Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2026 – 09:39 am BST

PDB ID	:	4C28 / pdb_00004c28
Title	:	Crystal structure of Trypanosoma cruzi CYP51 bound to the inhibitor (R)-N-(3-(1H-indol-3-yl)-1-oxo-1-(pyridin-4-ylamino)propan-2-yl)-4-(4-(4-chlorophenyl)piperazin-1-yl)-2-fluorobenzamide.
Authors	:	Vieira, D.F.; Calvet, C.M.; Choi, J.Y.; Cameron, M.D.; Gut, J.; Kellar, D.; Siqueira-Neto, J.L.; McKerrow, J.H.; Roush, W.R.; Podust, L.M.
Deposited on	:	2013-08-16
Resolution	:	2.03 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 (1)) were used in the production of this report:

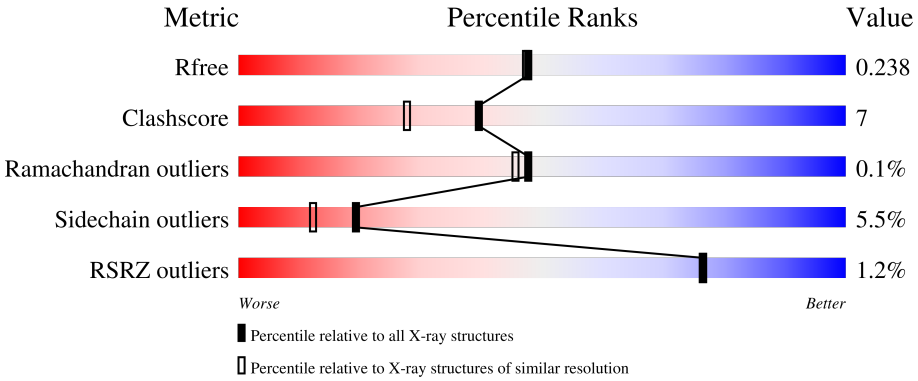
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 2.03 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	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (2.04-2.00)

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	467	83% 10% • 5%
1	B	467	77% 16% • 6%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7735 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
1	A	443	Total	C	N	O	S	0	1	0
			3536	2261	619	628	28			
1	B	441	Total	C	N	O	S	0	2	0
			3526	2256	618	624	28			

There are 28 discrepancies between the modelled and reference sequences:

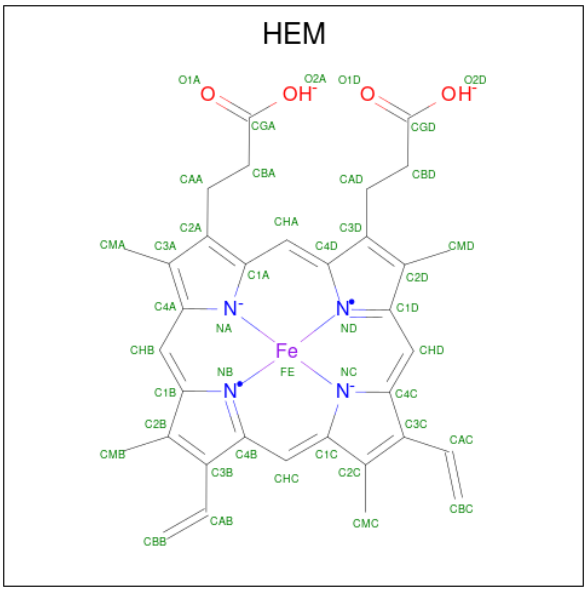
Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	expression tag	UNP Q7Z1V1
A	22	ALA	-	expression tag	UNP Q7Z1V1
A	23	LYS	-	expression tag	UNP Q7Z1V1
A	24	LYS	-	expression tag	UNP Q7Z1V1
A	25	THR	-	expression tag	UNP Q7Z1V1
A	26	SER	-	expression tag	UNP Q7Z1V1
A	27	SER	-	expression tag	UNP Q7Z1V1
A	28	LYS	-	expression tag	UNP Q7Z1V1
A	482	HIS	-	expression tag	UNP Q7Z1V1
A	483	HIS	-	expression tag	UNP Q7Z1V1
A	484	HIS	-	expression tag	UNP Q7Z1V1
A	485	HIS	-	expression tag	UNP Q7Z1V1
A	486	HIS	-	expression tag	UNP Q7Z1V1
A	487	HIS	-	expression tag	UNP Q7Z1V1
B	21	MET	-	expression tag	UNP Q7Z1V1
B	22	ALA	-	expression tag	UNP Q7Z1V1
B	23	LYS	-	expression tag	UNP Q7Z1V1
B	24	LYS	-	expression tag	UNP Q7Z1V1
B	25	THR	-	expression tag	UNP Q7Z1V1
B	26	SER	-	expression tag	UNP Q7Z1V1
B	27	SER	-	expression tag	UNP Q7Z1V1
B	28	LYS	-	expression tag	UNP Q7Z1V1
B	482	HIS	-	expression tag	UNP Q7Z1V1
B	483	HIS	-	expression tag	UNP Q7Z1V1
B	484	HIS	-	expression tag	UNP Q7Z1V1

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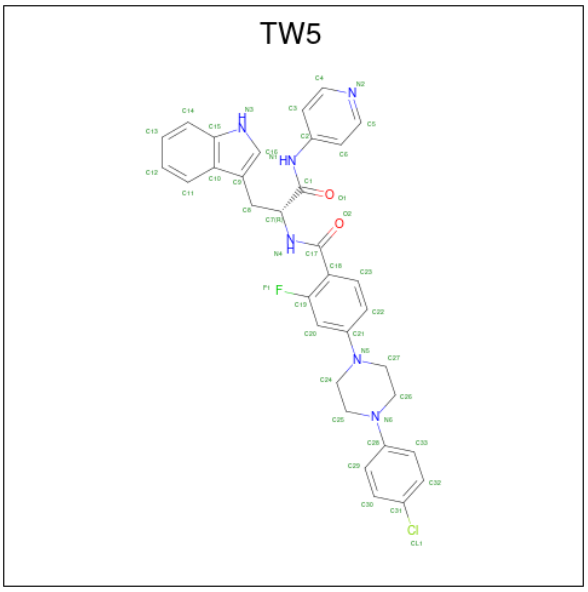
Chain	Residue	Modelled	Actual	Comment	Reference
B	485	HIS	-	expression tag	UNP Q7Z1V1
B	486	HIS	-	expression tag	UNP Q7Z1V1
B	487	HIS	-	expression tag	UNP Q7Z1V1

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



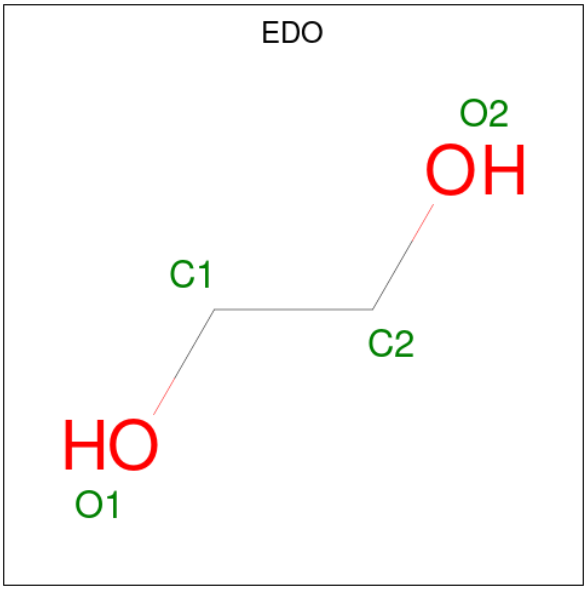
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is (R)-N-(3-(1H-indol-3-yl)-1-oxo-1-(pyridin-4-ylamino)propan-2-yl)-4-(4-(4-chlorophenyl)piperazin-1-yl)-2-fluorobenzamide (CCD ID: TW5) (formula: $C_{33}H_{30}ClFN_6O_2$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Cl	F	N	O	0	1
			86	66	2	2	12	4		
3	B	1	Total	C	Cl	F	N	O	0	1
			86	66	2	2	12	4		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0

- Molecule 6 is water.

