Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 06:17 pm GMT

PDB ID	:	4COH
Title	:	Crystal structure of Trypanosoma cruzi CYP51 bound to the sulfonamide derivative of the 4-aminopyridyl-based inhibitor
Authors	:	Vieira, D.F.; Choi, J.Y.; Roush, W.R.; Podust, L.M.
Deposited on	:	2014-01-28
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:

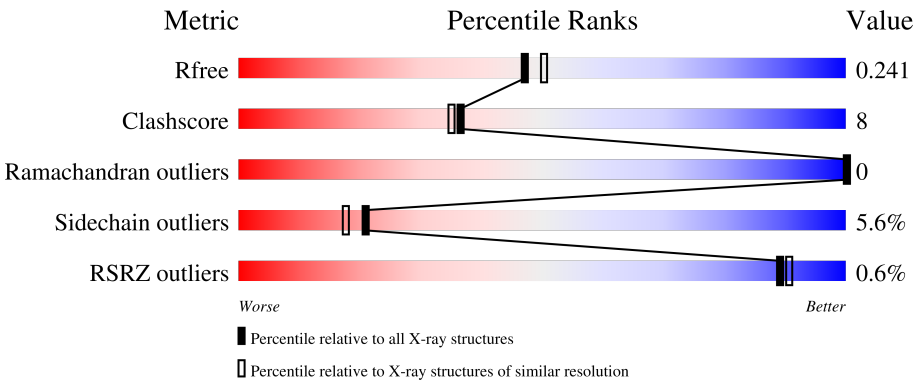
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (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	470	80% 11% • 6%
1	B	470	% 77% 14% • • 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7978 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 STEROL 14-ALPHA DEMETHYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	442	3520	2258	616	618	28	0	1	0
1	B	445	3564	2283	626	627	28	0	4	0

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	MET	-	expression tag	UNP Q5I4E1
A	19	ALA	-	expression tag	UNP Q5I4E1
A	20	LYS	-	expression tag	UNP Q5I4E1
A	21	LYS	-	expression tag	UNP Q5I4E1
A	22	THR	-	expression tag	UNP Q5I4E1
A	23	SER	-	expression tag	UNP Q5I4E1
A	24	SER	-	expression tag	UNP Q5I4E1
A	25	LYS	-	expression tag	UNP Q5I4E1
A	26	GLY	-	expression tag	UNP Q5I4E1
A	27	LYS	-	expression tag	UNP Q5I4E1
A	28	LEU	-	expression tag	UNP Q5I4E1
A	482	HIS	-	expression tag	UNP Q5I4E1
A	483	HIS	-	expression tag	UNP Q5I4E1
A	484	HIS	-	expression tag	UNP Q5I4E1
A	485	HIS	-	expression tag	UNP Q5I4E1
A	486	HIS	-	expression tag	UNP Q5I4E1
A	487	HIS	-	expression tag	UNP Q5I4E1
B	18	MET	-	expression tag	UNP Q5I4E1
B	19	ALA	-	expression tag	UNP Q5I4E1
B	20	LYS	-	expression tag	UNP Q5I4E1
B	21	LYS	-	expression tag	UNP Q5I4E1
B	22	THR	-	expression tag	UNP Q5I4E1
B	23	SER	-	expression tag	UNP Q5I4E1
B	24	SER	-	expression tag	UNP Q5I4E1
B	25	LYS	-	expression tag	UNP Q5I4E1

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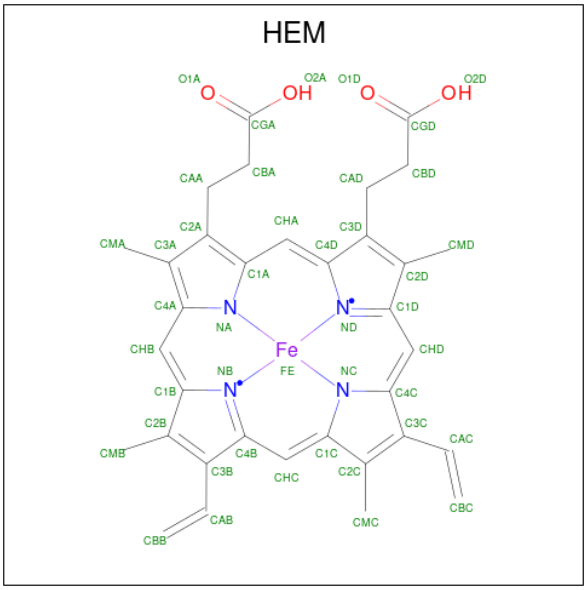
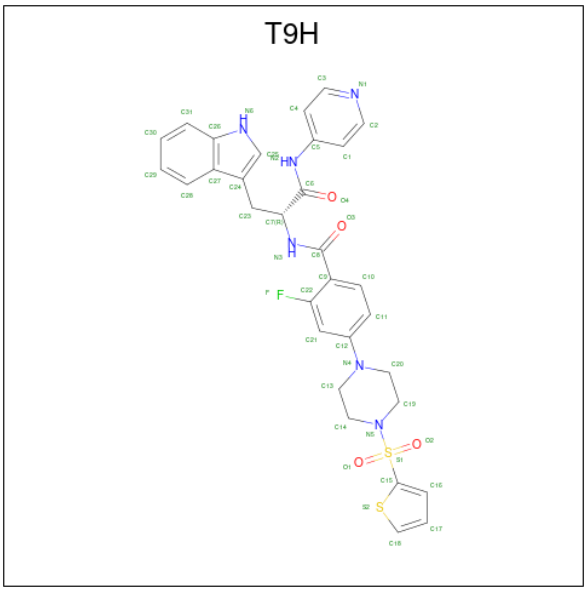
Chain	Residue	Modelled	Actual	Comment	Reference
B	26	GLY	-	expression tag	UNP Q5I4E1
B	27	LYS	-	expression tag	UNP Q5I4E1
B	28	LEU	-	expression tag	UNP Q5I4E1
B	482	HIS	-	expression tag	UNP Q5I4E1
B	483	HIS	-	expression tag	UNP Q5I4E1
B	484	HIS	-	expression tag	UNP Q5I4E1
B	485	HIS	-	expression tag	UNP Q5I4E1
B	486	HIS	-	expression tag	UNP Q5I4E1
B	487	HIS	-	expression tag	UNP Q5I4E1

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 3 is 2-fluoranyl-N-[(2R)-3-(1H-indol-3-yl)-1-oxidanylidene-1-(pyridin-4-ylamino) propan-2-yl]-4-(4-thiophen-2-ylsulfonylpiperazin-1-yl)benzamide (three-letter code: T9H) (formula: $C_{31}H_{29}FN_6O_4S_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	F	N	O	S		
3	A	1	44	31	1	6	4	2	0	0
			Total	C	F	N	O	S		
3	B	1	88	62	2	12	8	4	0	1

- Molecule 4 is water.

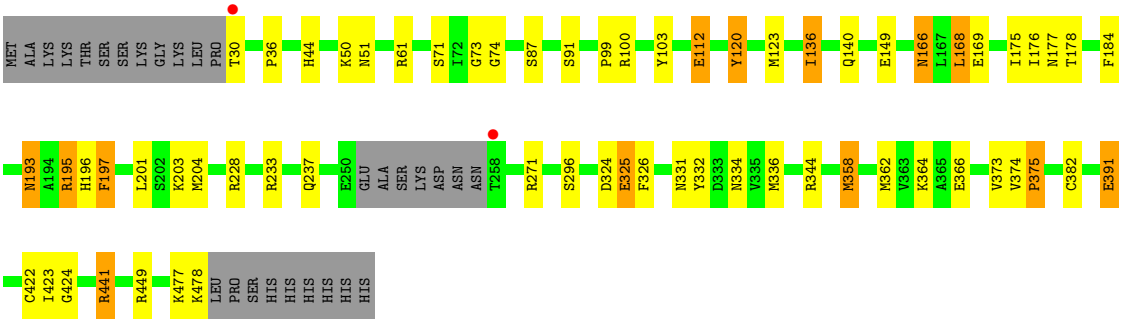
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	363	363	363	0	0
			Total	O		
4	B	313	313	313	0	0

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.

