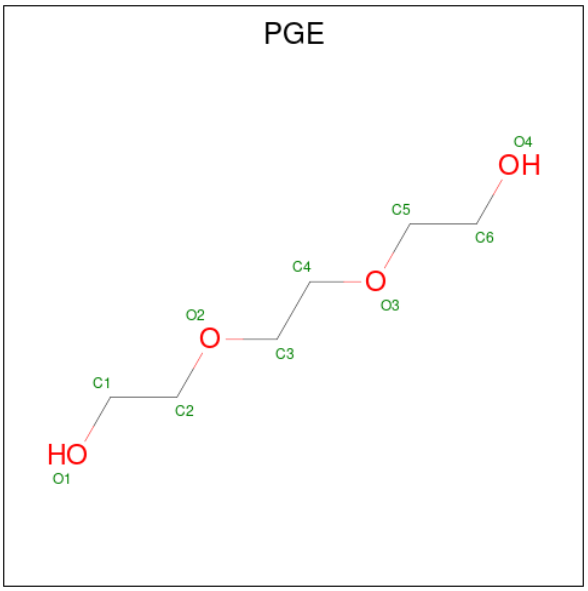
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
7	B	2	2	2	0	0

- Molecule 8 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



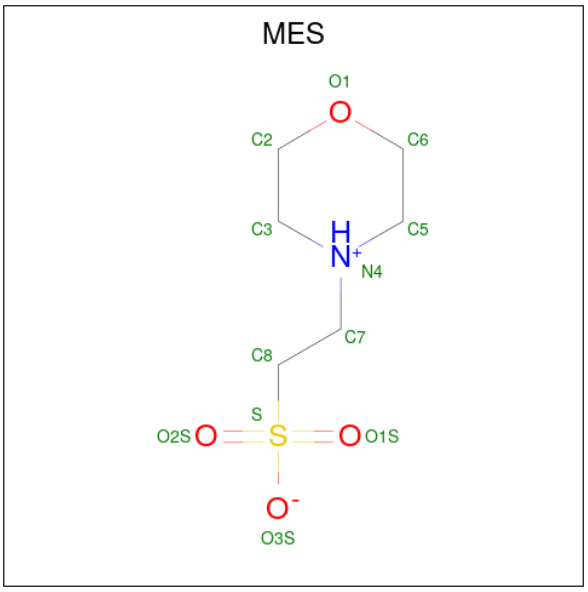
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
8	B	1	4	2	2	0	0

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C O 10 6 4	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	D	1	Total C N O S 12 6 1 4 1	0	0
10	F	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 11 is water.

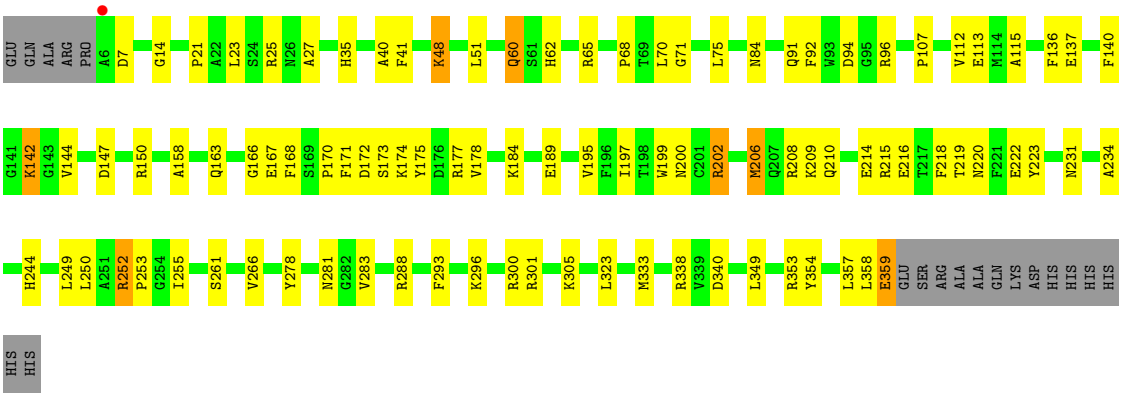
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
11	A	133	135	135	0	2
			Total	O		
11	B	243	246	246	0	3
			Total	O		
11	C	53	54	54	0	1
			Total	O		
11	D	149	152	152	0	3
			Total	O		
11	E	79	80	80	0	1
			Total	O		
11	F	268	270	270	0	2

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.

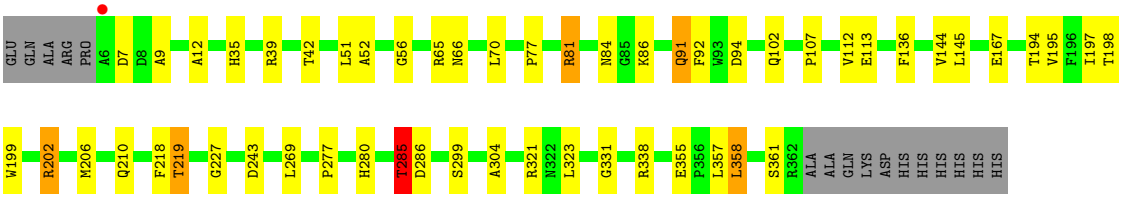
• Molecule 1: Methylamine utilization protein MauG

Chain A: 69% 24% • 5%



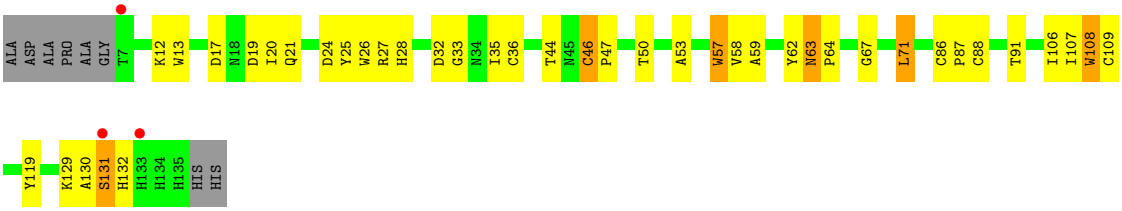
• Molecule 1: Methylamine utilization protein MauG

Chain B: 81% 13% • •



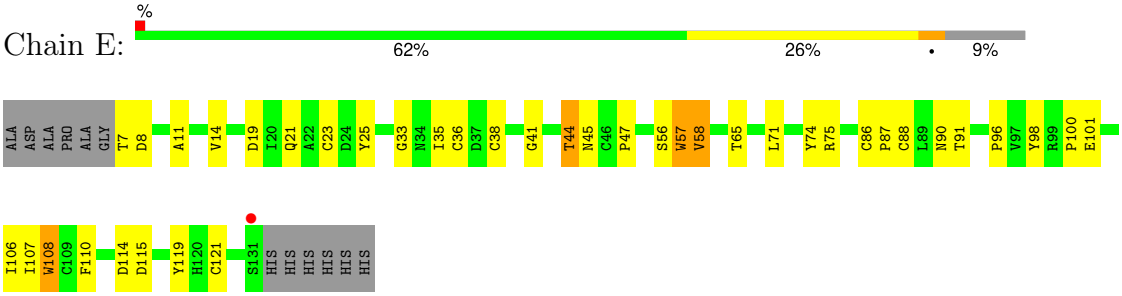
• Molecule 2: Methylamine dehydrogenase light chain

Chain C: 2% 64% 26% • 6%



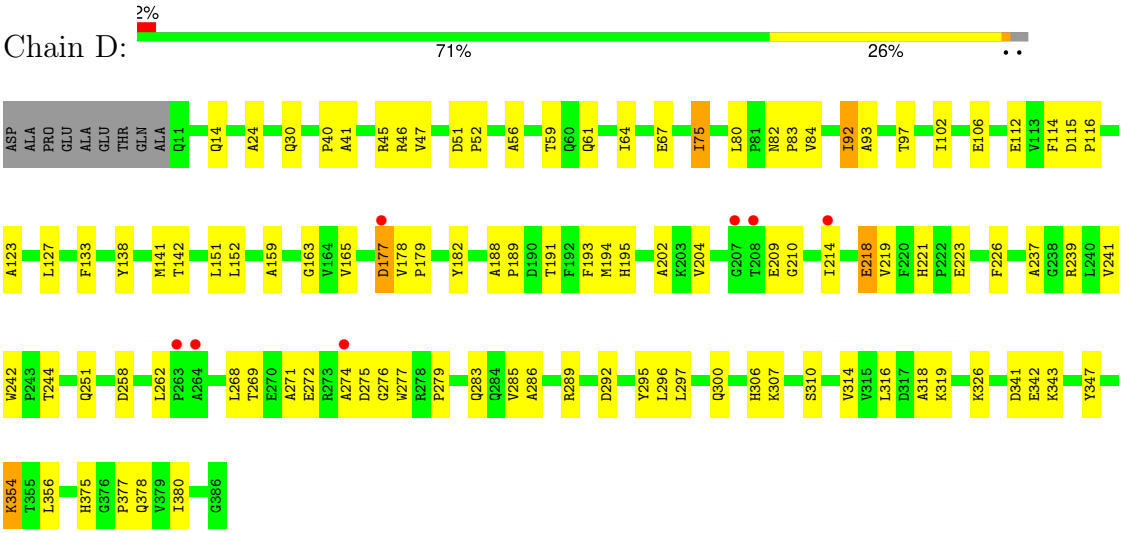
• Molecule 2: Methylamine dehydrogenase light chain

Chain E:



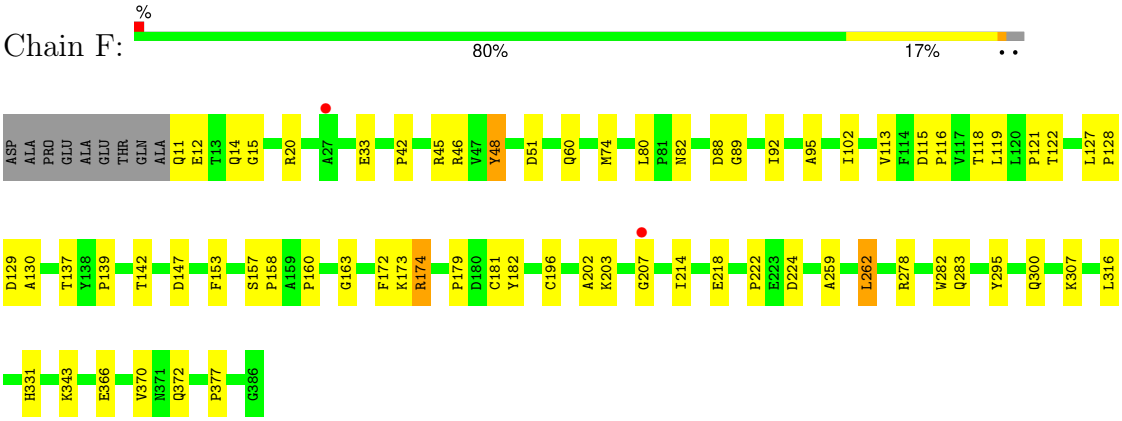
• Molecule 3: Methylamine dehydrogenase heavy chain