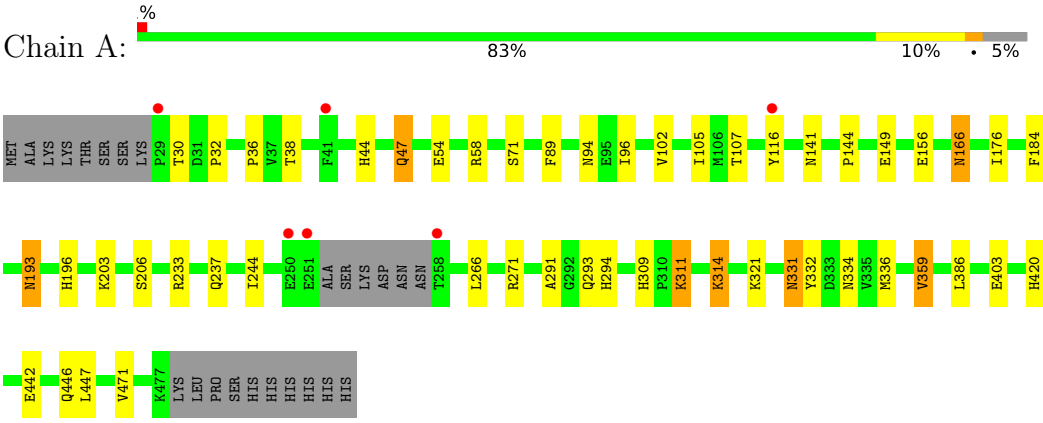
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	231	Total O 231 231	0	0
6	B	179	Total O 179 179	0	0

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.

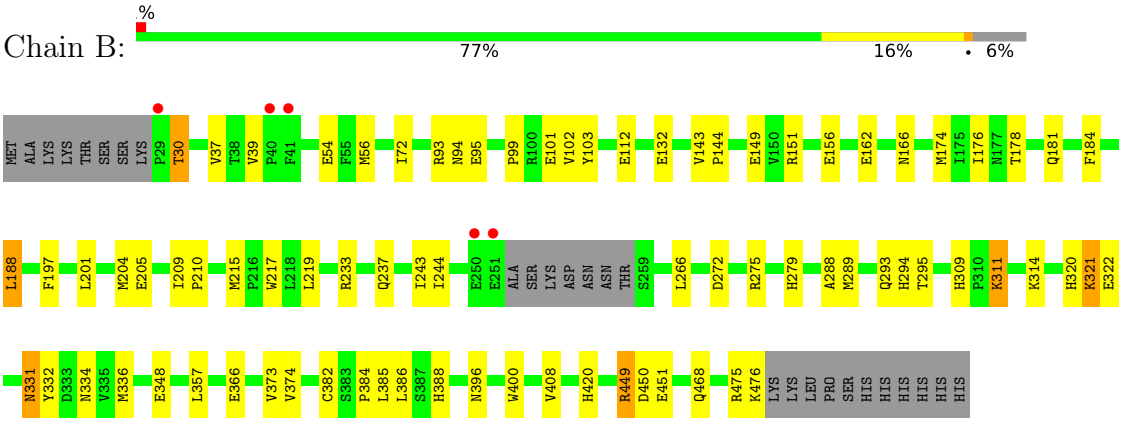
• Molecule 1: STEROL 14-ALPHA DEMETHYLASE

Chain A:



• Molecule 1: STEROL 14-ALPHA DEMETHYLASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.95Å 79.00Å 176.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.24 – 2.03 72.24 – 2.03	Depositor EDS
% Data completeness (in resolution range)	85.4 (72.24-2.03) 85.4 (72.24-2.03)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.186 , 0.238 0.191 , 0.238	Depositor DCC
R_{free} test set	2904 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 33.0	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	0.94	EDS
Total number of atoms	7735	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 3.30% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TW5, HEM, EDO, CL

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	1.15	3/3620 (0.1%)	1.12	2/4897 (0.0%)
1	B	1.15	3/3611 (0.1%)	1.13	6/4885 (0.1%)
All	All	1.15	6/7231 (0.1%)	1.13	8/9782 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	32	PRO	CA-C	8.18	1.56	1.51
1	A	206	SER	C-O	-6.00	1.16	1.24
1	A	107	THR	C-O	-5.93	1.18	1.24
1	B	396	ASN	C-O	-5.46	1.21	1.23
1	B	210	PRO	C-O	-5.45	1.17	1.24
1	B	272	ASP	C-O	-5.26	1.17	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	408	VAL	N-CA-C	-5.95	99.55	108.12
1	A	386	LEU	N-CA-C	5.47	117.05	111.14
1	B	30	THR	N-CA-C	5.42	117.80	109.07
1	B	322	GLU	N-CA-C	5.36	117.21	111.36
1	B	288	ALA	N-CA-C	5.34	116.78	111.07
1	A	94	ASN	N-CA-C	5.21	117.70	111.71
1	B	374	VAL	CA-C-N	-5.04	115.41	120.85
1	B	374	VAL	C-N-CA	-5.04	115.41	120.85

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	3536	0	3542	43	0
1	B	3526	0	3528	45	0
2	A	43	0	30	5	0
2	B	43	0	30	6	0
3	A	86	0	60	4	0
3	B	86	0	60	5	0
4	A	4	0	6	0	0
5	A	1	0	0	0	0
6	A	231	0	0	6	0
6	B	179	0	0	3	0
All	All	7735	0	7256	98	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 7.

