Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 06:56 pm GMT

PDB ID	:	4BJK
Title	:	CYP51 of Trypanosoma brucei bound to (S)-N-(3-(1H-indol-3-yl)-1-oxo-1- (pyridin-4-ylamino)propan-2-yl)-3,3'-difluoro-(1,1'-biphenyl)-4- carboxamide
Authors	:	Podust, L.M.
Deposited on	:	2013-04-18
Resolution	:	2.67 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:

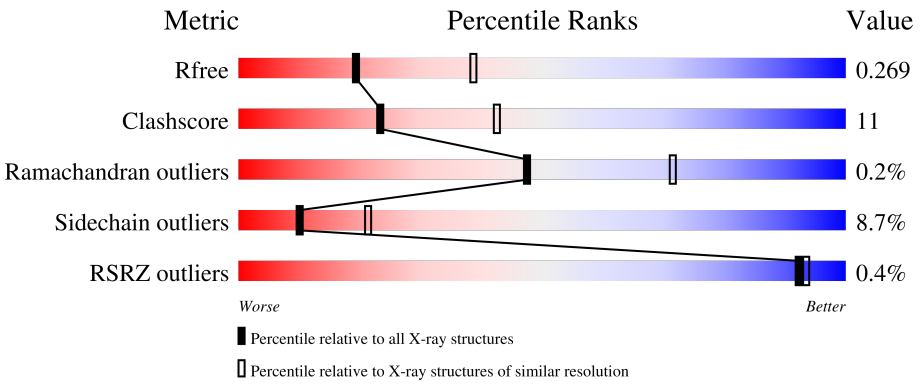
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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 2.67 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	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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	469	75% 19% • •
1	B	469	77% 17% • •
1	C	469	73% 19% • •
1	D	469	72% 19% • 5%

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
3	18I	B	1460	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 14491 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 LANOSTEROL 14-ALPHA-DEMETHYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	450	3539	2261	621	630	27	0	1	0
1	B	450	3524	2247	615	634	28	0	0	0
1	C	450	3536	2256	622	630	28	0	1	0
1	D	444	3484	2229	605	624	26	0	1	0

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	expression tag	UNP Q385E8
A	22	ALA	-	expression tag	UNP Q385E8
A	23	LYS	-	expression tag	UNP Q385E8
A	24	LYS	-	expression tag	UNP Q385E8
A	25	THR	-	expression tag	UNP Q385E8
A	26	SER	-	expression tag	UNP Q385E8
A	27	SER	-	expression tag	UNP Q385E8
A	28	LYS	-	expression tag	UNP Q385E8
A	29	GLY	-	expression tag	UNP Q385E8
A	30	LYS	-	expression tag	UNP Q385E8
A	31	LEU	-	expression tag	UNP Q385E8
A	482	HIS	-	expression tag	UNP Q385E8
A	483	HIS	-	expression tag	UNP Q385E8
A	484	HIS	-	expression tag	UNP Q385E8
A	485	HIS	-	expression tag	UNP Q385E8
A	486	HIS	-	expression tag	UNP Q385E8
A	487	HIS	-	expression tag	UNP Q385E8
A	488	HIS	-	expression tag	UNP Q385E8
A	489	HIS	-	expression tag	UNP Q385E8
A	34	MET	VAL	engineered mutation	UNP Q385E8
A	249	ALA	GLU	engineered mutation	UNP Q385E8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	250	ALA	GLU	engineered mutation	UNP Q385E8
A	251	ALA	GLU	engineered mutation	UNP Q385E8
B	21	MET	-	expression tag	UNP Q385E8
B	22	ALA	-	expression tag	UNP Q385E8
B	23	LYS	-	expression tag	UNP Q385E8
B	24	LYS	-	expression tag	UNP Q385E8
B	25	THR	-	expression tag	UNP Q385E8
B	26	SER	-	expression tag	UNP Q385E8
B	27	SER	-	expression tag	UNP Q385E8
B	28	LYS	-	expression tag	UNP Q385E8
B	29	GLY	-	expression tag	UNP Q385E8
B	30	LYS	-	expression tag	UNP Q385E8
B	31	LEU	-	expression tag	UNP Q385E8
B	482	HIS	-	expression tag	UNP Q385E8
B	483	HIS	-	expression tag	UNP Q385E8
B	484	HIS	-	expression tag	UNP Q385E8
B	485	HIS	-	expression tag	UNP Q385E8
B	486	HIS	-	expression tag	UNP Q385E8
B	487	HIS	-	expression tag	UNP Q385E8
B	488	HIS	-	expression tag	UNP Q385E8
B	489	HIS	-	expression tag	UNP Q385E8
B	34	MET	VAL	engineered mutation	UNP Q385E8
B	249	ALA	GLU	engineered mutation	UNP Q385E8
B	250	ALA	GLU	engineered mutation	UNP Q385E8
B	251	ALA	GLU	engineered mutation	UNP Q385E8
C	21	MET	-	expression tag	UNP Q385E8
C	22	ALA	-	expression tag	UNP Q385E8
C	23	LYS	-	expression tag	UNP Q385E8
C	24	LYS	-	expression tag	UNP Q385E8
C	25	THR	-	expression tag	UNP Q385E8
C	26	SER	-	expression tag	UNP Q385E8
C	27	SER	-	expression tag	UNP Q385E8
C	28	LYS	-	expression tag	UNP Q385E8
C	29	GLY	-	expression tag	UNP Q385E8
C	30	LYS	-	expression tag	UNP Q385E8
C	31	LEU	-	expression tag	UNP Q385E8
C	482	HIS	-	expression tag	UNP Q385E8
C	483	HIS	-	expression tag	UNP Q385E8
C	484	HIS	-	expression tag	UNP Q385E8
C	485	HIS	-	expression tag	UNP Q385E8
C	486	HIS	-	expression tag	UNP Q385E8
C	487	HIS	-	expression tag	UNP Q385E8

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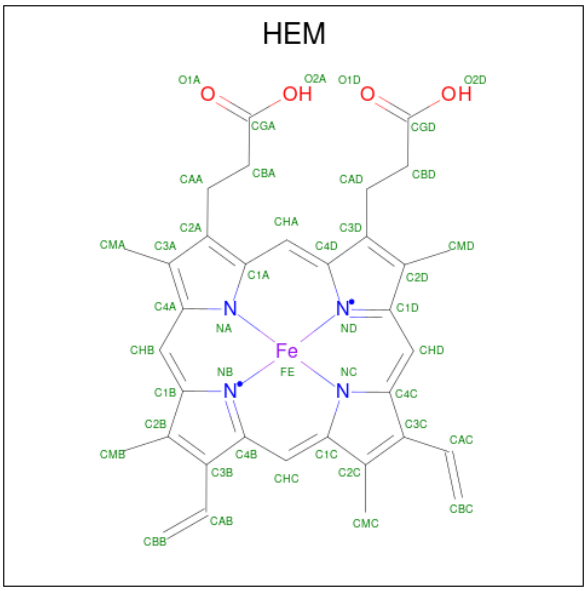
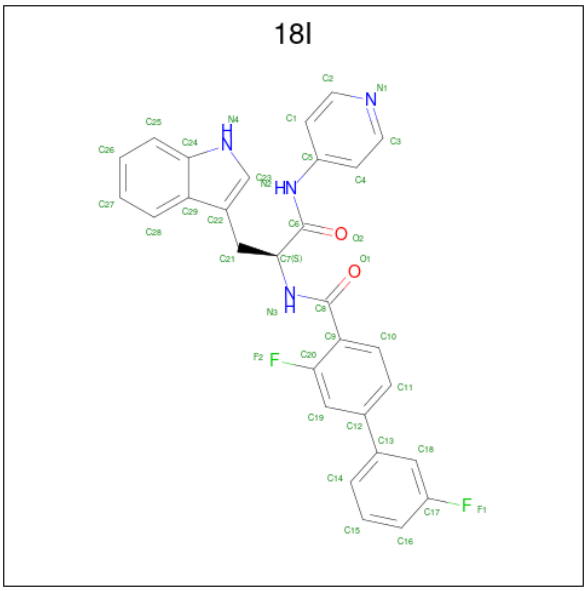
Chain	Residue	Modelled	Actual	Comment	Reference
C	488	HIS	-	expression tag	UNP Q385E8
C	489	HIS	-	expression tag	UNP Q385E8
C	34	MET	VAL	engineered mutation	UNP Q385E8
C	249	ALA	GLU	engineered mutation	UNP Q385E8
C	250	ALA	GLU	engineered mutation	UNP Q385E8
C	251	ALA	GLU	engineered mutation	UNP Q385E8
D	21	MET	-	expression tag	UNP Q385E8
D	22	ALA	-	expression tag	UNP Q385E8
D	23	LYS	-	expression tag	UNP Q385E8
D	24	LYS	-	expression tag	UNP Q385E8
D	25	THR	-	expression tag	UNP Q385E8
D	26	SER	-	expression tag	UNP Q385E8
D	27	SER	-	expression tag	UNP Q385E8
D	28	LYS	-	expression tag	UNP Q385E8
D	29	GLY	-	expression tag	UNP Q385E8
D	30	LYS	-	expression tag	UNP Q385E8
D	31	LEU	-	expression tag	UNP Q385E8
D	482	HIS	-	expression tag	UNP Q385E8
D	483	HIS	-	expression tag	UNP Q385E8
D	484	HIS	-	expression tag	UNP Q385E8
D	485	HIS	-	expression tag	UNP Q385E8
D	486	HIS	-	expression tag	UNP Q385E8
D	487	HIS	-	expression tag	UNP Q385E8
D	488	HIS	-	expression tag	UNP Q385E8
D	489	HIS	-	expression tag	UNP Q385E8
D	34	MET	VAL	engineered mutation	UNP Q385E8
D	249	ALA	GLU	engineered mutation	UNP Q385E8
D	250	ALA	GLU	engineered mutation	UNP Q385E8
D	251	ALA	GLU	engineered mutation	UNP Q385E8

- 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
			Total	C	Fe	N	O		
2	C	1	43	34	1	4	4	0	0
			Total	C	Fe	N	O		
2	D	1	43	34	1	4	4	0	0

- Molecule 3 is 3,3'-difluoro-N-[(2S)-3-(1H-indol-3-yl)-1-oxo-1-(pyridin-4-ylamino)propan-2-yl]biphenyl-4-carboxamide (three-letter code: 18I) (formula: $C_{29}H_{22}F_2N_4O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C F N O 37 29 2 4 2	0	0
3	B	1	Total C N O 21 16 4 1	0	0
3	C	1	Total C N O 21 16 4 1	0	0
3	D	1	Total C N O 21 16 4 1	0	0

- Molecule 4 is water.

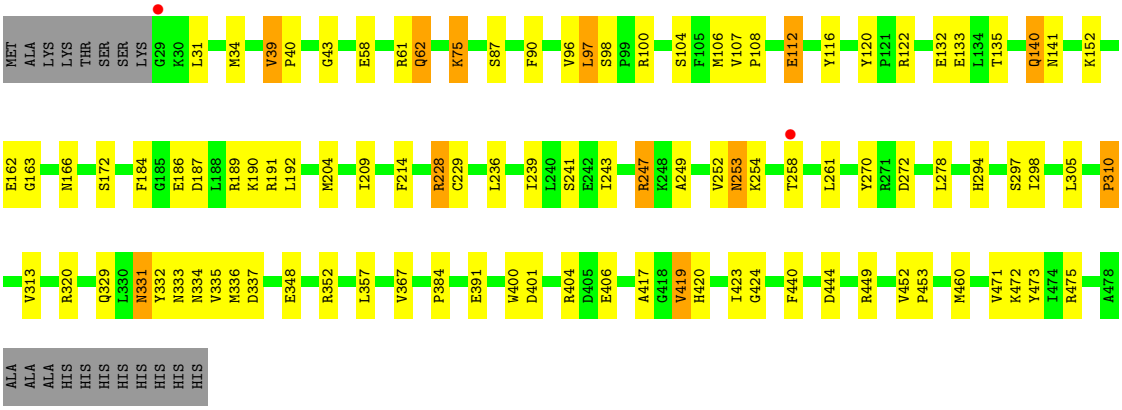
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	46	Total O 46 46	0	0
4	B	28	Total O 28 28	0	0
4	C	28	Total O 28 28	0	0
4	D	34	Total O 34 34	0	0

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.