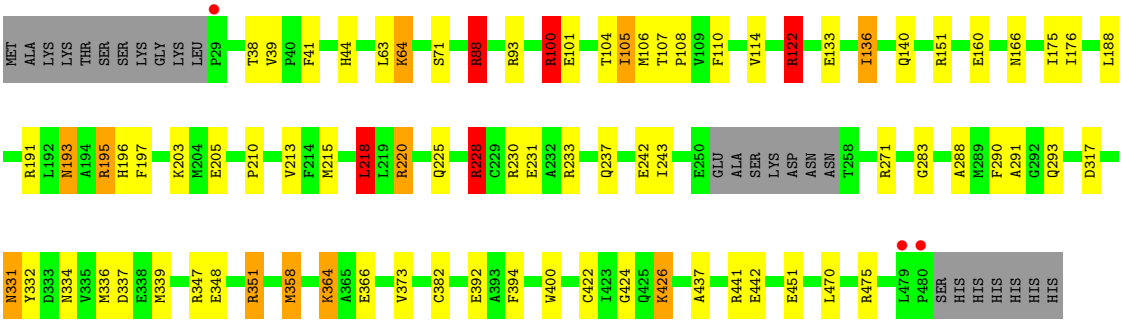
• Molecule 1: STEROL 14-ALPHA DEMETHYLASE

Chain A: 80% 11% • 6%



• Molecule 1: STEROL 14-ALPHA DEMETHYLASE

Chain B: % 77% 14% • • 5%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	79.22Å 96.39Å 137.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	137.11 – 2.08 68.59 – 2.08	Depositor EDS
% Data completeness (in resolution range)	94.3 (137.11-2.08) 94.4 (68.59-2.08)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.93 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.174 , 0.243 0.174 , 0.241	Depositor DCC
R_{free} test set	3024 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	27.1	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 38.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7978	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: T9H, HEM

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	1.05	4/3604 (0.1%)	0.97	14/4874 (0.3%)
1	B	1.00	1/3650 (0.0%)	0.97	13/4940 (0.3%)
All	All	1.03	5/7254 (0.1%)	0.97	27/9814 (0.3%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	GLU	CD-OE1	7.64	1.34	1.25
1	A	382	CYS	CB-SG	-7.58	1.69	1.82
1	A	120	TYR	CD1-CE1	5.11	1.47	1.39
1	A	112	GLU	CG-CD	5.08	1.59	1.51
1	B	392	GLU	CG-CD	5.04	1.59	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	441	ARG	NE-CZ-NH1	11.10	125.85	120.30
1	B	122	ARG	NE-CZ-NH2	-11.04	114.78	120.30
1	A	441	ARG	NE-CZ-NH2	-10.70	114.95	120.30
1	B	100	ARG	NE-CZ-NH2	-9.47	115.56	120.30
1	B	151	ARG	NE-CZ-NH1	8.65	124.63	120.30
1	A	73	GLY	N-CA-C	8.08	133.29	113.10
1	B	100	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	B	88	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	B	122	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	A	271	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	B	151	ARG	NE-CZ-NH2	-6.63	116.99	120.30
1	A	362	MET	CG-SD-CE	-5.98	90.64	100.20
1	B	228	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	73	GLY	CA-C-N	5.64	127.47	116.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	324	ASP	CB-CG-OD1	5.60	123.34	118.30
1	A	123	MET	CG-SD-CE	5.55	109.08	100.20
1	A	168	LEU	CA-CB-CG	5.55	128.06	115.30
1	A	176	ILE	CG1-CB-CG2	-5.41	99.50	111.40
1	A	449	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	218	LEU	CB-CG-CD1	5.37	120.12	111.00
1	B	122	ARG	CG-CD-NE	-5.28	100.72	111.80
1	B	351	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	B	441	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	344	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	100	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	364	LYS	CD-CE-NZ	5.05	123.31	111.70
1	A	358	MET	CG-SD-CE	-5.03	92.16	100.20

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	3520	0	3533	42	0
1	B	3564	0	3559	67	0
2	A	43	0	30	10	0
2	B	43	0	30	7	0
3	A	44	0	29	2	0
3	B	88	0	58	3	0
4	A	363	0	0	5	0
4	B	313	0	0	10	0
All	All	7978	0	7239	115	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 8.