All (98) 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:449[A]:ARG:CG	1:B:449[A]:ARG:HH11	1.74	0.98
1:A:47:GLN:HE21	1:A:47:GLN:H	1.21	0.87
1:B:449[A]:ARG:HG2	1:B:449[A]:ARG:NH1	1.93	0.81
1:A:336:MET:CE	1:A:430:LEU:HD13	2.10	0.81
1:A:44:HIS:HD2	1:A:71:SER:H	1.30	0.80
1:A:309:HIS:HD2	1:A:311:LYS:H	1.31	0.78
1:B:449[A]:ARG:CG	1:B:449[A]:ARG:NH1	2.36	0.77
1:B:449[B]:ARG:HD2	1:B:468:GLN:HB3	1.67	0.76
1:A:331:ASN:H	1:A:334:ASN:HD22	1.33	0.74
1:B:449[A]:ARG:HH11	1:B:449[A]:ARG:HG3	1.53	0.73
1:B:102:VAL:HG23	1:B:103:TYR:CE2	2.27	0.70
1:B:149:GLU:CG	1:B:181:GLN:HG3	2.22	0.70
1:B:102:VAL:HG23	1:B:103:TYR:CD2	2.27	0.69
1:B:149:GLU:HG2	1:B:181:GLN:HG3	1.74	0.67
1:B:451:GLU:HG2	6:B:2123:HOH:O	1.91	0.67
1:A:336:MET:HE3	1:A:430:LEU:HD13	1.75	0.67
1:A:309:HIS:CD2	1:A:311:LYS:HG2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ILE:HD12	1:B:219:LEU:HD23	1.81	0.63
1:A:291:ALA:HB2	3:A:1460[B]:TW5:H10	1.80	0.63
1:A:89:PHE:CE2	1:A:359:VAL:HG23	2.34	0.62
1:B:420:HIS:HD2	2:B:1450:HEM:O2D	1.86	0.58
1:A:89:PHE:CZ	1:A:359:VAL:HG23	2.40	0.57
1:B:215:MET:HE2	1:B:217:TRP:CZ2	2.40	0.56
1:A:193:ASN:ND2	1:A:196:HIS:H	2.03	0.56
1:B:366:GLU:HG2	1:B:373:VAL:HG13	1.88	0.55
1:B:309:HIS:HD2	1:B:311:LYS:H	1.53	0.55
1:B:366:GLU:HG2	1:B:373:VAL:CG1	2.37	0.55
1:A:184:PHE:CG	1:A:188:LEU:HD13	2.43	0.54
1:B:102:VAL:CG2	1:B:103:TYR:CE2	2.90	0.53
1:A:47:GLN:H	1:A:47:GLN:NE2	1.98	0.53
1:A:89:PHE:CE2	1:A:359:VAL:CG2	2.92	0.53
1:A:193:ASN:C	1:A:193:ASN:HD22	2.16	0.53
1:B:366:GLU:CG	1:B:373:VAL:CG1	2.87	0.53
1:A:44:HIS:CD2	1:A:71:SER:H	2.18	0.53
2:B:1450:HEM:HBB2	2:B:1450:HEM:HHC	1.91	0.53
1:A:331:ASN:HD22	1:A:331:ASN:C	2.16	0.52
1:B:244:ILE:HG12	1:B:266:LEU:HD11	1.91	0.52
1:A:309:HIS:CD2	1:A:311:LYS:H	2.21	0.51
1:A:420:HIS:HD2	2:A:1450:HEM:O2D	1.94	0.51
1:A:336:MET:CE	1:A:430:LEU:CD1	2.87	0.50
1:A:309:HIS:CD2	1:A:311:LYS:CG	2.94	0.50
1:A:176:ILE:HB	1:A:293[A]:GLN:OE1	2.12	0.50
1:B:99:PRO:O	1:B:102:VAL:HG22	2.11	0.50
1:A:96:ILE:N	1:A:96:ILE:HD12	2.26	0.50
2:A:1450:HEM:HBC2	2:A:1450:HEM:HHD	1.93	0.50
1:B:357:LEU:HD22	1:B:385:LEU:HD22	1.94	0.49
1:A:403:GLU:HG3	6:A:2165:HOH:O	2.12	0.49
1:A:233:ARG:HH12	1:A:237:GLN:NE2	2.12	0.48
1:A:54:GLU:OE2	1:A:58:ARG:HD3	2.13	0.48
2:B:1450:HEM:C1A	3:B:1460[A]:TW5:H3	2.49	0.48
1:B:56:MET:HB3	1:B:386:LEU:HD13	1.96	0.48
1:A:244:ILE:HG12	1:A:266:LEU:HD11	1.95	0.48
1:A:271:ARG:NH2	6:A:2135:HOH:O	2.47	0.48
2:B:1450:HEM:C1A	3:B:1460[B]:TW5:H3	2.49	0.48
1:A:47:GLN:HE21	1:A:47:GLN:N	2.01	0.48
1:B:93:ARG:HG2	6:B:2037:HOH:O	2.14	0.47
1:B:275:ARG:HD2	6:B:2102:HOH:O	2.14	0.47
1:B:332:TYR:CZ	1:B:336:MET:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1450:HEM:HBC2	2:B:1450:HEM:HHD	1.95	0.47
1:A:36:PRO:O	1:A:44:HIS:HE1	1.98	0.47
1:B:143:VAL:HB	1:B:144:PRO:HD3	1.96	0.47
1:A:314:LYS:HG2	6:A:2147:HOH:O	2.15	0.47
1:B:348:GLU:HG3	1:B:400:TRP:CD1	2.50	0.46
1:A:332:TYR:CZ	1:A:336:MET:HG3	2.51	0.46
1:A:336:MET:HE1	1:A:430:LEU:HD13	1.94	0.45
1:B:201:LEU:HD23	1:B:204:MET:CE	2.46	0.45
2:A:1450:HEM:C4D	3:A:1460[A]:TW5:H4	2.51	0.45
1:B:197:PHE:CE2	1:B:289:MET:HG3	2.51	0.45
1:B:205:GLU:OE1	1:B:294:HIS:HE1	1.99	0.45
1:B:331:ASN:H	1:B:334:ASN:HD22	1.63	0.45
1:B:311:LYS:HE3	1:B:311:LYS:HB3	1.75	0.44
1:B:449[A]:ARG:HD2	1:B:468:GLN:HB3	1.99	0.44
1:B:320:HIS:O	1:B:321:LYS:C	2.61	0.44
3:A:1460[A]:TW5:H17	3:A:1460[A]:TW5:H19	1.76	0.43
1:A:105:ILE:HG23	6:A:2048:HOH:O	2.17	0.43
1:A:141:ASN:O	1:A:144:PRO:HD2	2.18	0.43
1:B:384:PRO:O	1:B:388:HIS:CG	2.70	0.43
3:B:1460[B]:TW5:H17	3:B:1460[B]:TW5:H25	1.88	0.43
3:B:1460[B]:TW5:N1	3:B:1460[B]:TW5:C9	2.79	0.43
1:B:309:HIS:CD2	1:B:311:LYS:H	2.35	0.43
1:B:309:HIS:HE1	1:B:450:ASP:O	2.01	0.43
1:B:295:THR:HB	2:B:1450:HEM:CAB	2.49	0.43
1:B:233:ARG:HH12	1:B:237:GLN:NE2	2.17	0.43
1:A:193:ASN:HD21	1:A:196:HIS:H	1.67	0.42
1:A:331:ASN:H	1:A:334:ASN:ND2	2.09	0.42
1:B:184:PHE:CG	1:B:188:LEU:HD13	2.54	0.42
1:A:424:GLY:HA3	2:A:1450:HEM:C3C	2.54	0.42
1:A:294:HIS:HD2	6:A:2033:HOH:O	2.03	0.42
1:A:116:TYR:OH	3:A:1460[A]:TW5:H10	2.20	0.42
1:B:366:GLU:OE2	1:B:373:VAL:HG11	2.20	0.42
1:A:166:ASN:HD22	1:A:166:ASN:C	2.27	0.41
1:B:94:ASN:OD1	1:B:420:HIS:HE1	2.03	0.41
1:B:112:GLU:O	1:B:279:HIS:HE1	2.03	0.41
1:A:149:GLU:OE2	6:A:2079:HOH:O	2.22	0.41
1:A:424:GLY:HA3	2:A:1450:HEM:C2C	2.56	0.41
1:B:174:MET:O	1:B:178:THR:HG23	2.21	0.41
1:B:149:GLU:CG	1:B:181:GLN:CG	2.97	0.40
3:B:1460[B]:TW5:H2	3:B:1460[B]:TW5:C11	2.51	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	440/467 (94%)	432 (98%)	8 (2%)	0	100 100
1	B	439/467 (94%)	431 (98%)	6 (1%)	2 (0%)	24 17
All	All	879/934 (94%)	863 (98%)	14 (2%)	2 (0%)	48 40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	293[A]	GLN
1	B	293[B]	GLN

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	383/409 (94%)	364 (95%)	19 (5%)	22 15
1	B	380/409 (93%)	356 (94%)	24 (6%)	16 9
All	All	763/818 (93%)	720 (94%)	43 (6%)	19 12

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

Mol	Chain	Res	Type
1	A	30	THR
1	A	38	THR
1	A	47	GLN
1	A	102	VAL

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Mol	Chain	Res	Type
1	A	156	GLU
1	A	166	ASN
1	A	188	LEU
1	A	190	LYS
1	A	193	ASN
1	A	203	LYS
1	A	311	LYS
1	A	314	LYS
1	A	321	LYS
1	A	331	ASN
1	A	359	VAL
1	A	442	GLU
1	A	446	GLN
1	A	447	LEU
1	A	471	VAL
1	B	30	THR
1	B	37	VAL
1	B	39	VAL
1	B	54	GLU
1	B	72	ILE
1	B	95	GLU
1	B	101	GLU
1	B	132	GLU
1	B	151	ARG
1	B	156	GLU
1	B	162	GLU
1	B	166	ASN
1	B	176	ILE
1	B	188	LEU
1	B	243	ILE
1	B	311	LYS
1	B	314	LYS
1	B	321	LYS
1	B	331	ASN
1	B	382	CYS
1	B	449[A]	ARG
1	B	449[B]	ARG
1	B	475	ARG
1	B	476	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	A	47	GLN
1	A	94	ASN
1	A	128	ASN
1	A	166	ASN
1	A	181	GLN
1	A	193	ASN
1	A	237	GLN
1	A	279	HIS
1	A	294	HIS
1	A	309	HIS
1	A	331	ASN
1	A	334	ASN
1	A	420	HIS
1	B	57	GLN
1	B	237	GLN
1	B	279	HIS
1	B	294	HIS
1	B	309	HIS
1	B	331	ASN
1	B	334	ASN
1	B	420	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)