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 – 2.08 44.49 – 2.08	Depositor EDS
% Data completeness (in resolution range)	97.1 (44.49-2.08) 97.1 (44.49-2.08)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.170 , 0.234 0.186 , 0.245	Depositor DCC
R_{free} test set	5236 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.0	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	0.96	EDS
Total number of atoms	14569	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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: ACT, 0AF, PGE, MES, NA, EDO, HEC, 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	1.10	0/2844	1.12	3/3859 (0.1%)
1	B	1.33	5/2832 (0.2%)	1.19	3/3841 (0.1%)
2	C	1.19	1/1025 (0.1%)	1.18	5/1399 (0.4%)
2	E	1.47	4/990 (0.4%)	1.28	0/1352
3	D	1.11	3/3015 (0.1%)	1.13	8/4108 (0.2%)
3	F	1.36	8/3034 (0.3%)	1.23	7/4133 (0.2%)
All	All	1.25	21/13740 (0.2%)	1.18	26/18692 (0.1%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	370	VAL	CA-C	-6.77	1.44	1.52
3	F	80	LEU	N-CA	6.49	1.51	1.46
2	C	108	TRP	NE1-CE2	-6.47	1.30	1.37
3	D	24	ALA	CA-CB	6.36	1.63	1.53
3	F	130	ALA	C-O	-6.34	1.21	1.23
2	E	108	TRP	NE1-CE2	-6.07	1.30	1.37
2	E	106	ILE	CA-C	-6.01	1.45	1.52
3	F	95	ALA	CA-CB	-5.94	1.45	1.53
1	B	218	PHE	CA-C	-5.92	1.45	1.53
3	F	130	ALA	N-CA	5.87	1.50	1.46
3	D	83	PRO	N-CA	-5.60	1.40	1.46
3	F	137	THR	CA-CB	-5.59	1.45	1.53
2	E	44	THR	CA-C	5.49	1.59	1.52
1	B	91	GLN	C-O	5.42	1.30	1.23
2	E	11	ALA	CA-CB	5.32	1.62	1.53
3	D	80	LEU	C-O	5.30	1.26	1.23
3	F	130	ALA	CA-CB	-5.18	1.49	1.52
1	B	219	THR	CA-CB	5.16	1.62	1.53
3	F	259	ALA	CA-CB	-5.15	1.46	1.53
1	B	9	ALA	CA-C	5.03	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	227	GLY	N-CA	5.03	1.52	1.45

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	262	LEU	CA-C-N	-7.92	111.86	119.85
3	F	262	LEU	C-N-CA	-7.92	111.86	119.85
3	F	122	THR	N-CA-C	-7.66	103.77	113.72
3	F	118	THR	N-CA-C	-6.88	104.70	113.23
1	A	200	ASN	N-CA-C	6.85	119.58	111.71
2	C	63	ASN	CA-C-N	6.29	125.97	119.56
2	C	63	ASN	C-N-CA	6.29	125.97	119.56
2	C	132	HIS	N-CA-C	6.09	118.16	110.24
3	D	46	ARG	CA-C-N	-5.90	114.74	122.94
3	D	46	ARG	C-N-CA	-5.90	114.74	122.94
1	A	244	HIS	N-CA-C	5.89	118.80	110.25
1	B	285	THR	N-CA-C	5.54	117.39	111.36
3	D	115	ASP	CA-C-N	-5.53	114.32	120.45
3	D	115	ASP	C-N-CA	-5.53	114.32	120.45
1	B	12	ALA	N-CA-C	-5.36	105.52	111.36
1	A	278	TYR	N-CA-C	5.32	117.95	109.81
3	D	56	ALA	N-CA-C	-5.25	103.10	110.50
1	B	7	ASP	N-CA-C	-5.09	105.73	111.28
3	D	177	ASP	CB-CA-C	5.09	118.14	109.84
3	F	127	LEU	CA-C-N	-5.08	114.72	119.85
3	F	127	LEU	C-N-CA	-5.08	114.72	119.85
3	F	48	TYR	N-CA-C	-5.07	101.14	109.40
3	D	116	PRO	CA-C-N	-5.01	117.80	122.66
3	D	116	PRO	C-N-CA	-5.01	117.80	122.66
2	C	46	CYS	CA-C-N	-5.01	115.22	120.38
2	C	46	CYS	C-N-CA	-5.01	115.22	120.38

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	2777	0	2642	65	0
1	B	2768	0	2639	35	0
2	C	1009	0	898	34	0
2	E	972	0	878	35	0
3	D	2934	0	2814	60	0
3	F	2954	0	2835	39	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	86	0	60	4	0
5	B	86	0	60	3	0
6	A	4	0	3	0	0
7	B	2	0	0	0	0
8	B	4	0	6	0	0
9	B	10	0	14	1	0
10	D	12	0	12	0	0
10	F	12	0	12	0	0
11	A	135	0	0	3	0
11	B	246	0	0	2	0
11	C	54	0	0	2	0
11	D	152	0	0	4	0
11	E	80	0	0	3	0
11	F	270	0	0	3	0
All	All	14569	0	12873	246	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 9.