All (115) 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:293[B]:GLN:HE21	1:B:293[B]:GLN:CA	0.99	1.45
1:B:230[B]:ARG:HH11	1:B:230[B]:ARG:CG	1.64	1.09
1:B:230[B]:ARG:HG3	1:B:230[B]:ARG:NH1	1.64	1.04
1:B:293[B]:GLN:HA	1:B:293[B]:GLN:NE2	0.82	1.01
1:B:230[B]:ARG:HH11	1:B:230[B]:ARG:HG3	0.83	0.98
1:A:44:HIS:HD2	1:A:71:SER:H	1.10	0.97
1:B:230[B]:ARG:CG	1:B:230[B]:ARG:NH1	2.27	0.90
1:B:293[B]:GLN:CA	1:B:293[B]:GLN:NE2	1.77	0.89
1:B:288:ALA:HA	2:B:1450:HEM:CBC	2.04	0.87
1:A:61[A]:ARG:NE	4:A:2029:HOH:O	1.92	0.86
1:B:188:LEU:HD13	1:B:243:ILE:HD13	1.57	0.85
1:A:61[A]:ARG:NH2	4:A:2029:HOH:O	2.11	0.84
1:B:347[B]:ARG:NH1	4:B:2245:HOH:O	2.08	0.83
1:B:293[B]:GLN:HE21	1:B:293[B]:GLN:N	1.80	0.80
1:B:188:LEU:HD13	1:B:243:ILE:CD1	2.12	0.80
1:A:184:PHE:CE2	1:A:197:PHE:CE2	2.73	0.77
1:A:184:PHE:HE2	1:A:197:PHE:CE2	2.05	0.74
1:A:193:ASN:ND2	1:A:196:HIS:H	1.87	0.73
1:A:44:HIS:CD2	1:A:71:SER:H	2.02	0.71
1:A:61[A]:ARG:CZ	4:A:2029:HOH:O	2.31	0.68
1:B:44:HIS:HD2	1:B:71:SER:H	1.40	0.68
1:B:288:ALA:HA	2:B:1450:HEM:HBC1	1.76	0.68
1:B:230[B]:ARG:NH1	4:B:2163:HOH:O	2.27	0.67
2:A:1450:HEM:CMB	2:A:1450:HEM:HBB2	2.27	0.64
1:B:366:GLU:CD	1:B:373:VAL:HG11	2.18	0.62
1:A:477:LYS:O	1:A:478:LYS:HB2	1.98	0.62
1:A:184:PHE:CE2	1:A:197:PHE:HE2	2.15	0.62
1:A:423:ILE:HD11	2:A:1450:HEM:HMD2	1.80	0.62
1:B:176:ILE:HB	1:B:293[B]:GLN:OE1	2.01	0.61
1:B:160:GLU:O	1:B:475:ARG:HD2	2.01	0.61
1:B:288:ALA:HA	2:B:1450:HEM:HBC2	1.80	0.61
1:B:93:ARG:HG2	4:B:2051:HOH:O	2.01	0.60
1:B:332:TYR:CZ	1:B:336:MET:HG3	2.37	0.60
1:A:391:GLU:HG2	4:A:2281:HOH:O	2.02	0.58
1:A:332:TYR:CZ	1:A:336:MET:HG3	2.39	0.58
2:A:1450:HEM:HBB2	2:A:1450:HEM:HMB2	1.85	0.58
1:B:451:GLU:OE1	4:B:2299:HOH:O	2.16	0.57
1:B:195:ARG:HG3	1:B:196:HIS:N	2.19	0.57
1:B:331:ASN:H	1:B:334:ASN:ND2	2.03	0.57
1:A:87:SER:O	1:A:91:SER:HB2	2.05	0.57
1:A:201:LEU:HD23	1:A:204:MET:CE	2.34	0.57
1:B:188:LEU:CD1	1:B:243:ILE:CD1	2.81	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:GLU:HG3	1:B:373:VAL:CG1	2.35	0.57
1:B:233:ARG:HH12	1:B:237:GLN:NE2	2.04	0.56
2:A:1450:HEM:HMC1	2:A:1450:HEM:HBC2	1.86	0.56
1:B:63:LEU:C	1:B:64:LYS:HG2	2.25	0.55
1:B:63:LEU:O	1:B:64:LYS:HG2	2.06	0.55
1:A:44:HIS:HD2	1:A:71:SER:N	1.92	0.54
1:A:325:GLU:HG2	4:B:2035:HOH:O	2.08	0.54
1:B:44:HIS:CD2	1:B:71:SER:H	2.23	0.53
1:B:331:ASN:HD22	1:B:331:ASN:C	2.11	0.52
1:B:122:ARG:NH1	4:B:2085:HOH:O	2.41	0.52
1:B:422:CYS:HA	2:B:1450:HEM:C4D	2.44	0.52
1:B:100:ARG:HD3	4:B:2064:HOH:O	2.09	0.52
1:A:233:ARG:HH12	1:A:237:GLN:NE2	2.08	0.51
1:A:366:GLU:OE1	1:A:373:VAL:HG11	2.11	0.51
1:B:175:ILE:HG22	1:B:293[B]:GLN:HE22	1.75	0.51
1:B:317:ASP:OD2	4:B:2217:HOH:O	2.19	0.51
1:B:136:ILE:HD13	1:B:426:LYS:HD3	1.92	0.51
1:B:424:GLY:HA3	2:B:1450:HEM:C2C	2.46	0.50
1:B:331:ASN:H	1:B:334:ASN:HD22	1.59	0.50
1:A:193:ASN:HD22	1:A:196:HIS:H	1.59	0.50
1:B:290:PHE:CD1	3:B:1460[A]:T9H:H25	2.47	0.50
1:A:175:ILE:HD12	1:A:296:SER:HB3	1.94	0.49
1:B:291:ALA:HB2	3:B:1460[B]:T9H:H29	1.93	0.49
1:B:422:CYS:HA	2:B:1450:HEM:CHA	2.43	0.49
1:B:191:ARG:NH2	1:B:242:GLU:OE1	2.46	0.48
1:A:184:PHE:HE2	1:A:197:PHE:CD2	2.31	0.48
1:B:38:THR:HG22	1:B:39:VAL:HG23	1.96	0.47
4:A:2302:HOH:O	1:B:88:ARG:HD2	2.14	0.47
1:B:101:GLU:OE2	1:B:364:LYS:HE3	2.15	0.47
1:B:114:VAL:HG11	1:B:283:GLY:HA3	1.95	0.47
2:A:1450:HEM:HBC2	2:A:1450:HEM:CMC	2.45	0.47
1:A:36:PRO:O	1:A:44:HIS:HE1	1.98	0.46
1:B:110:PHE:HZ	3:B:1460[A]:T9H:C25	2.28	0.46
1:B:210:PRO:O	1:B:213:VAL:HG12	2.16	0.46
1:B:348:GLU:HG3	1:B:400:TRP:CD1	2.51	0.45
1:B:366:GLU:CG	1:B:373:VAL:CG1	2.93	0.45
1:B:220:ARG:N	1:B:220:ARG:HD2	2.31	0.45
1:B:351:ARG:HD3	1:B:394:PHE:CD1	2.51	0.45
1:A:177:ASN:OD1	1:A:195:ARG:NH1	2.50	0.45
1:A:193:ASN:HD22	1:A:193:ASN:C	2.20	0.45
1:B:100:ARG:HG2	1:B:101:GLU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ASN:HD22	1:A:169:GLU:H	1.63	0.44
1:B:331:ASN:ND2	1:B:334:ASN:H	2.14	0.44
1:A:422:CYS:HA	2:A:1450:HEM:CHA	2.48	0.44
1:B:105:ILE:HD13	1:B:106:MET:N	2.32	0.44
1:B:193:ASN:ND2	1:B:196:HIS:H	2.16	0.44
1:A:424:GLY:HA3	2:A:1450:HEM:C2C	2.52	0.43
1:A:71:SER:OG	1:A:74:GLY:CA	2.66	0.43
1:B:203:LYS:HD3	1:B:228:ARG:HG2	1.99	0.43
1:B:424:GLY:HA3	2:B:1450:HEM:C3C	2.54	0.43
3:A:1460:T9H:O4	3:A:1460:T9H:H1	2.19	0.43
1:A:364:LYS:HA	1:A:364:LYS:HD2	1.80	0.43
1:A:203:LYS:HE2	1:A:228:ARG:CZ	2.48	0.43
1:B:358:MET:HE3	1:B:358:MET:HB2	1.86	0.42
1:B:133:GLU:OE1	4:B:2101:HOH:O	2.22	0.42
1:B:196:HIS:HB2	4:B:2148:HOH:O	2.19	0.42
1:A:99:PRO:HD2	1:A:120:TYR:OH	2.19	0.42
1:A:149:GLU:HB3	1:A:178:THR:HG22	2.02	0.42
1:A:331:ASN:H	1:A:334:ASN:ND2	2.18	0.42
1:B:215:MET:HB2	1:B:218:LEU:HD22	2.02	0.42
2:A:1450:HEM:HMB2	2:A:1450:HEM:CBB	2.49	0.41
1:B:107:THR:HB	1:B:108:PRO:HD3	2.01	0.41
1:A:326:PHE:O	1:A:441:ARG:NH2	2.53	0.41
1:A:332:TYR:CE1	1:A:336:MET:HG3	2.55	0.41
1:B:105:ILE:HD13	1:B:105:ILE:C	2.41	0.41
1:B:332:TYR:CE1	1:B:336:MET:HG3	2.55	0.41
1:A:422:CYS:HA	2:A:1450:HEM:C4D	2.56	0.41
1:A:103:TYR:CE1	3:A:1460:T9H:N6	2.88	0.41
1:A:374:VAL:HA	1:A:375:PRO:HD3	1.90	0.41
1:A:136:ILE:HG23	1:A:332:TYR:OH	2.21	0.41
1:A:71:SER:OG	1:A:74:GLY:HA2	2.21	0.40
1:B:339:MET:HE3	1:B:437:ALA:HB2	2.03	0.40
1:A:423:ILE:CD1	2:A:1450:HEM:HMD2	2.49	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	439/470 (93%)	426 (97%)	13 (3%)	0	100	100
1	B	445/470 (95%)	432 (97%)	13 (3%)	0	100	100
All	All	884/940 (94%)	858 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	377/411 (92%)	362 (96%)	15 (4%)	31	31
1	B	381/411 (93%)	353 (93%)	28 (7%)	14	10
All	All	758/822 (92%)	715 (94%)	43 (6%)	21	17

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	THR
1	A	50	LYS
1	A	51	ASN
1	A	112	GLU
1	A	136	ILE
1	A	140	GLN
1	A	166	ASN
1	A	168	LEU
1	A	193	ASN
1	A	195	ARG
1	A	197	PHE
1	A	325	GLU
1	A	358	MET
1	A	375	PRO

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Mol	Chain	Res	Type
1	A	391	GLU
1	B	41	PHE
1	B	64	LYS
1	B	88	ARG
1	B	100	ARG
1	B	104[A]	THR
1	B	104[B]	THR
1	B	105	ILE
1	B	122	ARG
1	B	136	ILE
1	B	140	GLN
1	B	166	ASN
1	B	193	ASN
1	B	195	ARG
1	B	197	PHE
1	B	205	GLU
1	B	218	LEU
1	B	220	ARG
1	B	225	GLN
1	B	228	ARG
1	B	231	GLU
1	B	271	ARG
1	B	331	ASN
1	B	337	ASP
1	B	358	MET
1	B	382	CYS
1	B	426	LYS
1	B	442	GLU
1	B	470	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	51	ASN
1	A	166	ASN
1	A	193	ASN
1	A	237	GLN
1	A	334	ASN
1	B	44	HIS
1	B	166	ASN
1	B	193	ASN

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Mol	Chain	Res	Type
1	B	196	HIS
1	B	237	GLN
1	B	331	ASN
1	B	334	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 ligands 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	$\#\|Z\| > 2$
3	T9H	B	1460[B]	2	47,49,49	1.99	4 (8%)	61,70,70	2.60	18 (29%)
2	HEM	B	1450	3,1	41,50,50	2.11	12 (29%)	45,82,82	1.99	10 (22%)
2	HEM	A	1450	3,1	41,50,50	2.06	13 (31%)	45,82,82	2.31	18 (40%)
3	T9H	A	1460	2	47,49,49	1.93	7 (14%)	61,70,70	3.20	23 (37%)
3	T9H	B	1460[A]	2	47,49,49	1.94	3 (6%)	61,70,70	2.53	16 (26%)

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
3	T9H	B	1460[B]	2	-	3/29/46/46	0/6/6/6
2	HEM	B	1450	3,1	-	2/12/54/54	-
2	HEM	A	1450	3,1	-	0/12/54/54	-
3	T9H	A	1460	2	-	3/29/46/46	0/6/6/6
3	T9H	B	1460[A]	2	-	5/29/46/46	0/6/6/6