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	$\#\|Z\| > 2$
3	TW5	A	1460[B]	2	48,48,48	1.42	5 (10%)	67,67,67	1.55	10 (14%)
3	TW5	B	1460[B]	2	48,48,48	1.50	4 (8%)	67,67,67	1.58	10 (14%)
2	HEM	B	1450	3,1	50,50,50	1.66	14 (28%)	66,82,82	1.96	19 (28%)
3	TW5	B	1460[A]	2	48,48,48	1.48	3 (6%)	67,67,67	1.97	12 (17%)
4	EDO	A	1478	-	3,3,3	0.44	0	2,2,2	0.42	0
3	TW5	A	1460[A]	2	48,48,48	1.50	5 (10%)	67,67,67	1.52	8 (11%)
2	HEM	A	1450	3,1	50,50,50	1.60	9 (18%)	66,82,82	1.96	18 (27%)

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	TW5	A	1460[B]	2	-	0/28/38/38	0/6/6/6
3	TW5	B	1460[B]	2	-	8/28/38/38	0/6/6/6
2	HEM	B	1450	3,1	-	2/14/54/54	-
3	TW5	B	1460[A]	2	-	0/28/38/38	0/6/6/6
4	EDO	A	1478	-	-	0/1/1/1	-
3	TW5	A	1460[A]	2	-	2/28/38/38	0/6/6/6
2	HEM	A	1450	3,1	-	2/14/54/54	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1460[B]	TW5	C18-C19	7.18	1.48	1.38
3	A	1460[A]	TW5	C18-C19	7.15	1.48	1.38
3	B	1460[A]	TW5	C18-C19	7.07	1.48	1.38
3	A	1460[B]	TW5	C18-C19	7.07	1.48	1.38
2	B	1450	HEM	FE-NB	4.77	2.09	1.94
3	A	1460[A]	TW5	C10-C15	4.47	1.47	1.41
2	A	1450	HEM	C1B-NB	-4.37	1.32	1.40
3	B	1460[B]	TW5	C10-C15	4.36	1.47	1.41
3	B	1460[A]	TW5	C10-C15	4.33	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1450	HEM	FE-NB	3.74	2.06	1.94
2	A	1450	HEM	FE-NC	3.42	2.06	1.95
2	B	1450	HEM	C1B-NB	-3.28	1.34	1.40
2	A	1450	HEM	C1A-NA	-3.10	1.33	1.39
2	B	1450	HEM	C4D-ND	-2.98	1.35	1.40
3	A	1460[B]	TW5	C31-CL1	2.96	1.80	1.74
3	A	1460[A]	TW5	C31-CL1	2.87	1.80	1.74
3	A	1460[B]	TW5	C10-C15	2.78	1.45	1.41
2	B	1450	HEM	C4B-NB	-2.74	1.33	1.38
2	B	1450	HEM	CBD-CGD	2.72	1.56	1.50
2	B	1450	HEM	FE-NC	2.68	2.04	1.95
2	B	1450	HEM	C3C-C4C	-2.66	1.41	1.46
3	B	1460[A]	TW5	C2-N1	-2.65	1.36	1.41
2	B	1450	HEM	O1A-CGA	2.61	1.30	1.22
2	A	1450	HEM	CBD-CAD	-2.55	1.43	1.52
2	B	1450	HEM	C3D-C2D	-2.54	1.31	1.36
2	A	1450	HEM	C3D-C2D	-2.49	1.31	1.36
2	A	1450	HEM	C4D-ND	-2.48	1.36	1.40
3	B	1460[B]	TW5	C2-N1	-2.41	1.36	1.41
2	B	1450	HEM	C1C-C2C	-2.39	1.40	1.45
3	B	1460[B]	TW5	C31-CL1	2.36	1.79	1.74
2	A	1450	HEM	C4A-NA	-2.36	1.35	1.39
2	B	1450	HEM	C1C-NC	-2.35	1.35	1.39
2	A	1450	HEM	CHB-C1B	2.33	1.43	1.38
3	A	1460[B]	TW5	C10-C9	2.33	1.47	1.44
2	B	1450	HEM	C3B-C2B	-2.26	1.32	1.37
2	B	1450	HEM	O2A-CGA	-2.21	1.23	1.30
2	B	1450	HEM	O1D-CGD	2.14	1.29	1.22
3	A	1460[A]	TW5	C16-C9	2.11	1.40	1.36
3	A	1460[A]	TW5	C2-N1	-2.07	1.37	1.41
3	A	1460[B]	TW5	C2-N1	-2.04	1.37	1.41

