Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 11:52 AM EDT

PDB ID	:	3EBS
Title	:	Human Cytochrome P450 2A6 I208S/I300F/G301A/S369G in complex with Phenacetin
Authors	:	DeVore, N.M.; Scott, E.E.
Deposited on	:	2008-08-28
Resolution	:	2.15 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:

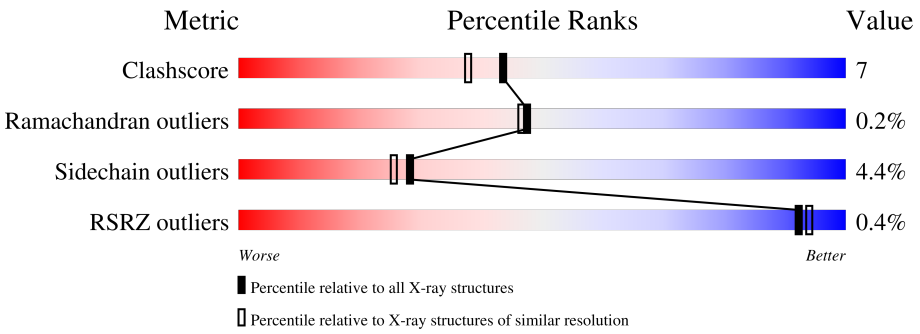
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.15 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))
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	476	86% 11% • •
1	B	476	% 80% 17% • •
1	C	476	86% 10% • •
1	D	476	82% 14% • •

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	N4E	D	1	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15520 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 Cytochrome P450 2A6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	465	3760	2414	650	678	18	0	0	0
1	B	466	3771	2420	654	679	18	0	0	0
1	C	464	3751	2408	648	677	18	0	0	0
1	D	464	3751	2408	648	677	18	0	0	0

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	expression tag	UNP P11509
A	24	ALA	-	expression tag	UNP P11509
A	25	LYS	-	expression tag	UNP P11509
A	26	LYS	-	expression tag	UNP P11509
A	27	THR	-	expression tag	UNP P11509
A	28	SER	-	expression tag	UNP P11509
A	208	SER	ILE	engineered mutation	UNP P11509
A	300	PHE	ILE	engineered mutation	UNP P11509
A	301	ALA	GLY	engineered mutation	UNP P11509
A	369	GLY	SER	engineered mutation	UNP P11509
A	495	HIS	-	expression tag	UNP P11509
A	496	HIS	-	expression tag	UNP P11509
A	497	HIS	-	expression tag	UNP P11509
A	498	HIS	-	expression tag	UNP P11509
B	23	MET	-	expression tag	UNP P11509
B	24	ALA	-	expression tag	UNP P11509
B	25	LYS	-	expression tag	UNP P11509
B	26	LYS	-	expression tag	UNP P11509
B	27	THR	-	expression tag	UNP P11509
B	28	SER	-	expression tag	UNP P11509
B	208	SER	ILE	engineered mutation	UNP P11509

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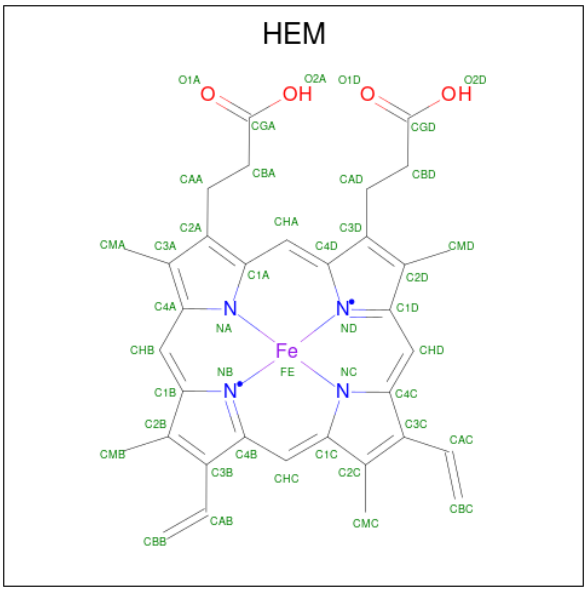
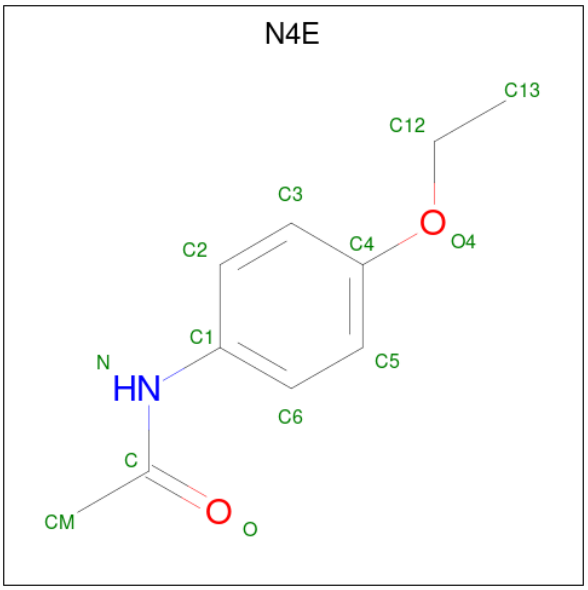
Chain	Residue	Modelled	Actual	Comment	Reference
B	300	PHE	ILE	engineered mutation	UNP P11509
B	301	ALA	GLY	engineered mutation	UNP P11509
B	369	GLY	SER	engineered mutation	UNP P11509
B	495	HIS	-	expression tag	UNP P11509
B	496	HIS	-	expression tag	UNP P11509
B	497	HIS	-	expression tag	UNP P11509
B	498	HIS	-	expression tag	UNP P11509
C	23	MET	-	expression tag	UNP P11509
C	24	ALA	-	expression tag	UNP P11509
C	25	LYS	-	expression tag	UNP P11509
C	26	LYS	-	expression tag	UNP P11509
C	27	THR	-	expression tag	UNP P11509
C	28	SER	-	expression tag	UNP P11509
C	208	SER	ILE	engineered mutation	UNP P11509
C	300	PHE	ILE	engineered mutation	UNP P11509
C	301	ALA	GLY	engineered mutation	UNP P11509
C	369	GLY	SER	engineered mutation	UNP P11509
C	495	HIS	-	expression tag	UNP P11509
C	496	HIS	-	expression tag	UNP P11509
C	497	HIS	-	expression tag	UNP P11509
C	498	HIS	-	expression tag	UNP P11509
D	23	MET	-	expression tag	UNP P11509
D	24	ALA	-	expression tag	UNP P11509
D	25	LYS	-	expression tag	UNP P11509
D	26	LYS	-	expression tag	UNP P11509
D	27	THR	-	expression tag	UNP P11509
D	28	SER	-	expression tag	UNP P11509
D	208	SER	ILE	engineered mutation	UNP P11509
D	300	PHE	ILE	engineered mutation	UNP P11509
D	301	ALA	GLY	engineered mutation	UNP P11509
D	369	GLY	SER	engineered mutation	UNP P11509
D	495	HIS	-	expression tag	UNP P11509
D	496	HIS	-	expression tag	UNP P11509
D	497	HIS	-	expression tag	UNP P11509
D	498	HIS	-	expression tag	UNP P11509

- 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 N-(4-ethoxyphenyl)acetamide (three-letter code: N4E) (formula: $C_{10}H_{13}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	13	10	1	2	0	0
3	B	1	13	10	1	2	0	0
3	D	1	13	10	1	2	0	0

- Molecule 4 is water.

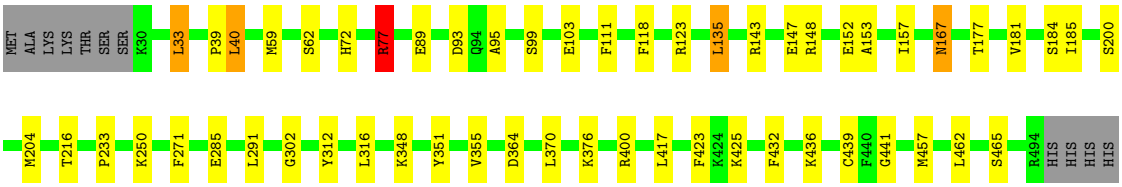
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	81	81	81	0	0
4	B	44	44	44	0	0
4	C	75	75	75	0	0
4	D	76	76	76	0	0

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.