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1460[B]	T9H	C15-S1	-8.09	1.64	1.76
3	B	1460[A]	T9H	C15-S1	-7.91	1.64	1.76
3	A	1460	T9H	C9-C22	7.35	1.49	1.38
2	A	1450	HEM	C3D-C2D	7.19	1.52	1.36
2	B	1450	HEM	C3D-C2D	6.96	1.51	1.36
3	B	1460[B]	T9H	C9-C22	6.59	1.47	1.38
3	B	1460[A]	T9H	C9-C22	6.46	1.47	1.38
3	A	1460	T9H	S1-N5	-6.29	1.54	1.63
2	B	1450	HEM	C3C-C2C	-6.22	1.31	1.40
3	B	1460[A]	T9H	S1-N5	-6.13	1.54	1.63
3	B	1460[B]	T9H	S1-N5	-6.04	1.54	1.63
3	A	1460	T9H	C15-S1	-4.46	1.69	1.76
2	A	1450	HEM	CMB-C2B	4.38	1.60	1.50
2	A	1450	HEM	C3C-CAC	4.08	1.56	1.47
2	B	1450	HEM	C3C-CAC	3.38	1.54	1.47
2	A	1450	HEM	CAB-C3B	3.04	1.55	1.47
3	A	1460	T9H	C17-C18	2.98	1.43	1.34
2	B	1450	HEM	CAA-C2A	2.91	1.56	1.52
2	A	1450	HEM	FE-ND	2.85	2.10	1.96
3	A	1460	T9H	C29-C28	2.83	1.43	1.36
2	A	1450	HEM	CMD-C2D	2.82	1.56	1.50
2	A	1450	HEM	C3C-C2C	-2.64	1.36	1.40
3	A	1460	T9H	C28-C27	-2.62	1.36	1.42
2	B	1450	HEM	CMC-C2C	2.60	1.57	1.51
2	B	1450	HEM	FE-NB	2.59	2.09	1.96
2	B	1450	HEM	CMA-C3A	2.47	1.56	1.51
2	A	1450	HEM	CMC-C2C	2.39	1.57	1.51
2	B	1450	HEM	C4A-NA	2.32	1.40	1.36
3	A	1460	T9H	C1-C2	2.19	1.43	1.38
2	B	1450	HEM	CBD-CGD	2.18	1.55	1.50
2	A	1450	HEM	CHB-C1B	2.17	1.40	1.35
2	B	1450	HEM	CHB-C1B	2.17	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1450	HEM	CHA-C4D	2.15	1.40	1.35
3	B	1460[B]	T9H	C27-C26	2.13	1.48	1.42
2	B	1450	HEM	CAB-C3B	2.10	1.53	1.47
2	A	1450	HEM	FE-NB	2.09	2.07	1.96
2	B	1450	HEM	O2A-CGA	-2.08	1.23	1.30
2	A	1450	HEM	O1D-CGD	2.04	1.28	1.22
2	A	1450	HEM	C1B-C2B	2.03	1.48	1.44

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1460	T9H	O1-S1-N5	10.84	116.57	106.69
3	A	1460	T9H	C20-C19-N5	9.42	116.12	108.91
3	B	1460[B]	T9H	O2-S1-N5	8.93	114.83	106.69
3	B	1460[A]	T9H	O2-S1-N5	8.32	114.27	106.69
3	A	1460	T9H	C17-C18-S2	-8.25	106.29	112.98
3	B	1460[A]	T9H	C14-N5-C19	7.61	120.59	112.17
3	B	1460[B]	T9H	C14-N5-C19	7.48	120.44	112.17
3	A	1460	T9H	C14-N5-C19	6.84	119.74	112.17
3	A	1460	T9H	O2-S1-N5	6.78	112.87	106.69
3	B	1460[A]	T9H	C17-C18-S2	-6.59	107.64	112.98
3	A	1460	T9H	C15-S1-N5	-6.07	95.61	106.81
3	B	1460[B]	T9H	O1-S1-N5	6.02	112.18	106.69
2	B	1450	HEM	C4D-ND-C1D	5.97	111.24	105.07
3	B	1460[A]	T9H	O1-S1-N5	5.92	112.08	106.69
2	A	1450	HEM	C4D-ND-C1D	5.74	111.00	105.07
3	B	1460[B]	T9H	C9-C8-N3	5.68	127.31	116.80
3	A	1460	T9H	C9-C8-N3	5.37	126.74	116.80
3	B	1460[A]	T9H	O2-S1-O1	-5.36	110.84	119.52
3	B	1460[B]	T9H	O2-S1-O1	-5.31	110.91	119.52
3	B	1460[B]	T9H	C17-C18-S2	-5.27	108.71	112.98
2	B	1450	HEM	C1B-NB-C4B	5.09	110.33	105.07
2	A	1450	HEM	C4B-C3B-C2B	4.80	110.92	107.11
3	A	1460	T9H	O2-S1-O1	-4.73	111.86	119.52
3	B	1460[A]	T9H	C13-N4-C20	4.66	121.81	111.52
3	B	1460[B]	T9H	C13-N4-C20	4.62	121.72	111.52
2	A	1450	HEM	CMA-C3A-C4A	-4.52	121.52	128.46
2	A	1450	HEM	C2C-C3C-C4C	4.44	110.00	106.90
3	B	1460[A]	T9H	C21-C12-N4	-4.37	116.63	121.33
2	A	1450	HEM	CHC-C4B-NB	4.33	129.14	124.43
3	B	1460[B]	T9H	C21-C12-N4	-3.96	117.07	121.33
2	A	1450	HEM	CMB-C2B-C1B	3.95	131.05	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1460	T9H	C28-C27-C26	3.86	123.29	118.17
3	B	1460[A]	T9H	C9-C8-N3	3.82	123.88	116.80
3	A	1460	T9H	C21-C22-C9	-3.77	119.51	123.53
3	A	1460	T9H	C13-N4-C20	3.74	119.78	111.52
2	B	1450	HEM	C2B-C1B-NB	-3.71	105.44	109.84
3	A	1460	T9H	O3-C8-C9	-3.65	114.35	121.01
3	A	1460	T9H	C29-C28-C27	-3.62	115.87	120.89
3	A	1460	T9H	C13-C14-N5	3.55	111.62	108.91
2	B	1450	HEM	CHC-C4B-NB	3.31	128.03	124.43
3	B	1460[A]	T9H	C15-S1-N5	-3.24	100.83	106.81
2	A	1450	HEM	O1D-CGD-CBD	-3.24	112.66	123.08
2	A	1450	HEM	C4A-C3A-C2A	3.24	109.25	107.00
3	B	1460[B]	T9H	O3-C8-C9	-3.19	115.19	121.01
2	B	1450	HEM	C4B-C3B-C2B	3.16	109.62	107.11
3	B	1460[B]	T9H	C28-C27-C26	3.15	122.35	118.17
3	A	1460	T9H	C19-C20-N4	3.15	116.81	110.70
3	B	1460[B]	T9H	C21-C22-C9	-3.11	120.21	123.53
3	B	1460[B]	T9H	C15-S1-N5	-3.10	101.09	106.81
3	B	1460[A]	T9H	C21-C22-C9	-3.07	120.25	123.53
2	A	1450	HEM	C4C-CHD-C1D	3.04	126.57	122.56
3	B	1460[B]	T9H	C13-C14-N5	2.87	111.11	108.91
2	B	1450	HEM	CMA-C3A-C4A	-2.84	124.10	128.46
3	B	1460[B]	T9H	O3-C8-N3	-2.75	117.40	122.45
3	B	1460[A]	T9H	C23-C7-N3	-2.74	105.01	110.79
3	A	1460	T9H	C21-C12-N4	-2.66	118.47	121.33
2	B	1450	HEM	C2C-C3C-C4C	2.64	108.74	106.90
2	B	1450	HEM	C4C-CHD-C1D	2.62	126.02	122.56
2	A	1450	HEM	C1B-NB-C4B	2.54	107.69	105.07
3	A	1460	T9H	C24-C23-C7	-2.53	108.49	113.45
2	B	1450	HEM	O2D-CGD-CBD	2.51	122.08	114.03
3	A	1460	T9H	C14-N5-S1	2.50	121.58	117.05
2	A	1450	HEM	O2D-CGD-CBD	2.43	121.85	114.03
2	A	1450	HEM	CBB-CAB-C3B	-2.41	115.62	127.62
3	B	1460[A]	T9H	O3-C8-C9	-2.38	116.66	121.01
3	B	1460[B]	T9H	C6-C7-N3	2.34	117.53	111.16
3	B	1460[B]	T9H	C31-C26-C27	-2.33	116.50	120.76
3	A	1460	T9H	C23-C24-C25	-2.32	125.11	127.97
2	A	1450	HEM	CMA-C3A-C2A	2.27	129.23	124.94
2	A	1450	HEM	C3B-C2B-C1B	-2.26	104.81	106.49
3	B	1460[A]	T9H	C22-C9-C8	-2.24	119.90	125.09
2	A	1450	HEM	C3C-C4C-NC	-2.24	106.72	110.94
3	A	1460	T9H	O3-C8-N3	-2.24	118.33	122.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1450	HEM	C1D-C2D-C3D	-2.18	104.66	106.96
2	A	1450	HEM	CAA-CBA-CGA	-2.17	107.67	113.76
3	B	1460[B]	T9H	C31-C26-N6	2.15	136.75	130.80
3	B	1460[B]	T9H	C20-C19-N5	2.13	110.54	108.91
3	A	1460	T9H	C22-C9-C8	-2.10	120.24	125.09
3	A	1460	T9H	C5-N2-C6	-2.06	122.46	127.40
3	B	1460[A]	T9H	C20-C19-N5	2.04	110.48	108.91
3	B	1460[A]	T9H	C28-C27-C26	2.04	120.87	118.17
3	A	1460	T9H	C12-C21-C22	2.03	121.74	119.21
2	B	1450	HEM	C4B-CHC-C1C	2.03	125.24	122.56
2	A	1450	HEM	CAD-CBD-CGD	-2.02	109.26	113.60
3	B	1460[A]	T9H	C19-N5-S1	2.02	120.71	117.05