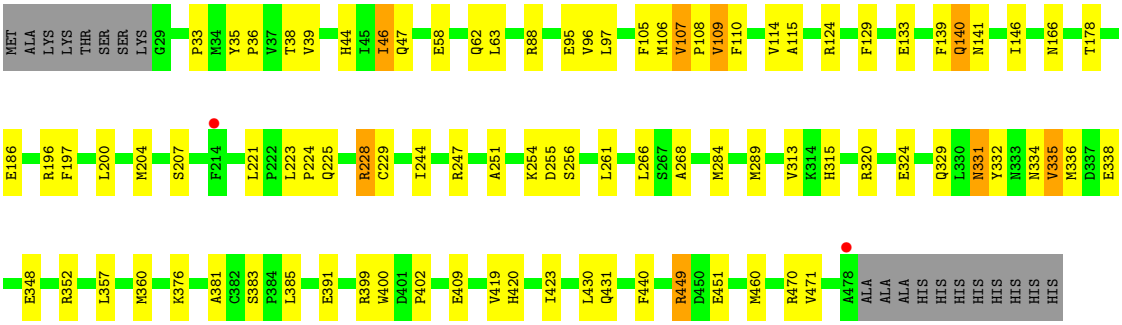
• Molecule 1: LANOSTEROL 14-ALPHA-DEMETHYLASE

Chain A: 75% 19%



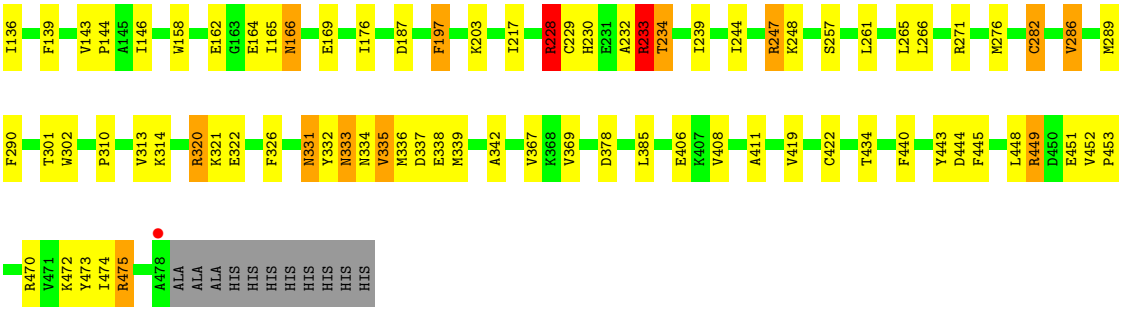
• Molecule 1: LANOSTEROL 14-ALPHA-DEMETHYLASE

Chain B: 77% 17%



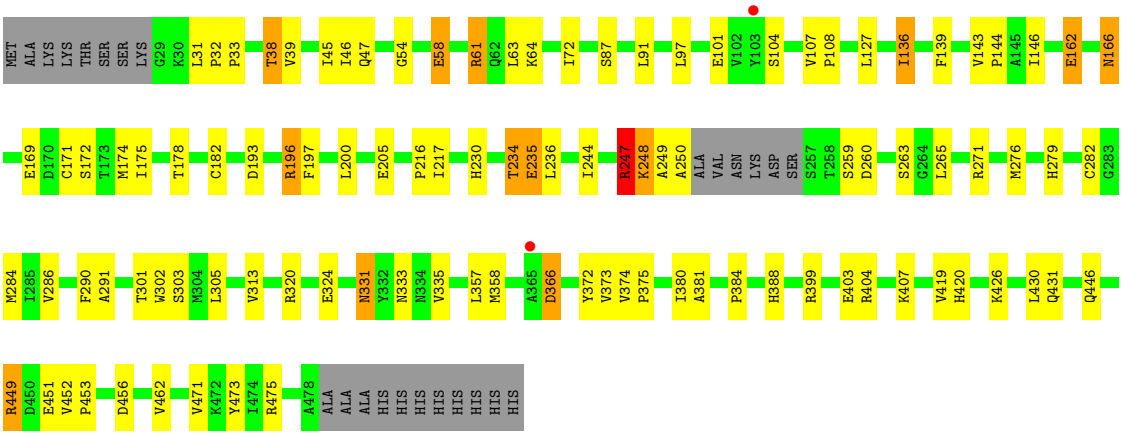
• Molecule 1: LANOSTEROL 14-ALPHA-DEMETHYLASE

Chain C: 73% 19%



- Molecule 1: LANOSTEROL 14-ALPHA-DEMETHYLASE

Chain D: 72% 19% • 5%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	199.29Å 114.67Å 136.22Å 90.00° 132.47° 90.00°	Depositor
Resolution (Å)	87.88 – 2.67 87.72 – 2.67	Depositor EDS
% Data completeness (in resolution range)	99.6 (87.88-2.67) 99.6 (87.72-2.67)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.194 , 0.274 0.195 , 0.269	Depositor DCC
R_{free} test set	3243 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	64.4	Xtriage
Anisotropy	0.112	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h-2*l,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14491	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: HEM, 18I

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.58	0/3621	0.75	0/4905
1	B	0.61	0/3606	0.76	1/4886 (0.0%)
1	C	0.54	0/3618	0.75	2/4900 (0.0%)
1	D	0.53	0/3564	0.74	1/4828 (0.0%)
All	All	0.56	0/14409	0.75	4/19519 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	233	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	D	247	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	C	228	ARG	NE-CZ-NH1	6.57	123.59	120.30
1	B	228	ARG	NE-CZ-NH1	5.97	123.29	120.30

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	3539	0	3545	66	0
1	B	3524	0	3511	65	0
1	C	3536	0	3534	87	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3484	0	3477	60	0
2	A	43	0	30	13	0
2	B	43	0	30	10	0
2	C	43	0	30	7	0
2	D	43	0	30	7	0
3	A	37	0	22	8	0
3	B	21	0	14	13	0
3	C	21	0	14	5	0
3	D	21	0	14	4	0
4	A	46	0	0	1	0
4	B	28	0	0	0	0
4	C	28	0	0	0	0
4	D	34	0	0	2	0
All	All	14491	0	14251	323	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 11.