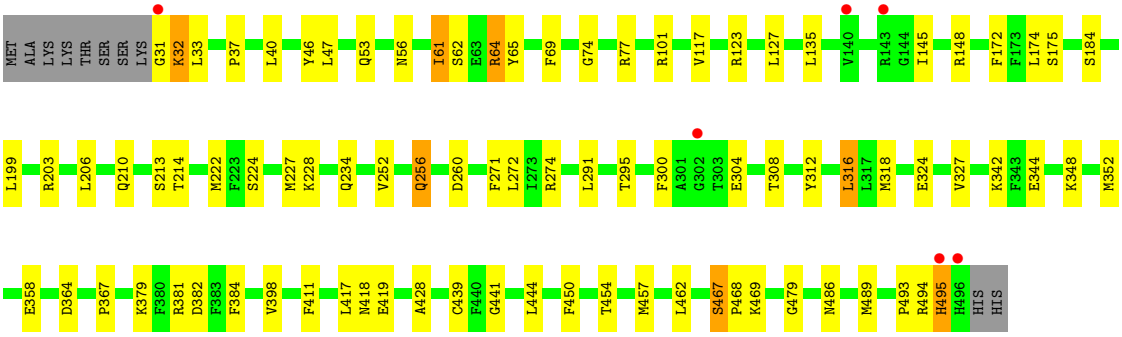
• Molecule 1: Cytochrome P450 2A6

Chain A: 86% 11% • •



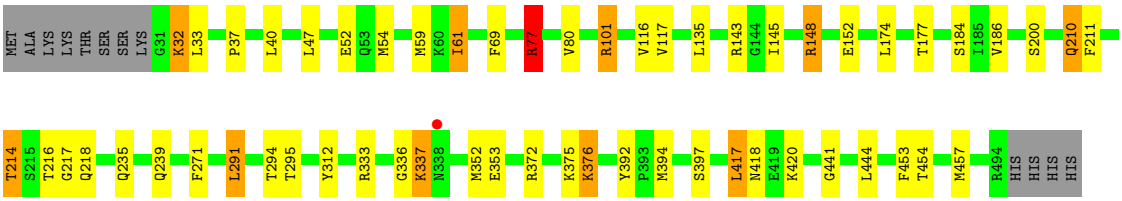
• Molecule 1: Cytochrome P450 2A6

Chain B: % 80% 17% • •



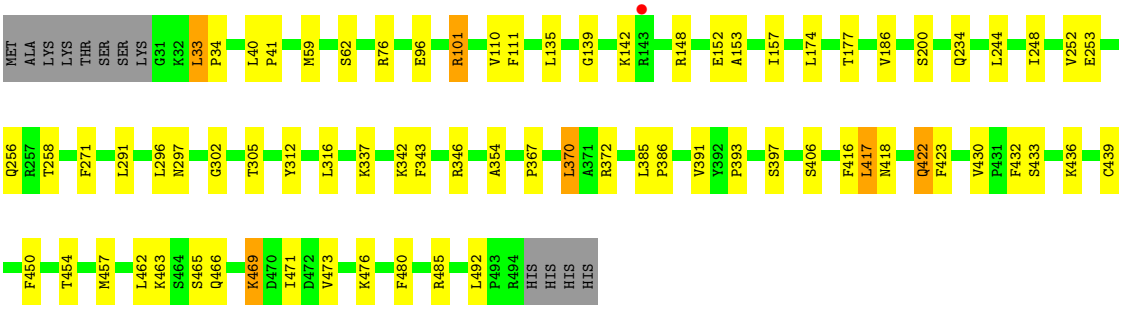
• Molecule 1: Cytochrome P450 2A6

Chain C: 86% 10% • •



• Molecule 1: Cytochrome P450 2A6

Chain D: 82% 14% • •


MET
ALA
LYS
LYS
THR
SER
SER
LYS
G31
K32
L33
P34
L40
P41
M59
S62
R76
E96
R101
V110
F111
L135
G139
K142
R143
R148
E152
A153
I157
L174
T177
V186
S200
Q234
L244
I248
V252
E253
Q256
R257
T258
F271
L291
L296
N297
G302
T305
Y312
L316
K337
K342
F343
R346
A354
P367
L370
A371
R372
L385
P386
V391
Y392
P393
S397
S406
F416
L417
N418
Q422
F423
V430
P431
F432
S433
K436
C439
F450
T454
M457
L462
K463
S464
S465
Q466
K469
D470
I471
D472
V473
K476
F480
R485
L492
P493
R494
HIS
HIS
HIS
HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	70.85Å 159.13Å 103.99Å 90.00° 92.08° 90.00°	Depositor
Resolution (Å)	87.04 – 2.15 87.01 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.7 (87.04-2.15) 97.7 (87.01-2.15)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.89 (at 2.14Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, R_{free}	0.211 , 0.269 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 53.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15520	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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: N4E, HEM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.72	0/3852	0.74	2/5187 (0.0%)
1	B	0.67	0/3865	0.70	0/5206
1	C	0.73	0/3843	0.75	2/5176 (0.0%)
1	D	0.69	0/3843	0.74	0/5176
All	All	0.70	0/15403	0.73	4/20745 (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	77	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	C	417	LEU	CA-CB-CG	5.45	127.83	115.30
1	A	77	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	33	LEU	CA-CB-CG	5.02	126.85	115.30