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1460[A]	T9H	C24-C23-C7-C6
3	B	1460[A]	T9H	C24-C23-C7-N3
3	B	1460[A]	T9H	C14-N5-S1-O2
3	B	1460[B]	T9H	C14-N5-S1-O2
3	B	1460[A]	T9H	C14-N5-S1-O1
3	A	1460	T9H	C19-N5-S1-O2
3	B	1460[B]	T9H	C14-N5-S1-O1
3	A	1460	T9H	C19-N5-S1-O1
3	A	1460	T9H	C19-N5-S1-C15
3	B	1460[A]	T9H	C14-N5-S1-C15
3	B	1460[B]	T9H	C14-N5-S1-C15
2	B	1450	HEM	CAD-CBD-CGD-O2D
2	B	1450	HEM	CAD-CBD-CGD-O1D

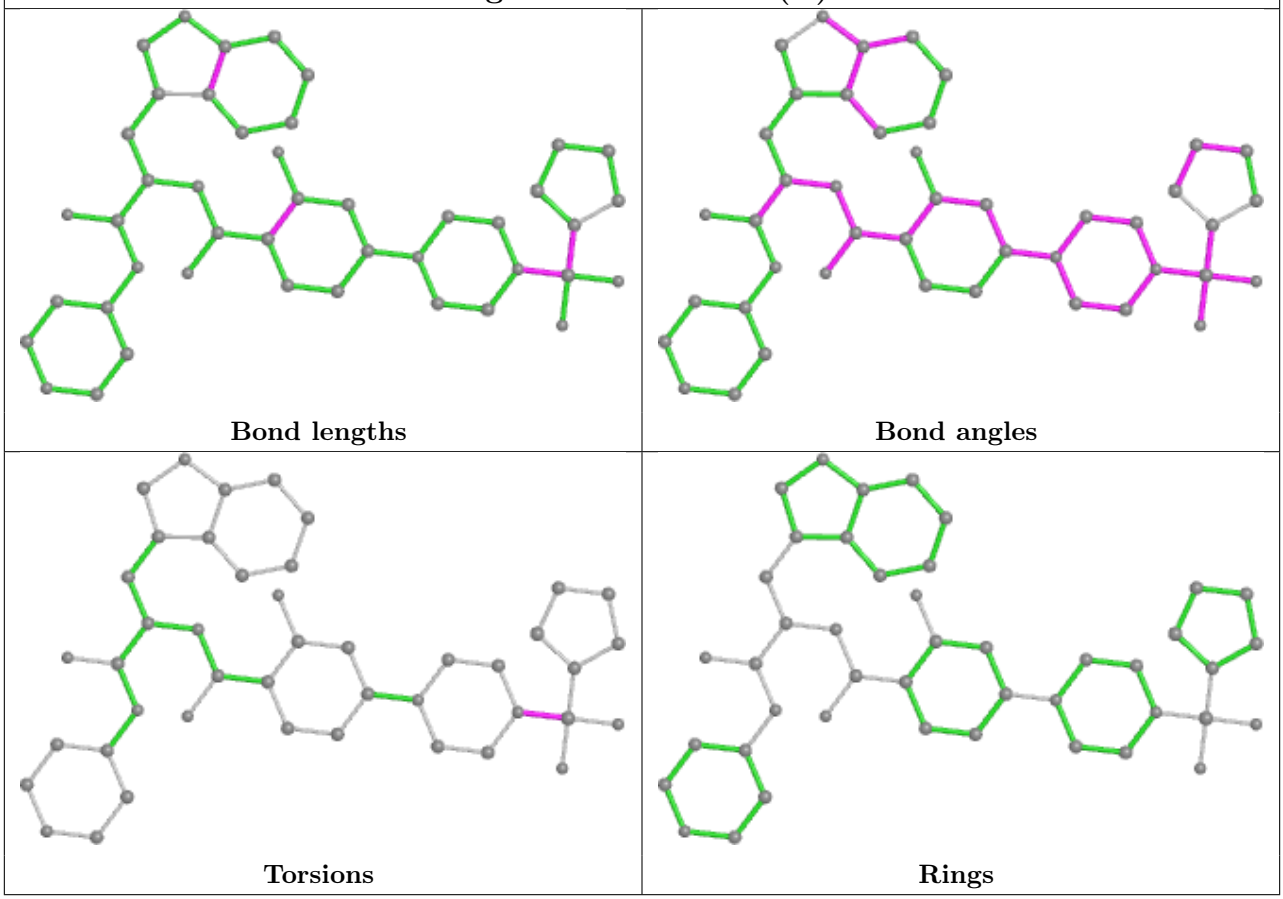
There are no ring outliers.

5 monomers are involved in 22 short contacts:

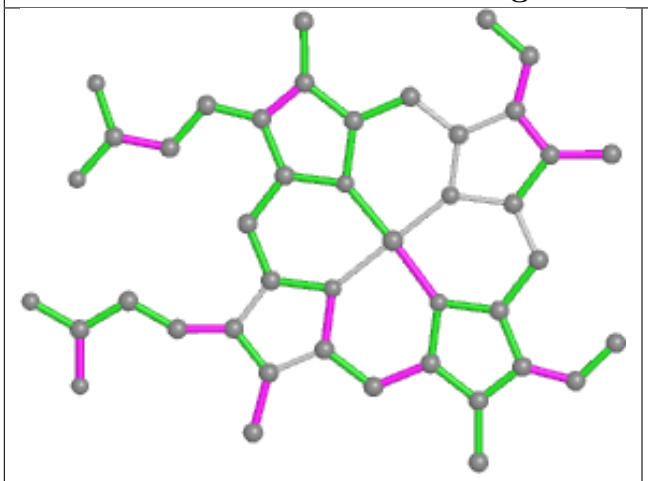
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1460[B]	T9H	1	0
2	B	1450	HEM	7	0
2	A	1450	HEM	10	0
3	A	1460	T9H	2	0
3	B	1460[A]	T9H	2	0

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.

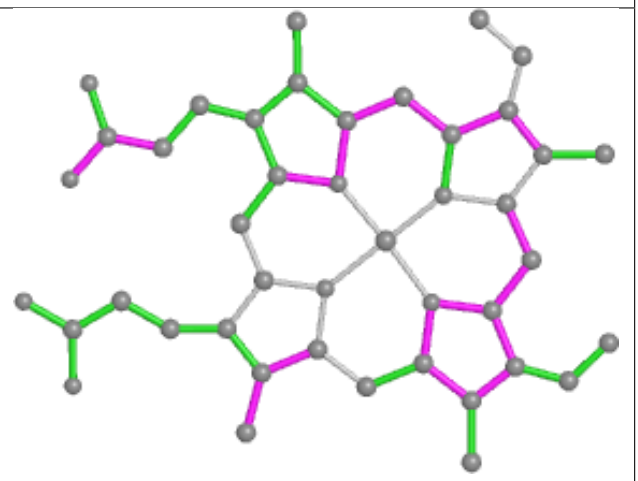
Ligand T9H B 1460 (B)