All (246) 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:285:THR:HG22	1:B:286:ASP:OD1	1.52	1.08
3:F:174[A]:ARG:HH21	3:F:174[A]:ARG:HG3	0.86	1.01
1:B:210:GLN:HE22	2:E:44:THR:HG21	1.24	1.00
3:F:174[A]:ARG:HH21	3:F:174[A]:ARG:CG	1.76	0.98
1:A:210:GLN:HE22	2:C:44:THR:HG21	1.27	0.97
2:E:35:ILE:HD12	2:E:86[B]:CYS:SG	2.08	0.94
2:C:57:0AF:HBC1	2:C:108:TRP:NE1	1.84	0.93
3:F:174[A]:ARG:HG3	3:F:174[A]:ARG:NH2	1.62	0.92
1:A:252:ARG:HG3	1:A:255:ILE:HG12	1.53	0.91
2:E:57:0AF:HBC1	2:E:108:TRP:NE1	1.86	0.91
1:B:197:ILE:HG22	1:B:206[B]:MET:HE1	1.52	0.89
2:C:36[B]:CYS:SG	2:C:47:PRO:HD3	2.12	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:57:0AF:HBC1	2:E:108:TRP:HE1	1.43	0.83
3:D:297:LEU:HD22	3:D:310:SER:HB2	1.59	0.81
1:B:210:GLN:NE2	2:E:44:THR:HG21	1.98	0.79
3:D:237:ALA:HB2	3:D:289:ARG:HG3	1.66	0.76
3:D:14:GLN:HE21	2:E:21:GLN:HE22	1.33	0.75
1:B:202:ARG:HB2	1:B:206[B]:MET:HE2	1.68	0.74
1:A:107:PRO:HG3	11:A:535[B]:HOH:O	1.87	0.73
2:E:56:SER:HB2	2:E:74:TYR:O	1.87	0.73
1:A:252:ARG:CG	1:A:255:ILE:HG12	2.18	0.73
3:D:314:VAL:HG12	3:D:326:LYS:HG3	1.71	0.72
1:B:113:GLU:HG2	5:B:402:HEC:HBC2	1.71	0.72
2:E:36[B]:CYS:SG	2:E:41:GLY:HA3	2.29	0.72
3:F:181[B]:CYS:HB3	3:F:196:CYS:SG	2.29	0.72
1:B:81:ARG:HD3	11:B:655:HOH:O	1.90	0.71
3:D:269:THR:OG1	3:D:272:GLU:HB2	1.91	0.71
1:A:210:GLN:NE2	2:C:44:THR:HG21	2.06	0.71
1:A:48:LYS:H	1:A:62:HIS:HE1	1.39	0.70
2:E:38:CYS:SG	2:E:86[B]:CYS:HB2	2.30	0.70
1:B:199:TRP:O	1:B:202:ARG:HD3	1.95	0.67
3:D:195:HIS:HD2	11:D:618:HOH:O	1.77	0.67
1:A:174:LYS:HE2	1:A:189:GLU:OE1	1.95	0.66
3:D:195:HIS:HE1	3:D:221:HIS:NE2	1.93	0.65
1:A:250:LEU:HD22	1:A:261:SER:HB2	1.78	0.65
2:E:36[B]:CYS:SG	2:E:45:ASN:O	2.55	0.64
1:B:39:ARG:HG3	1:B:42:THR:OG1	1.98	0.64
2:E:36[B]:CYS:SG	2:E:47:PRO:HD3	2.37	0.64
1:A:48:LYS:H	1:A:62:HIS:CE1	2.17	0.62
3:D:275:ASP:HB2	11:D:602:HOH:O	1.97	0.62
3:F:45:ARG:NH2	3:F:343:LYS:O	2.33	0.62
1:A:209:LYS:HE3	3:F:33:GLU:OE1	1.99	0.61
3:F:82:ASN:HB3	3:F:142:THR:HB	1.81	0.61
3:F:12:GLU:CD	3:F:20:ARG:HH11	2.09	0.61
2:C:57:0AF:HBC1	2:C:108:TRP:HE1	1.61	0.60
2:C:130:ALA:O	2:C:131[A]:SER:HB3	2.01	0.60
1:B:197:ILE:O	1:B:202:ARG:HD2	2.01	0.59
2:E:56:SER:CB	2:E:74:TYR:O	2.50	0.59
1:A:171:PHE:CZ	1:A:215[B]:ARG:HG3	2.38	0.59
2:E:36[B]:CYS:HB2	2:E:121:CYS:SG	2.43	0.59
1:B:84:ASN:HB2	1:B:86:LYS:HG2	1.84	0.59
1:B:39:ARG:HG3	1:B:39:ARG:O	2.03	0.59
1:A:40:ALA:HA	1:A:354:TYR:CZ	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:51:ASP:HA	3:F:377:PRO:HA	1.84	0.58
3:D:51:ASP:HA	3:D:377:PRO:HA	1.85	0.58
1:A:60:GLN:O	1:A:62:HIS:HD2	1.87	0.58
1:A:70:LEU:HD13	1:A:163:GLN:NE2	2.19	0.57
1:A:301:ARG:CZ	1:A:333:MET:HE1	2.34	0.57
1:A:197:ILE:C	1:A:202:ARG:HG2	2.29	0.57
2:E:21:GLN:O	2:E:86[B]:CYS:SG	2.63	0.57
1:A:48:LYS:HB2	1:A:62:HIS:CE1	2.40	0.56
3:D:341:ASP:OD1	3:D:341:ASP:N	2.39	0.55
1:B:299:SER:HB3	1:B:304:ALA:CB	2.37	0.55
3:F:89:GLY:HA2	11:F:626:HOH:O	2.06	0.55
1:A:206:MET:HE2	1:A:216:GLU:CD	2.31	0.55
2:E:96:PRO:HB2	2:E:98:TYR:CE1	2.42	0.55
2:C:58:VAL:HG22	2:C:59:ALA:N	2.22	0.54
1:A:96:ARG:HA	1:A:252:ARG:HB2	1.89	0.54
2:C:107:ILE:HD12	2:C:119:TYR:HB2	1.90	0.54
1:A:68:PRO:HG2	5:A:402:HEC:HBA1	1.90	0.54
2:E:38:CYS:SG	2:E:86[B]:CYS:CB	2.94	0.54
3:D:276:GLY:O	3:D:300:GLN:HA	2.07	0.54
2:C:91:THR:HB	3:D:306:HIS:CE1	2.43	0.53
2:C:86:CYS:H	3:F:372[A]:GLN:HE22	1.57	0.53
3:D:178:VAL:HG21	3:D:194:MET:HE1	1.91	0.53
2:C:32:ASP:C	2:C:32:ASP:OD1	2.52	0.53
1:B:198:THR:HG22	2:E:58:VAL:HG13	1.91	0.53
2:E:101[B]:GLU:HA	11:E:254:HOH:O	2.08	0.52
1:A:173:SER:O	1:A:177:ARG:HG3	2.09	0.52
2:C:21:GLN:HE22	3:F:14:GLN:HE21	1.57	0.52
1:A:113:GLU:HG2	5:A:402:HEC:HBC2	1.92	0.52
3:F:331:HIS:HE1	3:F:366:GLU:OE1	1.92	0.52
2:C:57:0AF:HBC1	2:C:108:TRP:CE2	2.45	0.52
2:C:71:LEU:HD13	2:C:130:ALA:HA	1.93	0.51
1:B:243:ASP:OD1	1:B:243:ASP:N	2.43	0.51
1:A:301:ARG:HD2	1:A:333:MET:SD	2.50	0.51
3:F:153:PHE:CZ	3:F:163:GLY:HA3	2.45	0.51
3:D:271:ALA:O	3:D:274:ALA:HB3	2.11	0.51
3:D:138:TYR:HB2	3:D:141:MET:HG2	1.93	0.51
3:D:218[A]:GLU:HG3	3:D:219:VAL:O	2.11	0.51
1:B:65:ARG:HH12	1:B:94:ASP:CG	2.18	0.51
1:A:147:ASP:OD2	1:A:150:ARG:HG3	2.11	0.51
2:E:75:ARG:HA	11:E:268:HOH:O	2.10	0.50
2:E:100:PRO:O	2:E:108:TRP:HZ2	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:45:ARG:NH1	3:D:67:GLU:OE1	2.45	0.50
1:B:39:ARG:NH1	1:B:51:LEU:HD23	2.27	0.50
2:C:46:CYS:HB3	2:C:50:THR:OG1	2.12	0.50
3:D:30:GLN:NE2	11:D:537:HOH:O	2.43	0.50
2:C:20:ILE:HG22	2:C:25:TYR:CZ	2.46	0.50
3:D:251:GLN:NE2	3:D:318:ALA:O	2.43	0.50
3:F:115:ASP:O	3:F:119:LEU:HA	2.12	0.49
1:A:252:ARG:HG3	1:A:255:ILE:CG1	2.34	0.49
1:B:35:HIS:CE1	1:B:70:LEU:HD21	2.47	0.49
1:A:293:PHE:O	1:A:296:LYS:HG2	2.13	0.49
3:F:196:CYS:SG	3:F:202:ALA:HB2	2.52	0.49
1:B:136:PHE:HB3	1:B:144:VAL:HG11	1.94	0.49
1:A:174:LYS:O	1:A:178:VAL:HG23	2.13	0.49
1:A:199:TRP:O	1:A:202:ARG:HG3	2.13	0.49
1:A:281:ASN:OD1	1:A:283:VAL:HG12	2.13	0.49
3:D:342:GLU:HA	11:D:631:HOH:O	2.13	0.49
1:A:222:GLU:O	1:A:266:VAL:HG23	2.13	0.48
1:B:52:ALA:O	1:B:66:ASN:HA	2.13	0.48
1:B:195:VAL:HG21	1:B:338:ARG:HG2	1.95	0.48
1:B:355:GLU:O	1:B:358:LEU:HB2	2.13	0.48
3:F:207:GLY:HA2	11:F:730:HOH:O	2.14	0.48
1:A:35:HIS:CE1	1:A:70:LEU:HD21	2.49	0.48
3:D:45:ARG:NH2	3:D:343:LYS:O	2.47	0.48
3:D:92:ILE:HG12	3:D:114:PHE:HB2	1.96	0.48
1:A:333:MET:HE2	3:D:159:ALA:HB2	1.96	0.47
2:E:91:THR:HG21	3:F:307:LYS:HD2	1.97	0.47
3:D:188:ALA:HB1	3:D:189:PRO:HD2	1.95	0.47
2:C:62:TYR:CE1	2:C:67:GLY:HA2	2.50	0.47
3:D:14:GLN:HG3	2:E:21:GLN:NE2	2.30	0.46
2:C:106:ILE:HG12	3:D:133:PHE:CZ	2.50	0.46
1:A:333:MET:HE2	3:D:159:ALA:CB	2.45	0.46
2:C:106:ILE:HG12	3:D:133:PHE:HZ	1.79	0.46
2:E:36[B]:CYS:HA	2:E:121:CYS:SG	2.55	0.46
1:A:140:PHE:O	1:A:150:ARG:NH2	2.48	0.46
3:D:179:PRO:HD3	3:D:214:ILE:HD13	1.98	0.46
1:A:65:ARG:HH12	1:A:94:ASP:CG	2.24	0.46
1:A:202:ARG:HG3	1:A:202:ARG:H	1.60	0.46
2:C:33:GLY:O	2:C:87:PRO:HA	2.16	0.46
3:D:152:LEU:HA	3:D:163:GLY:O	2.15	0.46
2:C:62:TYR:CZ	2:C:67:GLY:HA2	2.51	0.46
1:A:172:ASP:O	1:A:177:ARG:NH1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:60:GLN:NE2	3:F:74:MET:HE1	2.31	0.46
3:F:179:PRO:HD3	3:F:214:ILE:HD13	1.97	0.46
3:D:354:LYS:HE2	3:D:375:HIS:O	2.16	0.46
1:A:199:TRP:HH2	1:A:333:MET:O	1.99	0.46
2:C:91:THR:HG21	3:D:307:LYS:HD2	1.98	0.46
3:D:292:ASP:OD2	3:D:319:LYS:HG3	2.16	0.46
3:D:283:GLN:OE1	3:D:380:ILE:N	2.39	0.45
2:C:86:CYS:H	3:F:372[A]:GLN:NE2	2.14	0.45
1:A:175:TYR:C	1:A:175:TYR:CD2	2.94	0.45
3:F:88:ASP:OD1	3:F:88:ASP:C	2.60	0.45
2:C:19:ASP:OD1	3:F:15:GLY:HA3	2.16	0.45
1:A:359:GLU:CD	1:A:359:GLU:N	2.75	0.45
1:B:86:LYS:HE2	11:B:703:HOH:O	2.17	0.45
5:A:403:HEC:HBC3	5:A:403:HEC:CMC	2.46	0.45
2:C:13:TRP:HZ3	11:C:221:HOH:O	1.99	0.45
1:A:91:GLN:O	1:A:92:PHE:HB2	2.17	0.44
1:A:231:ASN:HB3	1:A:234:ALA:HB3	1.98	0.44
3:D:251:GLN:HB3	3:D:262:LEU:HD22	1.99	0.44
1:A:147:ASP:OD1	1:A:147:ASP:C	2.59	0.44
2:E:14:VAL:HG22	11:E:257:HOH:O	2.18	0.44
3:D:277:TRP:CE2	3:D:300:GLN:HG3	2.52	0.44
1:A:94:ASP:OD2	1:A:96:ARG:HG2	2.17	0.44
1:A:296:LYS:NZ	11:A:561:HOH:O	2.50	0.44
3:D:82:ASN:HB3	3:D:142:THR:HB	2.00	0.44
3:F:147:ASP:OD1	3:F:147:ASP:C	2.61	0.44
3:F:42:PRO:HG3	3:F:116:PRO:HB2	1.99	0.44
3:D:51:ASP:O	3:D:59:THR:HB	2.18	0.44
2:C:35:ILE:HD11	2:C:88[A]:CYS:SG	2.58	0.44
3:D:151:LEU:HB3	3:D:165:VAL:HB	2.00	0.43
3:D:271:ALA:O	3:D:274:ALA:N	2.51	0.43
1:A:252:ARG:CD	1:A:255:ILE:HG12	2.47	0.43
1:A:21:PRO:O	1:A:27:ALA:HA	2.18	0.43
1:A:195:VAL:HG21	1:A:338:ARG:HG2	2.00	0.43
3:D:209:GLU:HG2	3:D:210:GLY:N	2.34	0.43
2:E:7:THR:HG23	2:E:8:ASP:H	1.83	0.43
1:A:41:PHE:HB2	1:A:70:LEU:H	1.84	0.43
1:A:252:ARG:HA	1:A:253:PRO:HD3	1.90	0.43
3:D:40:PRO:O	3:D:41:ALA:C	2.60	0.43
3:D:142:THR:HG23	3:D:151:LEU:HD21	2.01	0.43
2:E:114:ASP:O	2:E:115:ASP:HB2	2.17	0.43
3:D:193:PHE:HA	3:D:202:ALA:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:25:TYR:CE2	2:C:27:ARG:HG3	2.54	0.43
1:A:71:GLY:HA2	1:A:168:PHE:O	2.19	0.43
3:D:286:ALA:HB3	3:D:295:TYR:HB2	2.00	0.43
1:B:51:LEU:HB3	1:B:277:PRO:HD3	2.01	0.42
3:D:226:PHE:O	3:D:244:THR:HA	2.19	0.42
3:D:347:TYR:HB3	3:D:356:LEU:HD11	2.00	0.42
3:F:128:PRO:O	3:F:129:ASP:HB2	2.19	0.42
3:F:203:LYS:O	3:F:214:ILE:HA	2.19	0.42
2:C:17:ASP:OD1	2:C:26:TRP:CD1	2.72	0.42
1:B:136:PHE:CG	1:B:145:LEU:HD21	2.55	0.42
1:B:280:HIS:HD1	5:B:403:HEC:CGD	2.32	0.42
3:D:239:ARG:HD2	3:D:251:GLN:OE1	2.18	0.42
1:A:163:GLN:HA	1:A:168:PHE:CD1	2.55	0.42
3:F:295:TYR:CD1	3:F:295:TYR:N	2.88	0.42
1:A:206:MET:O	1:A:220:ASN:HB3	2.19	0.42
1:A:359:GLU:HA	11:A:600:HOH:O	2.18	0.42
1:B:331:GLY:O	3:F:158:PRO:HA	2.19	0.42
1:A:25:ARG:HB2	1:A:115:ALA:O	2.20	0.42
2:C:53:ALA:HB2	2:C:109:CYS:HA	2.02	0.42
1:A:92:PHE:CD1	5:A:402:HEC:HBD1	2.55	0.42
1:B:77:PRO:HB3	9:B:406:PGE:H3	2.01	0.42
2:C:25:TYR:HB3	2:C:28:HIS:CD2	2.55	0.42
3:F:282:TRP:HB3	3:F:283:GLN:H	1.73	0.42
1:B:84:ASN:CB	1:B:86:LYS:HG2	2.48	0.42
1:A:60:GLN:O	1:A:62:HIS:CD2	2.70	0.41
1:B:91:GLN:O	1:B:92:PHE:HB2	2.19	0.41
3:F:46:ARG:HD3	3:F:48:TYR:CZ	2.55	0.41
1:A:137:GLU:OE1	1:A:142:LYS:HE2	2.20	0.41
2:E:33:GLY:O	2:E:87:PRO:HA	2.20	0.41
3:F:278:ARG:NH1	11:F:742:HOH:O	2.38	0.41
1:A:218:PHE:CD1	1:A:349:LEU:HD13	2.55	0.41
1:B:210:GLN:HE22	2:E:44:THR:CG2	2.12	0.41
3:D:47:VAL:HG13	3:D:64:ILE:HB	2.03	0.41
3:F:222:PRO:HB2	3:F:224:ASP:OD1	2.20	0.41
1:A:288:ARG:NH1	1:A:340:ASP:OD1	2.53	0.41
3:D:268:LEU:HD22	3:D:277:TRP:HB3	2.01	0.41
3:D:285:VAL:HA	3:D:295:TYR:O	2.20	0.41
1:B:107:PRO:HG2	5:B:402:HEC:C4B	2.51	0.41
3:D:61:GLN:HB3	3:D:75:ILE:HB	2.02	0.41
2:C:13:TRP:NE1	2:C:24:ASP:HA	2.36	0.41
3:D:112:GLU:HA	3:D:123:ALA:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:23:CYS:O	2:E:90:ASN:ND2	2.50	0.41
2:E:57:0AF:HZ3	2:E:108:TRP:HB2	2.03	0.41
2:E:110:PHE:CE1	3:F:157:SER:HB2	2.56	0.41
3:F:113:VAL:O	3:F:121:PRO:HA	2.21	0.41
1:A:14:GLY:N	1:A:158:ALA:HB1	2.36	0.41
3:D:84:VAL:HG23	3:D:93:ALA:HB3	2.02	0.41
2:E:107:ILE:HD12	2:E:119:TYR:HB2	2.03	0.41
1:B:194:THR:HG21	2:E:101[A]:GLU:HG3	2.03	0.40
2:C:12:LYS:NZ	11:C:208:HOH:O	2.47	0.40
1:B:299:SER:HB3	1:B:304:ALA:HB2	2.02	0.40
3:D:84:VAL:CG2	3:D:93:ALA:HB3	2.52	0.40
3:D:239:ARG:HG3	3:D:241:VAL:HG23	2.03	0.40
3:D:279:PRO:HB3	3:D:296:LEU:HD21	2.02	0.40
3:F:128:PRO:HD2	3:F:172:PHE:CG	2.56	0.40
3:F:174[A]:ARG:CG	3:F:174[A]:ARG:NH2	2.45	0.40
1:A:170:PRO:HG3	1:A:353:ARG:HH12	1.85	0.40
2:E:23:CYS:HB3	2:E:88[B]:CYS:SG	2.62	0.40
1:A:40:ALA:HA	1:A:354:TYR:CE1	2.56	0.40
3:D:191:THR:HA	3:D:204:VAL:O	2.21	0.40
1:A:136:PHE:HB3	1:A:144:VAL:HG11	2.02	0.40
1:A:223:TYR:CG	1:A:249:LEU:HD22	2.56	0.40
1:B:56:GLY:HA3	1:B:112:VAL:O	2.21	0.40
2:C:13:TRP:HE1	2:C:24:ASP:HA	1.86	0.40
2:C:63:ASN:HA	2:C:64:PRO:HD2	1.93	0.40
3:D:52:PRO:HG2	3:D:378:GLN:OE1	2.21	0.40
2:E:19:ASP:O	2:E:25:TYR:HB2	2.21	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	357/373 (96%)	343 (96%)	13 (4%)	1 (0%)	36	36
1	B	356/373 (95%)	347 (98%)	9 (2%)	0	100	100
2	C	129/137 (94%)	121 (94%)	6 (5%)	2 (2%)	7	4
2	E	126/137 (92%)	124 (98%)	2 (2%)	0	100	100
3	D	376/385 (98%)	358 (95%)	17 (4%)	1 (0%)	36	36
3	F	378/385 (98%)	364 (96%)	13 (3%)	1 (0%)	36	36
All	All	1722/1790 (96%)	1657 (96%)	60 (4%)	5 (0%)	43	36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	131[A]	SER
2	C	131[B]	SER
3	D	102	ILE
1	A	166	GLY
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	281/292 (96%)	258 (92%)	23 (8%)	10	7
1	B	280/292 (96%)	268 (96%)	12 (4%)	26	26
2	C	111/112 (99%)	109 (98%)	2 (2%)	51	58
2	E	108/112 (96%)	105 (97%)	3 (3%)	38	42
3	D	306/310 (99%)	293 (96%)	13 (4%)	26	26
3	F	308/310 (99%)	297 (96%)	11 (4%)	31	32
All	All	1394/1428 (98%)	1330 (95%)	64 (5%)	24	23