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1460[A]	TW5	C26-N6-C25	6.08	124.94	111.52
3	B	1460[A]	TW5	C27-N5-C24	5.94	124.64	111.52
3	B	1460[A]	TW5	C14-C15-C10	-5.44	116.73	122.19
3	A	1460[A]	TW5	C26-N6-C25	5.43	123.50	111.52
3	B	1460[B]	TW5	C26-N6-C25	5.33	123.28	111.52
3	A	1460[B]	TW5	C26-N6-C25	5.25	123.11	111.52
2	B	1450	HEM	C4C-NC-C1C	5.14	110.38	105.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1450	HEM	O2D-CGD-CBD	5.04	130.22	114.03
2	B	1450	HEM	C1B-NB-C4B	4.95	110.19	105.07
3	B	1460[A]	TW5	C18-C17-N4	4.54	125.21	116.80
2	A	1450	HEM	CHC-C4B-NB	4.53	129.34	124.42
3	A	1460[A]	TW5	C14-C15-C10	-4.48	117.69	122.19
2	A	1450	HEM	O1D-CGD-CBD	-4.48	108.69	123.08
3	B	1460[A]	TW5	O2-C17-N4	-4.44	114.28	122.45
3	A	1460[B]	TW5	C14-C15-C10	-4.41	117.77	122.19
2	A	1450	HEM	C1B-NB-C4B	4.24	109.45	105.07
2	A	1450	HEM	CMD-C2D-C1D	4.23	131.49	125.04
3	B	1460[B]	TW5	C14-C15-C10	-4.09	118.09	122.19
3	B	1460[A]	TW5	C11-C10-C15	3.82	122.93	118.83
2	B	1450	HEM	CAB-C3B-C2B	-3.62	116.67	128.60
3	B	1460[B]	TW5	C20-C19-C18	-3.57	119.72	123.53
2	A	1450	HEM	C4C-NC-C1C	3.50	108.78	105.35
2	B	1450	HEM	CHD-C4C-NC	3.49	128.22	124.44
2	B	1450	HEM	CMC-C2C-C1C	3.44	130.78	124.71
2	B	1450	HEM	CMD-C2D-C1D	3.44	130.28	125.04
3	A	1460[A]	TW5	C11-C10-C15	3.27	122.34	118.83
2	B	1450	HEM	CHB-C1B-NB	3.27	128.41	124.37
2	B	1450	HEM	CBD-CAD-C3D	3.25	121.67	112.63
2	A	1450	HEM	CAD-CBD-CGD	-3.23	106.65	113.60
2	B	1450	HEM	CMB-C2B-C1B	3.21	129.93	125.04
2	A	1450	HEM	CAC-C3C-C4C	3.19	132.59	124.90
3	B	1460[B]	TW5	C8-C7-N4	-3.17	104.39	110.60
3	A	1460[B]	TW5	C18-C17-N4	3.14	122.61	116.80
2	A	1450	HEM	CHD-C1D-C2D	-3.09	120.15	124.98
3	B	1460[B]	TW5	C11-C10-C15	3.05	122.10	118.83
3	B	1460[A]	TW5	C14-C15-N3	3.03	135.84	130.79
3	B	1460[B]	TW5	C27-C26-N6	3.01	116.56	110.70
3	A	1460[A]	TW5	C20-C19-C18	-3.00	120.33	123.53
3	A	1460[B]	TW5	C20-C19-C18	-2.94	120.39	123.53
2	B	1450	HEM	CAC-C3C-C4C	2.89	131.87	124.90
3	A	1460[A]	TW5	C27-N5-C24	2.85	117.82	111.52
2	B	1450	HEM	CAC-C3C-C2C	-2.84	119.24	128.60
2	A	1450	HEM	CAC-C3C-C2C	-2.83	119.27	128.60
3	B	1460[A]	TW5	C22-C21-N5	-2.81	117.51	121.38
3	A	1460[B]	TW5	C15-N3-C16	2.78	111.69	109.07
2	B	1450	HEM	CMC-C2C-C3C	-2.69	121.71	128.30
2	B	1450	HEM	CHA-C4D-ND	2.60	127.58	124.37
2	A	1450	HEM	CHA-C4D-ND	2.60	127.58	124.37
3	A	1460[B]	TW5	C14-C15-N3	2.57	135.08	130.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1460[A]	TW5	C7-N4-C17	-2.55	115.35	121.60
3	B	1460[A]	TW5	C20-C19-C18	-2.51	120.85	123.53
2	B	1450	HEM	CHA-C4D-C3D	-2.51	120.62	125.33
3	A	1460[B]	TW5	C11-C10-C15	2.47	121.48	118.83
2	A	1450	HEM	C1D-C2D-C3D	-2.44	104.39	106.96
3	B	1460[A]	TW5	C8-C7-N4	-2.44	105.82	110.60
2	A	1450	HEM	C2D-C1D-ND	2.40	112.76	109.88
2	A	1450	HEM	CMC-C2C-C1C	2.39	128.92	124.71
3	B	1460[B]	TW5	C27-N5-C24	2.39	116.78	111.52
3	B	1460[B]	TW5	C6-C2-N1	2.37	128.39	120.40
3	A	1460[B]	TW5	C27-N5-C24	2.37	116.74	111.52
3	A	1460[A]	TW5	C14-C15-N3	2.35	134.70	130.79
2	B	1450	HEM	CAD-CBD-CGD	-2.33	108.59	113.60
3	A	1460[A]	TW5	C8-C7-N4	-2.27	106.16	110.60
2	B	1450	HEM	CHD-C1D-C2D	-2.25	121.46	124.98
2	A	1450	HEM	CHD-C1D-ND	2.22	126.83	124.42
2	A	1450	HEM	O2A-CGA-O1A	-2.21	117.79	123.30
2	B	1450	HEM	CAB-C3B-C4B	2.18	134.63	124.47
3	B	1460[B]	TW5	C14-C15-N3	2.17	134.41	130.79
3	A	1460[B]	TW5	O1-C1-N1	2.13	128.50	123.93
2	A	1450	HEM	C1A-CHA-C4D	-2.13	121.30	126.34
2	B	1450	HEM	CBA-CAA-C2A	-2.12	106.74	112.63
3	A	1460[B]	TW5	C1-C7-N4	2.12	116.92	111.16
3	B	1460[A]	TW5	C25-C24-N5	2.09	114.77	110.70
3	A	1460[A]	TW5	C3-C2-N1	2.08	127.40	120.40
2	A	1450	HEM	O2A-CGA-CBA	2.06	120.64	114.03
2	B	1450	HEM	C4C-CHD-C1D	-2.06	121.62	126.06
3	B	1460[B]	TW5	C15-C10-C9	-2.01	105.03	107.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1460[A]	TW5	C1-C7-C8-C9
3	B	1460[B]	TW5	C1-C7-C8-C9
3	A	1460[A]	TW5	N4-C7-C8-C9
3	B	1460[B]	TW5	N4-C7-C8-C9
3	B	1460[B]	TW5	N1-C1-C7-C8
3	B	1460[B]	TW5	O1-C1-C7-C8
2	A	1450	HEM	C4C-C3C-CAC-CBC
2	B	1450	HEM	C4B-C3B-CAB-CBB
3	B	1460[B]	TW5	C1-C7-N4-C17

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Mol	Chain	Res	Type	Atoms
3	B	1460[B]	TW5	O1-C1-C7-N4
3	B	1460[B]	TW5	N1-C1-C7-N4
2	B	1450	HEM	C4C-C3C-CAC-CBC
3	B	1460[B]	TW5	C7-C8-C9-C16
2	A	1450	HEM	CAD-CBD-CGD-O2D

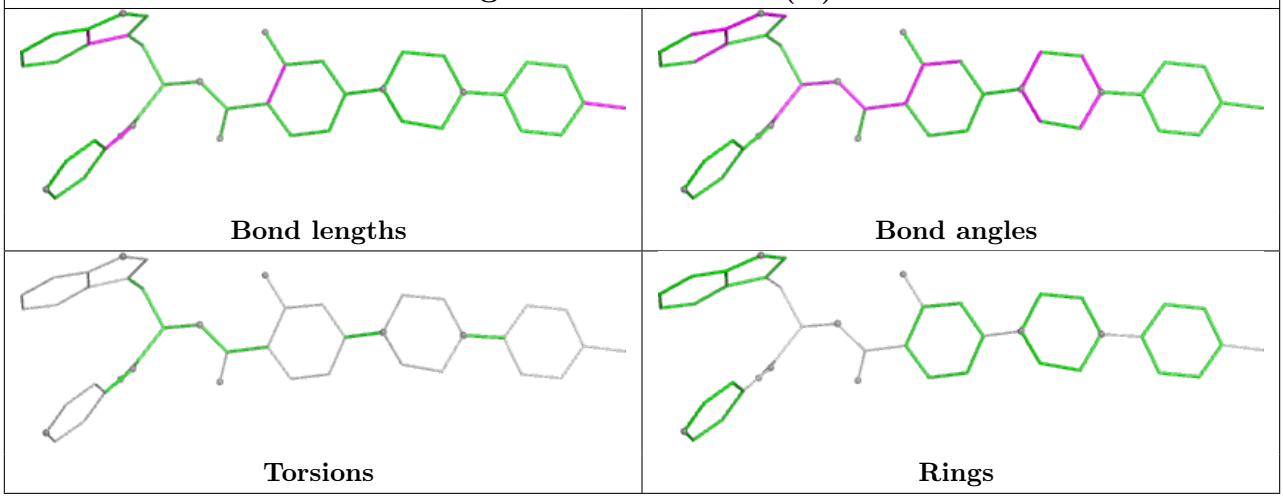
There are no ring outliers.

6 monomers are involved in 17 short contacts:

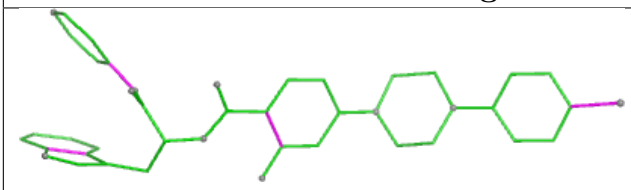
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1460[B]	TW5	1	0
3	B	1460[B]	TW5	4	0
2	B	1450	HEM	6	0
3	B	1460[A]	TW5	1	0
3	A	1460[A]	TW5	3	0
2	A	1450	HEM	5	0

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.