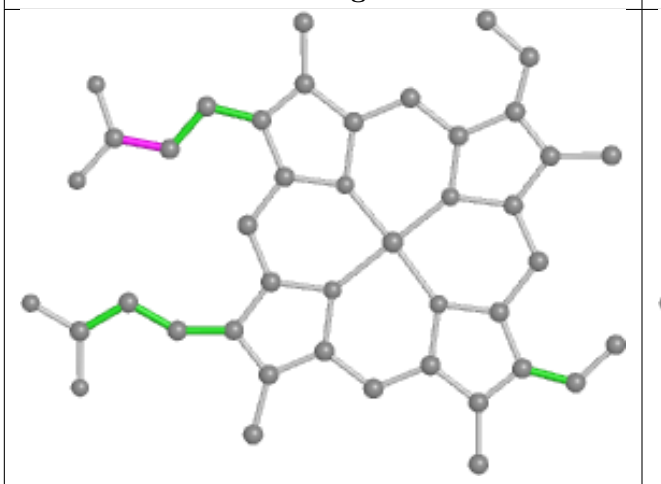
Ligand HEM B 1450



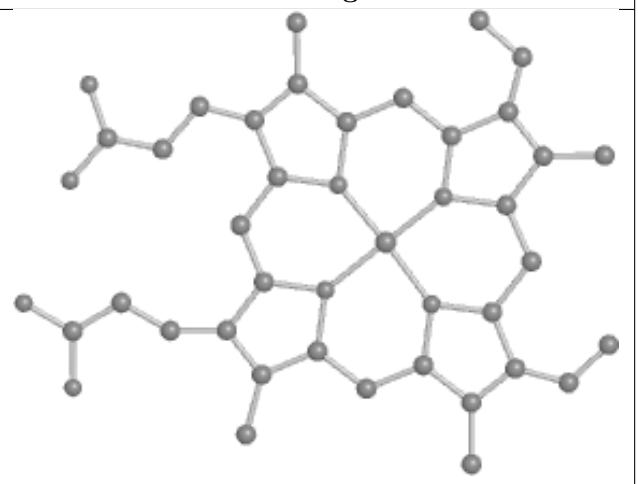
Bond lengths



Bond angles

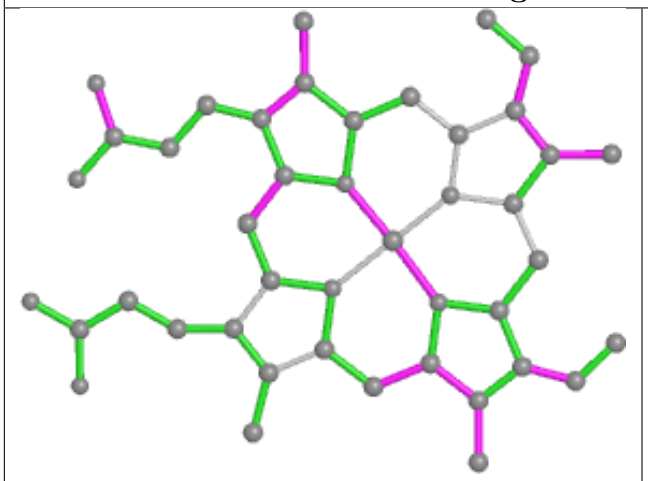


Torsions

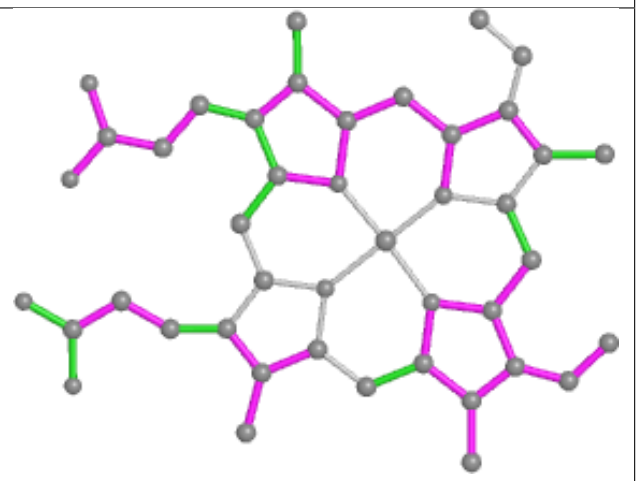


Rings

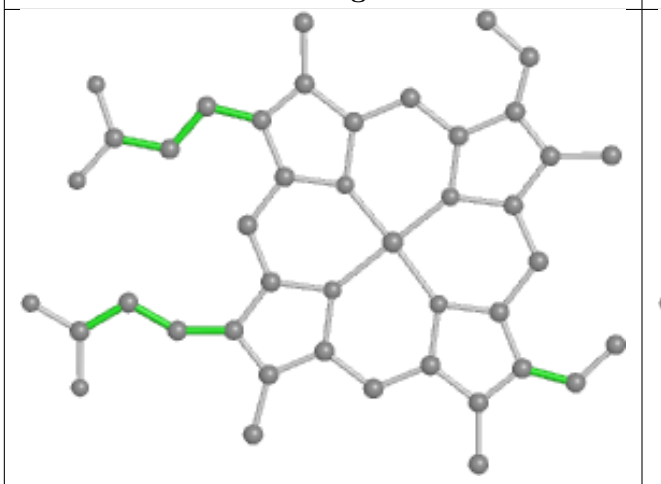
Ligand HEM A 1450



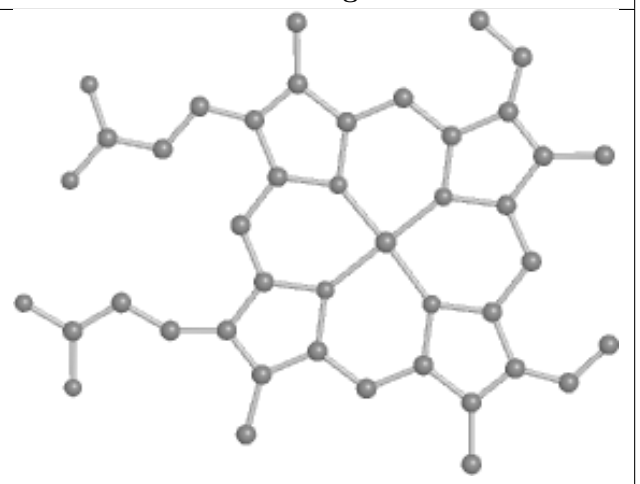
Bond lengths



Bond angles

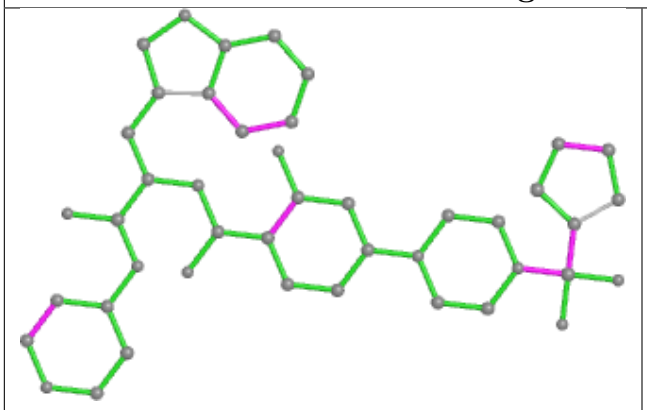


Torsions

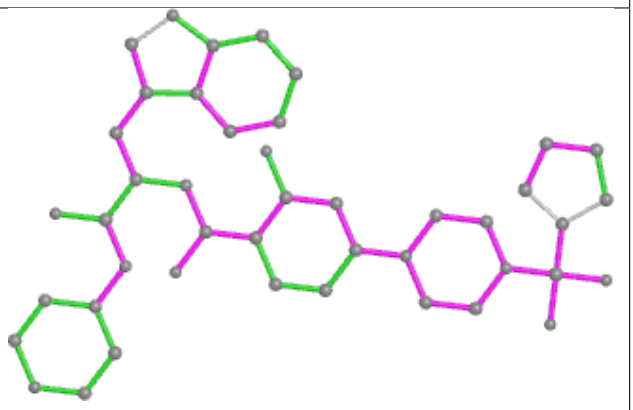


Rings

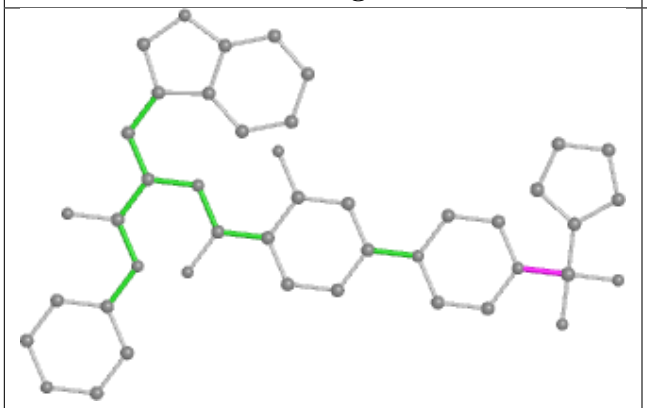
Ligand T9H A 1460



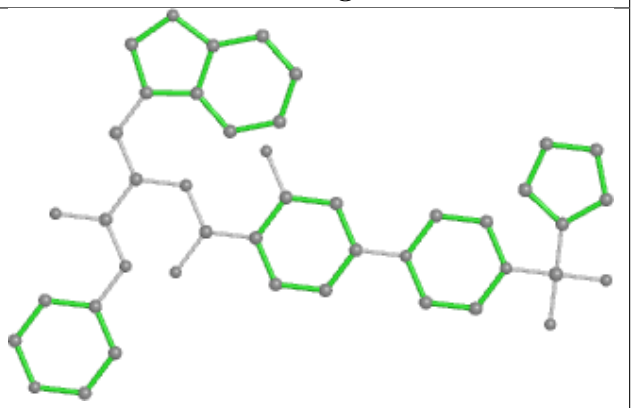
Bond lengths



Bond angles

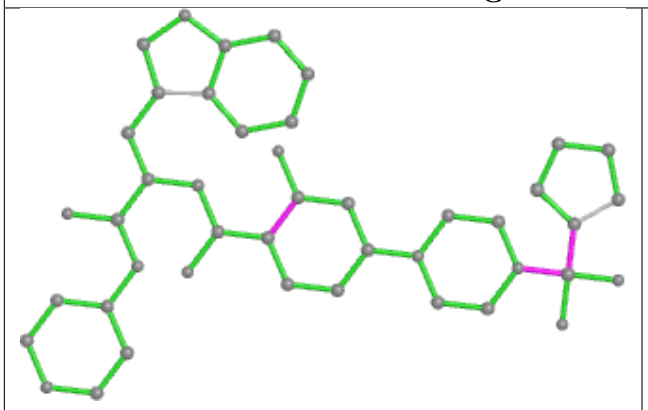


Torsions

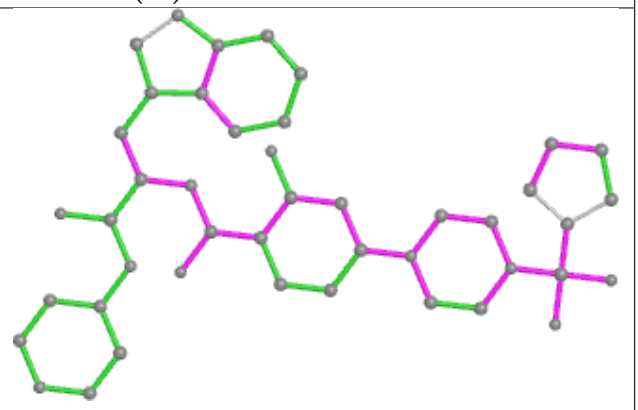


Rings

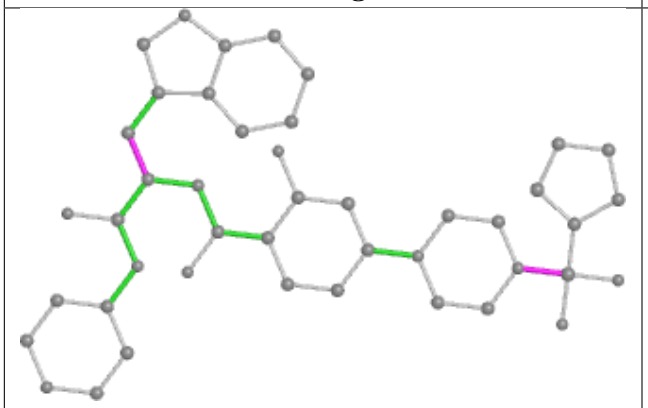
Ligand T9H B 1460 (A)



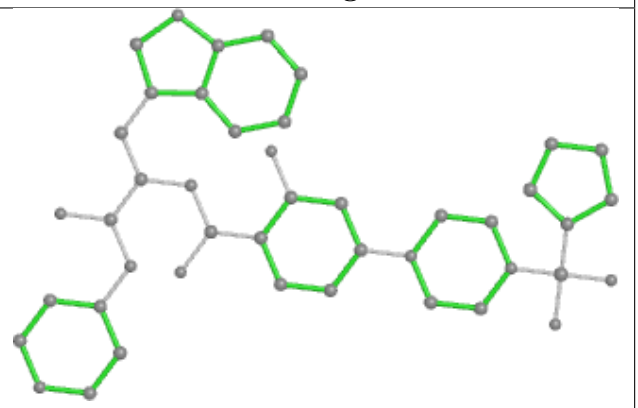
Bond lengths



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	442/470 (94%)	-0.55	2 (0%)	91	92	12, 22, 35, 54	0