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASP
1	A	23	LEU
1	A	48	LYS
1	A	51	LEU
1	A	60	GLN
1	A	75	LEU
1	A	84	ASN
1	A	112	VAL
1	A	142	LYS
1	A	167	GLU
1	A	184	LYS
1	A	202	ARG
1	A	206	MET
1	A	208	ARG
1	A	214	GLU
1	A	219	THR
1	A	252	ARG
1	A	300	ARG
1	A	305	LYS
1	A	323	LEU
1	A	357	LEU
1	A	358	LEU
1	A	359	GLU
1	B	81	ARG
1	B	102	GLN
1	B	167	GLU
1	B	202	ARG
1	B	219	THR
1	B	269	LEU
1	B	285	THR
1	B	321	ARG
1	B	323	LEU
1	B	357	LEU
1	B	358	LEU
1	B	361	SER
2	C	71	LEU
2	C	129	LYS
3	D	75	ILE
3	D	92	ILE
3	D	97	THR
3	D	106	GLU
3	D	127	LEU
3	D	177	ASP

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Mol	Chain	Res	Type
3	D	218[A]	GLU
3	D	218[B]	GLU
3	D	223	GLU
3	D	242	TRP
3	D	258	ASP
3	D	316	LEU
3	D	354	LYS
2	E	58	VAL
2	E	65	THR
2	E	71	LEU
3	F	11	GLN
3	F	92	ILE
3	F	139	PRO
3	F	160	PRO
3	F	173	LYS
3	F	174[A]	ARG
3	F	174[B]	ARG
3	F	218	GLU
3	F	262	LEU
3	F	300	GLN
3	F	316	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	62	HIS
1	A	84	ASN
1	A	91	GLN
1	A	163	GLN
1	A	210	GLN
1	A	244	HIS
1	B	91	GLN
1	B	163	GLN
1	B	210	GLN
2	C	21	GLN
2	C	68	GLN
2	C	135	HIS
3	D	30	GLN
3	D	195	HIS
3	D	216	HIS
2	E	21	GLN

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Mol	Chain	Res	Type
2	E	68	GLN
3	F	60	GLN
3	F	61	GLN
3	F	155	GLN
3	F	300	GLN
3	F	375	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	0AF	E	57	2	15,16,17	2.03	5 (33%)	14,22,24	0.95	0
2	0AF	C	57	2	15,16,17	2.20	5 (33%)	14,22,24	1.34	2 (14%)

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	-	0/5/6/8	0/2/2/2
2	0AF	C	57	2	-	0/5/6/8	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	57	0AF	CB-CA	4.45	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	57	0AF	CE2-NE1	-4.24	1.30	1.37
2	C	57	0AF	CD1-NE1	-4.10	1.30	1.37
2	C	57	0AF	CD2-CE2	-3.62	1.36	1.41
2	E	57	0AF	CD1-NE1	-3.43	1.31	1.37
2	E	57	0AF	CE2-NE1	-3.37	1.32	1.37
2	C	57	0AF	CD2-CG	-2.77	1.39	1.44
2	C	57	0AF	CA-N	-2.64	1.40	1.48
2	E	57	0AF	CD2-CG	-2.62	1.39	1.44
2	E	57	0AF	CD2-CE2	-2.52	1.38	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	57	0AF	CB-CG-CD1	-2.51	122.07	126.97
2	C	57	0AF	CB-CG-CD2	2.22	130.96	126.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 13 ligands modelled in this entry, 4 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	402	1,11	50,50,50	2.54	23 (46%)	68,82,82	2.12	28 (41%)
5	HEC	B	403	1	50,50,50	2.36	22 (44%)	68,82,82	2.19	26 (38%)
5	HEC	B	402	1	50,50,50	2.47	23 (46%)	68,82,82	2.17	30 (44%)
8	EDO	B	405	-	3,3,3	0.45	0	2,2,2	0.43	0
6	ACT	A	404	-	3,3,3	0.90	0	3,3,3	1.20	0
10	MES	F	401	-	12,12,12	2.03	1 (8%)	15,16,16	3.07	9 (60%)
5	HEC	A	403	1	50,50,50	2.51	22 (44%)	68,82,82	2.11	24 (35%)
10	MES	D	401	-	12,12,12	1.87	1 (8%)	15,16,16	2.62	9 (60%)
9	PGE	B	406	-	9,9,9	0.72	0	8,8,8	0.84	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
5	HEC	A	402	1,11	1/1/3/7	2/14/54/54	-
5	HEC	B	403	1	1/1/3/7	6/14/54/54	-
5	HEC	B	402	1	1/1/3/7	5/14/54/54	-
8	EDO	B	405	-	-	1/1/1/1	-
10	MES	F	401	-	-	2/6/14/14	0/1/1/1
5	HEC	A	403	1	1/1/3/7	6/14/54/54	-
10	MES	D	401	-	-	5/6/14/14	0/1/1/1
9	PGE	B	406	-	-	4/7/7/7	-