All (323) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:VAL:HG13	1:A:253:ASN:OD1	1.11	1.25
1:B:107:VAL:HG12	1:B:108:PRO:CD	1.68	1.21
1:C:335:VAL:HA	1:C:339:MET:HE3	1.20	1.11
1:C:93[A]:ARG:HH11	1:C:93[A]:ARG:HG3	1.00	1.11
1:A:104:SER:O	1:A:107:VAL:HG23	1.58	1.03
1:B:107:VAL:HG12	1:B:108:PRO:HD3	1.02	1.02
1:A:252:VAL:CG1	1:A:253:ASN:OD1	2.08	1.01
1:C:333:ASN:ND2	1:C:333:ASN:H	1.60	0.99
1:B:107:VAL:CG1	1:B:108:PRO:HD3	1.92	0.98
1:C:331:ASN:C	1:C:331:ASN:HD22	1.66	0.97
1:B:109:VAL:HG12	1:B:110:PHE:CD1	2.00	0.97
1:D:320:ARG:O	1:D:324:GLU:HG3	1.67	0.95
2:A:1450:HEM:C4D	3:A:1460:18I:H2	2.03	0.93
1:C:93[A]:ARG:HG3	1:C:93[A]:ARG:NH1	1.80	0.92
2:B:1450:HEM:C4D	3:B:1460:18I:H3	2.06	0.91
1:B:320:ARG:O	1:B:324:GLU:HG2	1.72	0.89
1:C:475:ARG:CG	1:C:475:ARG:HH11	1.86	0.88
1:C:333:ASN:H	1:C:333:ASN:HD22	1.18	0.87
3:B:1460:18I:C22	3:B:1460:18I:HN2	1.87	0.87
3:B:1460:18I:H1	3:B:1460:18I:O2	1.76	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:SER:O	1:A:107:VAL:CG2	2.23	0.85
1:C:228:ARG:HG3	1:C:228:ARG:HH11	1.41	0.85
1:A:252:VAL:HG13	1:A:253:ASN:CG	1.95	0.85
1:A:252:VAL:O	4:A:2018:HOH:O	1.95	0.84
1:A:140[B]:GLN:OE1	1:A:141:ASN:N	2.09	0.84
1:B:46:ILE:HG22	1:B:47:GLN:N	1.93	0.83
1:A:253:ASN:O	1:A:254:LYS:HG2	1.80	0.82
1:C:93[A]:ARG:HH11	1:C:93[A]:ARG:CG	1.89	0.82
1:B:46:ILE:CG2	1:B:47:GLN:N	2.43	0.79
1:C:335:VAL:CG1	1:C:336:MET:N	2.44	0.79
1:C:475:ARG:HH11	1:C:475:ARG:HG2	1.45	0.79
1:B:107:VAL:CG1	1:B:108:PRO:CD	2.54	0.78
1:A:107:VAL:N	1:A:108:PRO:HD2	1.99	0.77
1:C:133:GLU:HG2	1:C:261:LEU:HD12	1.67	0.77
1:A:140[B]:GLN:OE1	1:A:140[B]:GLN:N	2.17	0.76
1:C:331:ASN:C	1:C:331:ASN:ND2	2.39	0.76
1:A:310:PRO:O	1:A:313:VAL:HG23	1.86	0.75
2:C:1450:HEM:HBC2	2:C:1450:HEM:HMC2	1.68	0.75
1:D:366:ASP:HB3	1:D:375:PRO:HA	1.67	0.75
3:B:1460:18I:N2	3:B:1460:18I:C29	2.49	0.74
2:A:1450:HEM:CHA	3:A:1460:18I:H2	2.16	0.74
1:D:249:ALA:O	1:D:250:ALA:HB2	1.87	0.74
2:D:1450:HEM:HBC2	2:D:1450:HEM:HMC2	1.68	0.74
1:C:335:VAL:CA	1:C:339:MET:HE3	2.10	0.73
1:C:333:ASN:O	1:C:337:ASP:HB2	1.89	0.73
2:C:1450:HEM:C1A	3:C:1460:18I:C3	2.72	0.72
1:B:107:VAL:N	1:B:108:PRO:HD2	2.05	0.72
1:C:335:VAL:HA	1:C:339:MET:CE	2.12	0.71
1:B:107:VAL:HG12	1:B:108:PRO:N	2.01	0.71
1:C:331:ASN:ND2	1:C:334:ASN:H	1.88	0.71
1:A:249:ALA:O	1:A:252:VAL:HG12	1.91	0.71
2:A:1450:HEM:C1A	3:A:1460:18I:H2	2.26	0.70
1:A:204:MET:HA	1:A:229:CYS:HB3	1.74	0.69
1:C:187:ASP:OD2	1:C:247:ARG:HD2	1.92	0.69
1:B:109:VAL:HG12	1:B:110:PHE:N	2.08	0.69
1:B:106:MET:HB3	1:B:110:PHE:CE2	2.28	0.69
1:B:335:VAL:HG22	1:B:430:LEU:HD12	1.75	0.69
1:B:105:PHE:O	1:B:108:PRO:HD2	1.93	0.68
1:D:230:HIS:O	1:D:234:THR:HG23	1.94	0.68
1:A:112:GLU:CD	1:A:112:GLU:H	1.98	0.68
1:B:107:VAL:CG1	1:B:108:PRO:N	2.54	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1460:18I:HN2	3:B:1460:18I:C29	2.07	0.67
1:C:102:VAL:HG23	1:C:103:TYR:CD1	2.29	0.67
1:C:136:ILE:HA	1:C:139:PHE:CD2	2.29	0.67
2:B:1450:HEM:CHA	3:B:1460:18I:H3	2.25	0.67
1:C:475:ARG:HG2	1:C:475:ARG:NH1	2.06	0.67
1:C:143:VAL:HB	1:C:144:PRO:HD3	1.75	0.66
1:A:133:GLU:HG2	1:A:261:LEU:HD12	1.77	0.66
1:D:33:PRO:HB2	1:D:63:LEU:HD13	1.77	0.66
1:D:249:ALA:O	1:D:250:ALA:CB	2.44	0.66
3:B:1460:18I:C22	3:B:1460:18I:N2	2.48	0.66
1:C:332:TYR:O	1:C:336:MET:HB2	1.96	0.65
1:D:166:ASN:ND2	1:D:169:GLU:H	1.94	0.65
1:C:331:ASN:HD21	1:C:334:ASN:H	1.45	0.65
3:B:1460:18I:O2	3:B:1460:18I:C1	2.42	0.65
2:A:1450:HEM:HMC1	2:A:1450:HEM:HBC2	1.79	0.64
1:C:335:VAL:HG12	1:C:336:MET:N	2.11	0.64
1:A:419:VAL:HG22	1:A:420:HIS:CD2	2.34	0.63
2:A:1450:HEM:ND	3:A:1460:18I:H2	2.13	0.63
1:B:331:ASN:C	1:B:331:ASN:HD22	2.02	0.63
2:C:1450:HEM:CHA	3:C:1460:18I:H3	1.92	0.63
1:A:163:GLY:HA3	1:A:473:TYR:CE2	2.34	0.62
1:C:331:ASN:ND2	1:C:333:ASN:HD22	1.96	0.62
1:A:228:ARG:HG3	1:A:228:ARG:HH11	1.65	0.62
1:C:230:HIS:O	1:C:234:THR:HG23	2.00	0.62
1:B:109:VAL:CG1	1:B:110:PHE:CD1	2.80	0.62
1:A:192:LEU:HD13	1:A:239:ILE:HD13	1.82	0.62
1:A:184:PHE:O	1:A:189:ARG:NH1	2.33	0.61
1:C:310:PRO:O	1:C:313:VAL:HG13	2.00	0.61
1:C:37:VAL:HG22	1:C:44:HIS:CE1	2.36	0.61
1:D:205:GLU:HB2	1:D:290:PHE:HZ	1.66	0.60
1:D:166:ASN:HD22	1:D:169:GLU:H	1.48	0.60
1:A:39:VAL:HG13	1:A:43:GLY:O	2.02	0.60
1:B:140:GLN:HG3	1:B:141:ASN:N	2.16	0.60
1:B:223:LEU:HB3	1:B:224:PRO:HD2	1.84	0.60
1:D:107:VAL:N	1:D:108:PRO:CD	2.63	0.60
1:C:106:MET:HE3	1:C:110:PHE:CZ	2.37	0.59
2:D:1450:HEM:HBC2	2:D:1450:HEM:CMC	2.32	0.59
1:B:320:ARG:NH1	1:B:440:PHE:O	2.36	0.59
1:C:320:ARG:NH1	1:C:440:PHE:O	2.36	0.59
3:D:1460:18I:H1	3:D:1460:18I:O2	2.02	0.59
1:A:100:ARG:HG3	1:A:116:TYR:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:ARG:NH1	1:A:440:PHE:O	2.36	0.59
1:C:39:VAL:HG23	1:C:40:PRO:HD2	1.85	0.58
1:B:46:ILE:HG22	1:B:47:GLN:H	1.68	0.58
1:D:143:VAL:HG22	1:D:430:LEU:HD11	1.85	0.58
1:A:191:ARG:HG3	1:A:243:ILE:HD11	1.84	0.58
1:B:133:GLU:HG2	1:B:261:LEU:HD12	1.86	0.58
1:B:204:MET:HA	1:B:229:CYS:CB	2.33	0.58
1:C:475:ARG:HH11	1:C:475:ARG:HG3	1.67	0.58
1:C:333:ASN:HD22	1:C:333:ASN:N	1.95	0.57
1:A:107:VAL:N	1:A:108:PRO:CD	2.67	0.57
1:D:107:VAL:N	1:D:108:PRO:HD2	2.19	0.57
1:C:333:ASN:ND2	1:C:333:ASN:N	2.39	0.56
1:A:305:LEU:HD13	1:A:453:PRO:HG2	1.86	0.56
1:B:449:ARG:HD3	1:B:451:GLU:O	2.05	0.56
1:B:107:VAL:N	1:B:108:PRO:CD	2.68	0.56
1:D:244:ILE:CG2	1:D:248:LYS:HE2	2.35	0.56
1:A:98:SER:HG	1:A:120:TYR:HH	1.54	0.56
1:C:107:VAL:HG22	1:C:117:ALA:HB2	1.88	0.56
3:C:1460:18I:HN2	3:C:1460:18I:C23	2.18	0.56
2:B:1450:HEM:HBB2	2:B:1450:HEM:HMB2	1.86	0.56
1:B:331:ASN:ND2	1:B:334:ASN:H	2.03	0.56
2:B:1450:HEM:HBC2	2:B:1450:HEM:CMC	2.37	0.55
1:C:335:VAL:HG13	1:C:336:MET:N	2.19	0.55
2:B:1450:HEM:HBC2	2:B:1450:HEM:HMC2	1.87	0.55
1:B:419:VAL:HG23	1:B:420:HIS:CD2	2.42	0.55
1:D:174:MET:O	1:D:178:THR:HG23	2.07	0.55
2:B:1450:HEM:HBB2	2:B:1450:HEM:CMB	2.37	0.55
1:A:249:ALA:O	1:A:252:VAL:CG1	2.54	0.55
1:A:253:ASN:OD1	1:A:253:ASN:N	2.39	0.55
1:D:449:ARG:HD3	1:D:451:GLU:O	2.07	0.55
1:B:114:VAL:CG1	1:B:284:MET:CE	2.86	0.54
1:C:233:ARG:HH11	1:C:233:ARG:CG	2.20	0.54
1:C:334:ASN:HA	1:C:338:GLU:OE1	2.08	0.54
1:B:244:ILE:HG12	1:B:266:LEU:HD11	1.88	0.54
1:C:88:ARG:HG2	1:C:369:VAL:HA	1.89	0.54
1:D:178:THR:OG1	1:D:431:GLN:NE2	2.40	0.54
1:B:332:TYR:CE2	1:B:336:MET:HG3	2.43	0.54
1:C:166:ASN:C	1:C:166:ASN:HD22	2.10	0.54
1:D:193:ASP:OD1	1:D:193:ASP:C	2.47	0.53
2:A:1450:HEM:HBC2	2:A:1450:HEM:CMC	2.39	0.53
1:A:75:LYS:HE2	1:A:214:PHE:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1450:HEM:HMB2	2:A:1450:HEM:HBB2	1.90	0.53
1:D:97:LEU:HD22	1:D:380:ILE:HG21	1.89	0.53
1:C:449:ARG:HD3	1:C:451:GLU:O	2.10	0.52
1:D:265:LEU:HB3	1:D:276:MET:CE	2.39	0.52
1:A:253:ASN:C	1:A:254:LYS:HG2	2.29	0.52
1:C:106:MET:CE	1:C:110:PHE:CZ	2.91	0.52
1:C:332:TYR:CD1	1:C:332:TYR:C	2.82	0.52
1:B:204:MET:HA	1:B:229:CYS:HB2	1.91	0.52
1:A:320:ARG:NH2	1:A:444:ASP:OD1	2.37	0.52
1:C:143:VAL:HG21	1:C:332:TYR:HA	1.91	0.52
1:D:38:THR:HG23	1:D:47:GLN:HE22	1.75	0.52
1:B:335:VAL:CG2	1:B:430:LEU:HD12	2.38	0.51
1:A:58:GLU:O	1:A:62:GLN:HB2	2.11	0.51
1:C:233:ARG:HH11	1:C:233:ARG:HG2	1.74	0.51
1:C:233:ARG:HG2	1:C:233:ARG:NH1	2.26	0.51
1:C:322:GLU:OE1	1:C:339:MET:HG3	2.11	0.51
1:D:61:ARG:O	1:D:64:LYS:N	2.44	0.51
1:C:335:VAL:HG12	1:C:336:MET:H	1.76	0.50
3:C:1460:18I:C22	3:C:1460:18I:N2	2.74	0.50
1:A:162:GLU:OE2	1:A:472:LYS:NZ	2.37	0.50
1:B:255:ASP:OD1	1:B:255:ASP:N	2.44	0.50
1:A:106:MET:SD	3:A:1460:18I:H21A	2.51	0.50