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	3760	0	3739	38	0
1	B	3771	0	3740	63	0
1	C	3751	0	3726	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3751	0	3726	43	0
2	A	43	0	30	4	0
2	B	43	0	30	4	0
2	C	43	0	30	6	0
2	D	43	0	30	4	0
3	A	13	0	13	5	0
3	B	13	0	13	5	0
3	D	13	0	13	9	0
4	A	81	0	0	0	0
4	B	44	0	0	0	0
4	C	75	0	0	0	0
4	D	76	0	0	3	0
All	All	15520	0	15090	202	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 (202) 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:D:111:PHE:CZ	3:D:1:N4E:HMA	1.82	1.13
3:B:1:N4E:HM	3:B:1:N4E:H2	1.15	1.08
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.24	1.01
1:C:214:THR:HG22	1:C:217:GLY:H	1.30	0.95
1:B:318:MET:HE3	1:B:489:MET:HB2	1.49	0.95
3:B:1:N4E:HM	3:B:1:N4E:C2	1.93	0.95
1:D:111:PHE:HZ	3:D:1:N4E:HMA	1.24	0.92
1:B:46:TYR:HB2	1:B:222:MET:HE1	1.53	0.90
1:B:64:ARG:HG2	1:B:64:ARG:HH11	1.39	0.87
1:C:392:TYR:HB3	1:C:394:MET:HE2	1.57	0.86
1:B:318:MET:CE	1:B:489:MET:HB2	2.04	0.86
1:D:457:MET:HA	1:D:457:MET:HE2	1.56	0.86
1:B:462:LEU:HD22	1:B:489:MET:HE1	1.62	0.82
1:C:392:TYR:HB3	1:C:394:MET:CE	2.09	0.82
1:C:54:MET:HG3	1:C:218:GLN:HE21	1.45	0.81
1:B:46:TYR:HB2	1:B:222:MET:CE	2.10	0.81
1:D:111:PHE:CE1	3:D:1:N4E:HMA	2.17	0.80
1:D:367:PRO:HD2	1:D:480:PHE:O	1.82	0.80
1:C:61:ILE:HD11	1:C:69:PHE:CD1	2.19	0.78
1:C:77:ARG:HH11	1:C:77:ARG:HG2	1.50	0.77
1:B:61:ILE:HD11	1:B:69:PHE:CD1	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:MET:CE	1:A:462:LEU:HD21	2.16	0.75
1:B:64:ARG:HH11	1:B:64:ARG:CG	2.01	0.74
1:B:117:VAL:HG21	3:B:1:N4E:H6	1.72	0.71
1:A:457:MET:HE3	1:A:462:LEU:HD21	1.71	0.71
1:C:392:TYR:HD1	1:C:394:MET:HE1	1.55	0.71
1:A:271:PHE:HB3	1:A:291:LEU:HD13	1.74	0.69
1:C:375:LYS:HB3	1:C:376:LYS:HE2	1.73	0.69
1:A:77:ARG:HH11	1:A:77:ARG:CG	2.05	0.68
1:D:457:MET:HA	1:D:457:MET:CE	2.24	0.67
1:B:37:PRO:HD3	1:B:61:ILE:HD13	1.76	0.66
1:B:318:MET:HE3	1:B:489:MET:CE	2.26	0.66
1:D:450:PHE:O	1:D:454:THR:HG23	1.96	0.65
1:D:457:MET:HE2	1:D:457:MET:CA	2.27	0.64
1:C:392:TYR:CD1	1:C:394:MET:HE1	2.31	0.64
1:A:33:LEU:HD21	1:A:77:ARG:HD2	1.80	0.63
1:A:111:PHE:CZ	3:A:1:N4E:HMA	2.34	0.63
1:D:457:MET:HE3	1:D:462:LEU:HD21	1.81	0.63
1:C:101:ARG:HD2	1:C:117:VAL:O	1.98	0.62
1:C:352:MET:CE	1:C:454:THR:HG22	2.29	0.62
1:C:336:GLY:O	1:C:337:LYS:HG3	1.99	0.62
1:D:372:ARG:NH2	4:D:717:HOH:O	2.33	0.61
1:D:152:GLU:HG3	1:D:177:THR:HG23	1.83	0.61
1:D:305:THR:HG21	3:D:1:N4E:H13	1.83	0.60
1:C:61:ILE:HG12	1:C:69:PHE:CE1	2.36	0.60
1:C:101:ARG:NH1	2:C:500:HEM:O2A	2.33	0.60
1:A:432:PHE:HB3	1:A:439:CYS:HB3	1.84	0.60
1:B:64:ARG:HG2	1:B:64:ARG:NH1	2.13	0.60
1:C:186:VAL:HG13	1:C:295:THR:HG23	1.83	0.60
1:A:111:PHE:CE1	3:A:1:N4E:HMA	2.36	0.59
1:A:40:LEU:HD11	1:C:47:LEU:HD11	1.84	0.59
1:B:213:SER:HA	1:B:479:GLY:HA3	1.85	0.59
1:C:453:PHE:O	1:C:457:MET:HG2	2.01	0.59
1:C:148:ARG:HD3	1:C:184:SER:OG	2.03	0.59
1:A:271:PHE:CD2	1:A:291:LEU:HB2	2.37	0.59
1:A:77:ARG:HG2	1:A:77:ARG:NH1	2.03	0.58
3:D:1:N4E:H2	3:D:1:N4E:O	2.04	0.58
1:B:327:VAL:HG13	1:B:352:MET:HE2	1.85	0.57
1:B:300:PHE:CG	3:B:1:N4E:HMB	2.39	0.57
1:A:457:MET:HE1	1:A:462:LEU:HD21	1.86	0.57
1:C:211:PHE:O	1:C:214:THR:HB	2.04	0.57
1:B:318:MET:HE3	1:B:489:MET:HE2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:CYS:HB2	2:B:500:HEM:NA	2.20	0.56
1:D:480:PHE:CZ	3:D:1:N4E:H5	2.41	0.55
1:C:235:GLN:O	1:C:239:GLN:HG3	2.04	0.55
1:A:143:ARG:O	1:A:147:GLU:HG2	2.05	0.55
1:C:80:VAL:HG13	1:C:394:MET:CE	2.36	0.55
1:B:450:PHE:O	1:B:454:THR:HG23	2.08	0.54
1:D:139:GLY:O	1:D:142:LYS:HG2	2.06	0.54
1:B:304:GLU:O	1:B:308:THR:OG1	2.25	0.54
1:A:216:THR:HG21	1:A:233:PRO:HG2	1.90	0.54
1:C:80:VAL:HG13	1:C:394:MET:HE2	1.89	0.54
1:C:392:TYR:HB3	1:C:394:MET:HE1	1.88	0.54
1:D:343:PHE:O	1:D:346:ARG:HG2	2.08	0.53
1:B:352:MET:HE3	1:B:454:THR:HG22	1.91	0.53
1:A:135:LEU:HD12	1:A:185:ILE:HG21	1.89	0.53
1:D:59:MET:CE	1:D:397:SER:HB3	2.38	0.53
1:B:327:VAL:HG13	1:B:352:MET:CE	2.37	0.53
2:C:500:HEM:HMB2	2:C:500:HEM:HBB2	1.90	0.53
1:C:152:GLU:HG3	1:C:177:THR:HG23	1.91	0.53
1:B:318:MET:CE	1:B:489:MET:CB	2.84	0.52
1:B:148:ARG:HD3	1:B:184:SER:CB	2.39	0.52
1:B:148:ARG:HD3	1:B:184:SER:HB3	1.91	0.52
1:D:59:MET:HE1	1:D:397:SER:HB3	1.90	0.52
1:C:418:ASN:HB3	1:C:420:LYS:H	1.75	0.52
1:B:318:MET:HE1	1:B:489:MET:HB2	1.91	0.51
1:A:118:PHE:HE2	1:A:370:LEU:HD11	1.74	0.51
3:A:1:N4E:H2	3:A:1:N4E:O	2.08	0.51
1:B:61:ILE:HD12	1:B:65:TYR:CD2	2.46	0.51
1:B:441:GLY:HA3	2:B:500:HEM:C3C	2.45	0.51
2:D:500:HEM:HMB2	2:D:500:HEM:HBB2	1.91	0.51
1:A:39:PRO:HG3	1:A:72:HIS:CE1	2.45	0.51
1:C:352:MET:HE3	1:C:454:THR:HG22	1.92	0.51
1:D:153:ALA:O	1:D:157:ILE:HG12	2.11	0.51
1:D:430:VAL:HA	4:D:709:HOH:O	2.12	0.50
1:B:381:ARG:O	1:B:382:ASP:HB2	2.12	0.50
1:A:181:VAL:O	1:A:184:SER:HB2	2.11	0.50
1:B:494:ARG:O	1:B:495:HIS:HB2	2.12	0.50
1:D:466:GLN:HG3	1:D:471:ILE:HG12	1.93	0.50
1:B:318:MET:HE3	1:B:489:MET:HE3	1.94	0.50
1:B:398:VAL:O	1:B:428:ALA:HB1	2.12	0.49
1:C:214:THR:CG2	1:C:217:GLY:H	2.15	0.49
2:C:500:HEM:HHA	2:C:500:HEM:HBA2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:MET:CE	1:C:397:SER:HB3	2.42	0.49
1:B:145:ILE:HD12	1:B:148:ARG:HD2	1.94	0.49
1:D:463:LYS:HD3	1:D:492:LEU:HD11	1.95	0.49
1:D:480:PHE:HZ	3:D:1:N4E:H5	1.77	0.49
1:A:153:ALA:O	1:A:157:ILE:HG12	2.13	0.48
1:A:167:ASN:HD21	1:A:465:SER:HB3	1.78	0.48
1:D:432:PHE:HB3	1:D:439:CYS:HB3	1.94	0.48
1:A:99:SER:HB2	1:A:436:LYS:HB2	1.96	0.48
1:A:351:TYR:O	1:A:355:VAL:HG23	2.13	0.48
1:B:210:GLN:O	1:B:214:THR:HG23	2.13	0.48
1:D:111:PHE:HZ	3:D:1:N4E:CM	2.09	0.48
1:A:423:PHE:HE1	1:A:425:LYS:HG2	1.79	0.48
1:D:96:GLU:OE1	1:D:436:LYS:NZ	2.44	0.48
1:B:53:GLN:HB3	1:B:56:ASN:HB2	1.96	0.48
1:C:392:TYR:CB	1:C:394:MET:CE	2.89	0.48
1:B:316:LEU:HG	1:B:411:PHE:CD1	2.48	0.48
1:B:61:ILE:HD12	1:B:65:TYR:HD2	1.79	0.47
1:D:244:LEU:HB3	1:D:296:LEU:HD11	1.95	0.47
1:B:462:LEU:HD22	1:B:489:MET:CE	2.39	0.47
1:D:457:MET:CE	1:D:462:LEU:HD21	2.44	0.47
1:B:32:LYS:O	1:B:384:PHE:N	2.41	0.47
1:A:370:LEU:HB2	3:A:1:N4E:H13	1.96	0.47
1:A:200:SER:O	1:A:204:MET:HG3	2.15	0.47
1:B:364:ASP:OD1	1:B:367:PRO:HA	2.14	0.47
1:C:61:ILE:CG1	1:C:69:PHE:CE1	2.98	0.47
3:B:1:N4E:C2	3:B:1:N4E:CM	2.77	0.47
1:A:118:PHE:CE2	1:A:370:LEU:HD11	2.51	0.46
1:C:116:VAL:HG12	1:C:294:THR:HG23	1.96	0.46
1:C:37:PRO:HD3	1:C:61:ILE:HD12	1.97	0.46
1:D:469:LYS:HG2	4:D:729:HOH:O	2.14	0.46
1:D:297:ASN:HA	3:D:1:N4E:O	2.14	0.46
1:B:227:MET:HB3	1:B:234:GLN:HE21	1.81	0.46
1:A:95:ALA:O	1:A:99:SER:HB3	2.15	0.46
1:A:364:ASP:OD2	1:A:400:ARG:NH2	2.47	0.46
1:B:252:VAL:O	1:B:256:GLN:HG3	2.16	0.46
1:C:441:GLY:HA3	2:C:500:HEM:C3C	2.51	0.46
1:B:33:LEU:HD21	1:B:77:ARG:HD2	1.98	0.46
1:D:33:LEU:HD23	1:D:34:PRO:HD2	1.98	0.46
1:B:46:TYR:HB2	1:B:222:MET:HE3	1.95	0.46
1:B:172:PHE:HA	1:B:175:SER:OG	2.16	0.45
1:C:392:TYR:CB	1:C:394:MET:HE2	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:MET:HE3	1:C:397:SER:HB3	1.97	0.45
1:C:210:GLN:HE21	1:C:210:GLN:HB2	1.61	0.45
1:B:222:MET:HB3	1:B:222:MET:HE2	1.74	0.45
1:B:324:GLU:HG3	1:B:457:MET:CE	2.47	0.45
1:C:117:VAL:HG22	2:C:500:HEM:HAD1	1.97	0.45
1:D:391:VAL:O	1:D:393:PRO:HD3	2.17	0.45
1:B:31:GLY:N	1:B:379:LYS:HE3	2.32	0.45
1:B:123:ARG:O	1:B:127:LEU:HG	2.17	0.45
1:B:206:LEU:O	1:B:210:GLN:HB2	2.17	0.45
2:D:500:HEM:HBB2	2:D:500:HEM:CMB	2.47	0.44
1:B:199:LEU:HD21	1:B:203:ARG:NH2	2.33	0.44
1:B:342:LYS:HG3	1:B:344:GLU:HG2	1.98	0.44
1:B:444:LEU:HD23	2:B:500:HEM:HBC2	1.99	0.44
1:A:441:GLY:HA3	2:A:500:HEM:C3C	2.51	0.44
1:C:271:PHE:CD2	1:C:291:LEU:HB2	2.53	0.44
1:B:467:SER:O	1:B:469:LYS:N	2.51	0.44
1:B:439:CYS:HB2	2:B:500:HEM:C1A	2.52	0.44
1:C:77:ARG:HG2	1:C:77:ARG:NH1	2.27	0.44
1:D:101:ARG:NH2	1:D:370:LEU:HB3	2.33	0.44
1:D:302:GLY:HA2	2:D:500:HEM:HMC2	1.99	0.44
1:D:148:ARG:NH2	1:D:152:GLU:OE2	2.49	0.44
1:A:59:MET:O	1:A:62:SER:HB3	2.18	0.43
1:A:152:GLU:HG3	1:A:177:THR:HG23	1.99	0.43
1:D:354:ALA:HB2	1:D:417:LEU:HD13	2.00	0.43
1:D:418:ASN:OD1	1:D:422:GLN:HG3	2.18	0.43
1:A:72:HIS:NE2	1:A:77:ARG:HD3	2.32	0.43
2:A:500:HEM:HBB2	2:A:500:HEM:HMB2	2.00	0.43
1:B:74:GLY:N	1:B:222:MET:HE2	2.34	0.43
1:D:433:SER:HB3	2:D:500:HEM:HBA1	2.01	0.43
1:B:47:LEU:HB3	1:D:41:PRO:HD2	2.01	0.43
1:A:271:PHE:CE2	1:A:291:LEU:HB2	2.54	0.43
1:D:416:PHE:HB3	1:D:423:PHE:CE2	2.54	0.43
1:C:52:GLU:O	1:C:52:GLU:HG2	2.18	0.43
1:D:248:ILE:O	1:D:252:VAL:HG23	2.19	0.42
1:B:32:LYS:HD3	1:B:32:LYS:HA	1.28	0.42
1:B:62:SER:HB3	1:B:69:PHE:CE2	2.54	0.42
1:C:186:VAL:HG13	1:C:295:THR:CG2	2.48	0.42
1:B:358:GLU:HA	1:B:358:GLU:OE1	2.20	0.42
1:D:476:LYS:HB2	1:D:485:ARG:HA	2.00	0.42
1:A:148:ARG:HD3	1:A:184:SER:OG	2.20	0.42
1:A:123:ARG:HA	1:A:285:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:PRO:HD3	1:C:61:ILE:CD1	2.50	0.42
2:C:500:HEM:HBB2	2:C:500:HEM:CMB	2.50	0.42
1:D:385:LEU:HA	1:D:386:PRO:HD2	1.97	0.42
1:B:271:PHE:CD2	1:B:291:LEU:HB2	2.55	0.41
1:C:32:LYS:HZ2	1:C:32:LYS:HG3	1.40	0.41
1:D:271:PHE:CG	1:D:291:LEU:HD13	2.54	0.41
2:A:500:HEM:C1A	3:A:1:N4E:H12	2.55	0.41
1:B:493:PRO:C	1:B:495:HIS:H	2.22	0.41
1:C:61:ILE:HD11	1:C:69:PHE:CE1	2.54	0.41
1:C:145:ILE:HG12	1:C:444:LEU:HD13	2.02	0.41
1:C:372:ARG:HH11	1:C:372:ARG:HG3	1.85	0.41
1:B:224:SER:O	1:B:228:LYS:HD2	2.19	0.41
1:B:256:GLN:HB3	1:B:272:LEU:HD13	2.02	0.41
1:C:333:ARG:HG2	1:C:333:ARG:HH11	1.86	0.41
1:C:214:THR:HG23	1:C:216:THR:H	1.86	0.40
1:A:89:GLU:O	1:A:93:ASP:HB2	2.22	0.40
1:A:302:GLY:HA2	2:A:500:HEM:HMC2	2.03	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	463/476 (97%)	445 (96%)	18 (4%)	0	100	100
1	B	464/476 (98%)	441 (95%)	21 (4%)	2 (0%)	34	29
1	C	462/476 (97%)	447 (97%)	14 (3%)	1 (0%)	47	46
1	D	462/476 (97%)	442 (96%)	20 (4%)	0	100	100
All	All	1851/1904 (97%)	1775 (96%)	73 (4%)	3 (0%)	47	46