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	F	401	MES	C8-S	-6.57	1.68	1.77
10	D	401	MES	C8-S	-5.90	1.69	1.77
5	B	402	HEC	C1D-ND	-5.34	1.31	1.40
5	B	402	HEC	CHA-C1A	5.23	1.48	1.38
5	B	402	HEC	FE-ND	4.95	2.10	1.94
5	A	402	HEC	FE-NA	4.76	2.10	1.95
5	B	403	HEC	CHB-C4A	4.76	1.47	1.38
5	A	402	HEC	CHD-C1D	4.65	1.47	1.38
5	A	403	HEC	CHC-C4B	4.63	1.47	1.38
5	A	403	HEC	CHB-C4A	4.56	1.47	1.38
5	A	403	HEC	C4C-NC	-4.53	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	402	HEC	CHC-C4B	4.48	1.47	1.38
5	A	402	HEC	C1D-ND	-4.40	1.32	1.40
5	A	403	HEC	C4B-NB	-4.40	1.32	1.40
5	A	403	HEC	CHD-C1D	4.39	1.47	1.38
5	A	402	HEC	CHA-C4D	4.36	1.49	1.39
5	B	403	HEC	CHC-C4B	4.34	1.47	1.38
5	A	402	HEC	CHA-C1A	4.25	1.46	1.38
5	A	403	HEC	C1A-NA	-4.24	1.31	1.39
5	B	402	HEC	C4C-NC	-4.24	1.31	1.39
5	A	403	HEC	C4A-NA	-4.22	1.31	1.39
5	A	402	HEC	FE-ND	4.20	2.07	1.94
5	A	403	HEC	CHA-C1A	4.20	1.46	1.38
5	B	403	HEC	C4C-NC	-4.15	1.31	1.39
5	B	402	HEC	CHC-C4B	4.11	1.46	1.38
5	A	403	HEC	FE-NA	4.06	2.08	1.95
5	A	402	HEC	C4A-NA	-4.06	1.32	1.39
5	B	403	HEC	C1D-ND	-3.94	1.33	1.40
5	B	403	HEC	CHA-C4D	3.86	1.48	1.39
5	A	402	HEC	FE-NC	3.84	2.07	1.95
5	B	403	HEC	C1A-NA	-3.81	1.32	1.39
5	B	402	HEC	CHD-C4C	3.77	1.47	1.39
5	B	403	HEC	FE-NB	3.70	2.06	1.94
5	B	402	HEC	CHB-C4A	3.68	1.45	1.38
5	A	402	HEC	CHC-C1C	3.63	1.47	1.39
5	B	403	HEC	C4B-NB	-3.63	1.34	1.40
5	B	403	HEC	C1C-NC	-3.62	1.32	1.39
5	B	403	HEC	C4D-ND	-3.62	1.31	1.38
5	A	402	HEC	CHB-C1B	3.59	1.47	1.39
5	B	403	HEC	C4A-NA	-3.55	1.32	1.39
5	B	402	HEC	CHA-C4D	3.55	1.47	1.39
5	A	402	HEC	CHD-C4C	3.50	1.47	1.39
5	B	402	HEC	CHD-C1D	3.48	1.45	1.38
5	A	403	HEC	FE-NB	3.45	2.05	1.94
5	B	402	HEC	FE-NC	3.43	2.06	1.95
5	A	403	HEC	C1B-NB	-3.42	1.32	1.38
5	A	403	HEC	CHC-C1C	3.40	1.47	1.39
5	A	403	HEC	C1D-ND	-3.39	1.34	1.40
5	A	402	HEC	C4C-NC	-3.37	1.33	1.39
5	A	403	HEC	FE-NC	3.36	2.06	1.95
5	B	402	HEC	C1B-NB	-3.36	1.32	1.38
5	B	403	HEC	FE-NA	3.35	2.06	1.95
5	B	402	HEC	C4A-NA	-3.32	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	402	HEC	FE-NB	3.29	2.05	1.94
5	B	402	HEC	CHB-C1B	3.28	1.46	1.39
5	B	402	HEC	C4B-NB	-3.27	1.34	1.40
5	A	403	HEC	FE-ND	3.25	2.04	1.94
5	B	403	HEC	CHC-C1C	3.24	1.46	1.39
5	A	403	HEC	CHB-C1B	3.24	1.46	1.39
5	A	402	HEC	C1A-NA	-3.24	1.33	1.39
5	A	403	HEC	C4D-ND	-3.18	1.32	1.38
5	B	402	HEC	C1C-NC	-3.11	1.33	1.39
5	A	402	HEC	CHB-C4A	3.06	1.44	1.38
5	A	402	HEC	FE-NB	3.03	2.04	1.94
5	A	403	HEC	CHA-C4D	3.02	1.46	1.39
5	B	403	HEC	CHD-C1D	3.01	1.44	1.38
5	B	402	HEC	FE-NA	2.95	2.04	1.95
5	A	402	HEC	C4C-C3C	2.91	1.50	1.44
5	B	403	HEC	C3B-C2B	2.79	1.42	1.36
5	A	403	HEC	C1C-NC	-2.79	1.34	1.39
5	B	403	HEC	FE-NC	2.71	2.04	1.95
5	A	402	HEC	C1C-NC	-2.71	1.34	1.39
5	B	402	HEC	CHC-C1C	2.69	1.45	1.39
5	B	403	HEC	CBD-CAD	2.63	1.61	1.51
5	B	403	HEC	CHB-C1B	2.63	1.45	1.39
5	A	403	HEC	CHD-C4C	2.60	1.45	1.39
5	B	402	HEC	C1D-C2D	2.52	1.49	1.44
5	B	403	HEC	C4C-C3C	2.44	1.49	1.44
5	A	402	HEC	C1A-C2A	2.40	1.49	1.45
5	A	402	HEC	C4D-ND	-2.36	1.34	1.38
5	A	402	HEC	C4B-NB	-2.32	1.36	1.40
5	A	403	HEC	C4A-C3A	2.31	1.49	1.45
5	A	402	HEC	C1D-C2D	2.26	1.49	1.44
5	A	403	HEC	C1A-C2A	2.23	1.49	1.45
5	A	402	HEC	CBA-CGA	2.21	1.55	1.50
5	B	402	HEC	C4D-C3D	2.20	1.48	1.45
5	B	402	HEC	O2A-CGA	-2.18	1.23	1.30
5	B	403	HEC	FE-ND	2.17	2.01	1.94
5	B	402	HEC	C1B-C2B	2.09	1.48	1.44
5	B	403	HEC	CHD-C4C	2.08	1.44	1.39
5	B	402	HEC	C3B-C2B	2.05	1.41	1.36
5	B	403	HEC	C1C-C2C	2.03	1.47	1.43

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	402	HEC	C3D-C4D-ND	6.15	116.30	110.35
10	F	401	MES	C5-N4-C3	6.14	122.07	108.84
10	F	401	MES	C2-C3-N4	-5.47	101.81	110.12
5	A	403	HEC	CBD-CAD-C3D	-5.05	98.56	112.53
5	B	402	HEC	C2D-C1D-ND	5.01	115.60	109.84
10	D	401	MES	C5-N4-C3	4.97	119.55	108.84
5	B	403	HEC	C3C-C4C-NC	4.63	115.29	110.15
5	A	402	HEC	C3D-C4D-ND	4.56	114.76	110.35
5	B	403	HEC	C1B-C2B-C3B	-4.54	102.20	106.98
5	B	403	HEC	C2A-C1A-NA	4.49	114.65	110.32
5	A	403	HEC	CAD-CBD-CGD	-4.42	101.95	113.67
5	A	403	HEC	C2B-C1B-NB	4.33	114.91	109.90
5	A	402	HEC	C2D-C1D-ND	4.25	114.72	109.84
5	A	402	HEC	C3C-C4C-NC	4.21	114.83	110.15
5	B	403	HEC	CBD-CAD-C3D	-4.16	101.04	112.53
5	A	403	HEC	CBB-CAB-C3B	-4.13	101.22	112.42
10	D	401	MES	C6-C5-N4	-4.06	103.94	110.12
5	A	402	HEC	C2A-C1A-NA	4.06	114.24	110.32
5	A	403	HEC	C1D-C2D-C3D	-4.05	102.72	106.98
5	B	403	HEC	C2B-C1B-NB	4.03	114.56	109.90
10	F	401	MES	O2S-S-C8	4.01	112.78	106.73
5	B	402	HEC	C3B-C4B-NB	3.89	114.44	110.17
5	A	403	HEC	C1B-C2B-C3B	-3.85	102.93	106.98
5	B	402	HEC	CHD-C1D-ND	-3.84	119.61	124.37
5	B	403	HEC	C3B-C4B-NB	3.73	114.26	110.17
10	D	401	MES	C2-C3-N4	-3.69	104.52	110.12
5	B	402	HEC	C4D-C3D-C2D	-3.68	101.53	106.89
5	A	403	HEC	C4A-C3A-C2A	-3.58	101.66	106.97
5	A	403	HEC	C2D-C1D-ND	3.56	113.94	109.84
5	B	402	HEC	CMC-C2C-C3C	3.51	133.07	125.62
5	A	403	HEC	C3B-C4B-NB	3.50	114.01	110.17
5	B	403	HEC	CAD-C3D-C4D	3.50	130.79	124.70
10	F	401	MES	C6-C5-N4	-3.48	104.84	110.12
10	D	401	MES	C7-N4-C3	3.38	120.24	111.24
5	A	403	HEC	CBA-CAA-C2A	-3.37	103.22	112.53
10	D	401	MES	C7-N4-C5	3.36	120.20	111.24
5	A	402	HEC	C1D-C2D-C3D	-3.36	103.45	106.98
5	A	402	HEC	CHD-C1D-ND	-3.29	120.29	124.37
5	B	403	HEC	C3D-C4D-ND	3.28	113.52	110.35
5	B	403	HEC	C1A-C2A-C3A	-3.26	102.82	107.11
5	B	403	HEC	CAD-CBD-CGD	-3.25	105.04	113.67
5	A	402	HEC	C3B-C4B-NB	3.25	113.73	110.17
5	B	403	HEC	CAC-C3C-C2C	3.24	132.01	126.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	403	HEC	CBC-CAC-C3C	-3.19	103.78	112.42
5	B	402	HEC	C1D-ND-C4D	-3.10	101.53	105.21
5	A	402	HEC	O2A-CGA-CBA	3.08	123.73	114.00
5	B	402	HEC	C1C-C2C-C3C	-3.06	103.31	106.82
5	A	402	HEC	CAB-C3B-C4B	3.06	128.77	124.79
5	B	403	HEC	C1D-C2D-C3D	-3.04	103.78	106.98
5	A	402	HEC	C2B-C1B-NB	3.04	113.41	109.90
5	B	403	HEC	C4C-C3C-C2C	-3.03	102.17	106.87
5	B	402	HEC	CBD-CAD-C3D	-3.00	104.23	112.53
5	B	402	HEC	C3C-C4C-NC	2.99	113.47	110.15
5	A	402	HEC	C3A-C4A-NA	2.99	115.16	109.64
5	B	402	HEC	O2A-CGA-CBA	2.98	123.43	114.00
5	A	403	HEC	C3C-C4C-NC	2.97	113.45	110.15
10	F	401	MES	C7-N4-C3	2.97	119.15	111.24
5	B	402	HEC	C4B-C3B-C2B	-2.95	102.60	106.89
5	A	402	HEC	CMC-C2C-C3C	2.92	131.83	125.62
5	A	402	HEC	CBD-CAD-C3D	-2.92	104.45	112.53
5	A	402	HEC	C4C-C3C-C2C	-2.90	102.38	106.87
5	A	403	HEC	C3A-C4A-NA	2.88	114.96	109.64
5	A	403	HEC	C2A-C1A-NA	2.88	113.10	110.32
10	F	401	MES	C7-N4-C5	2.83	118.78	111.24
5	A	402	HEC	CHD-C4C-NC	-2.82	118.75	123.86
10	F	401	MES	O3S-S-C8	2.80	111.49	106.00
5	B	402	HEC	CBA-CAA-C2A	-2.80	104.80	112.53
5	B	402	HEC	CBB-CAB-C3B	-2.80	104.84	112.42
5	A	402	HEC	C2C-C1C-NC	2.78	114.59	110.14
5	B	403	HEC	CMC-C2C-C3C	2.77	131.50	125.62
5	A	403	HEC	CMC-C2C-C3C	2.76	131.48	125.62
5	B	403	HEC	CAB-C3B-C2B	2.76	132.63	127.56
5	B	402	HEC	CHA-C4D-C3D	-2.75	120.77	124.77
5	B	402	HEC	C2B-C1B-NB	2.70	113.03	109.90
5	B	403	HEC	C2D-C1D-ND	2.70	112.94	109.84
5	B	403	HEC	CHC-C1C-C2C	-2.68	119.64	127.43
5	A	403	HEC	C1C-C2C-C3C	-2.67	103.75	106.82
5	B	402	HEC	C2C-C1C-NC	2.66	114.40	110.14
5	A	402	HEC	CMD-C2D-C1D	2.54	129.00	125.03
5	B	403	HEC	C2C-C1C-NC	2.54	114.21	110.14
5	A	402	HEC	CHB-C4A-NA	-2.54	121.69	124.45
5	B	402	HEC	CHC-C4B-C3B	-2.54	120.55	125.23
5	A	402	HEC	CAD-C3D-C4D	2.53	129.11	124.70
5	B	402	HEC	CAA-C2A-C1A	2.52	129.97	124.85
5	B	402	HEC	C1A-C2A-C3A	-2.52	103.80	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	402	HEC	CAA-CBA-CGA	-2.51	107.01	113.67
5	A	402	HEC	C1A-C2A-C3A	-2.50	103.81	107.11
5	A	402	HEC	CHA-C4D-ND	-2.48	121.75	124.42
5	B	403	HEC	O2A-CGA-CBA	2.44	121.72	114.00
5	B	402	HEC	CAC-C3C-C2C	2.44	130.75	126.89
5	A	402	HEC	C4A-C3A-C2A	-2.41	103.40	106.97
10	D	401	MES	O1S-S-C8	2.38	110.33	106.73
5	A	402	HEC	CAC-C3C-C2C	2.37	130.64	126.89
5	B	402	HEC	CAB-C3B-C2B	2.35	131.87	127.56
5	B	403	HEC	CMB-C2B-C3B	2.29	132.34	126.15
10	D	401	MES	C6-O1-C2	2.29	117.28	109.88
5	A	402	HEC	C4B-C3B-C2B	-2.26	103.61	106.89
5	B	403	HEC	CMD-C2D-C1D	2.25	128.55	125.03
5	A	403	HEC	CMA-C3A-C2A	2.23	132.19	126.15
5	A	403	HEC	O2A-CGA-CBA	2.22	121.03	114.00
10	D	401	MES	O3S-S-C8	2.20	110.31	106.00
10	F	401	MES	O1-C6-C5	-2.19	107.04	111.77
5	A	403	HEC	CHD-C1D-ND	-2.19	121.66	124.37
5	B	402	HEC	O1A-CGA-CBA	-2.18	116.19	123.09
5	B	402	HEC	C2A-C1A-NA	2.17	112.42	110.32
5	B	403	HEC	CBA-CAA-C2A	-2.15	106.58	112.53
5	B	402	HEC	C1D-C2D-C3D	-2.15	104.72	106.98
5	A	403	HEC	O1A-CGA-CBA	-2.15	116.29	123.09
5	B	403	HEC	CBB-CAB-C3B	-2.10	106.72	112.42
5	B	403	HEC	CHC-C4B-C3B	-2.10	121.36	125.23
5	A	403	HEC	CAA-C2A-C3A	2.09	131.78	127.87
5	B	402	HEC	O1D-CGD-CBD	-2.08	116.49	123.09
5	A	402	HEC	C4D-C3D-C2D	-2.08	103.86	106.89
10	F	401	MES	C8-C7-N4	-2.07	104.52	112.36
5	B	403	HEC	CHA-C1A-NA	-2.06	122.21	124.45
5	A	402	HEC	CMA-C3A-C2A	2.05	131.70	126.15
5	B	402	HEC	CMB-C2B-C3B	2.04	131.68	126.15
5	B	402	HEC	O2D-CGD-CBD	2.04	120.45	114.00
5	B	402	HEC	C1B-C2B-C3B	-2.04	104.84	106.98
5	A	403	HEC	C2C-C1C-NC	2.04	113.41	110.14
5	B	403	HEC	CAB-C3B-C4B	-2.03	122.14	124.79
10	D	401	MES	O3S-S-O1S	-2.03	106.32	111.40
5	A	403	HEC	CHC-C1C-C2C	-2.03	121.54	127.43
5	A	403	HEC	CMD-C2D-C1D	2.03	128.20	125.03
5	B	402	HEC	CAD-C3D-C2D	2.01	131.62	127.87
5	A	402	HEC	CHC-C1C-C2C	-2.00	121.62	127.43

