Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2023 – 03:08 PM EDT

PDB ID	:	2PG7
Title	:	Crystal Structure of Human Microsomal P450 2A6 N297Q/I300V
Authors	:	Sansen, S.; Hsu, M.H.; Stout, C.D.; Johnson, E.F.
Deposited on	:	2007-04-06
Resolution	:	2.80 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:

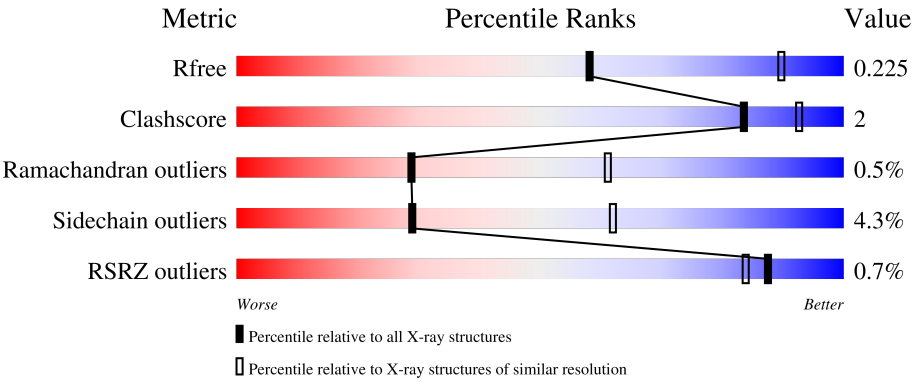
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	87% 10%
1	B	476	% 88% 9%
1	C	476	87% 10%
1	D	476	% 86% 11%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15273 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
1	A	464	Total	C	N	O	S	0	0	0
			3751	2408	648	677	18			
1	B	464	Total	C	N	O	S	0	0	0
			3757	2412	650	677	18			
1	C	464	Total	C	N	O	S	0	0	0
			3751	2408	648	677	18			
1	D	464	Total	C	N	O	S	0	0	0
			3751	2408	648	677	18			

There are 52 discrepancies between the modelled and reference sequences:

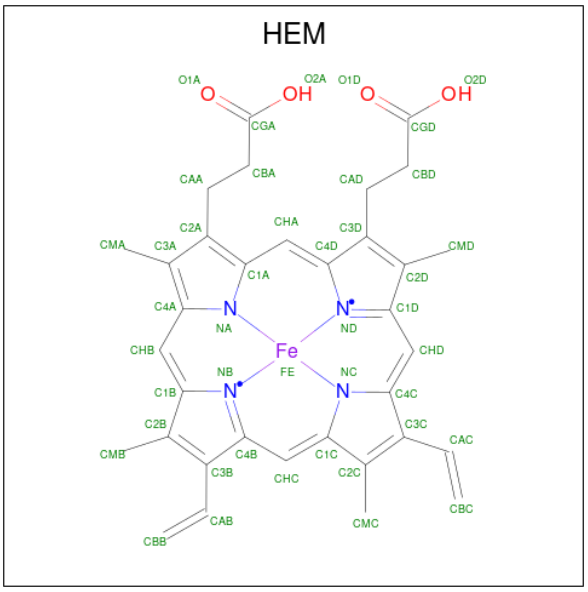
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	cloning artifact	UNP P11509
A	24	ALA	-	cloning artifact	UNP P11509
A	25	LYS	-	cloning artifact	UNP P11509
A	26	LYS	-	cloning artifact	UNP P11509
A	27	THR	-	cloning artifact	UNP P11509
A	28	SER	-	cloning artifact	UNP P11509
A	160	LEU	HIS	variant	UNP P11509
A	297	GLN	ASN	engineered mutation	UNP P11509
A	300	VAL	ILE	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	-	cloning artifact	UNP P11509
B	24	ALA	-	cloning artifact	UNP P11509
B	25	LYS	-	cloning artifact	UNP P11509
B	26	LYS	-	cloning artifact	UNP P11509
B	27	THR	-	cloning artifact	UNP P11509
B	28	SER	-	cloning artifact	UNP P11509
B	160	LEU	HIS	variant	UNP P11509
B	297	GLN	ASN	engineered mutation	UNP P11509