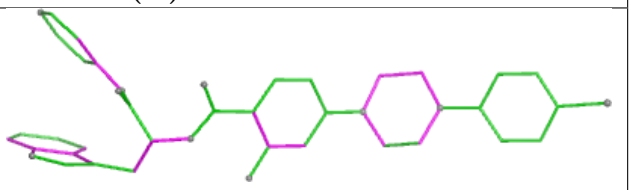
Ligand TW5 A 1460 (B)



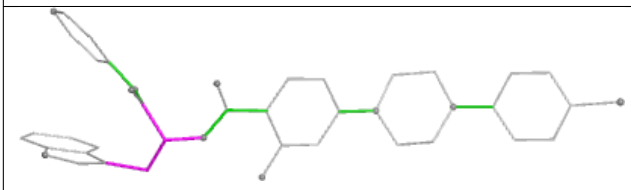
Ligand TW5 B 1460 (B)



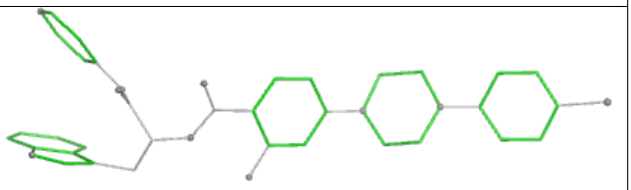
Bond lengths



Bond angles

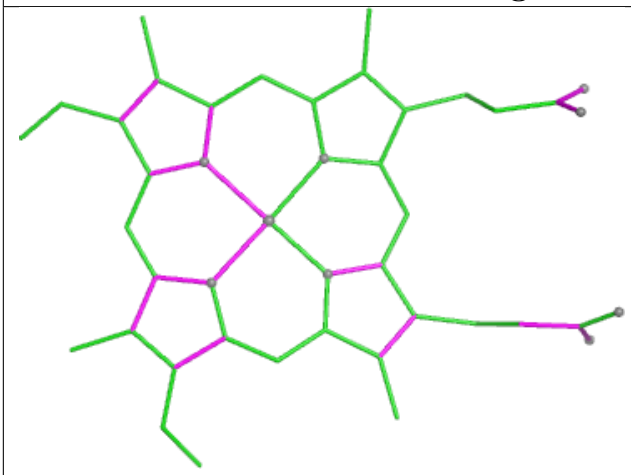


Torsions

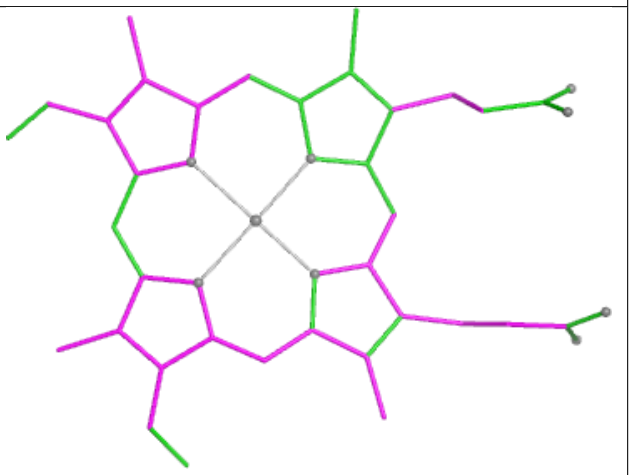


Rings

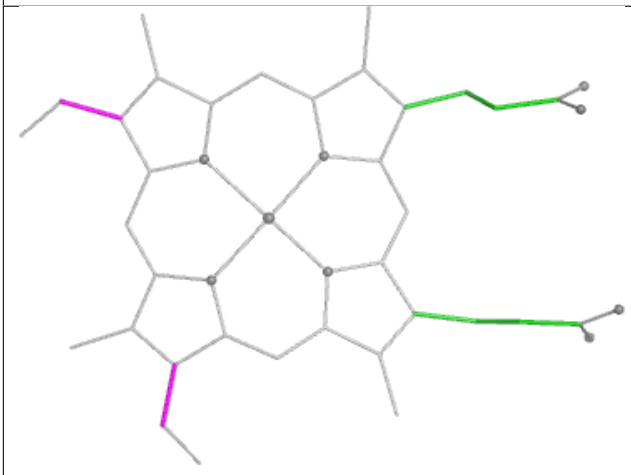
Ligand HEM B 1450



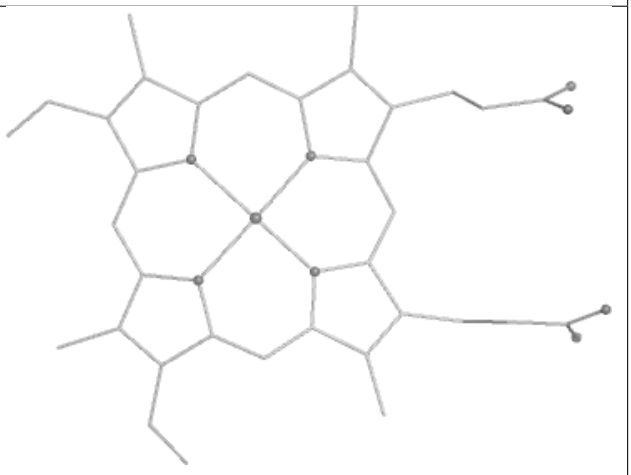
Bond lengths



Bond angles

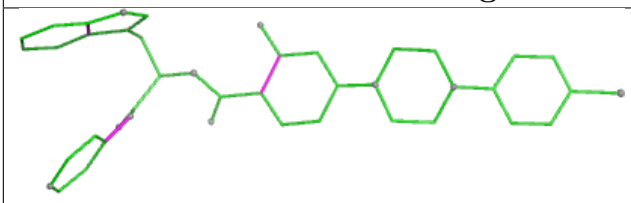


Torsions

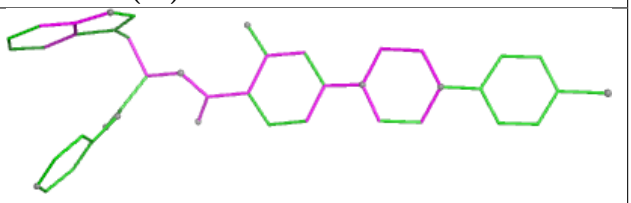


Rings

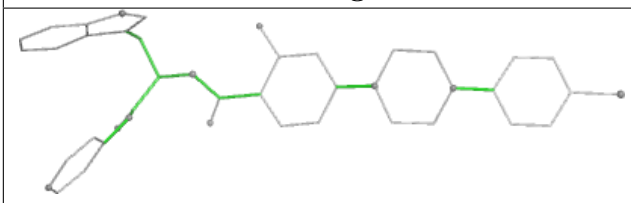
Ligand TW5 B 1460 (A)



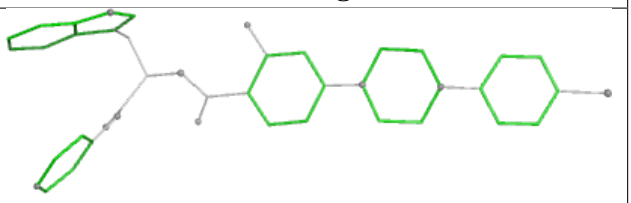
Bond lengths



Bond angles

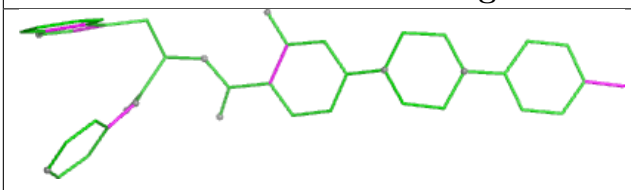


Torsions

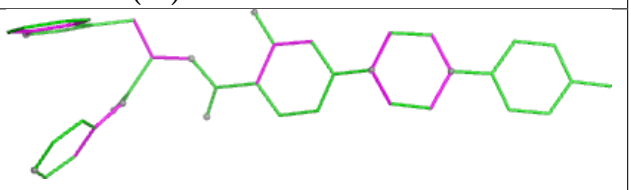


Rings

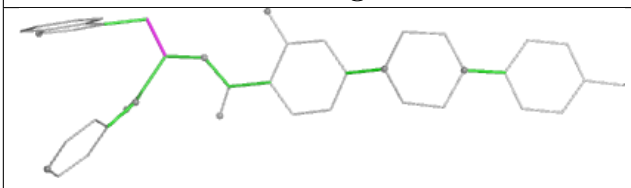
Ligand TW5 A 1460 (A)