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	468	PRO
1	B	495	HIS
1	C	337	LYS

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	411/421 (98%)	400 (97%)	11 (3%)	44	46
1	B	412/421 (98%)	393 (95%)	19 (5%)	27	23
1	C	410/421 (97%)	392 (96%)	18 (4%)	28	25
1	D	410/421 (97%)	385 (94%)	25 (6%)	18	14
All	All	1643/1684 (98%)	1570 (96%)	73 (4%)	28	25

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	77	ARG
1	A	103	GLU
1	A	135	LEU
1	A	167	ASN
1	A	250	LYS
1	A	312	TYR
1	A	316	LEU
1	A	348	LYS
1	A	376	LYS
1	A	417	LEU
1	B	32	LYS
1	B	40	LEU
1	B	61	ILE
1	B	64	ARG
1	B	101	ARG
1	B	135	LEU
1	B	174	LEU
1	B	256	GLN

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Mol	Chain	Res	Type
1	B	260	ASP
1	B	274	ARG
1	B	295	THR
1	B	312	TYR
1	B	316	LEU
1	B	348	LYS
1	B	417	LEU
1	B	418	ASN
1	B	419	GLU
1	B	467	SER
1	B	486	ASN
1	C	32	LYS
1	C	33	LEU
1	C	40	LEU
1	C	61	ILE
1	C	77	ARG
1	C	101	ARG
1	C	135	LEU
1	C	143	ARG
1	C	148	ARG
1	C	174	LEU
1	C	200	SER
1	C	210	GLN
1	C	214	THR
1	C	291	LEU
1	C	312	TYR
1	C	353	GLU
1	C	376	LYS
1	C	417	LEU
1	D	33	LEU
1	D	40	LEU
1	D	62	SER
1	D	76	ARG
1	D	101	ARG
1	D	110	VAL
1	D	135	LEU
1	D	174	LEU
1	D	186	VAL
1	D	200	SER
1	D	234	GLN
1	D	253	GLU
1	D	256	GLN

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Mol	Chain	Res	Type
1	D	258	THR
1	D	312	TYR
1	D	316	LEU
1	D	337	LYS
1	D	342	LYS
1	D	370	LEU
1	D	406	SER
1	D	417	LEU
1	D	422	GLN
1	D	465	SER
1	D	469	LYS
1	D	473	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	B	340	GLN
1	B	418	ASN
1	B	422	GLN
1	C	218	GLN
1	C	477	HIS
1	D	276	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)