1:D:87:SER:HB2	1:D:91:LEU:HD12	1.94	0.50
1:A:140[B]:GLN:OE1	1:A:140[B]:GLN:CA	2.59	0.50
1:B:114:VAL:HG12	1:B:115:ALA:N	2.25	0.50
1:C:282:CYS:O	1:C:286:VAL:HG12	2.11	0.50
1:C:93[A]:ARG:NH1	1:C:93[A]:ARG:CG	2.57	0.50
1:A:424:GLY:HA3	2:A:1450:HEM:C2C	2.47	0.50
1:A:294:HIS:O	1:A:298:ILE:HD12	2.12	0.49
2:A:1450:HEM:C1A	3:A:1460:18I:C2	2.95	0.49
1:A:252:VAL:C	1:A:253:ASN:OD1	2.51	0.49
1:A:140[B]:GLN:N	1:A:140[B]:GLN:CD	2.66	0.49
2:D:1450:HEM:C1A	3:D:1460:18I:H3	2.48	0.49
1:A:204:MET:HA	1:A:229:CYS:CB	2.40	0.48
1:B:109:VAL:CG1	1:B:110:PHE:N	2.76	0.48
1:B:251:ALA:HA	1:B:254:LYS:O	2.13	0.48
1:D:54:GLY:O	1:D:58:GLU:HG2	2.14	0.48
1:D:260:ASP:N	1:D:263:SER:OG	2.47	0.48
2:D:1450:HEM:HMD1	2:D:1450:HEM:CBD	2.44	0.48
2:D:1450:HEM:HMD1	2:D:1450:HEM:HBD1	1.95	0.48
1:A:424:GLY:HA3	2:A:1450:HEM:C3C	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:ILE:HG13	1:D:182:CYS:SG	2.54	0.48
1:B:228:ARG:HG3	1:B:228:ARG:HH11	1.78	0.48
2:A:1450:HEM:HBB2	2:A:1450:HEM:CMB	2.44	0.48
1:C:422:CYS:HA	2:C:1450:HEM:C4D	2.48	0.47
3:B:1460:18I:C24	3:B:1460:18I:H4	2.44	0.47
1:D:127:LEU:HD13	2:D:1450:HEM:CGD	2.44	0.47
1:D:247:ARG:NH2	1:D:260:ASP:OD1	2.46	0.47
1:C:109:VAL:HG12	1:C:110:PHE:CD1	2.49	0.47
1:D:384:PRO:O	1:D:388:HIS:CG	2.68	0.47
1:D:45:ILE:CD1	1:D:72:ILE:HG23	2.43	0.47
1:D:419:VAL:HG23	1:D:420:HIS:CD2	2.50	0.47
1:A:90:PHE:CG	1:A:417:ALA:HB3	2.50	0.47
1:A:96:VAL:HG12	1:A:97:LEU:HD13	1.97	0.47
1:A:253:ASN:C	1:A:254:LYS:CG	2.82	0.47
1:A:332:TYR:CZ	1:A:336:MET:HG3	2.49	0.47
1:A:357:LEU:O	1:A:384:PRO:HD2	2.15	0.47
3:B:1460:18I:HN2	3:B:1460:18I:C23	2.27	0.47
2:B:1450:HEM:C4D	3:B:1460:18I:C3	2.87	0.47
1:A:332:TYR:CE2	1:A:336:MET:HG3	2.50	0.47
1:B:204:MET:HG2	1:B:229:CYS:HB2	1.96	0.47
1:D:200:LEU:HD21	1:D:235:GLU:HG2	1.97	0.47
1:B:348:GLU:HG3	1:B:400:TRP:CD1	2.50	0.46
1:C:131:ALA:O	1:C:135:THR:HG23	2.15	0.46
1:C:408:VAL:HB	1:C:411:ALA:HB2	1.97	0.46
1:C:452:VAL:HG13	1:C:453:PRO:HD2	1.95	0.46
1:D:305:LEU:HD13	1:D:453:PRO:HG2	1.97	0.46
1:B:146:ILE:HG23	1:B:178:THR:HG21	1.96	0.46
2:B:1450:HEM:ND	3:B:1460:18I:C3	2.78	0.46
1:C:333:ASN:O	1:C:337:ASP:N	2.44	0.46
2:C:1450:HEM:CMB	2:C:1450:HEM:HBB2	2.45	0.46
1:A:108:PRO:HB2	1:A:229:CYS:SG	2.55	0.46
1:A:333:ASN:O	1:A:337:ASP:HB2	2.16	0.46
1:B:423:ILE:HD11	2:B:1450:HEM:HMD2	1.96	0.46
1:C:60:LYS:HG3	1:C:66:GLY:HA2	1.98	0.46
1:B:146:ILE:HG12	1:B:178:THR:HB	1.98	0.46
1:C:107:VAL:N	1:C:108:PRO:CD	2.78	0.46
1:D:357:LEU:HD21	1:D:462:VAL:HG21	1.97	0.46
1:A:423:ILE:HD11	2:A:1450:HEM:HMD2	1.99	0.45
2:C:1450:HEM:HBB2	2:C:1450:HEM:HMB2	1.98	0.45
1:C:133:GLU:CG	1:C:261:LEU:HD12	2.41	0.45
3:D:1460:18I:O2	3:D:1460:18I:C1	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LEU:CD1	1:A:239:ILE:HD13	2.47	0.45
1:D:196:ARG:HD3	4:D:2017:HOH:O	2.17	0.45
1:A:140[B]:GLN:CD	1:A:140[B]:GLN:H	2.20	0.45
2:B:1450:HEM:C1A	3:B:1460:18I:H3	2.52	0.45
1:C:158:TRP:O	1:C:443:TYR:OH	2.26	0.45
1:A:140[A]:GLN:HE21	1:A:140[A]:GLN:HB3	1.58	0.45
1:C:166:ASN:C	1:C:166:ASN:ND2	2.70	0.45
1:C:197:PHE:CE2	1:C:289:MET:HG3	2.50	0.45
1:B:105:PHE:O	1:B:108:PRO:HG2	2.17	0.45
1:D:101:GLU:O	1:D:104:SER:HB3	2.17	0.45
1:D:162:GLU:HA	1:D:473:TYR:O	2.17	0.45
1:D:205:GLU:CB	1:D:290:PHE:HZ	2.29	0.45
1:B:95:GLU:OE1	1:B:95:GLU:N	2.50	0.45
1:B:114:VAL:HG13	1:B:284:MET:CE	2.47	0.45
1:B:196:ARG:NH2	1:B:200:LEU:HD21	2.32	0.45
3:A:1460:18I:C22	3:A:1460:18I:N2	2.80	0.44
1:C:93[A]:ARG:HD2	1:C:93[A]:ARG:N	2.32	0.44
1:C:313:VAL:HG23	1:C:314:LYS:N	2.31	0.44
1:D:366:ASP:HA	1:D:374:VAL:O	2.17	0.44
1:B:129:PHE:CE1	1:B:268:ALA:HB1	2.51	0.44
1:D:216:PRO:HD2	4:D:2019:HOH:O	2.17	0.44
1:B:114:VAL:CG1	1:B:115:ALA:N	2.80	0.44
2:D:1450:HEM:HBB2	2:D:1450:HEM:HMB2	1.99	0.44
1:B:35:TYR:CD1	1:B:36:PRO:HD2	2.52	0.44
1:D:301:THR:O	1:D:305:LEU:HG	2.17	0.44
1:C:244:ILE:HG12	1:C:266:LEU:HD11	2.00	0.44
1:A:348:GLU:HG3	1:A:400:TRP:CD1	2.53	0.44
1:B:107:VAL:CB	1:B:108:PRO:CD	2.94	0.44
3:C:1460:18I:O2	3:C:1460:18I:H1	2.18	0.44
1:D:291:ALA:HB1	3:D:1460:18I:C2	2.48	0.44
1:D:358:MET:HE3	1:D:381:ALA:HB1	1.99	0.44
1:A:460:MET:CB	3:A:1460:18I:C10	2.96	0.43
1:B:33:PRO:HB2	1:B:63:LEU:HD13	2.00	0.43
1:B:44:HIS:HA	1:B:47:GLN:NE2	2.33	0.43
1:C:120:TYR:O	1:C:121:PRO:C	2.56	0.43
1:C:339:MET:HG2	1:C:342:ALA:HB3	2.00	0.43
1:C:162:GLU:HG2	1:C:472:LYS:HE2	1.99	0.43
1:D:136:ILE:HA	1:D:139:PHE:CD2	2.54	0.43
1:D:143:VAL:HB	1:D:144:PRO:HD3	2.00	0.43
1:A:187:ASP:OD2	1:A:247:ARG:HD2	2.17	0.43
1:D:31:LEU:HD23	1:D:31:LEU:HA	1.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:CYS:O	1:D:175:ILE:HG12	2.19	0.43
1:C:136:ILE:HA	1:C:139:PHE:CE2	2.54	0.43
1:C:265:LEU:HD22	1:C:276:MET:HE1	2.01	0.43
1:C:228:ARG:HG3	1:C:228:ARG:NH1	2.19	0.43
1:D:456:ASP:C	1:D:456:ASP:OD1	2.56	0.43
1:B:105:PHE:HD1	1:B:105:PHE:H	1.67	0.42
1:D:403:GLU:OE1	1:D:403:GLU:HA	2.19	0.42
1:D:107:VAL:HB	1:D:108:PRO:HD3	2.01	0.42
1:D:282:CYS:O	1:D:286:VAL:HG13	2.19	0.42
1:B:197:PHE:CE2	1:B:289:MET:HG3	2.54	0.42
1:D:32:PRO:HD3	1:D:372:TYR:HB3	2.00	0.42
1:C:176:ILE:CD1	1:C:289:MET:CE	2.98	0.42
1:B:207:SER:HB3	1:B:225:GLN:O	2.19	0.42
1:B:334:ASN:HA	1:B:338:GLU:HB2	2.02	0.42
1:B:360:MET:HG2	1:B:381:ALA:HB2	2.02	0.42
1:D:45:ILE:HD13	1:D:72:ILE:HG23	2.00	0.42
1:D:331:ASN:HD22	1:D:333:ASN:H	1.68	0.42
1:B:178:THR:OG1	1:B:431:GLN:NE2	2.52	0.42
2:C:1450:HEM:HBC2	2:C:1450:HEM:CMC	2.44	0.42
1:B:58:GLU:OE1	1:B:62:GLN:NE2	2.53	0.42
1:C:301:THR:O	1:C:302:TRP:C	2.58	0.42
1:D:358:MET:CE	1:D:381:ALA:HB1	2.50	0.42
1:D:419:VAL:CG2	1:D:420:HIS:CD2	3.02	0.42
1:B:139:PHE:N	1:B:139:PHE:CD1	2.86	0.42
1:C:33:PRO:HB2	1:C:63:LEU:HD22	2.01	0.42
1:C:164:GLU:HG2	1:C:470:ARG:HH11	1.84	0.42
1:C:203:LYS:HD3	1:C:232:ALA:HB2	2.02	0.41
1:B:357:LEU:HD22	1:B:385:LEU:HD22	2.02	0.41
1:A:122:ARG:CD	1:A:270:TYR:CE1	3.03	0.41
1:B:204:MET:HA	1:B:229:CYS:HB3	2.01	0.41
1:D:302:TRP:O	1:D:303:SER:C	2.58	0.41
1:B:315:HIS:CE1	1:B:402:PRO:HD2	2.55	0.41
1:D:335:VAL:CG2	1:D:430:LEU:HD12	2.50	0.41
1:C:445:PHE:HA	1:C:472:LYS:O	2.21	0.41
1:C:473:TYR:C	1:C:474:ILE:HG13	2.40	0.41
2:A:1450:HEM:HBD1	2:A:1450:HEM:HHA	2.02	0.41
1:A:272:ASP:C	1:A:272:ASP:OD1	2.59	0.41
1:D:31:LEU:CD2	1:D:373:VAL:O	2.69	0.41
1:A:331:ASN:HD22	1:A:331:ASN:C	2.23	0.41
1:C:385:LEU:HA	1:C:385:LEU:HD12	1.82	0.41
1:A:331:ASN:ND2	1:A:334:ASN:H	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:ARG:HD3	1:A:400:TRP:HB2	2.01	0.41
1:A:401:ASP:O	1:A:404:ARG:HG2	2.21	0.41
1:C:176:ILE:HD12	1:C:289:MET:HE3	2.03	0.41
1:D:284:MET:HA	1:D:284:MET:CE	2.50	0.41
1:B:106:MET:CB	1:B:110:PHE:CE2	3.02	0.41
1:C:166:ASN:ND2	1:C:169:GLU:H	2.19	0.41
1:C:331:ASN:O	1:C:334:ASN:HB2	2.21	0.41
1:B:96:VAL:HG12	1:B:97:LEU:HD13	2.03	0.40
1:C:44:HIS:HB3	1:C:55:PHE:CZ	2.56	0.40
1:D:33:PRO:CB	1:D:63:LEU:HD13	2.49	0.40
1:C:158:TRP:NE1	1:C:165:ILE:HD13	2.37	0.40
1:A:278:LEU:HD12	1:A:278:LEU:HA	1.93	0.40
1:C:228:ARG:HD2	1:C:228:ARG:HA	1.86	0.40
1:A:172:SER:HA	1:A:297:SER:OG	2.22	0.40
1:A:106:MET:C	1:A:108:PRO:HD2	2.41	0.40
1:C:146:ILE:HG22	1:C:434:THR:HG21	2.04	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	449/469 (96%)	430 (96%)	17 (4%)	2 (0%)	34 58
1	B	448/469 (96%)	421 (94%)	27 (6%)	0	100 100
1	C	449/469 (96%)	425 (95%)	23 (5%)	1 (0%)	47 71
1	D	441/469 (94%)	413 (94%)	28 (6%)	0	100 100
All	All	1787/1876 (95%)	1689 (94%)	95 (5%)	3 (0%)	47 71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	PRO
1	A	40	PRO
1	C	40	PRO