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	402	HEC	NA
5	A	403	HEC	NA
5	B	402	HEC	NA
5	B	403	HEC	NA

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	D	401	MES	C7-C8-S-O1S
10	D	401	MES	C7-C8-S-O2S
10	D	401	MES	C7-C8-S-O3S
9	B	406	PGE	C4-C3-O2-C2
5	B	402	HEC	C2B-C3B-CAB-CBB
5	A	402	HEC	C2C-C3C-CAC-CBC
5	A	403	HEC	C2C-C3C-CAC-CBC
9	B	406	PGE	O2-C3-C4-O3
5	A	402	HEC	C4C-C3C-CAC-CBC
5	A	403	HEC	C4C-C3C-CAC-CBC
9	B	406	PGE	O1-C1-C2-O2
9	B	406	PGE	O3-C5-C6-O4
5	B	403	HEC	C2B-C3B-CAB-CBB
5	A	403	HEC	C2B-C3B-CAB-CBB
5	B	403	HEC	C2C-C3C-CAC-CBC
5	B	402	HEC	C4B-C3B-CAB-CBB
10	F	401	MES	C8-C7-N4-C3
5	B	403	HEC	C4B-C3B-CAB-CBB
10	F	401	MES	N4-C7-C8-S
8	B	405	EDO	O1-C1-C2-O2
10	D	401	MES	C8-C7-N4-C3
10	D	401	MES	C8-C7-N4-C5
5	B	403	HEC	C4C-C3C-CAC-CBC
5	B	402	HEC	CAD-CBD-CGD-O2D
5	A	403	HEC	CAD-CBD-CGD-O2D
5	B	403	HEC	CAD-CBD-CGD-O2D
5	B	403	HEC	CAD-CBD-CGD-O1D
5	A	403	HEC	CAD-CBD-CGD-O1D
5	A	403	HEC	C4B-C3B-CAB-CBB
5	B	402	HEC	CAD-CBD-CGD-O1D
5	B	402	HEC	CAA-CBA-CGA-O2A

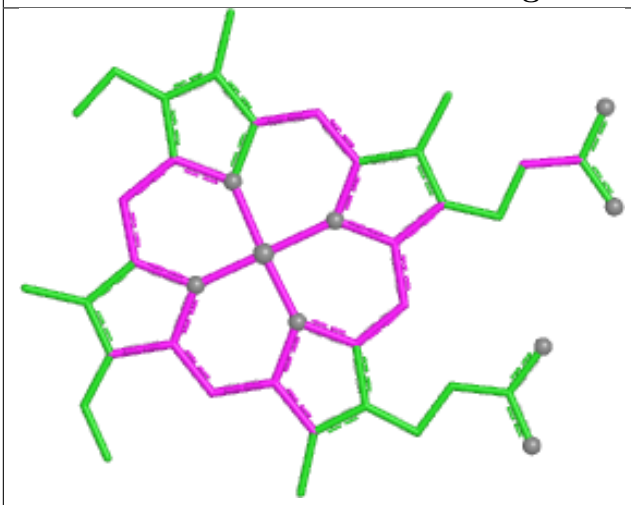
There are no ring outliers.

5 monomers are involved in 8 short contacts:

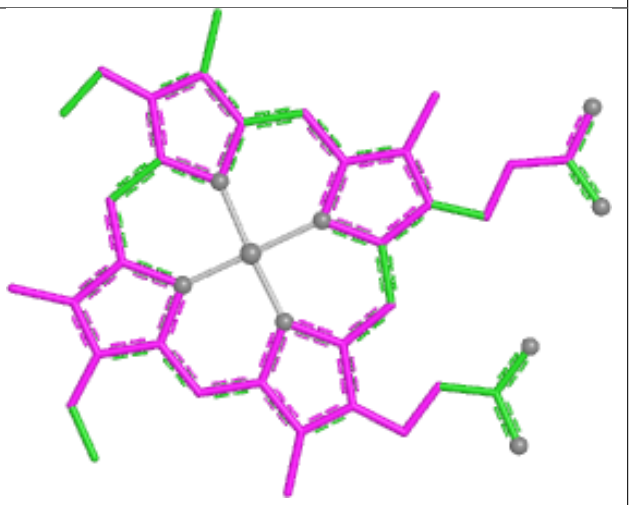
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	402	HEC	3	0
5	B	403	HEC	1	0
5	B	402	HEC	2	0
5	A	403	HEC	1	0
9	B	406	PGE	1	0

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.