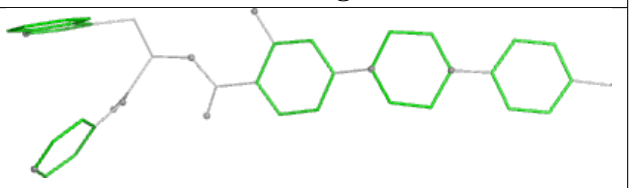
Bond lengths



Bond angles

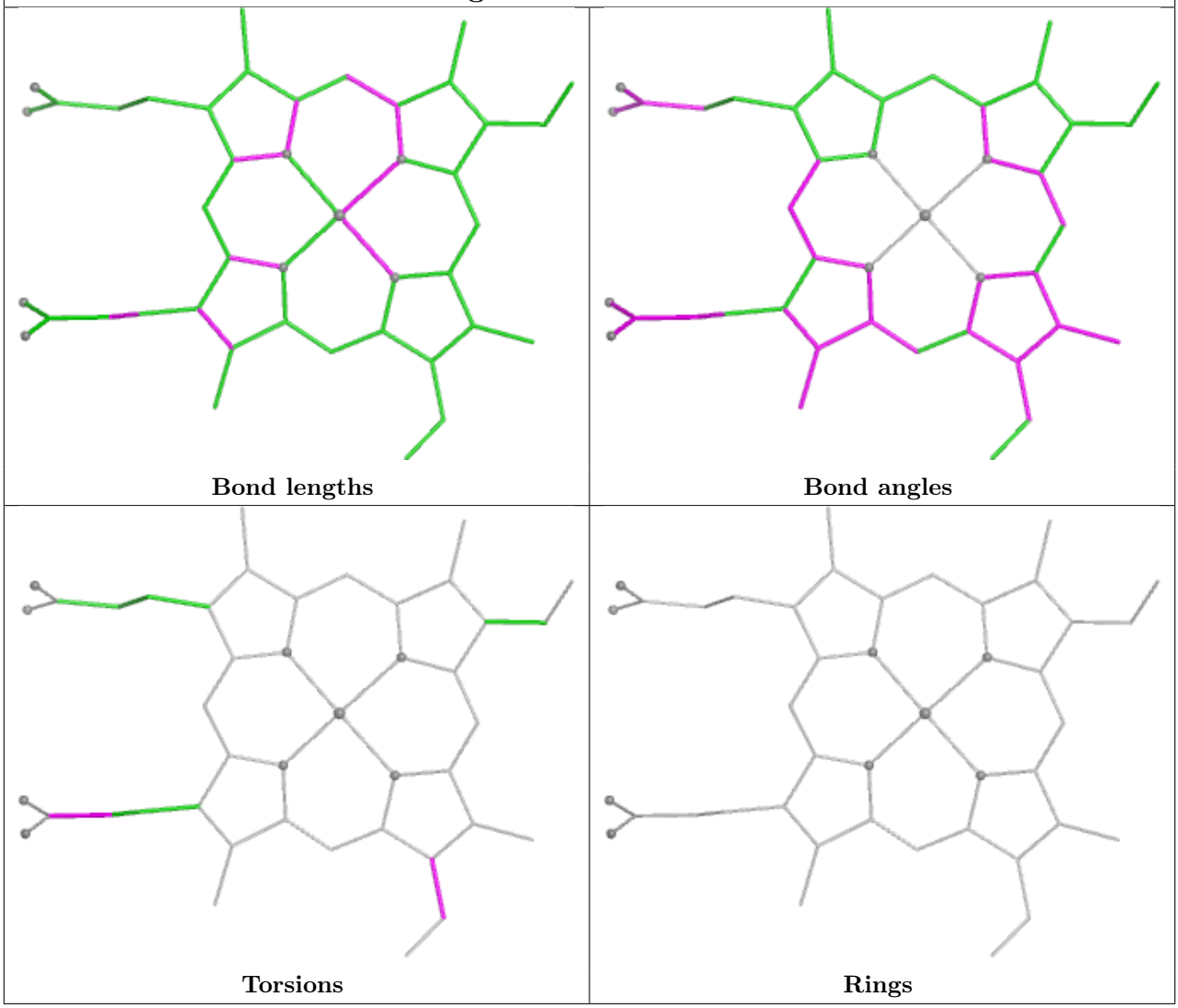


Torsions



Rings

Ligand HEM A 1450



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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	443/467 (94%)	-0.28	6 (1%)	73	73	11, 22, 39, 65	1 (0%)
1	B	441/467 (94%)	-0.19	5 (1%)	78	78	9, 24, 42, 63	2 (0%)
All	All	884/934 (94%)	-0.24	11 (1%)	76	76	9, 23, 41, 65	3 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	116	TYR	5.1
1	B	29	PRO	4.8
1	A	258	THR	4.4
1	B	40	PRO	3.2
1	A	29	PRO	3.2
1	B	250	GLU	2.9
1	B	251	GLU	2.7
1	B	41	PHE	2.7
1	A	41	PHE	2.2
1	A	250	GLU	2.1
1	A	251	GLU	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands (i)

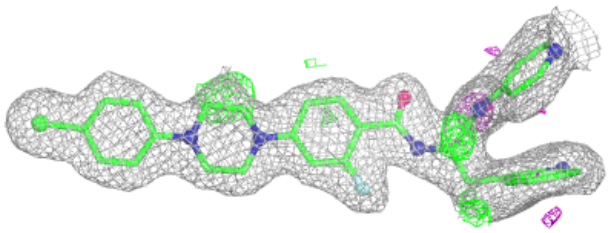
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

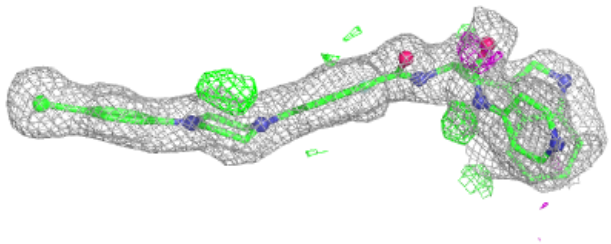
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	1478	4/4	0.90	0.13	33,38,40,47	0
5	CL	A	1479	1/1	0.90	0.12	53,53,53,53	0
3	TW5	A	1460[A]	43/43	0.93	0.07	15,19,22,28	43
3	TW5	A	1460[B]	43/43	0.93	0.07	15,18,22,28	43
3	TW5	B	1460[A]	43/43	0.95	0.07	12,15,17,18	43
3	TW5	B	1460[B]	43/43	0.95	0.07	14,17,21,25	43
2	HEM	B	1450	43/43	0.97	0.07	15,18,24,28	0
2	HEM	A	1450	43/43	0.98	0.06	12,15,22,25	0

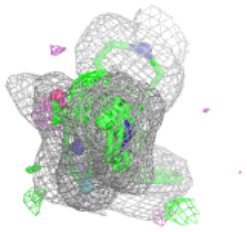
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TW5 A 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)

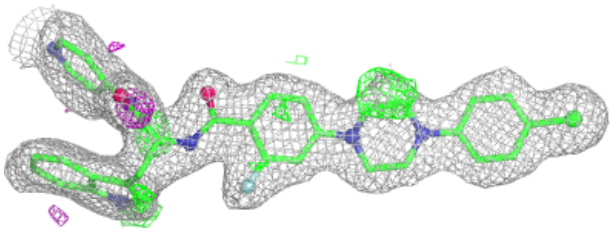


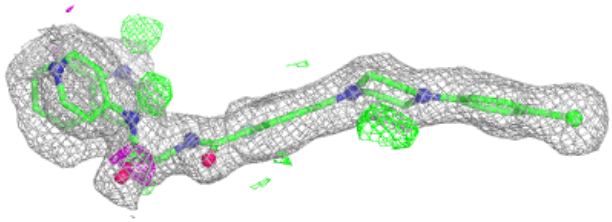


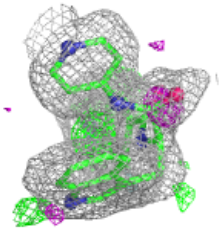


Electron density around TW5 A 1460 (B):