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	378/403 (94%)	343 (91%)	35 (9%)	9 19
1	B	378/403 (94%)	351 (93%)	27 (7%)	14 31
1	C	378/403 (94%)	340 (90%)	38 (10%)	7 16
1	D	371/403 (92%)	339 (91%)	32 (9%)	10 22
All	All	1505/1612 (93%)	1373 (91%)	132 (9%)	10 21

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	34	MET
1	A	39	VAL
1	A	61	ARG
1	A	62	GLN
1	A	75	LYS
1	A	87	SER
1	A	97	LEU
1	A	112	GLU
1	A	132	GLU
1	A	135	THR
1	A	140[A]	GLN
1	A	140[B]	GLN
1	A	152	LYS
1	A	166	ASN
1	A	186	GLU
1	A	190	LYS
1	A	209	ILE
1	A	228	ARG

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Mol	Chain	Res	Type
1	A	236	LEU
1	A	241	SER
1	A	247	ARG
1	A	253	ASN
1	A	258	THR
1	A	329	GLN
1	A	331	ASN
1	A	335	VAL
1	A	367	VAL
1	A	391	GLU
1	A	406	GLU
1	A	419	VAL
1	A	449	ARG
1	A	452	VAL
1	A	471	VAL
1	A	475	ARG
1	B	38	THR
1	B	39	VAL
1	B	46	ILE
1	B	88	ARG
1	B	107	VAL
1	B	109	VAL
1	B	124	ARG
1	B	140	GLN
1	B	166	ASN
1	B	186	GLU
1	B	221	LEU
1	B	247	ARG
1	B	256	SER
1	B	313	VAL
1	B	329	GLN
1	B	331	ASN
1	B	335	VAL
1	B	352	ARG
1	B	376	LYS
1	B	383	SER
1	B	391	GLU
1	B	399	ARG
1	B	409	GLU
1	B	449	ARG
1	B	460	MET
1	B	470	ARG

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Mol	Chain	Res	Type
1	B	471	VAL
1	C	72	ILE
1	C	75	LYS
1	C	88	ARG
1	C	93[A]	ARG
1	C	93[B]	ARG
1	C	97	LEU
1	C	109	VAL
1	C	112	GLU
1	C	124	ARG
1	C	166	ASN
1	C	197	PHE
1	C	217	ILE
1	C	228	ARG
1	C	229	CYS
1	C	233	ARG
1	C	234	THR
1	C	239	ILE
1	C	247	ARG
1	C	248	LYS
1	C	257	SER
1	C	271	ARG
1	C	282	CYS
1	C	286	VAL
1	C	290	PHE
1	C	320	ARG
1	C	321	LYS
1	C	326	PHE
1	C	331	ASN
1	C	333	ASN
1	C	335	VAL
1	C	367	VAL
1	C	378	ASP
1	C	406	GLU
1	C	419	VAL
1	C	444	ASP
1	C	448	LEU
1	C	449	ARG
1	C	475	ARG
1	D	38	THR
1	D	39	VAL
1	D	46	ILE

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Mol	Chain	Res	Type
1	D	58	GLU
1	D	61	ARG
1	D	136	ILE
1	D	162	GLU
1	D	166	ASN
1	D	172	SER
1	D	196	ARG
1	D	197	PHE
1	D	217	ILE
1	D	234	THR
1	D	235	GLU
1	D	236	LEU
1	D	247	ARG
1	D	248	LYS
1	D	259	SER
1	D	271	ARG
1	D	279	HIS
1	D	313	VAL
1	D	331	ASN
1	D	366	ASP
1	D	399	ARG
1	D	404	ARG
1	D	407	LYS
1	D	426	LYS
1	D	446	GLN
1	D	449	ARG
1	D	452	VAL
1	D	471	VAL
1	D	475	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	A	225	GLN
1	A	293	GLN
1	A	306	HIS
1	A	331	ASN
1	A	431	GLN
1	B	47	GLN
1	B	141	ASN
1	B	166	ASN

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Mol	Chain	Res	Type
1	B	293	GLN
1	B	294	HIS
1	B	315	HIS
1	B	331	ASN
1	B	333	ASN
1	B	334	ASN
1	B	431	GLN
1	C	166	ASN
1	C	279	HIS
1	C	293	GLN
1	C	306	HIS
1	C	331	ASN
1	C	333	ASN
1	C	334	ASN
1	D	47	GLN
1	D	166	ASN
1	D	279	HIS
1	D	293	GLN
1	D	331	ASN
1	D	333	ASN
1	D	334	ASN
1	D	431	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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)

8 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	$\#\|Z\| > 2$
2	HEM	B	1450	3,1	41,50,50	1.53	5 (12%)	45,82,82	2.06	14 (31%)
2	HEM	C	1450	3,1	41,50,50	1.41	4 (9%)	45,82,82	2.00	9 (20%)
3	18I	B	1460	2	22,23,41	1.18	1 (4%)	25,31,57	1.41	5 (20%)
3	18I	C	1460	2	22,23,41	1.10	1 (4%)	25,31,57	1.16	2 (8%)
2	HEM	A	1450	3,1	41,50,50	1.44	5 (12%)	45,82,82	2.30	9 (20%)
2	HEM	D	1450	3,1	41,50,50	1.53	7 (17%)	45,82,82	1.99	11 (24%)
3	18I	D	1460	2	22,23,41	1.20	2 (9%)	25,31,57	1.34	5 (20%)
3	18I	A	1460	2	40,41,41	1.58	2 (5%)	53,57,57	1.55	11 (20%)

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	HEM	B	1450	3,1	-	1/12/54/54	-
2	HEM	C	1450	3,1	-	0/12/54/54	-
3	18I	B	1460	2	-	4/11/12/24	0/3/3/5
3	18I	C	1460	2	-	0/11/12/24	0/3/3/5
2	HEM	A	1450	3,1	-	4/12/54/54	-
2	HEM	D	1450	3,1	-	4/12/54/54	-
3	18I	D	1460	2	-	1/11/12/24	0/3/3/5
3	18I	A	1460	2	-	2/23/24/24	0/5/5/5