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	300	VAL	ILE	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	-	cloning artifact	UNP P11509
C	24	ALA	-	cloning artifact	UNP P11509
C	25	LYS	-	cloning artifact	UNP P11509
C	26	LYS	-	cloning artifact	UNP P11509
C	27	THR	-	cloning artifact	UNP P11509
C	28	SER	-	cloning artifact	UNP P11509
C	160	LEU	HIS	variant	UNP P11509
C	297	GLN	ASN	engineered mutation	UNP P11509
C	300	VAL	ILE	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	-	cloning artifact	UNP P11509
D	24	ALA	-	cloning artifact	UNP P11509
D	25	LYS	-	cloning artifact	UNP P11509
D	26	LYS	-	cloning artifact	UNP P11509
D	27	THR	-	cloning artifact	UNP P11509
D	28	SER	-	cloning artifact	UNP P11509
D	160	LEU	HIS	variant	UNP P11509
D	297	GLN	ASN	engineered mutation	UNP P11509
D	300	VAL	ILE	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
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is water.

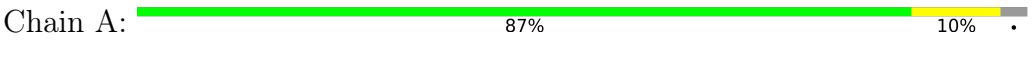
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	23	Total	O	0	0
			23	23		
3	C	25	Total	O	0	0
			25	25		
3	D	23	Total	O	0	0
			23	23		

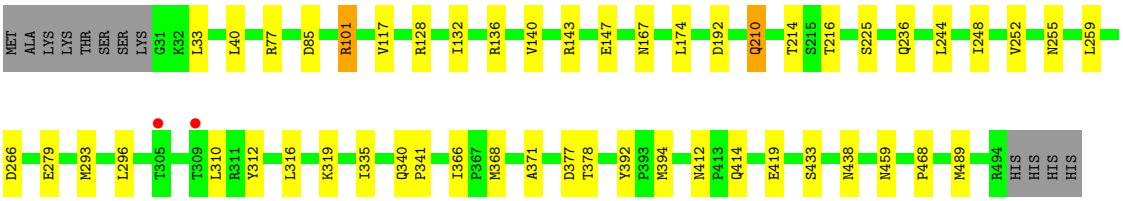
3 Residue-property plots (i)

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

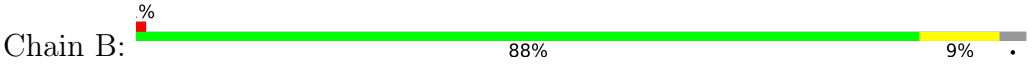
Chain A:

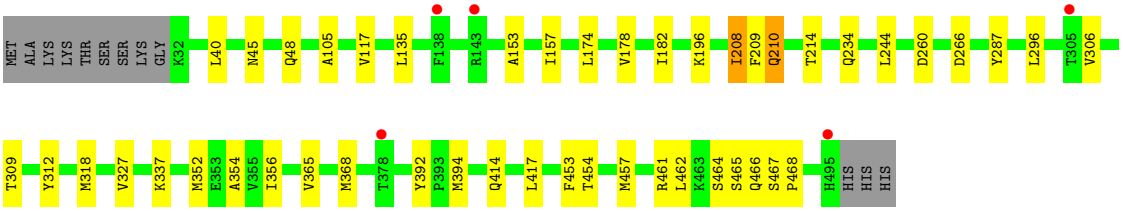




• Molecule 1: Cytochrome P450 2A6

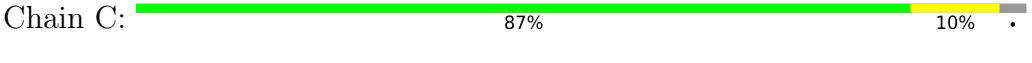
Chain B:

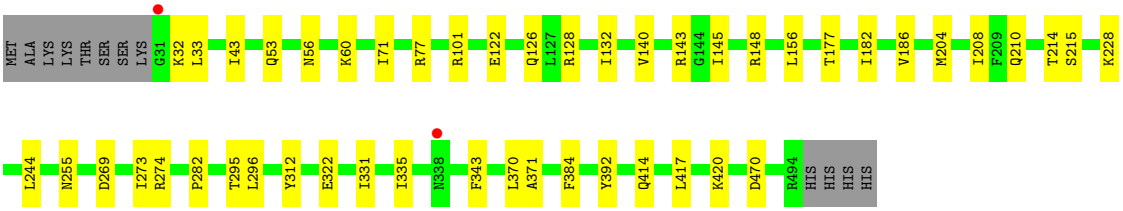




• Molecule 1: Cytochrome P450 2A6

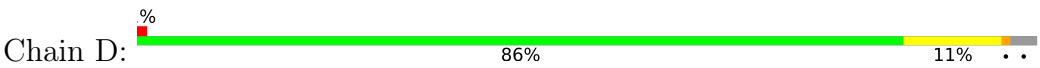
Chain C:

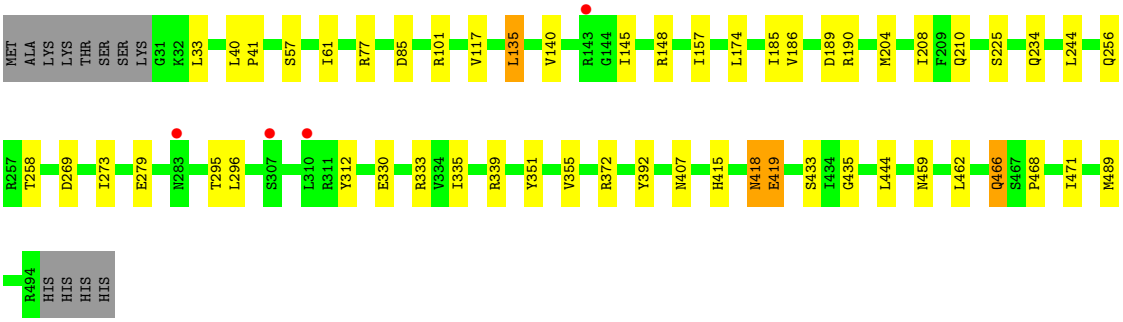




• Molecule 1: Cytochrome P450 2A6

Chain D:




MET ALA LYS LYS THR SER SER LYS G31 K32 L33 L40 P41 S57 I61 R77 D85 R101 V117 L135 V140 R143 G144 I145 R148 I157 L174 I185 V186 D189 R190 M204 I208 F209 Q210 S225 Q234 L244 Q256
R257 T258 D269 I273 E279 N283 T295 L296 S307 L310 R311 Y312 E330 R333 V334 I335 R339 Y351 V355 R372 Y392 N407 H415 N418 E419 S433 I434 G435 L444 N459 L462 Q466 S467 P468 I471 M489
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	70.89Å 159.39Å 104.10Å 90.00° 91.92° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80 36.65 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.00-2.80) 99.6 (36.65-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.235 , 0.289 0.226 , 0.225	Depositor DCC
R_{free} test set	2865 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	52.3	Xtriage
Anisotropy	0.849	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 35.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.041 for h,-k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	15273	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.68	0/3842	0.74	2/5175 (0.0%)
1	B	0.70	0/3849	0.75	0/5185
1	C	0.69	0/3842	0.75	1/5175 (0.0%)
1	D	0.68	0/3842	0.74	1/5175 (0.0%)
All	All	0.69	0/15375	0.75	4/20710 (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	33	LEU	CA-CB-CG	6.04	129.20	115.30
1	D	135	LEU	CA-CB-CG	5.19	127.23	115.30
1	A	366	ILE	CG1-CB-CG2	-5.14	100.08	111.40
1	A	33	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3751	0	3734	19	0
1	B	3757	0	3738	16	0
1	C	3751	0	3734	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	3751	0	3734	25	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
2	C	43	0	30	0	0
2	D	43	0	30	2	0
3	A	20	0	0	0	0
3	B	23	0	0	0	0
3	C	25	0	0	0	0
3	D	23	0	0	0	0
All	All	15273	0	15060	73	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 2.