7 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	A	500	1	41,50,50	2.24	8 (19%)	45,82,82	1.63	6 (13%)
2	HEM	C	500	1	41,50,50	2.04	7 (17%)	45,82,82	1.85	13 (28%)
3	N4E	A	1	-	13,13,13	0.90	1 (7%)	16,16,16	0.60	0
2	HEM	D	500	-	41,50,50	1.94	7 (17%)	45,82,82	2.01	15 (33%)
3	N4E	B	1	-	13,13,13	1.03	1 (7%)	16,16,16	1.21	2 (12%)
2	HEM	B	500	1	41,50,50	2.02	8 (19%)	45,82,82	1.45	8 (17%)
3	N4E	D	1	-	13,13,13	0.95	1 (7%)	16,16,16	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	500	1	-	2/12/54/54	-
2	HEM	C	500	1	-	4/12/54/54	-
3	N4E	A	1	-	-	3/7/7/7	0/1/1/1
2	HEM	D	500	-	-	4/12/54/54	-
3	N4E	B	1	-	-	5/7/7/7	0/1/1/1
2	HEM	B	500	1	-	4/12/54/54	-
3	N4E	D	1	-	-	2/7/7/7	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3D-C2D	8.29	1.54	1.36
2	C	500	HEM	C3D-C2D	8.06	1.53	1.36
2	D	500	HEM	C3D-C2D	7.68	1.53	1.36
2	B	500	HEM	C3D-C2D	7.22	1.52	1.36
2	A	500	HEM	C3C-C2C	-5.01	1.33	1.40
2	C	500	HEM	C3C-CAC	4.76	1.57	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C3C-C2C	-4.34	1.34	1.40
2	A	500	HEM	C3C-CAC	4.28	1.56	1.47
2	B	500	HEM	C3C-CAC	4.16	1.56	1.47
2	C	500	HEM	C3C-C2C	-4.11	1.34	1.40
2	D	500	HEM	C3C-CAC	4.08	1.56	1.47
2	A	500	HEM	FE-ND	4.03	2.16	1.96
2	A	500	HEM	CAB-C3B	3.44	1.56	1.47
2	B	500	HEM	CAB-C3B	3.41	1.56	1.47
2	C	500	HEM	CAB-C3B	3.40	1.56	1.47
2	D	500	HEM	CAB-C3B	3.30	1.56	1.47
2	D	500	HEM	FE-ND	3.18	2.12	1.96
2	D	500	HEM	C3C-C2C	-3.08	1.36	1.40
2	A	500	HEM	CMD-C2D	2.98	1.57	1.50
2	B	500	HEM	CMB-C2B	2.83	1.56	1.50
2	C	500	HEM	FE-NB	2.80	2.10	1.96
2	C	500	HEM	CAA-C2A	2.77	1.56	1.52
3	D	1	N4E	C1-N	-2.71	1.36	1.41
2	D	500	HEM	CAA-C2A	2.70	1.56	1.52
2	A	500	HEM	CMA-C3A	2.68	1.57	1.51
2	B	500	HEM	FE-ND	2.62	2.09	1.96
2	B	500	HEM	CMD-C2D	2.59	1.56	1.50
3	A	1	N4E	C1-N	-2.56	1.36	1.41
3	B	1	N4E	C1-N	-2.41	1.36	1.41
2	B	500	HEM	CAA-C2A	2.35	1.55	1.52
2	A	500	HEM	CMB-C2B	2.27	1.55	1.50
2	D	500	HEM	FE-NB	2.09	2.07	1.96
2	C	500	HEM	CMD-C2D	2.06	1.55	1.50

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	500	HEM	C4D-ND-C1D	6.33	111.61	105.07
2	C	500	HEM	C4D-ND-C1D	6.33	111.61	105.07
2	A	500	HEM	C4D-ND-C1D	6.08	111.35	105.07
2	A	500	HEM	C4C-CHD-C1D	4.46	128.45	122.56
2	D	500	HEM	C4C-CHD-C1D	4.37	128.32	122.56
2	B	500	HEM	C4D-ND-C1D	3.83	109.03	105.07
2	C	500	HEM	C4B-CHC-C1C	3.78	127.55	122.56
2	C	500	HEM	C4C-CHD-C1D	3.64	127.36	122.56
2	B	500	HEM	C1D-C2D-C3D	-3.49	103.29	106.96
2	B	500	HEM	CBA-CAA-C2A	-3.43	106.76	112.62
2	D	500	HEM	CBA-CAA-C2A	-3.41	106.81	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	500	HEM	CMA-C3A-C4A	-3.07	123.74	128.46
2	D	500	HEM	CAD-C3D-C4D	2.98	129.87	124.66
2	D	500	HEM	CMD-C2D-C1D	2.86	129.40	125.04
2	C	500	HEM	CAD-CBD-CGD	-2.85	107.47	113.60
2	C	500	HEM	C1D-C2D-C3D	-2.75	104.06	106.96
2	D	500	HEM	C3B-C2B-C1B	2.75	108.53	106.49
2	D	500	HEM	CMC-C2C-C3C	2.74	129.81	124.68
2	A	500	HEM	CAD-CBD-CGD	-2.71	107.76	113.60
2	D	500	HEM	C4B-CHC-C1C	2.67	126.08	122.56
2	D	500	HEM	C4A-C3A-C2A	2.62	108.82	107.00
2	D	500	HEM	CAD-CBD-CGD	-2.61	107.98	113.60
2	C	500	HEM	CMC-C2C-C3C	2.56	129.48	124.68
2	B	500	HEM	CAD-CBD-CGD	-2.49	108.24	113.60
2	B	500	HEM	CMD-C2D-C1D	2.47	128.80	125.04
2	B	500	HEM	C4B-CHC-C1C	2.44	125.77	122.56
3	B	1	N4E	CM-C-N	2.44	118.56	114.98
2	D	500	HEM	C1B-NB-C4B	2.40	107.55	105.07
2	C	500	HEM	CHD-C1D-ND	2.38	127.02	124.43
2	C	500	HEM	C1B-NB-C4B	2.35	107.50	105.07
2	C	500	HEM	C3D-C4D-ND	-2.29	107.62	110.17
2	A	500	HEM	O2A-CGA-CBA	2.24	121.23	114.03
2	C	500	HEM	CHA-C4D-ND	2.23	127.13	124.38
2	C	500	HEM	C4A-C3A-C2A	2.22	108.54	107.00
2	D	500	HEM	O2A-CGA-CBA	2.17	121.01	114.03
3	B	1	N4E	O-C-N	-2.17	120.19	123.04
2	B	500	HEM	C4C-CHD-C1D	2.16	125.41	122.56
2	D	500	HEM	O1D-CGD-CBD	-2.15	116.18	123.08
2	B	500	HEM	CAD-C3D-C4D	2.11	128.34	124.66
2	C	500	HEM	CMA-C3A-C4A	-2.10	125.23	128.46
2	A	500	HEM	C1B-NB-C4B	2.06	107.20	105.07
2	C	500	HEM	O1D-CGD-CBD	-2.04	116.54	123.08
2	A	500	HEM	CHC-C4B-C3B	2.03	127.68	124.57
2	D	500	HEM	O2D-CGD-CBD	2.00	120.47	114.03

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	500	HEM	C1A-C2A-CAA-CBA
2	C	500	HEM	C3A-C2A-CAA-CBA
3	B	1	N4E	C13-C12-O4-C4
3	B	1	N4E	CM-C-N-C1

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Mol	Chain	Res	Type	Atoms
3	D	1	N4E	C3-C4-O4-C12
3	B	1	N4E	C5-C4-O4-C12
3	D	1	N4E	C5-C4-O4-C12
3	B	1	N4E	C3-C4-O4-C12
3	B	1	N4E	O-C-N-C1
3	A	1	N4E	C5-C4-O4-C12
3	A	1	N4E	C3-C4-O4-C12
3	A	1	N4E	C13-C12-O4-C4
2	B	500	HEM	CAA-CBA-CGA-O1A
2	A	500	HEM	CAA-CBA-CGA-O2A
2	C	500	HEM	CAA-CBA-CGA-O1A
2	A	500	HEM	CAA-CBA-CGA-O1A
2	C	500	HEM	CAA-CBA-CGA-O2A
2	B	500	HEM	CAA-CBA-CGA-O2A
2	D	500	HEM	CAD-CBD-CGD-O1D
2	B	500	HEM	CAD-CBD-CGD-O1D
2	D	500	HEM	CAD-CBD-CGD-O2D
2	B	500	HEM	CAD-CBD-CGD-O2D
2	D	500	HEM	CAA-CBA-CGA-O2A
2	D	500	HEM	CAA-CBA-CGA-O1A

There are no ring outliers.