1	B	445/470 (94%)	-0.51	3 (0%)	87	89	15, 24, 38, 54	0
All	All	887/940 (94%)	-0.53	5 (0%)	89	91	12, 23, 36, 54	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	479	LEU	3.2
1	B	29	PRO	2.8
1	B	480	PRO	2.6
1	A	258	THR	2.2
1	A	30	THR	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

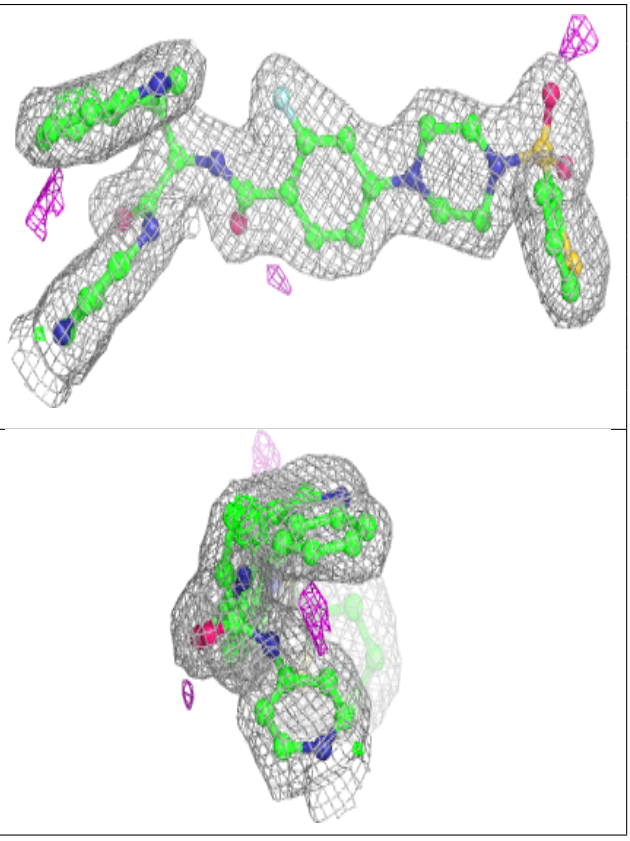
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	T9H	A	1460	44/44	0.96	0.09	14,21,27,30	0
3	T9H	B	1460[A]	44/44	0.97	0.10	12,22,26,30	44
3	T9H	B	1460[B]	44/44	0.97	0.10	10,21,25,29	44
2	HEM	B	1450	43/43	0.98	0.10	10,17,23,27	0
2	HEM	A	1450	43/43	0.98	0.10	8,15,23,24	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.

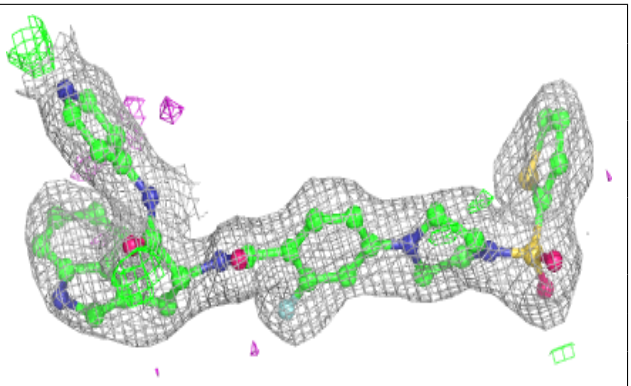
Electron density around T9H A 1460:

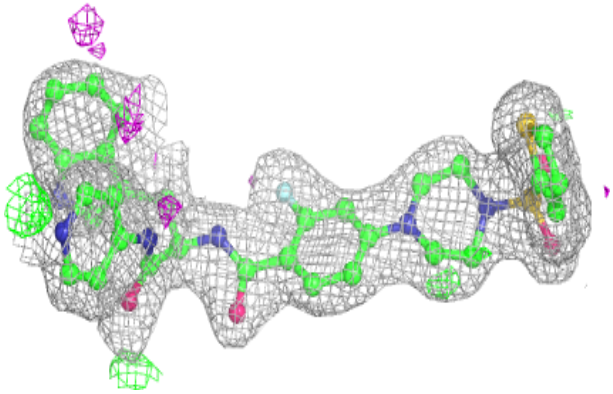
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