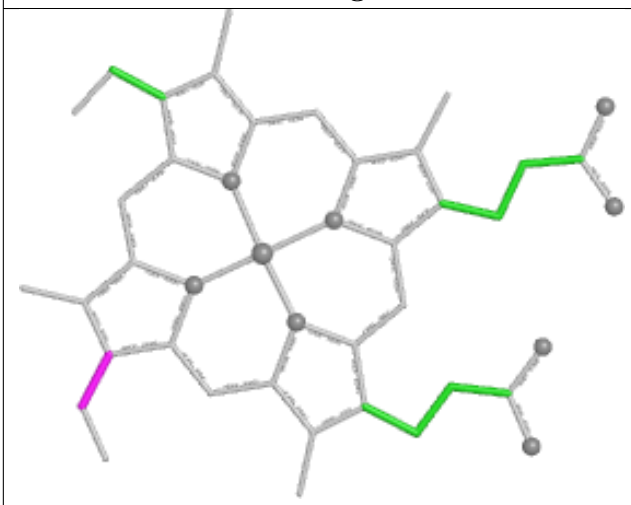
Ligand HEC A 402



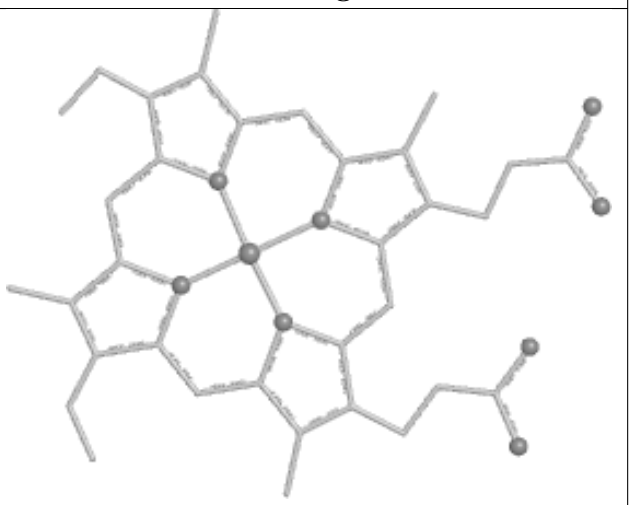
Bond lengths



Bond angles

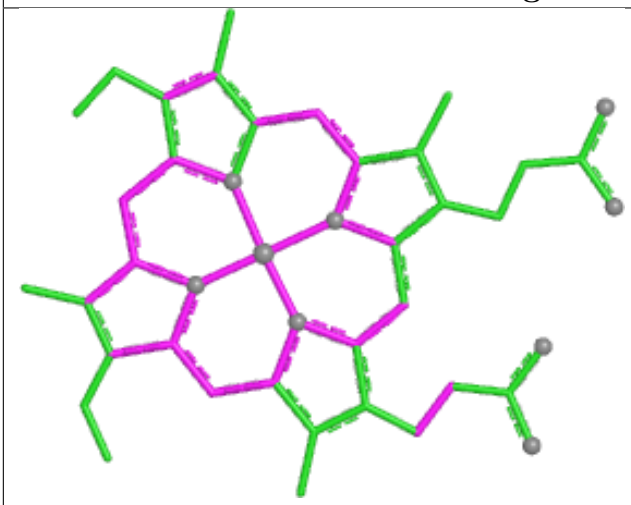


Torsions

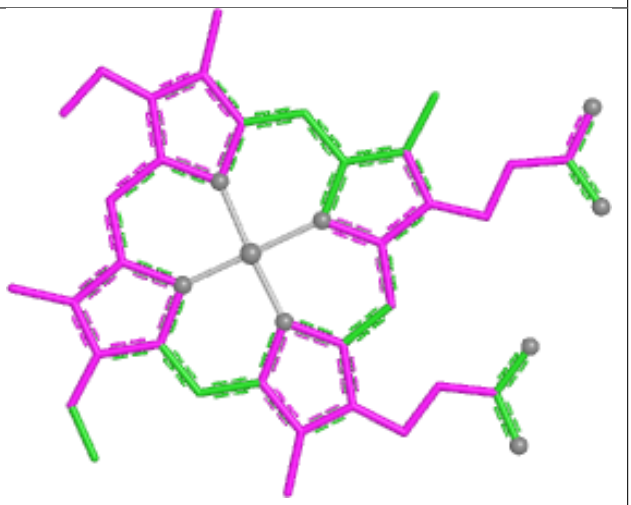


Rings

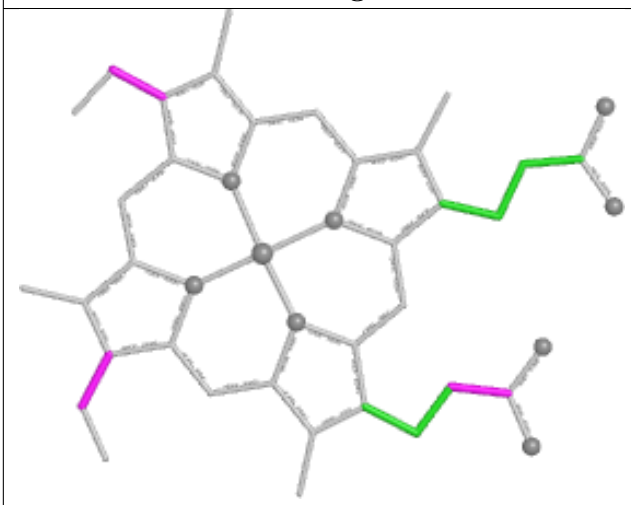
Ligand HEC B 403



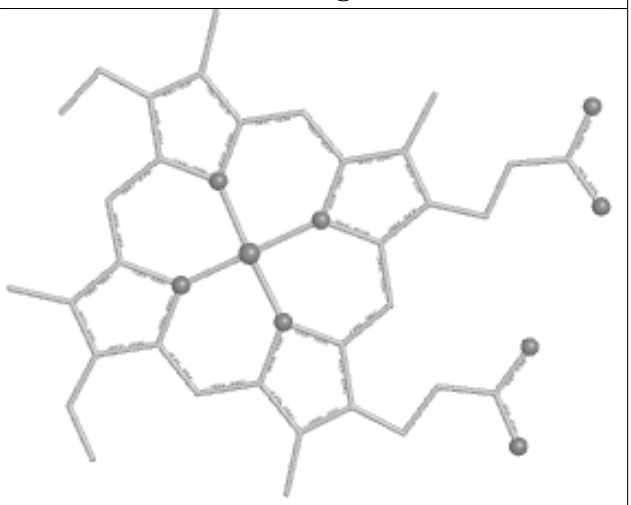
Bond lengths



Bond angles

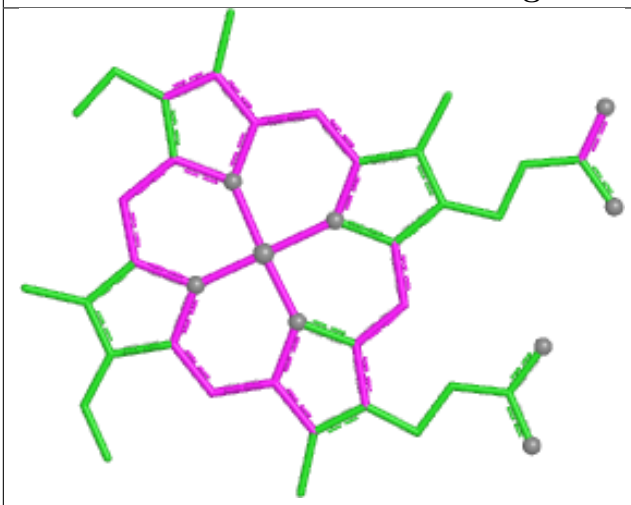


Torsions

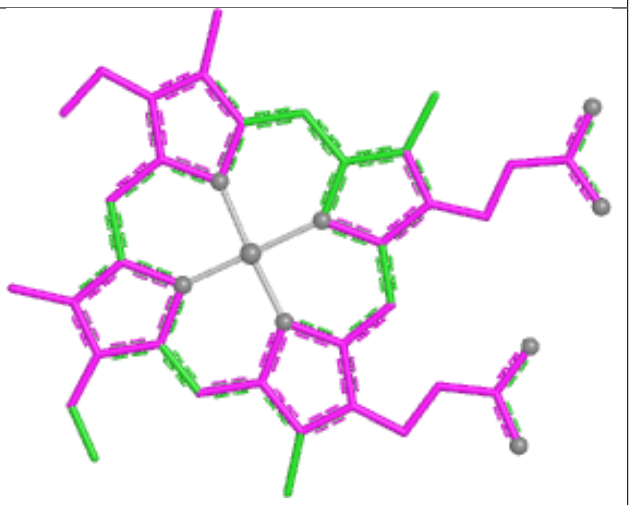


Rings

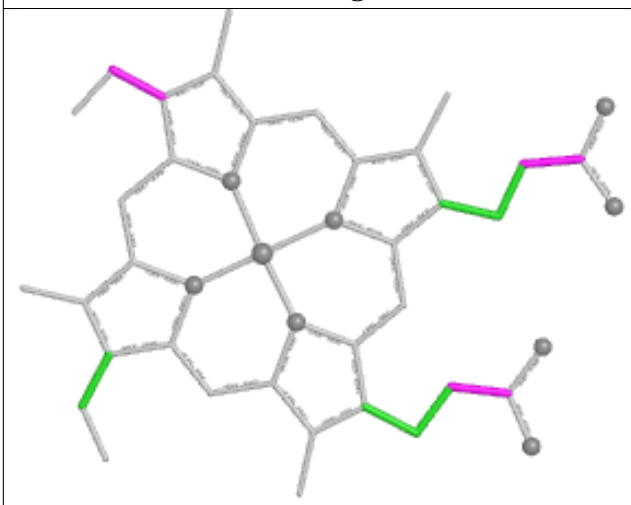
Ligand HEC B 402



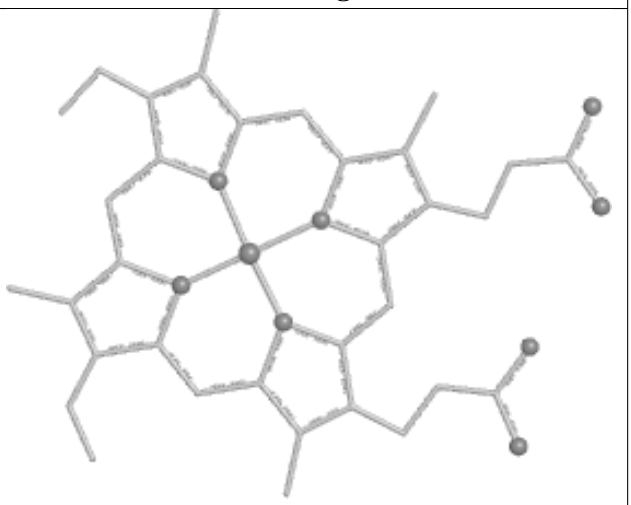
Bond lengths



Bond angles

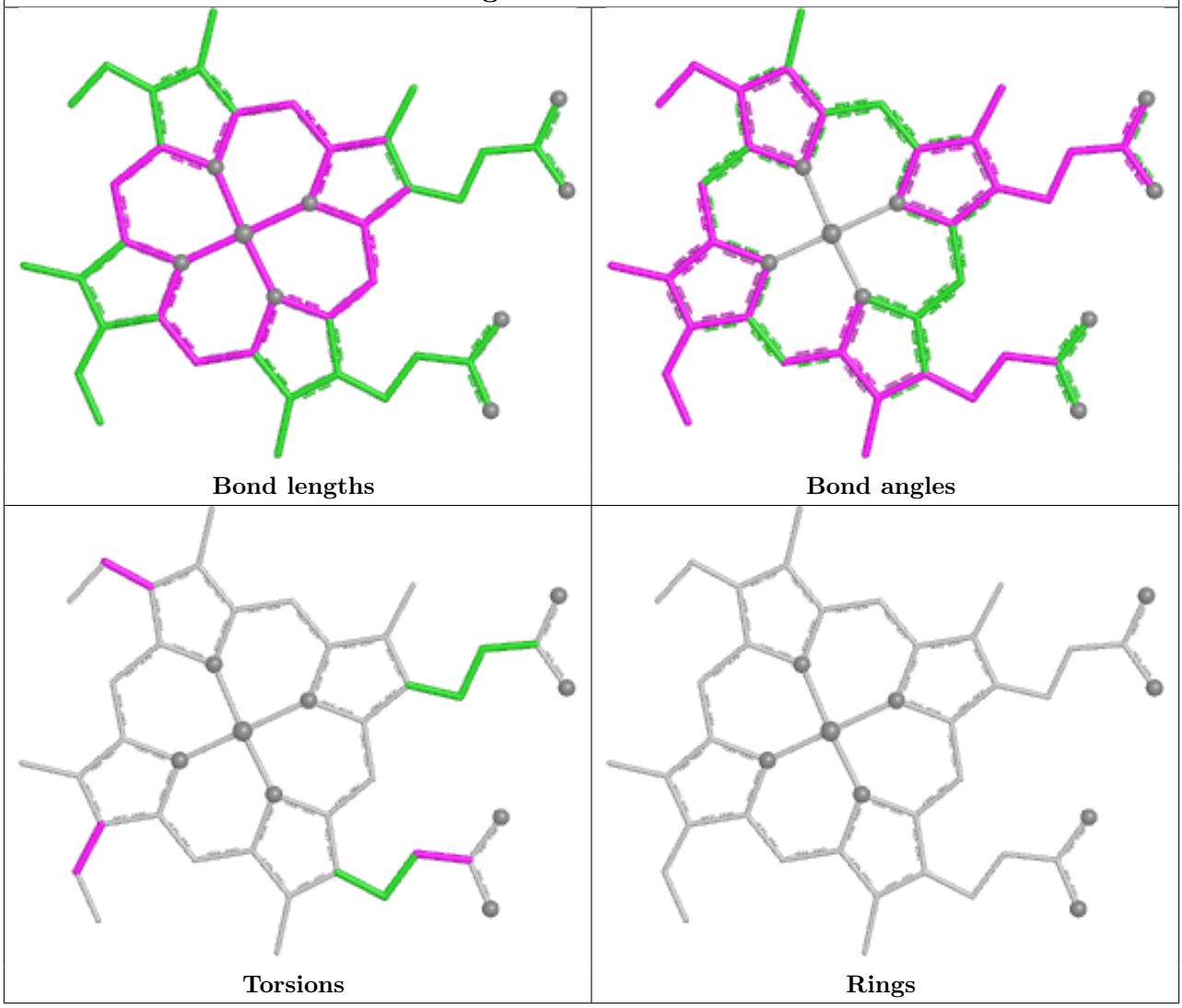


Torsions



Rings

Ligand HEC A 403



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%)	0.18	1 (0%)	90	91	21, 46, 66, 77	5 (1%)
1	B	357/373 (95%)	-0.21	1 (0%)	90	91	16, 36, 57, 79	1 (0%)
2	C	128/137 (93%)	0.18	3 (2%)	61	64	16, 42, 69, 92	3 (2%)
2	E	124/137 (90%)	-0.19	1 (0%)	82	84	14, 30, 44, 67	4 (3%)
3	D	376/385 (97%)	0.28	7 (1%)	66	69	28, 50, 80, 88	2 (0%)
3	F	376/385 (97%)	-0.29	2 (0%)	87	89	15, 33, 52, 70	4 (1%)
All	All	1715/1790 (95%)	-0.01	15 (0%)	81	83	14, 40, 70, 92	19 (1%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	131[A]	SER	3.8
3	D	207	GLY	3.5
1	B	6	ALA	2.9
3	F	207	GLY	2.8
1	A	6	ALA	2.8
3	D	274	ALA	2.6
2	E	131	SER	2.3
3	D	208	THR	2.2
2	C	133	HIS	2.1
3	D	264	ALA	2.1
2	C	7	THR	2.1
3	D	263	PRO	2.1
3	D	214	ILE	2.1
3	F	27	ALA	2.1
3	D	177	ASP	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	0AF	E	57	15/16	0.87	0.10	31,35,38,38	0
2	0AF	C	57	15/16	0.89	0.10	44,46,48,48	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