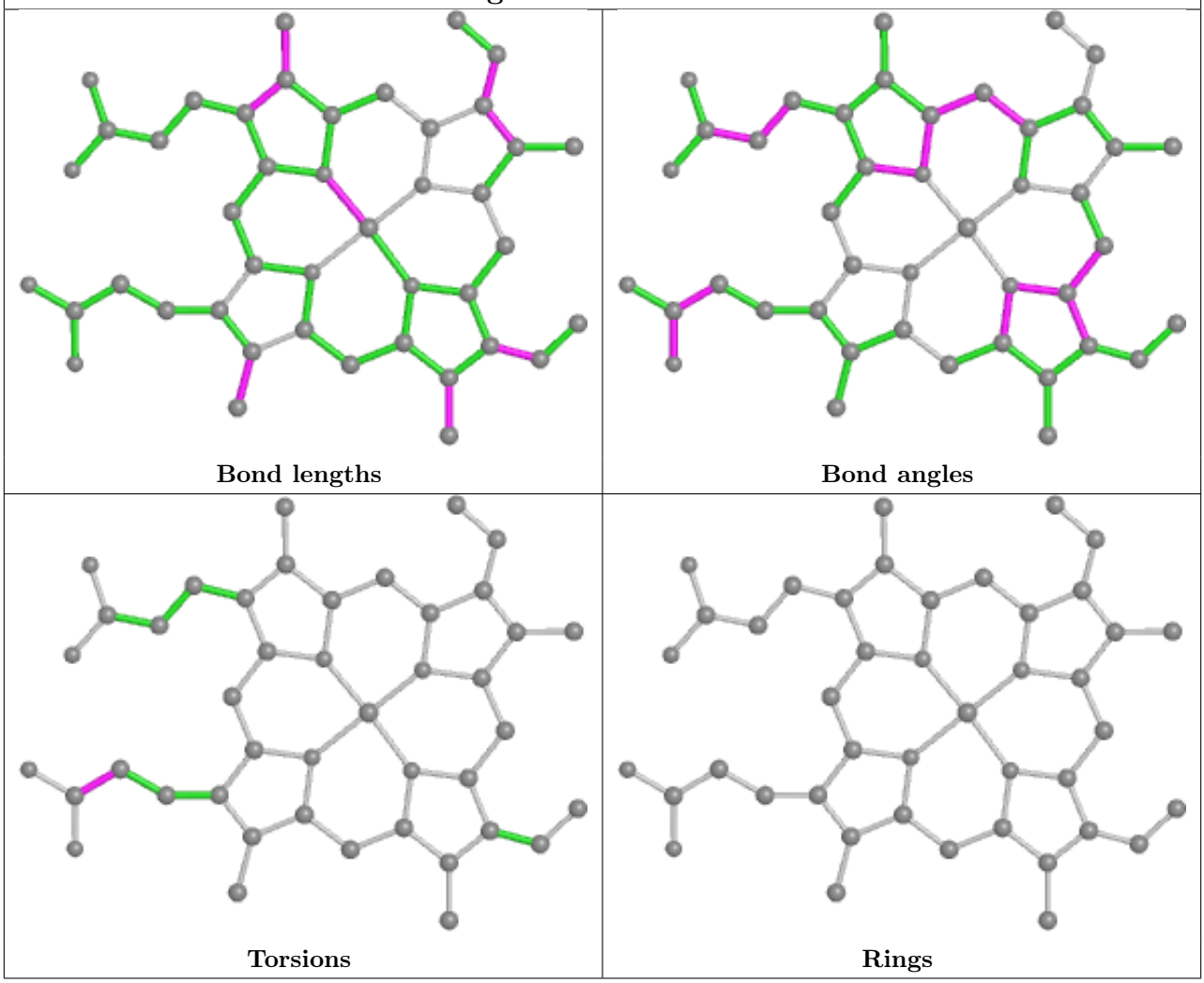
7 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	4	0
2	C	500	HEM	6	0
3	A	1	N4E	5	0
2	D	500	HEM	4	0
3	B	1	N4E	5	0
2	B	500	HEM	4	0
3	D	1	N4E	9	0

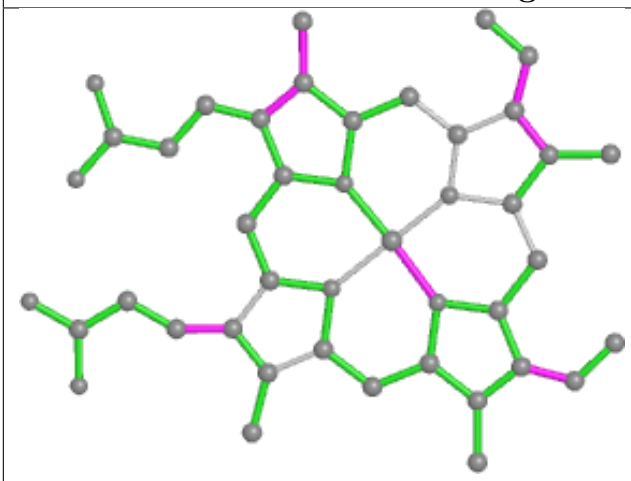
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