All (73) 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:145:ILE:HD13	1:D:185:ILE:HD11	1.75	0.69
1:C:32:LYS:HB3	1:C:384:PHE:HB3	1.75	0.67
1:D:244:LEU:HB3	1:D:296:LEU:HD11	1.79	0.64
1:B:368:MET:HG2	1:B:394:MET:SD	2.40	0.62
1:A:244:LEU:HB3	1:A:296:LEU:HD11	1.83	0.60
1:D:101:ARG:HD3	1:D:117:VAL:O	2.01	0.60
1:D:117:VAL:HG22	2:D:500:HEM:HAD1	1.84	0.60
1:C:128:ARG:HE	1:C:132:ILE:HD11	1.67	0.59
1:D:335:ILE:HA	1:D:339:ARG:HH21	1.70	0.56
1:A:132:ILE:HG22	1:A:136:ARG:NH1	2.21	0.55
1:C:53:GLN:HB3	1:C:56:ASN:HB2	1.89	0.55
1:A:40:LEU:HD21	1:C:43:ILE:HD13	1.89	0.55
1:A:225:SER:HB2	1:D:225:SER:HB2	1.88	0.55
1:A:433:SER:HB3	2:A:500:HEM:HBA1	1.89	0.54
1:C:156:LEU:HB2	1:C:177:THR:HG21	1.90	0.54
1:B:352:MET:HE3	1:B:454:THR:HG22	1.90	0.54
1:D:407:ASN:H	1:D:415:HIS:HE1	1.55	0.53
1:A:128:ARG:O	1:A:132:ILE:HG13	2.08	0.52
1:D:140:VAL:HG22	1:D:444:LEU:HD13	1.92	0.52
1:D:433:SER:HB3	2:D:500:HEM:HBA1	1.92	0.52
1:D:204:MET:O	1:D:208:ILE:HG12	2.11	0.51
1:D:330:GLU:HG3	1:D:333:ARG:NH2	2.27	0.50
1:B:244:LEU:HB3	1:B:296:LEU:HD11	1.94	0.50
1:C:269:ASP:O	1:C:273:ILE:HG12	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:269:ASP:O	1:D:273:ILE:HG12	2.11	0.49
1:A:412:ASN:HD21	1:A:414:GLN:HB2	1.78	0.49
1:C:214:THR:HG22	1:C:215:SER:H	1.77	0.49
1:A:248:ILE:O	1:A:252:VAL:HG23	2.13	0.49
1:D:462:LEU:HD22	1:D:489:MET:HE1	1.93	0.49
1:B:153:ALA:O	1:B:157:ILE:HG12	2.13	0.49
1:B:45:ASN:HD22	1:B:48:GLN:NE2	2.10	0.49
1:A:132:ILE:HG22	1:A:136:ARG:HH12	1.78	0.48
1:B:414:GLN:NE2	1:B:417:LEU:HD23	2.29	0.48
1:C:77:ARG:HH11	1:C:77:ARG:HG2	1.78	0.48
1:B:327:VAL:HG13	1:B:352:MET:HE1	1.96	0.47
1:D:419:GLU:H	1:D:419:GLU:CD	2.17	0.47
1:C:122:GLU:O	1:C:126:GLN:HB2	2.15	0.47
1:D:466:GLN:HG3	1:D:471:ILE:HG12	1.96	0.47
1:D:157:ILE:HG21	1:D:459:ASN:HD22	1.80	0.47
1:D:351:TYR:O	1:D:355:VAL:HG23	2.15	0.47
1:C:186:VAL:HG13	1:C:295:THR:HG23	1.96	0.46
1:C:331:ILE:HG23	1:C:335:ILE:HD12	1.97	0.46
1:B:352:MET:O	1:B:356:ILE:HG12	2.17	0.45
1:B:117:VAL:HG22	2:B:500:HEM:HAD1	1.98	0.45
1:A:210:GLN:O	1:A:214:THR:HG23	2.16	0.45
1:B:210:GLN:O	1:B:214:THR:HG23	2.17	0.44