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

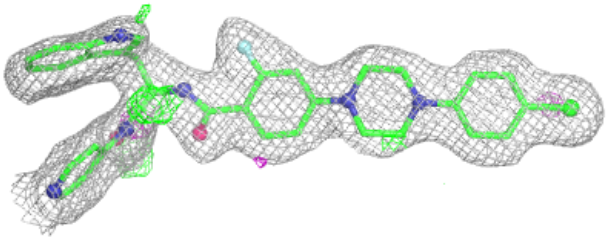


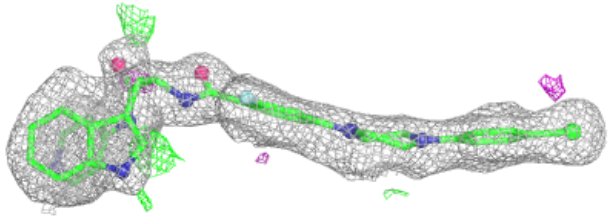


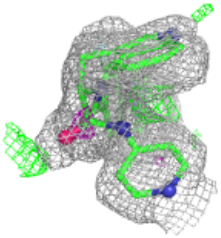


Electron density around TW5 B 1460 (A):

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

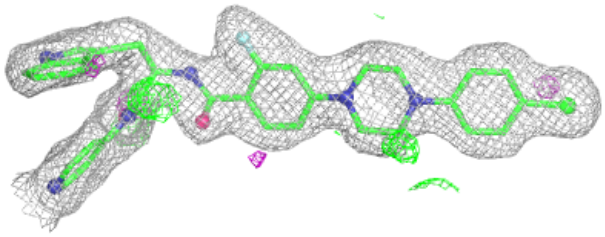


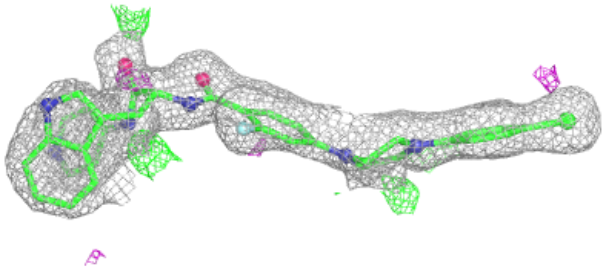


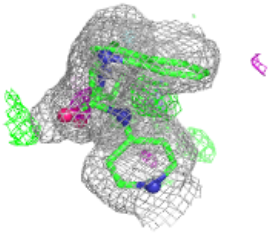


Electron density around TW5 B 1460 (B):

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

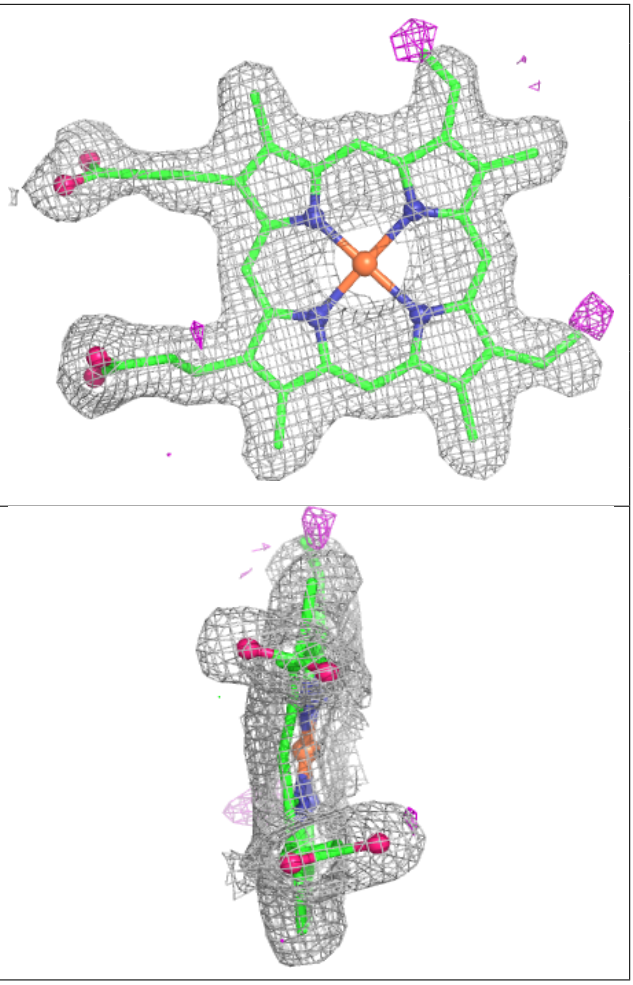






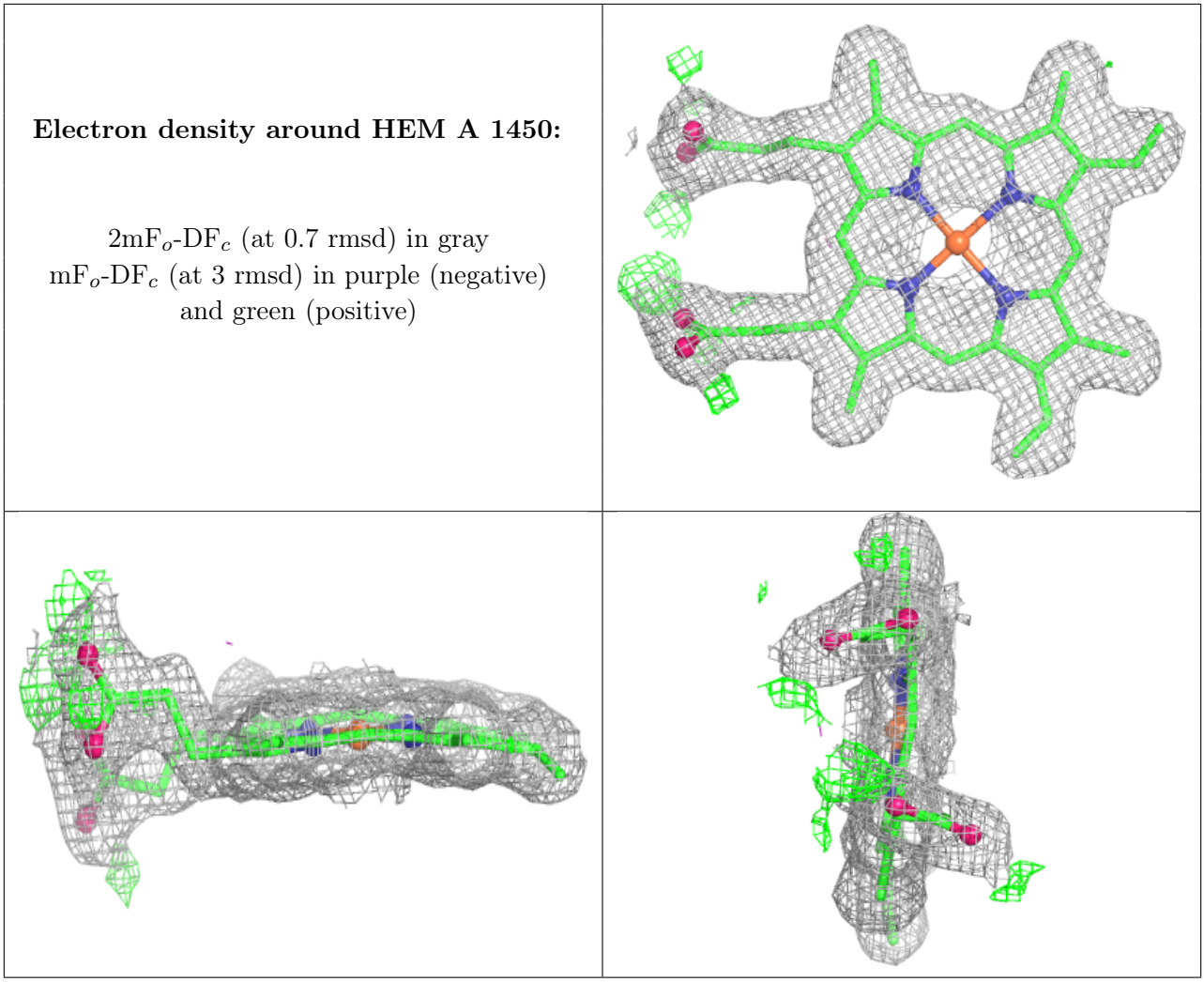
Electron density around HEM B 1450:

$2mF_o$-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

There are no such residues in this entry.