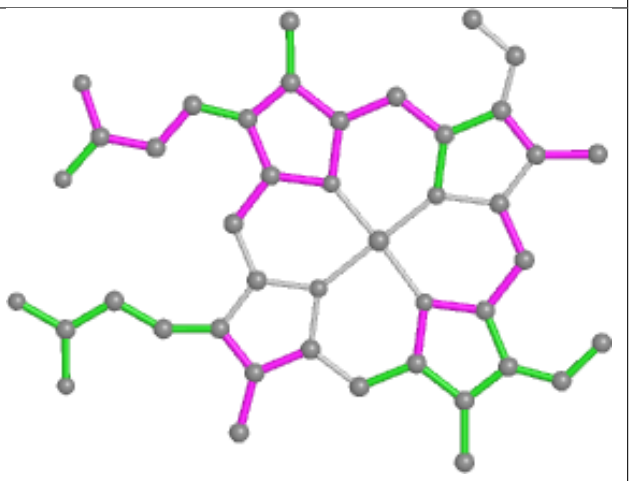
Ligand HEM A 500



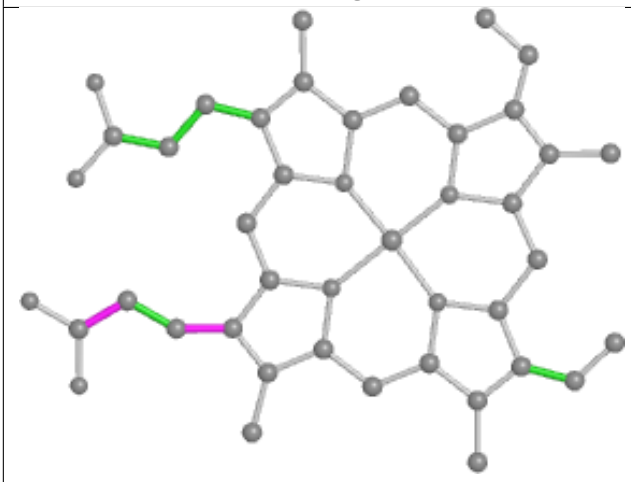
Ligand HEM C 500



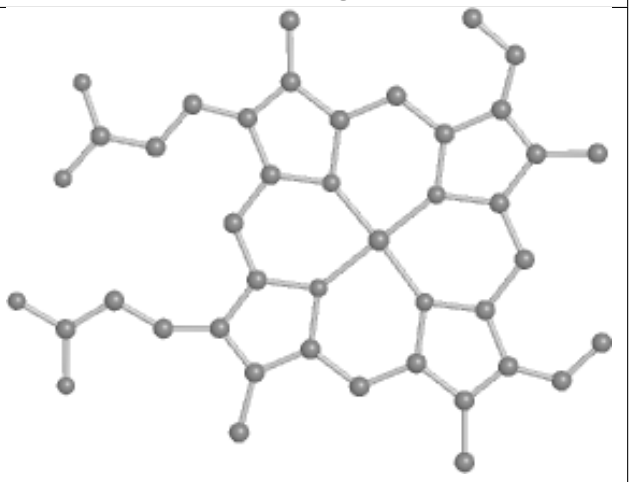
Bond lengths



Bond angles

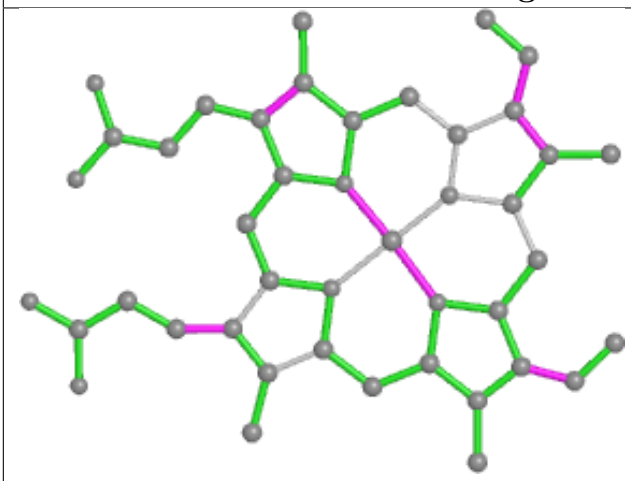


Torsions

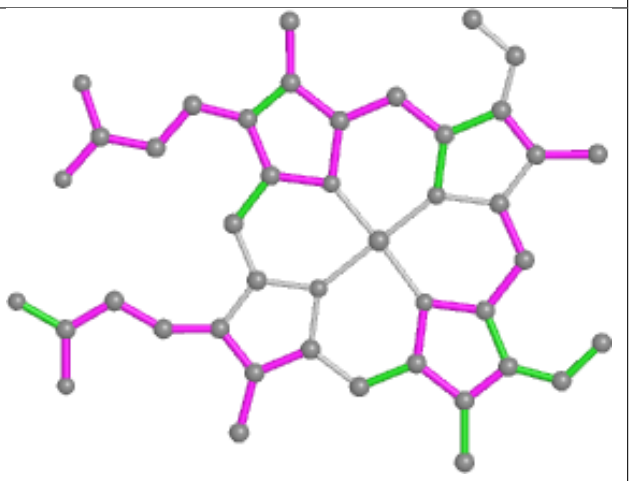


Rings

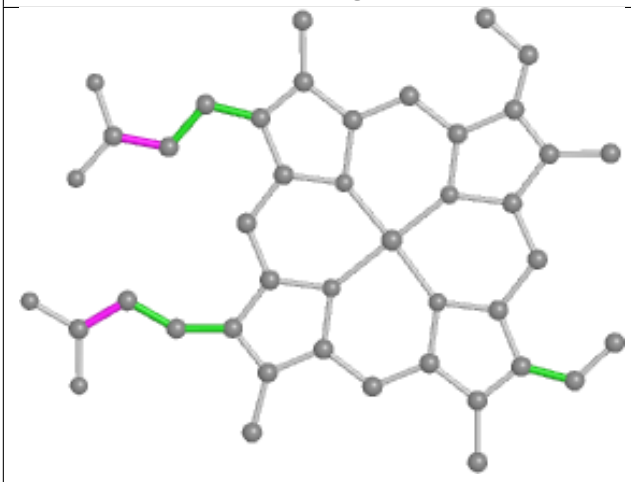
Ligand HEM D 500



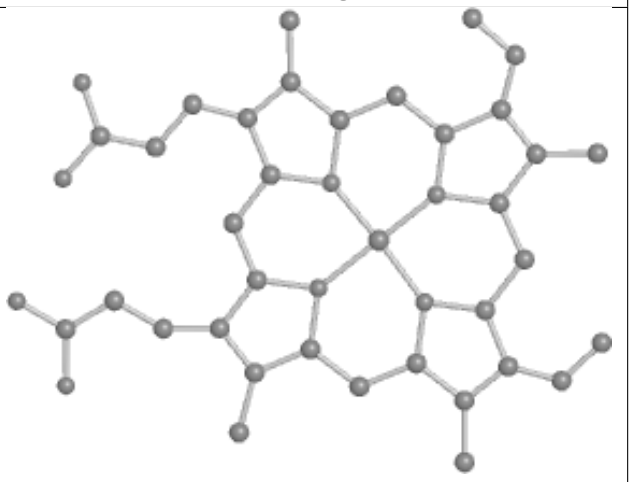
Bond lengths



Bond angles

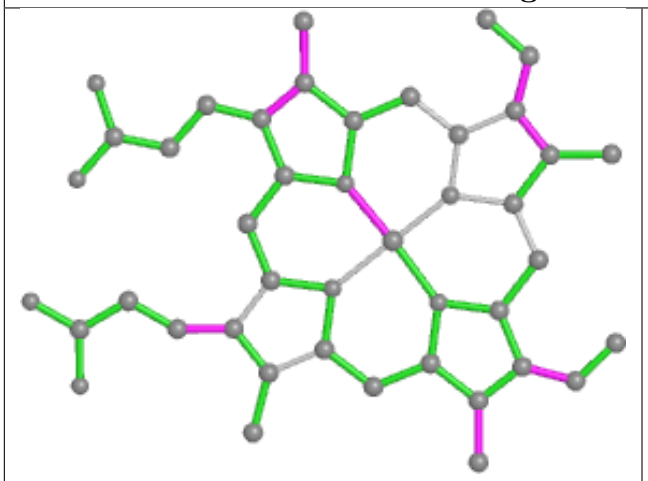


Torsions

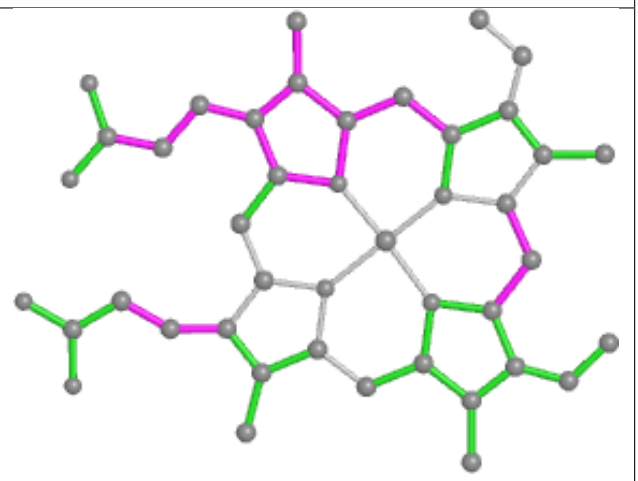


Rings

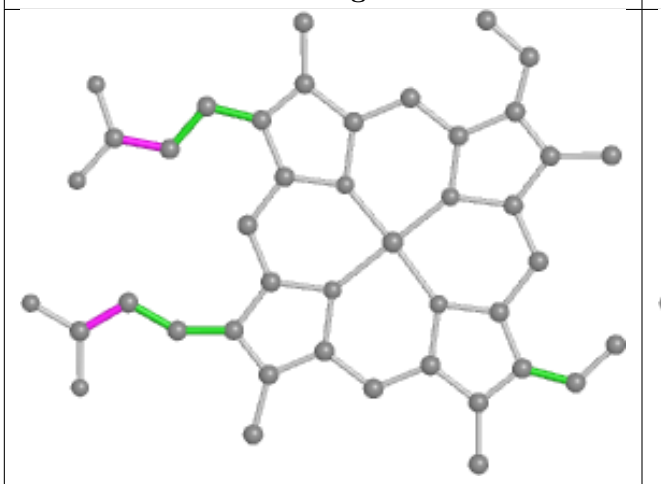
Ligand HEM B 500



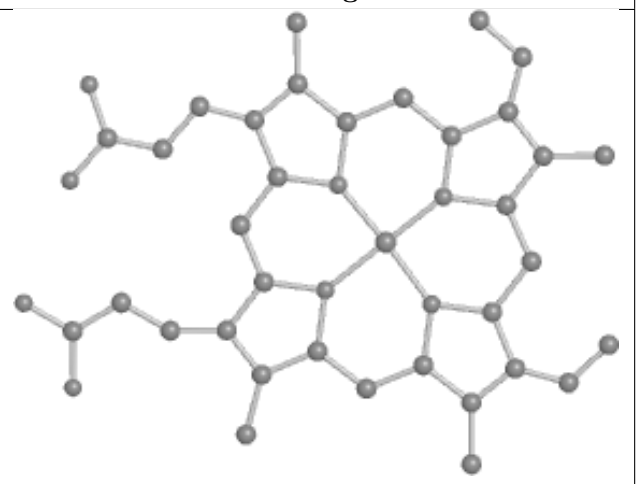
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	465/476 (97%)	-0.15	0	100	100	24, 35, 50, 64	0
1	B	466/476 (97%)	0.05	6 (1%)	77	82	20, 42, 61, 71	0
1	C	464/476 (97%)	-0.08	1 (0%)	95	96	20, 37, 53, 59	0
1	D	464/476 (97%)	-0.08	1 (0%)	95	96	24, 37, 57, 68	0
All	All	1859/1904 (97%)	-0.07	8 (0%)	92	94	20, 38, 55, 71	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	495	HIS	4.0
1	B	496	HIS	3.8
1	B	31	GLY	3.7
1	B	140	VAL	2.8
1	D	143	ARG	2.7
1	C	338	ASN	2.7
1	B	302	GLY	2.2
1	B	143	ARG	2.2