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1460	18I	C9-C20	8.02	1.49	1.38
2	B	1450	HEM	C1B-NB	-5.02	1.31	1.40
2	A	1450	HEM	C1B-NB	-4.79	1.32	1.40
2	D	1450	HEM	C1B-NB	-4.54	1.32	1.40
2	C	1450	HEM	C1B-NB	-4.51	1.32	1.40
2	B	1450	HEM	C4B-NB	-3.79	1.31	1.38
2	D	1450	HEM	C4D-ND	-3.68	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1450	HEM	C4B-NB	-3.66	1.31	1.38
3	B	1460	18I	C5-N2	-3.32	1.34	1.41
3	D	1460	18I	C5-N2	-3.16	1.35	1.41
2	C	1450	HEM	C4D-ND	-3.14	1.34	1.40
2	C	1450	HEM	C4B-NB	-3.02	1.32	1.38
2	B	1450	HEM	C4D-ND	-3.00	1.35	1.40
2	A	1450	HEM	C4B-NB	-2.89	1.32	1.38
2	A	1450	HEM	C4D-ND	-2.87	1.35	1.40
3	C	1460	18I	C5-N2	-2.75	1.36	1.41
2	C	1450	HEM	C1D-ND	-2.38	1.33	1.38
2	D	1450	HEM	FE-NB	2.24	2.07	1.96
2	A	1450	HEM	C1D-ND	-2.24	1.34	1.38
3	D	1460	18I	C29-C24	2.22	1.48	1.42
2	B	1450	HEM	CHB-C1B	2.20	1.40	1.35
2	D	1450	HEM	C1A-CHA	-2.18	1.34	1.41
3	A	1460	18I	C18-C17	2.17	1.41	1.37
2	A	1450	HEM	CHB-C1B	2.16	1.40	1.35
2	B	1450	HEM	C1A-CHA	-2.14	1.35	1.41
2	D	1450	HEM	FE-ND	-2.01	1.86	1.96
2	D	1450	HEM	C3B-C4B	2.01	1.48	1.44

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1450	HEM	C1B-NB-C4B	6.83	112.13	105.07
2	B	1450	HEM	CHC-C4B-NB	5.77	130.70	124.43
2	A	1450	HEM	CAD-CBD-CGD	-5.66	101.43	113.60
2	A	1450	HEM	CHC-C4B-NB	5.63	130.54	124.43
2	A	1450	HEM	C1B-NB-C4B	5.52	110.78	105.07
2	B	1450	HEM	C1B-NB-C4B	5.50	110.75	105.07
2	A	1450	HEM	CAD-C3D-C4D	5.49	134.25	124.66
2	C	1450	HEM	CHC-C4B-NB	5.45	130.36	124.43
2	D	1450	HEM	C1B-NB-C4B	5.11	110.35	105.07
3	A	1460	18I	C4-C5-C1	-4.60	112.74	119.03
2	A	1450	HEM	CHD-C1D-ND	4.55	129.37	124.43
2	A	1450	HEM	CAD-C3D-C2D	-4.29	119.89	127.88
2	D	1450	HEM	CHD-C1D-ND	4.17	128.96	124.43
2	B	1450	HEM	CHA-C4D-ND	4.12	129.47	124.38
2	A	1450	HEM	CHD-C1D-C2D	-4.07	118.61	124.98
2	D	1450	HEM	CHA-C4D-ND	4.01	129.33	124.38
2	C	1450	HEM	CHD-C1D-ND	3.98	128.75	124.43
2	D	1450	HEM	CHC-C4B-NB	3.81	128.56	124.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1450	HEM	CBA-CAA-C2A	3.68	118.90	112.62
2	D	1450	HEM	CAD-CBD-CGD	-3.65	105.74	113.60
3	A	1460	18I	C28-C29-C24	3.63	122.98	118.17
2	D	1450	HEM	CHA-C4D-C3D	-3.54	118.69	125.33
2	B	1450	HEM	CHD-C1D-ND	3.49	128.22	124.43
2	C	1450	HEM	CHA-C4D-ND	3.47	128.67	124.38
2	B	1450	HEM	CAD-CBD-CGD	-3.32	106.47	113.60
3	B	1460	18I	C28-C29-C24	3.12	122.31	118.17
2	C	1450	HEM	CHD-C1D-C2D	-3.08	120.16	124.98
2	D	1450	HEM	CHD-C1D-C2D	-3.02	120.27	124.98
3	A	1460	18I	C19-C20-C9	-2.96	120.37	123.53
2	C	1450	HEM	CHB-C1B-NB	2.92	127.99	124.38
2	B	1450	HEM	C2C-C3C-C4C	2.88	108.91	106.90
2	B	1450	HEM	CHA-C4D-C3D	-2.87	119.93	125.33
3	A	1460	18I	C2-C1-C5	2.87	122.86	118.93
2	B	1450	HEM	CMD-C2D-C1D	2.86	129.39	125.04
2	C	1450	HEM	CHA-C4D-C3D	-2.85	119.98	125.33
3	D	1460	18I	C21-C7-C6	-2.81	102.39	108.97
2	A	1450	HEM	CMD-C2D-C1D	2.70	129.15	125.04
2	B	1450	HEM	CMC-C2C-C3C	2.70	129.73	124.68
3	A	1460	18I	C22-C21-C7	-2.68	108.20	113.45
2	C	1450	HEM	CAD-CBD-CGD	-2.68	107.84	113.60
3	B	1460	18I	C21-C7-C6	2.67	115.22	108.97
3	B	1460	18I	C5-N2-C6	-2.63	121.10	127.40
2	D	1450	HEM	C4B-CHC-C1C	2.62	126.01	122.56
2	C	1450	HEM	O2D-CGD-CBD	2.56	122.27	114.03
3	A	1460	18I	C27-C28-C29	-2.54	117.38	120.89
2	B	1450	HEM	CBD-CAD-C3D	2.51	119.61	112.63
2	B	1450	HEM	CHD-C1D-C2D	-2.47	121.12	124.98
2	B	1450	HEM	O2A-CGA-O1A	-2.43	117.24	123.30
2	B	1450	HEM	C3B-C2B-C1B	-2.40	104.71	106.49
3	A	1460	18I	C9-C8-N3	2.36	121.17	116.80
3	C	1460	18I	C4-C5-C1	-2.34	115.84	119.03
3	D	1460	18I	C27-C28-C29	-2.33	117.66	120.89
2	D	1450	HEM	CAD-C3D-C2D	2.31	132.19	127.88
3	A	1460	18I	O2-C6-C7	-2.28	115.65	120.45
3	D	1460	18I	C21-C22-C29	2.27	129.78	126.25
3	C	1460	18I	C28-C29-C24	2.27	121.18	118.17
2	D	1450	HEM	C4C-CHD-C1D	-2.25	119.58	122.56
3	D	1460	18I	C21-C22-C23	-2.20	125.25	127.97
3	D	1460	18I	C28-C29-C24	2.20	121.08	118.17
3	B	1460	18I	C25-C24-C29	-2.18	116.78	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1460	18I	C21-C7-N3	-2.15	106.27	110.79
3	A	1460	18I	C25-C24-C29	-2.14	116.84	120.76
3	B	1460	18I	C27-C28-C29	-2.10	117.98	120.89
3	A	1460	18I	C4-C5-N2	2.10	127.46	120.40
2	B	1450	HEM	O2D-CGD-CBD	2.07	120.68	114.03
2	A	1450	HEM	CBA-CAA-C2A	-2.07	109.09	112.62

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1450	HEM	C2D-C3D-CAD-CBD
3	B	1460	18I	N2-C6-C7-C21
3	B	1460	18I	O2-C6-C7-C21
3	B	1460	18I	C22-C21-C7-N3
3	B	1460	18I	C22-C21-C7-C6
2	A	1450	HEM	C4D-C3D-CAD-CBD
2	D	1450	HEM	C4D-C3D-CAD-CBD
2	A	1450	HEM	C2D-C3D-CAD-CBD
2	D	1450	HEM	CAD-CBD-CGD-O2D
2	A	1450	HEM	CAD-CBD-CGD-O2D
2	D	1450	HEM	CAD-CBD-CGD-O1D
2	A	1450	HEM	CAD-CBD-CGD-O1D
3	A	1460	18I	O2-C6-C7-N3
3	D	1460	18I	C7-C21-C22-C23
3	A	1460	18I	N2-C6-C7-N3
2	B	1450	HEM	CAD-CBD-CGD-O2D

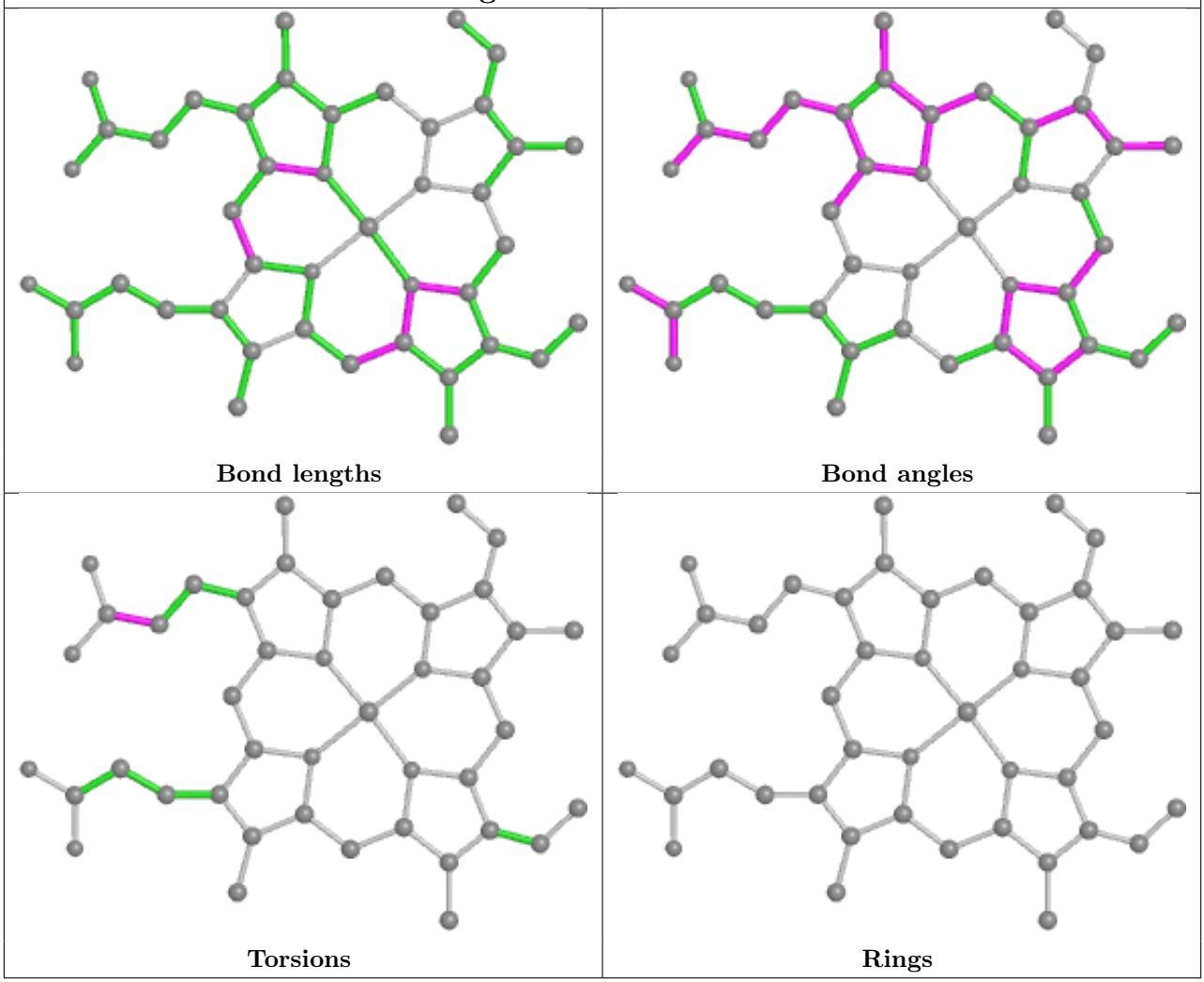
There are no ring outliers.

8 monomers are involved in 54 short contacts:

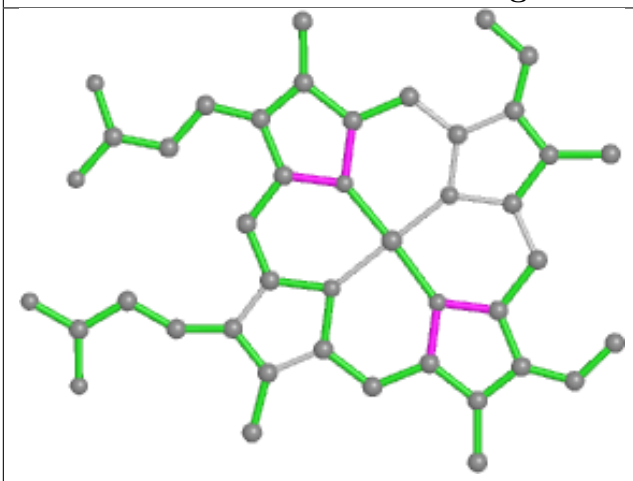
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1450	HEM	10	0
2	C	1450	HEM	7	0
3	B	1460	18I	13	0
3	C	1460	18I	5	0
2	A	1450	HEM	13	0
2	D	1450	HEM	7	0
3	D	1460	18I	4	0
3	A	1460	18I	8	0

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.