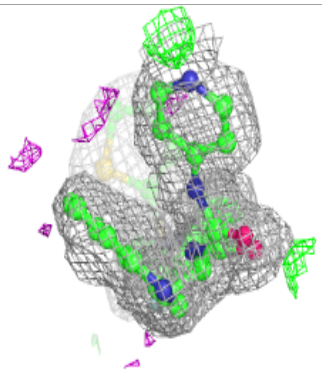


Electron density around T9H B 1460 (A):

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

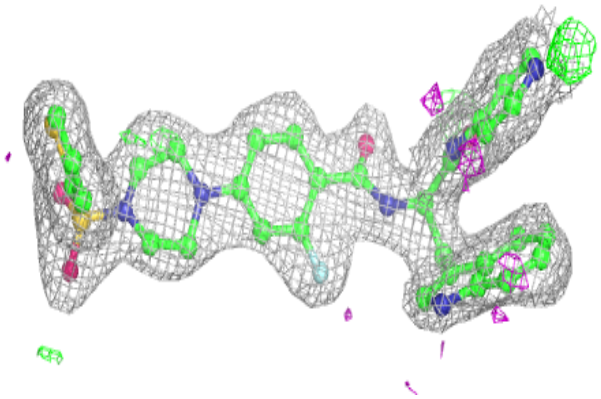


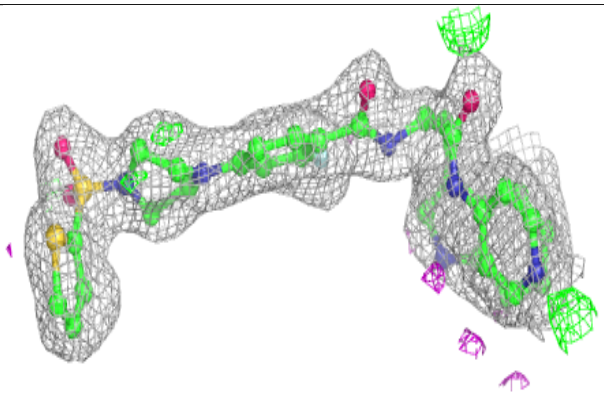


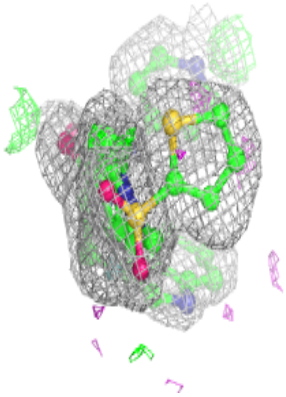


Electron density around T9H B 1460 (B):

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

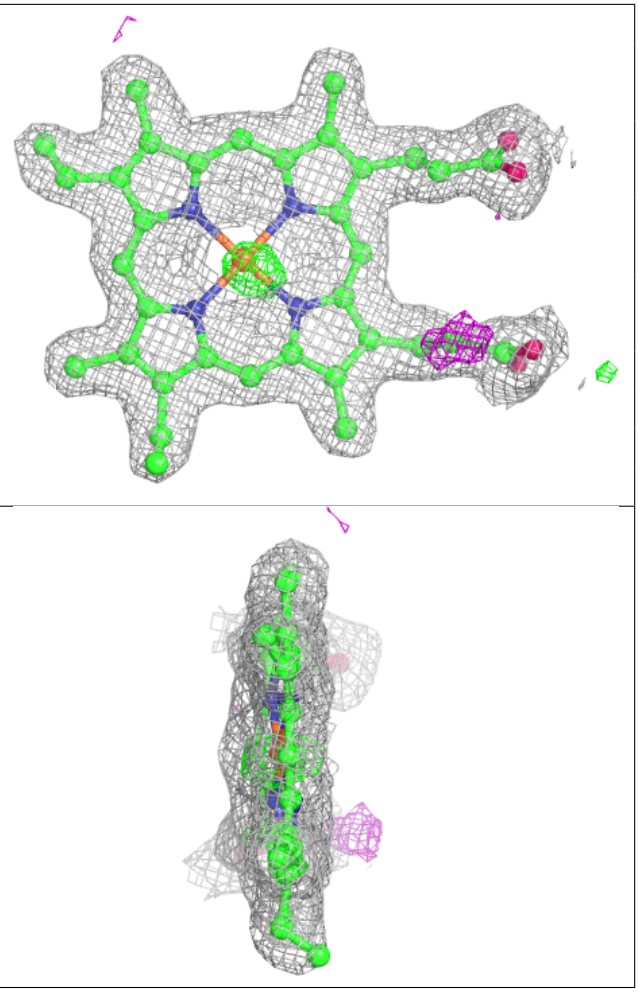






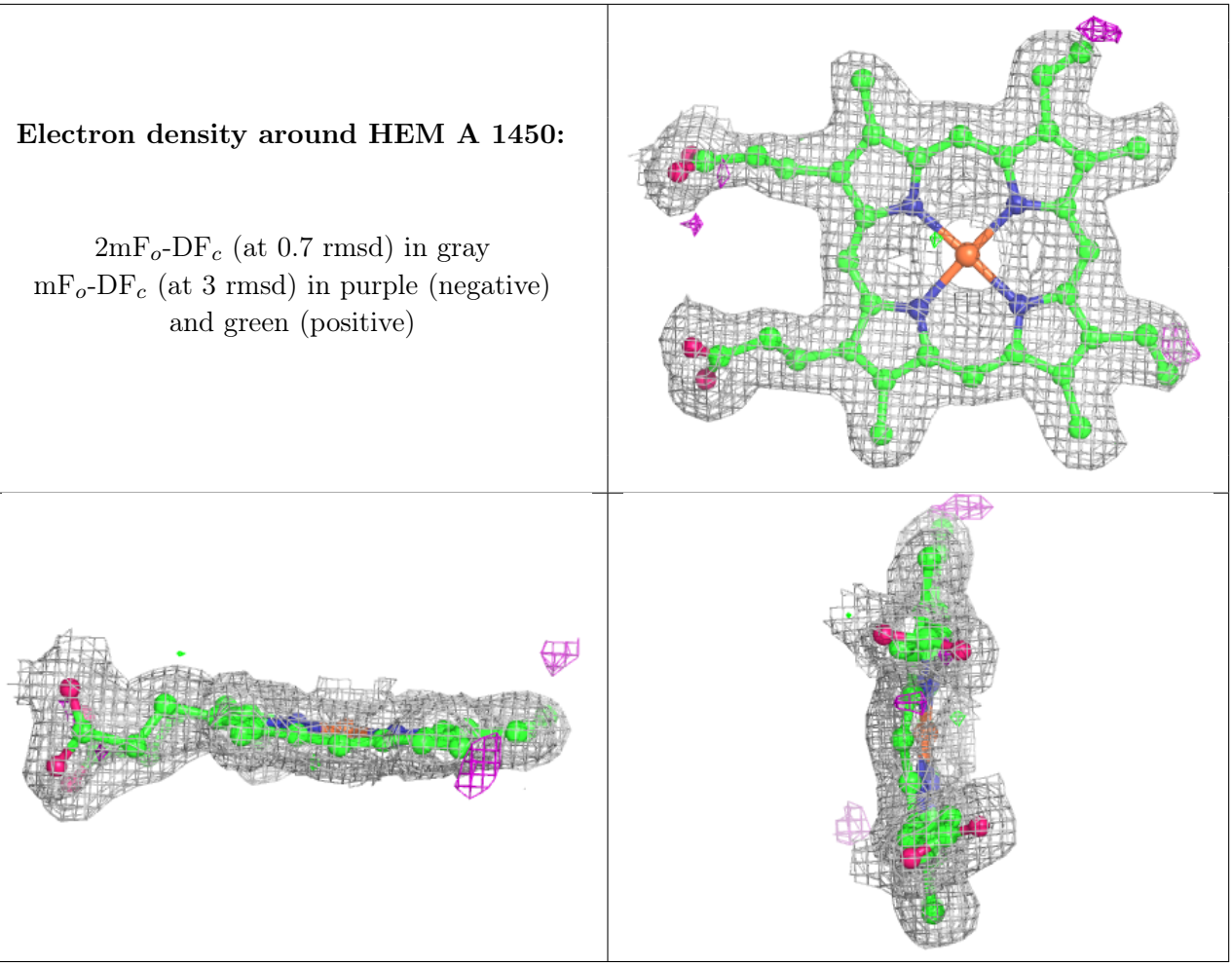
Electron density around HEM B 1450:

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



Electron density around HEM A 1450:

$2mF_o$-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.