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)

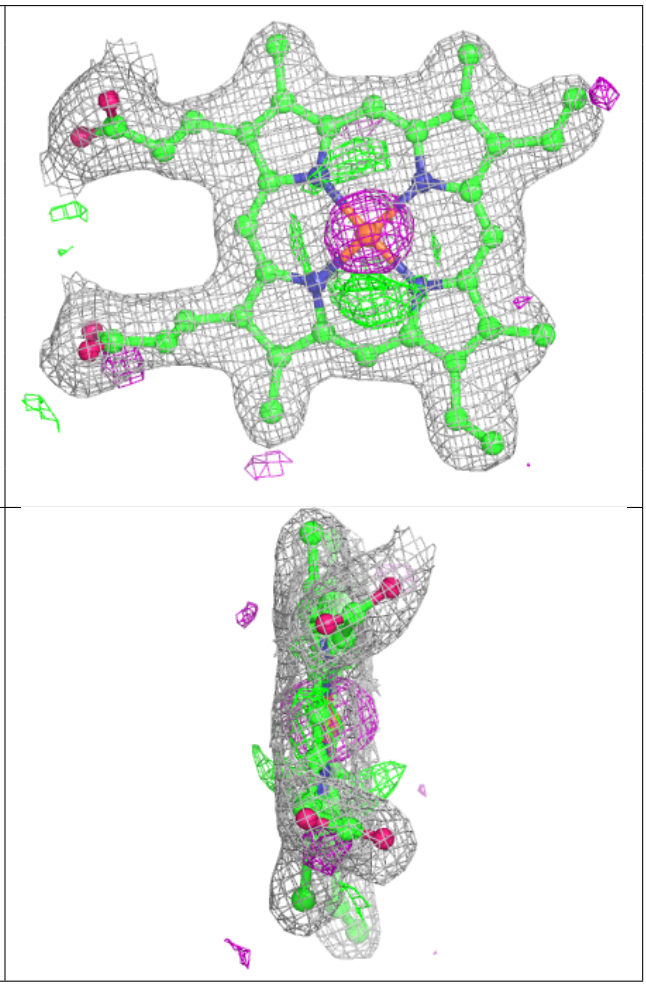
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	N4E	B	1	13/13	0.82	0.21	55,58,58,58	0
3	N4E	A	1	13/13	0.89	0.23	72,72,72,72	0
3	N4E	D	1	13/13	0.91	0.23	69,69,69,70	0
2	HEM	C	500	43/43	0.94	0.12	10,25,30,31	0
2	HEM	B	500	43/43	0.95	0.10	15,27,32,34	0
2	HEM	A	500	43/43	0.95	0.10	2,20,30,32	0
2	HEM	D	500	43/43	0.95	0.10	15,27,31,32	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.

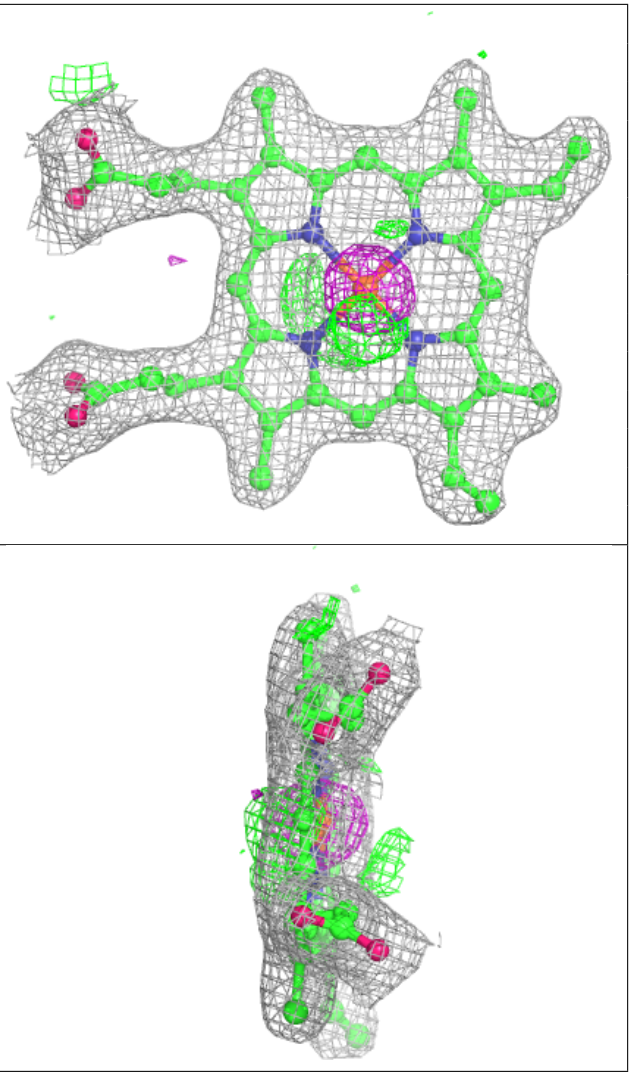
Electron density around HEM C 500:

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



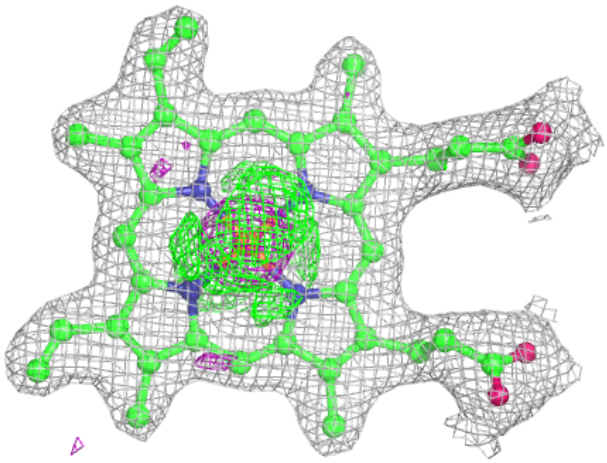
Electron density around HEM B 500:

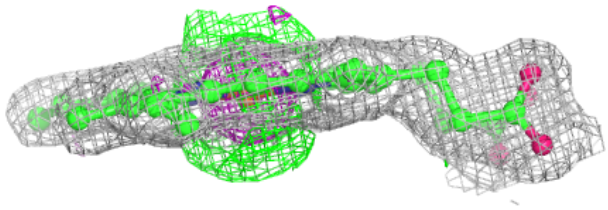
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

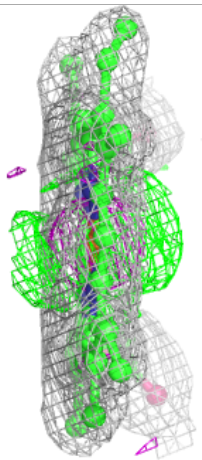


Electron density around HEM A 500:

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

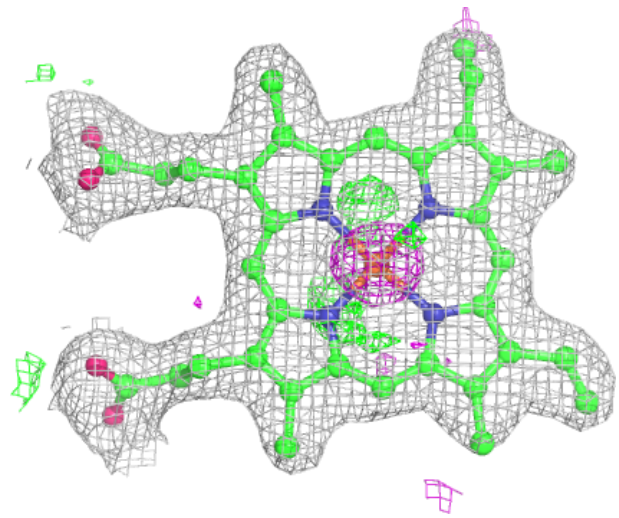


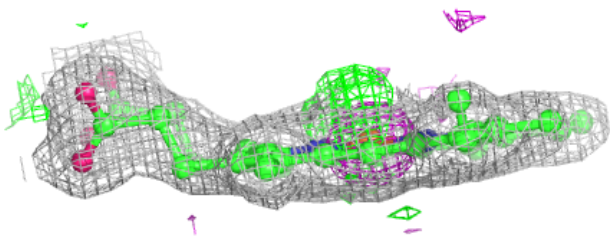




Electron density around HEM D 500:

$2mF_o$-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.