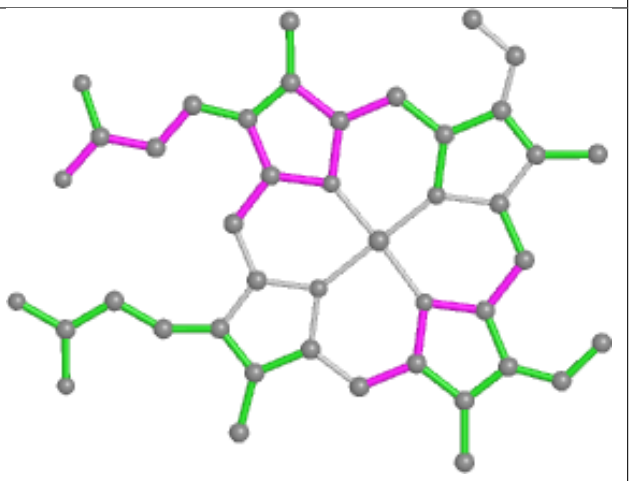
Ligand HEM B 1450



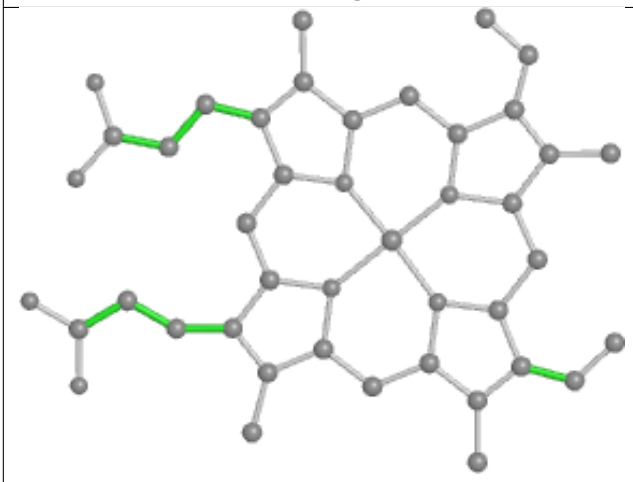
Ligand HEM C 1450



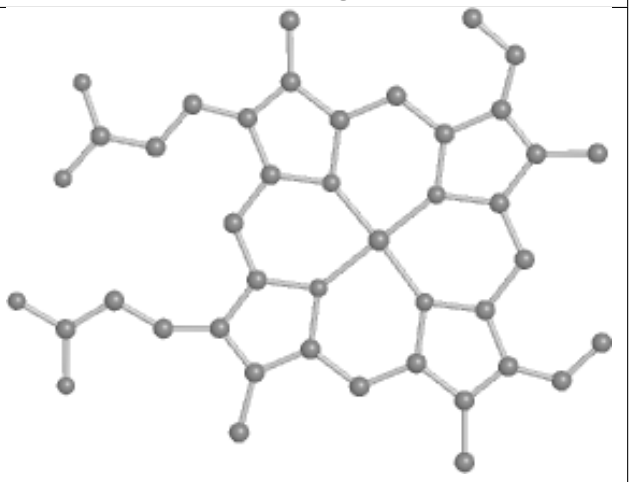
Bond lengths



Bond angles

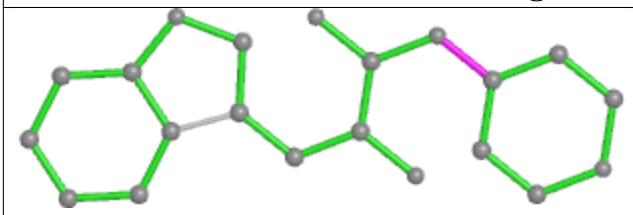


Torsions

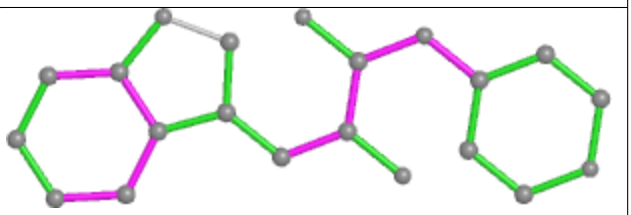


Rings

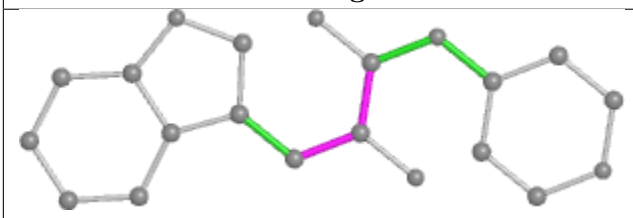
Ligand 18I B 1460



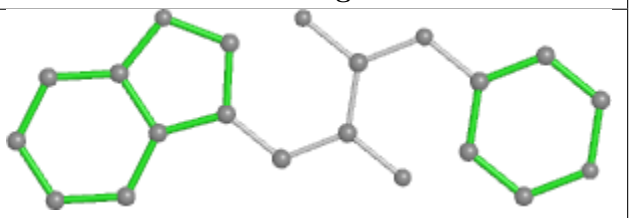
Bond lengths



Bond angles

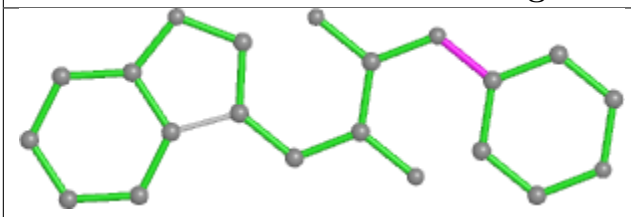


Torsions

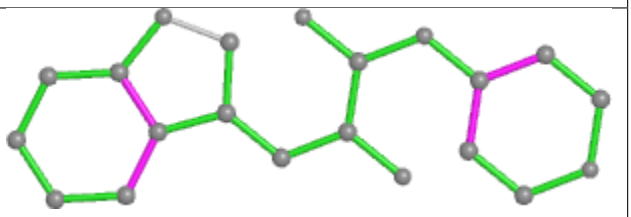


Rings

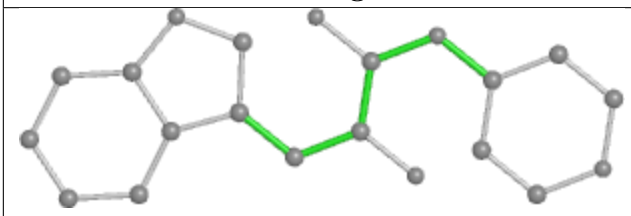
Ligand 18I C 1460



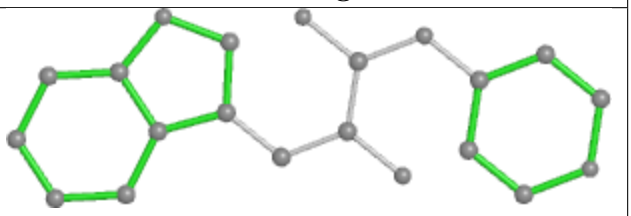
Bond lengths



Bond angles

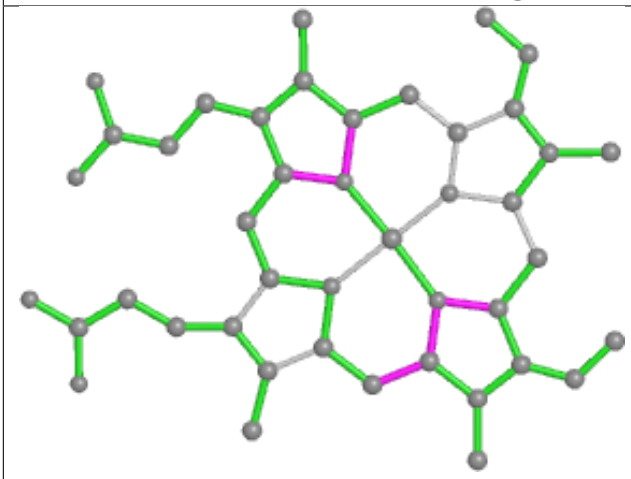


Torsions

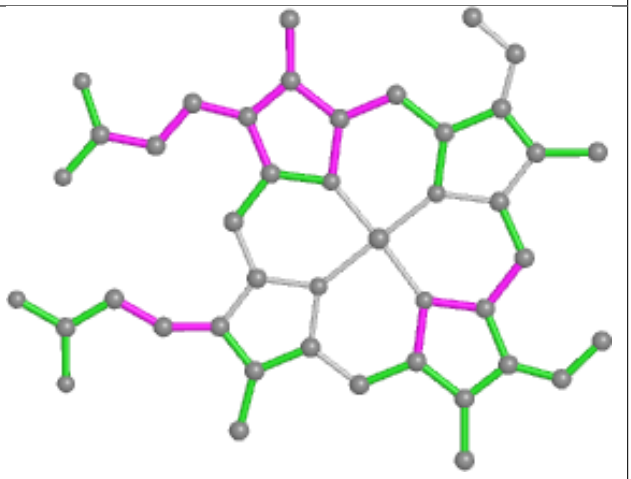


Rings

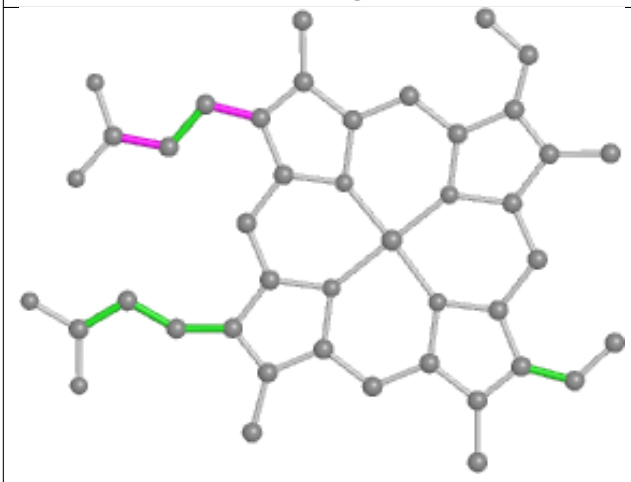
Ligand HEM A 1450



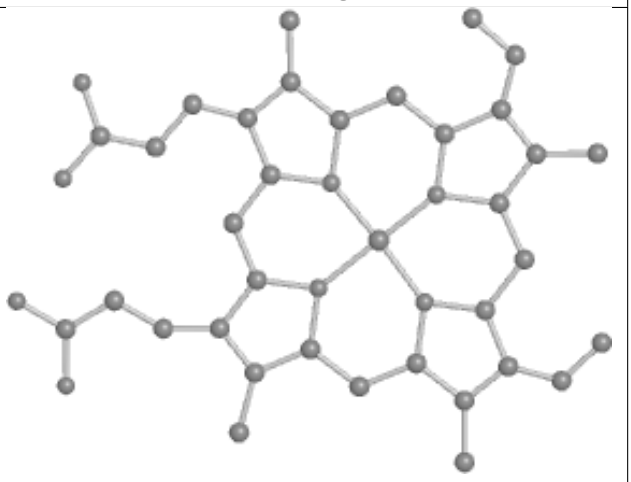
Bond lengths



Bond angles

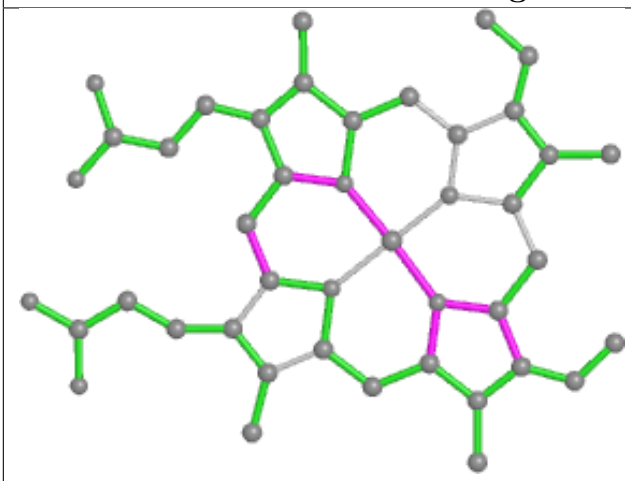


Torsions

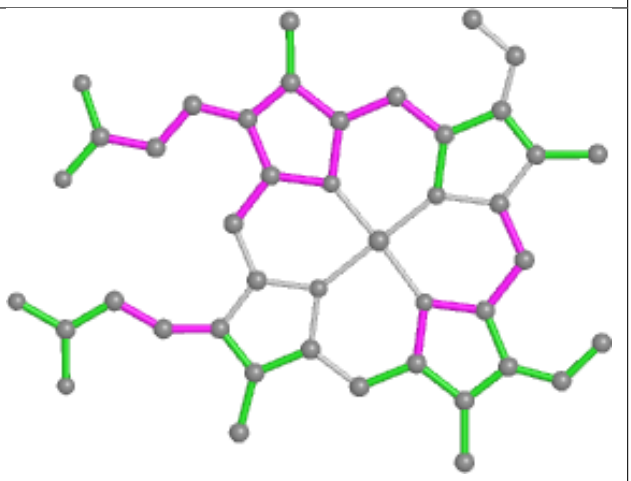


Rings

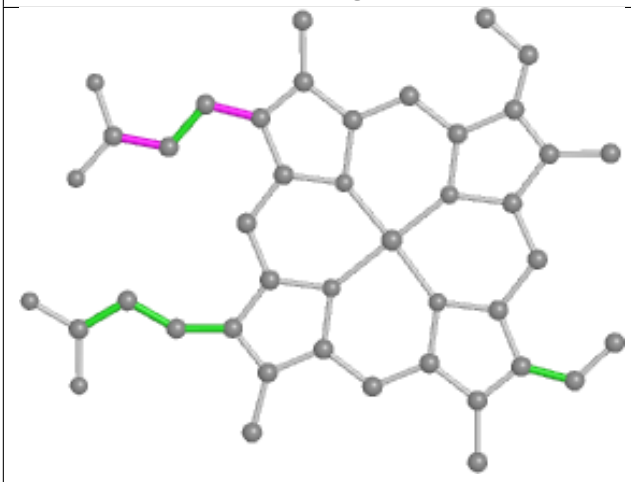
Ligand HEM D 1450



Bond lengths



Bond angles



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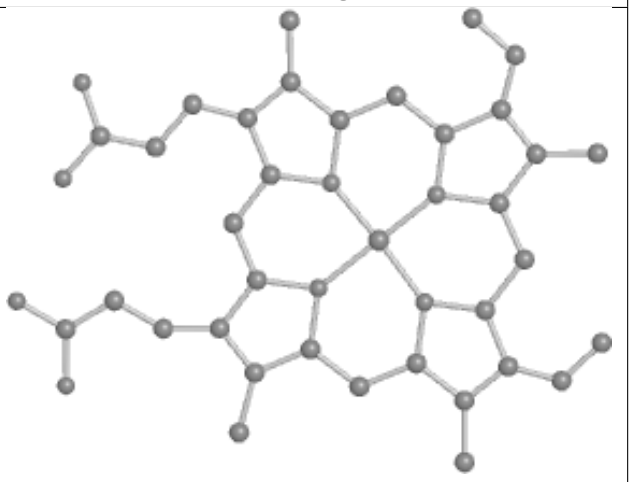
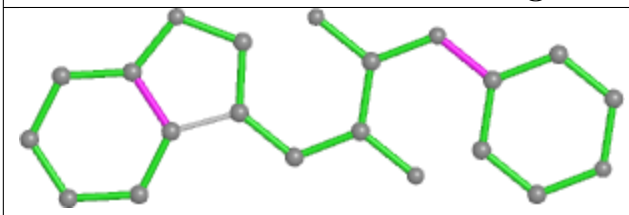
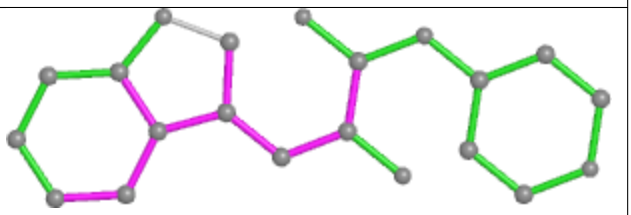


Rings

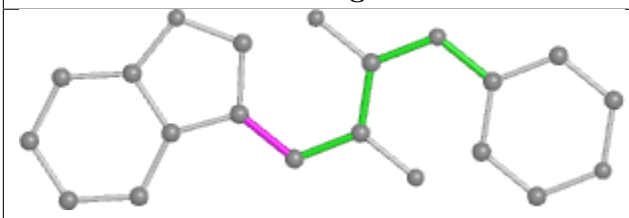
Ligand 18I D 1460



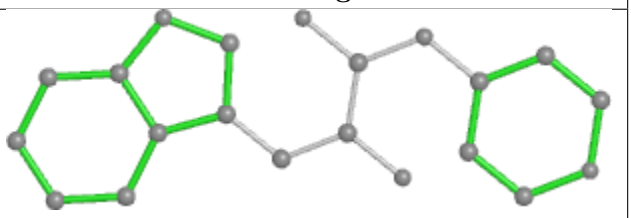
Bond lengths



Bond angles

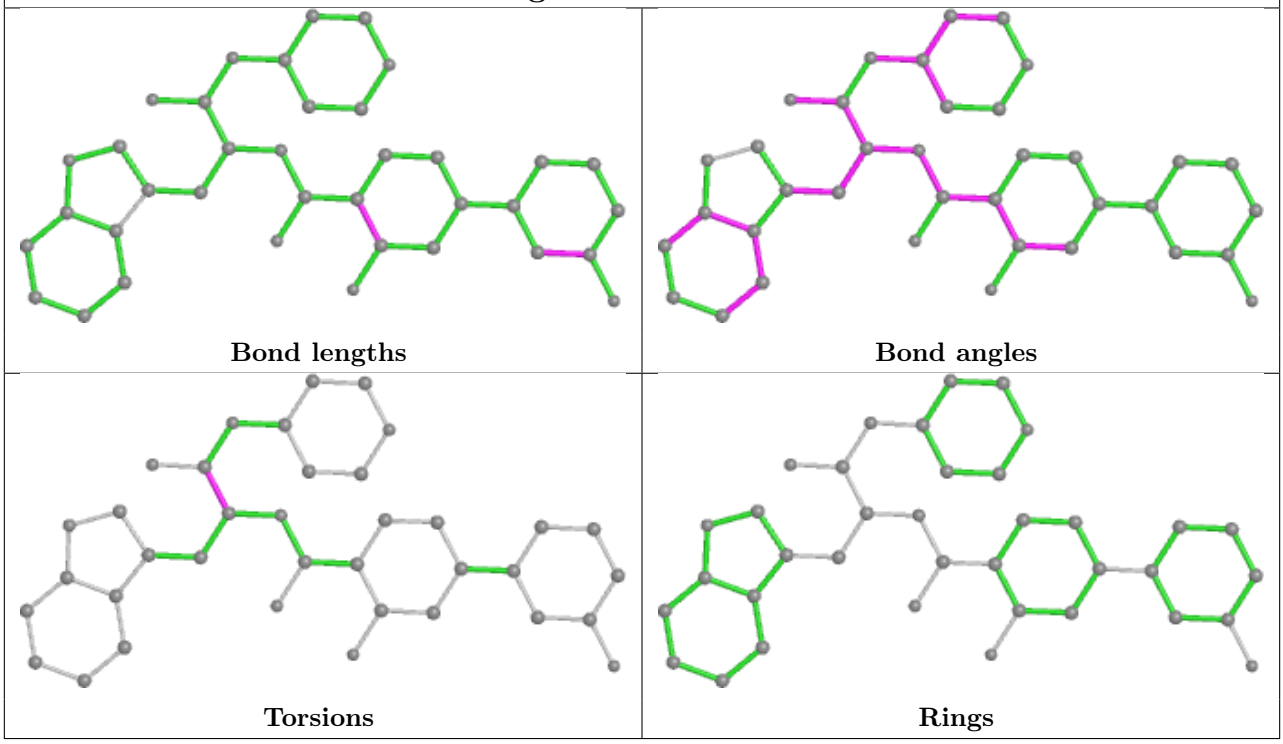


Torsions



Rings

Ligand 18I A 1460



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	450/469 (95%)	-0.26	2 (0%)	92	93	40, 58, 84, 138	0
1	B	450/469 (95%)	-0.21	2 (0%)	92	93	41, 62, 90, 119	0
1	C	450/469 (95%)	-0.21	1 (0%)	95	96	45, 70, 98, 126	0
1	D	444/469 (94%)	-0.16	2 (0%)	91	92	48, 68, 99, 117	0
All	All	1794/1876 (95%)	-0.21	7 (0%)	92	93	40, 65, 95, 138	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214	PHE	2.9
1	D	365	ALA	2.8
1	A	29	GLY	2.6
1	A	258	THR	2.3
1	B	478	ALA	2.2
1	D	103	TYR	2.1
1	C	478	ALA	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)

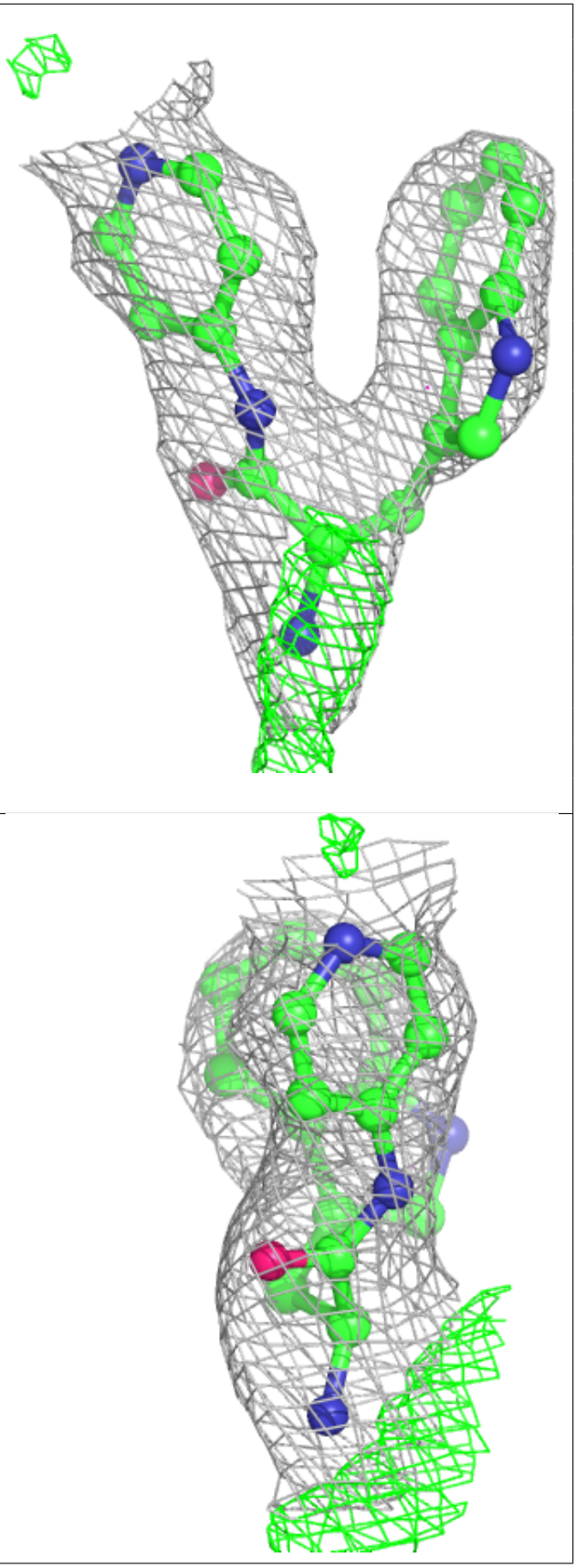
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	18I	D	1460	21/37	0.86	0.28	73,86,96,100	0
3	18I	A	1460	37/37	0.92	0.25	55,74,93,96	0
3	18I	B	1460	21/37	0.93	0.21	70,87,105,106	0
3	18I	C	1460	21/37	0.95	0.21	67,93,108,111	0
2	HEM	A	1450	43/43	0.97	0.17	41,48,55,63	0
2	HEM	C	1450	43/43	0.98	0.16	42,51,58,69	0
2	HEM	D	1450	43/43	0.98	0.19	53,61,71,79	0
2	HEM	B	1450	43/43	0.98	0.17	40,46,60,62	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.

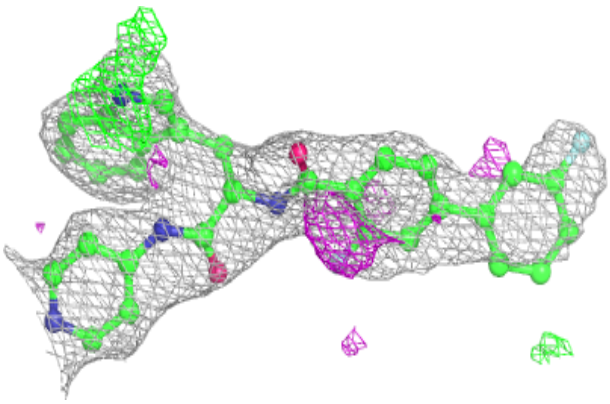
Electron density around 18I D 1460:

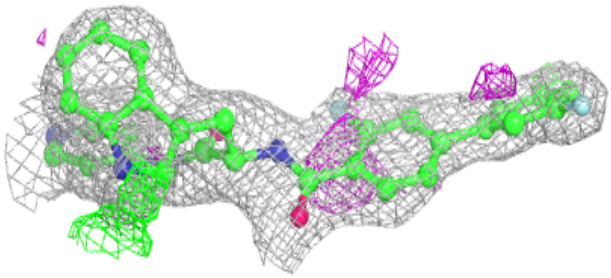
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

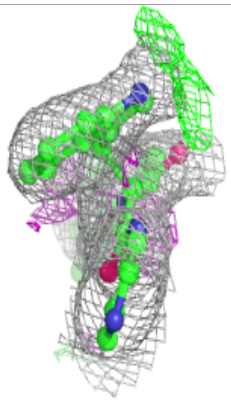


Electron density around 18I A 1460:

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

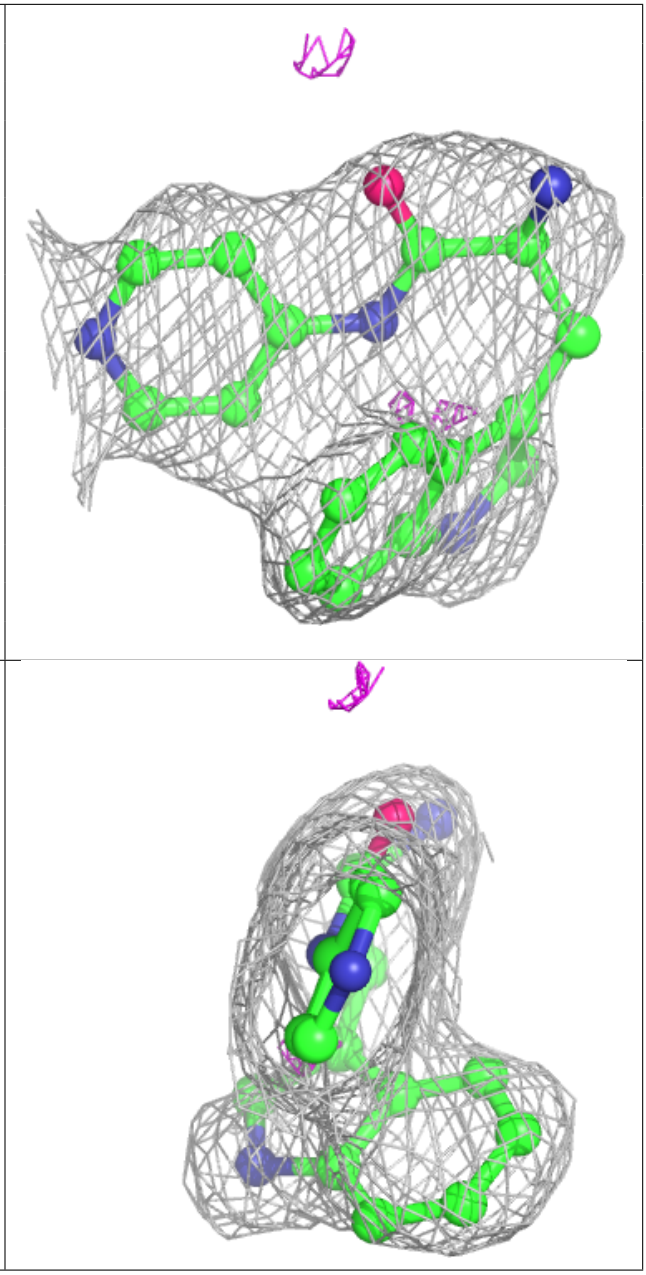






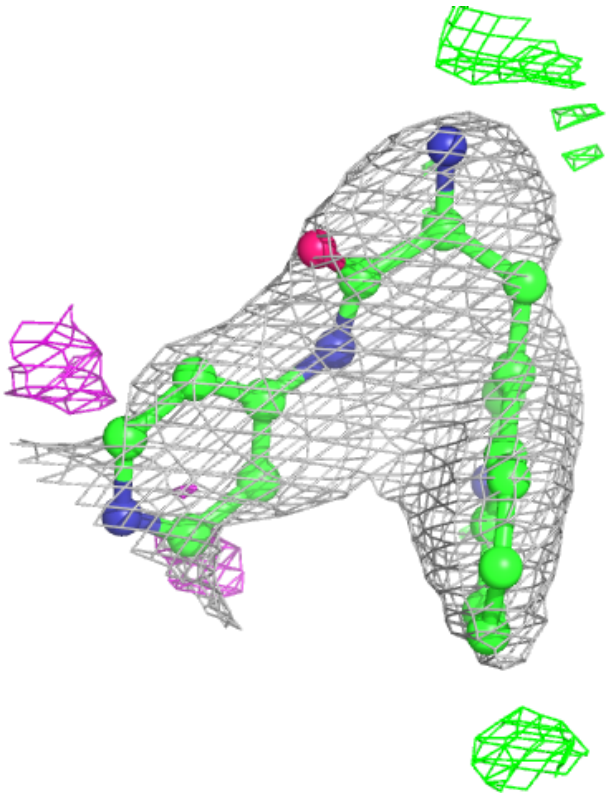
Electron density around 18I B 1460:

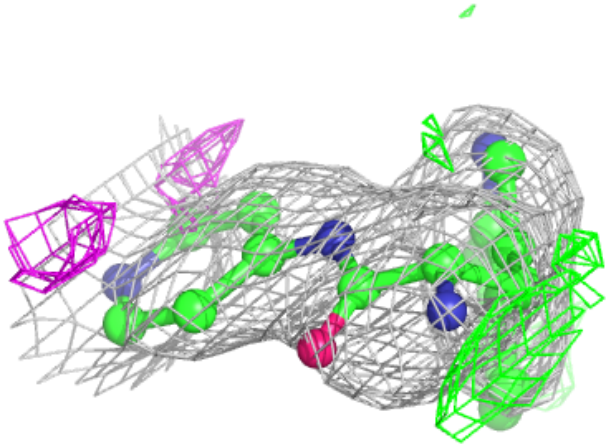
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

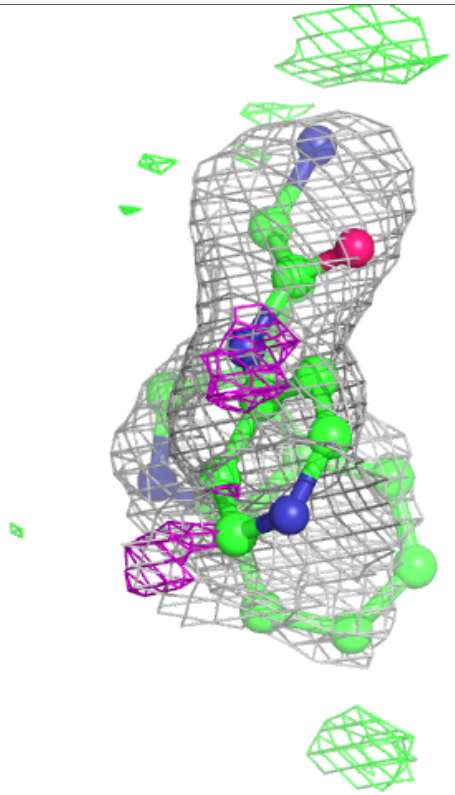


Electron density around 18I C 1460:

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

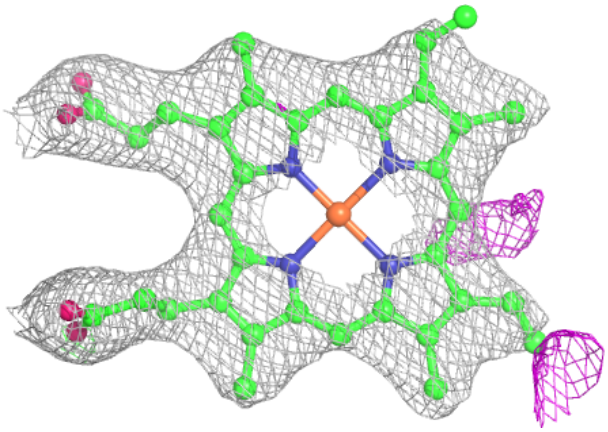


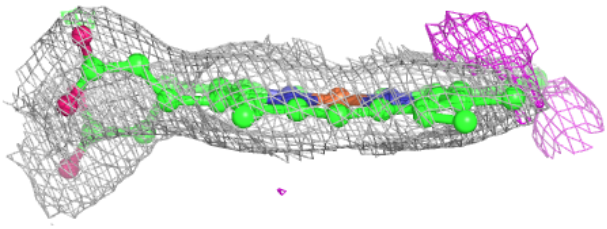


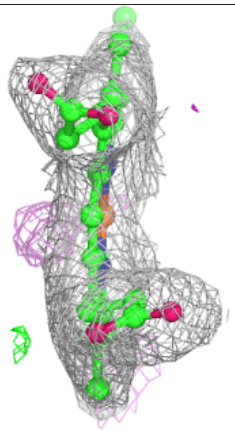


Electron density around HEM A 1450:

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

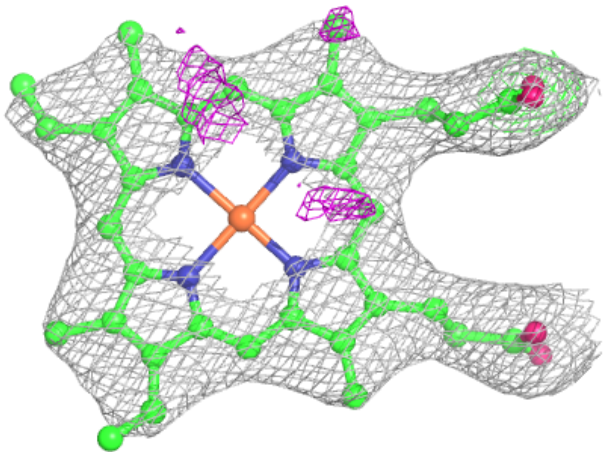


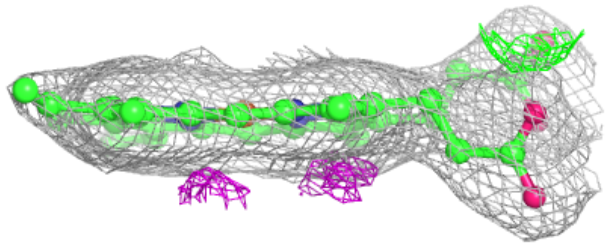


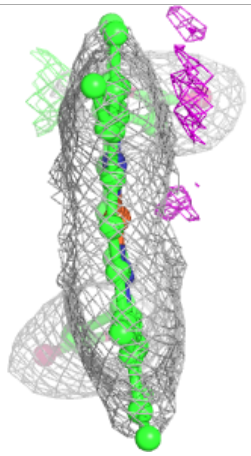


Electron density around HEM C 1450:

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

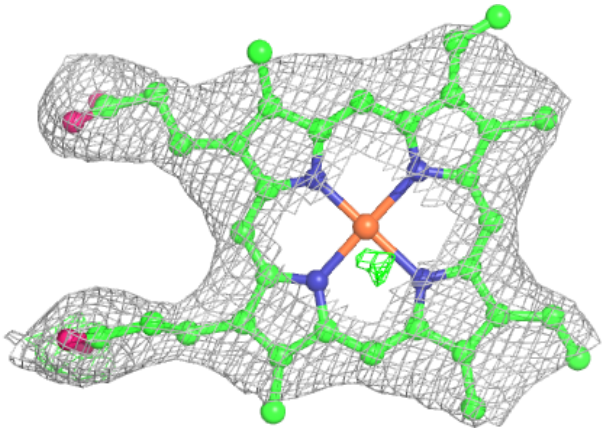


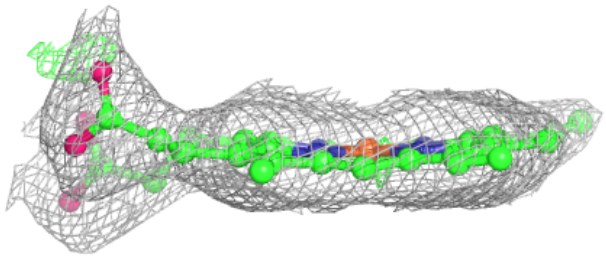


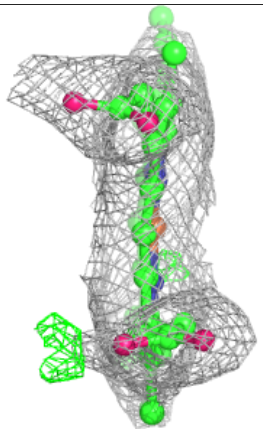


Electron density around HEM D 1450:

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

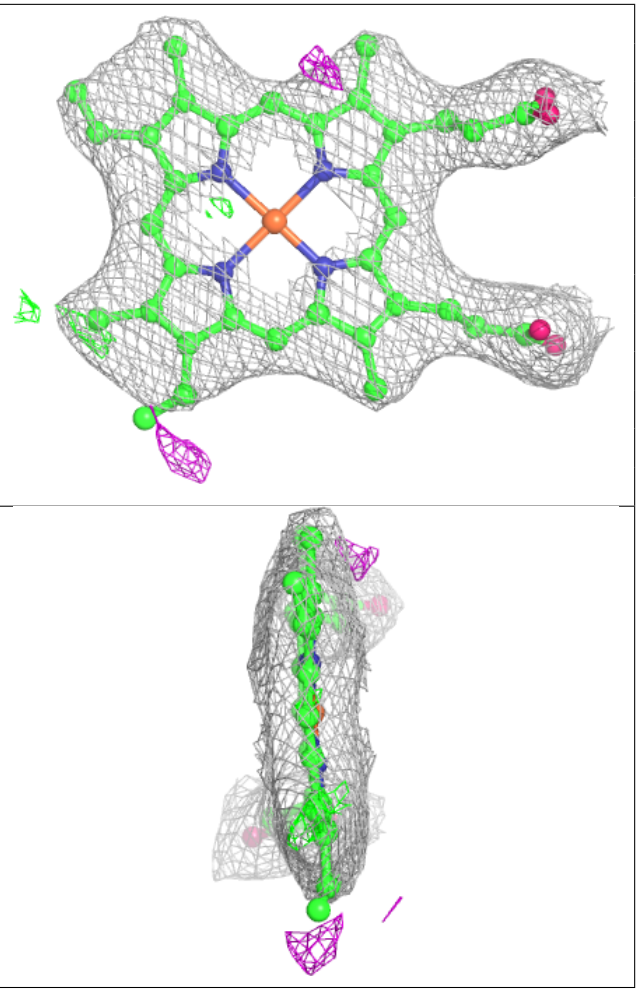






Electron density around HEM B 1450:

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



6.5 Other polymers (i)

There are no such residues in this entry.