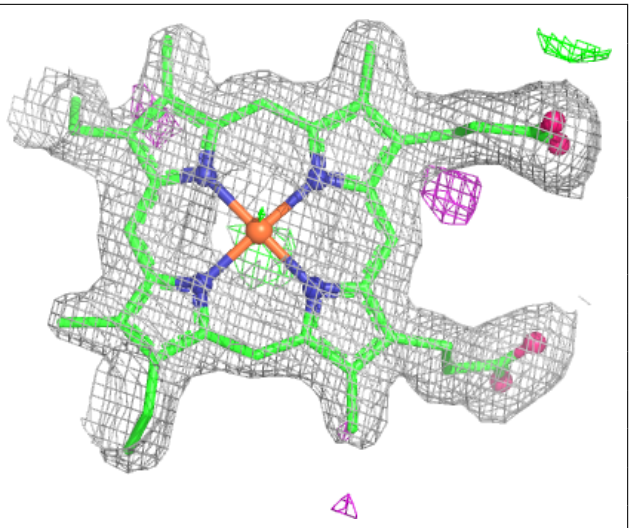
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

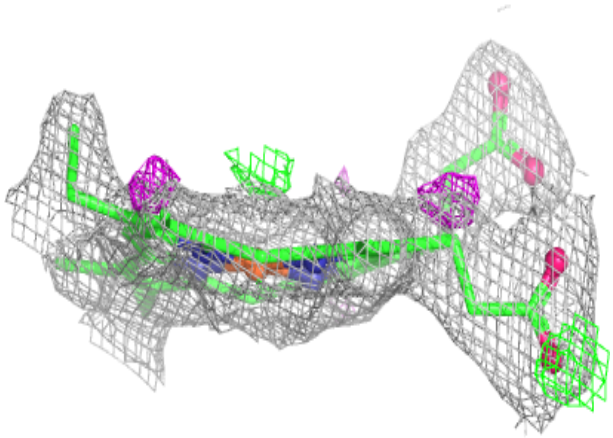
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	PGE	B	406	10/10	0.77	0.17	61,66,69,69	0
10	MES	D	401	12/12	0.78	0.19	80,90,93,93	0
6	ACT	A	404	4/4	0.79	0.19	75,76,76,76	0
10	MES	F	401	12/12	0.81	0.17	72,80,82,83	0
7	NA	B	407	1/1	0.91	0.11	46,46,46,46	0
8	EDO	B	405	4/4	0.92	0.11	53,53,54,57	0
7	NA	B	404	1/1	0.93	0.05	39,39,39,39	0
4	CA	A	401	1/1	0.96	0.04	45,45,45,45	0
5	HEC	B	402	43/43	0.97	0.07	23,29,33,34	0
5	HEC	A	402	43/43	0.97	0.08	31,39,43,44	0
5	HEC	B	403	43/43	0.98	0.05	18,22,26,28	0
5	HEC	A	403	43/43	0.98	0.07	35,39,42,45	0
4	CA	B	401	1/1	0.99	0.03	25,25,25,25	0

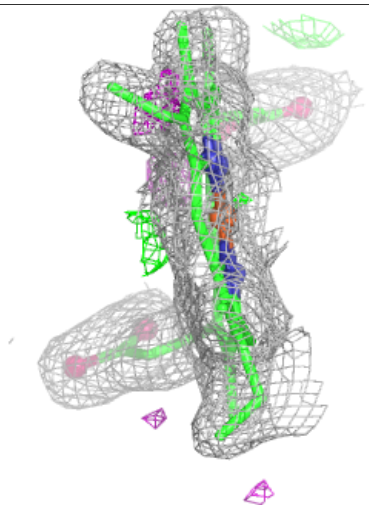
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEC B 402:

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

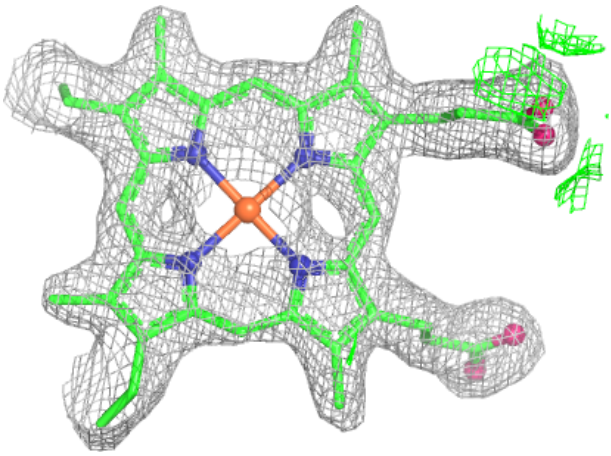


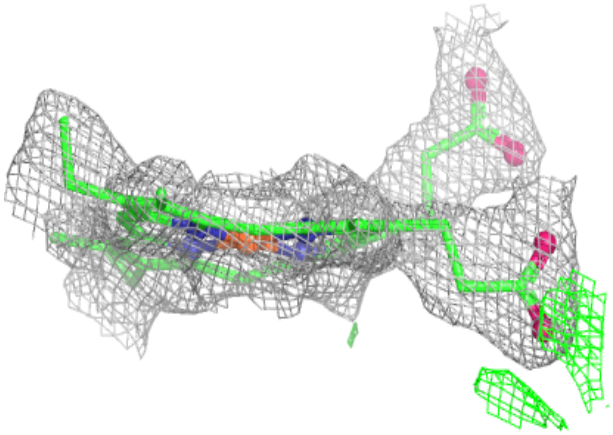


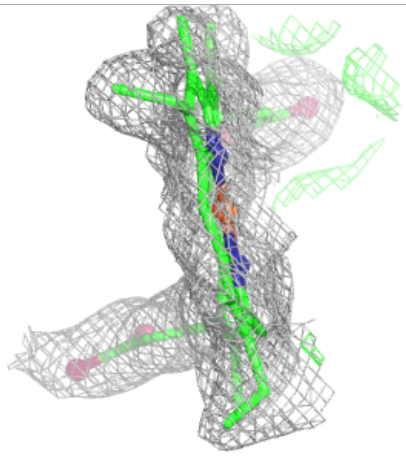


Electron density around HEC A 402:

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

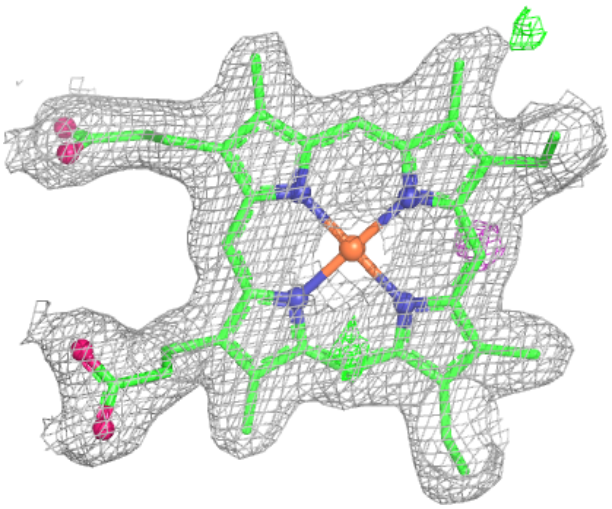


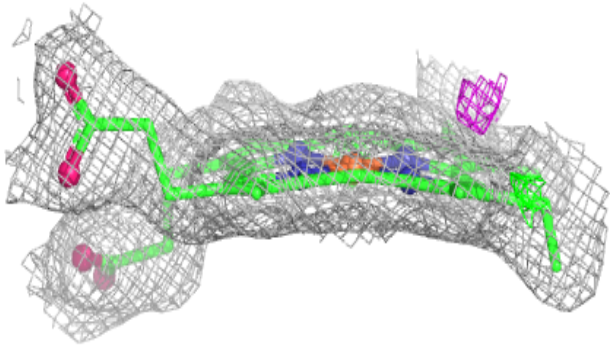


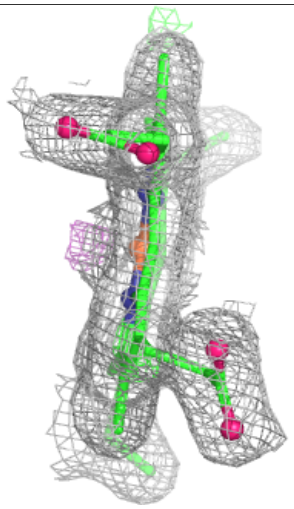


Electron density around HEC B 403:

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

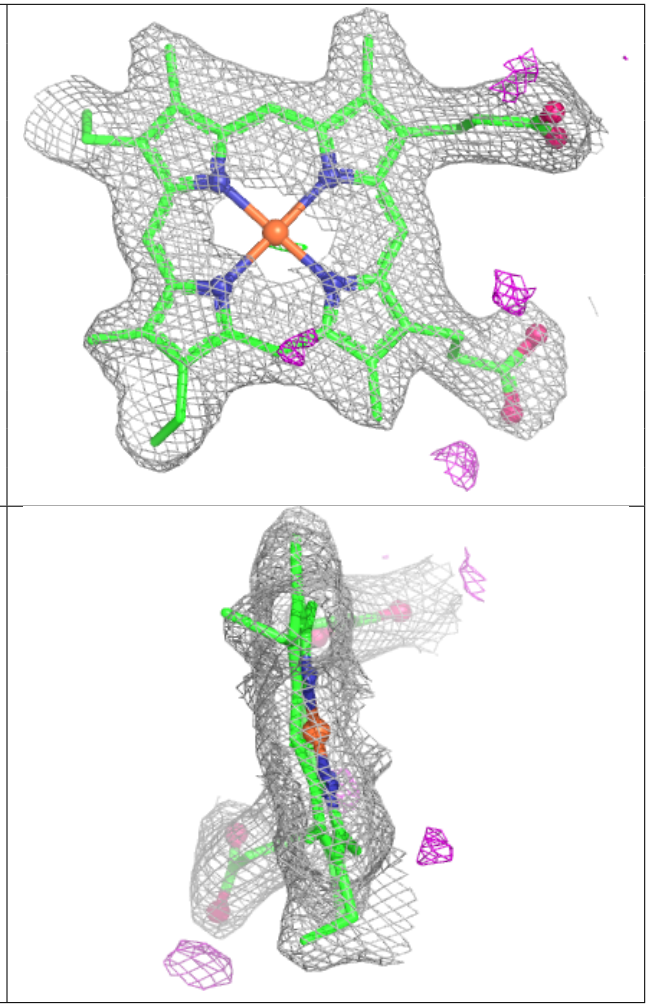






Electron density around HEC A 403:

$2mF_o$-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.