1:A:117:VAL:HG22	2:A:500:HEM:HAD1	2.00	0.44
1:B:178:VAL:HG11	1:B:306:VAL:HB	2.00	0.44
1:C:244:LEU:HB3	1:C:296:LEU:HD11	1.98	0.44
1:D:33:LEU:HD11	1:D:77:ARG:NH1	2.33	0.44
1:D:57:SER:O	1:D:61:ILE:HG12	2.18	0.44
1:C:204:MET:O	1:C:208:ILE:HG12	2.17	0.43
1:D:148:ARG:HH21	1:D:190:ARG:HB3	1.83	0.43
1:A:319:LYS:HD2	1:A:468:PRO:O	2.18	0.43
1:B:318:MET:HE3	1:B:462:LEU:HB3	1.99	0.43
1:A:335:ILE:HG21	1:A:341:PRO:HG3	2.00	0.43
1:D:462:LEU:HD22	1:D:489:MET:CE	2.49	0.42
1:D:189:ASP:CG	1:D:190:ARG:H	2.23	0.42
1:A:143:ARG:O	1:A:147:GLU:HG2	2.19	0.42
1:B:208:ILE:HD13	1:B:208:ILE:HA	1.93	0.42
1:D:186:VAL:HG13	1:D:295:THR:HG23	2.02	0.42
1:C:214:THR:HG22	1:C:215:SER:N	2.34	0.42
1:B:453:PHE:O	1:B:457:MET:HG2	2.20	0.41
1:D:372:ARG:HH22	1:D:435:GLY:HA3	1.84	0.41
1:A:368:MET:HG2	1:A:394:MET:SD	2.60	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:MET:HB2	1:A:489:MET:HE2	1.90	0.41
1:B:309:THR:OG1	1:B:365:VAL:HG21	2.20	0.41
1:C:101:ARG:NH2	1:C:370:LEU:O	2.53	0.41
1:A:174:LEU:HD22	1:A:310:LEU:HD13	2.03	0.41
1:D:135:LEU:HG	1:D:140:VAL:HG21	2.03	0.41
1:A:101:ARG:HD2	1:A:117:VAL:O	2.22	0.40
1:B:354:ALA:HB2	1:B:417:LEU:HD13	2.03	0.40
1:A:255:ASN:O	1:A:259:LEU:HB2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	462/476 (97%)	436 (94%)	23 (5%)	3 (1%)	25	56
1	B	462/476 (97%)	429 (93%)	31 (7%)	2 (0%)	34	66
1	C	462/476 (97%)	440 (95%)	19 (4%)	3 (1%)	25	56
1	D	462/476 (97%)	430 (93%)	30 (6%)	2 (0%)	34	66
All	All	1848/1904 (97%)	1735 (94%)	103 (6%)	10 (0%)	29	61

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	VAL
1	C	371	ALA
1	A	371	ALA
1	B	468	PRO
1	A	438	ASN
1	B	105	ALA
1	C	282	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	418	ASN
1	D	468	PRO
1	C	140	VAL

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	411/422 (97%)	392 (95%)	19 (5%)	27	60
1	B	412/422 (98%)	392 (95%)	20 (5%)	25	57
1	C	411/422 (97%)	393 (96%)	18 (4%)	28	61
1	D	411/422 (97%)	397 (97%)	14 (3%)	37	71
All	All	1645/1688 (98%)	1574 (96%)	71 (4%)	29	62

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ARG
1	A	85	ASP
1	A	101	ARG
1	A	167	ASN
1	A	192	ASP
1	A	210	GLN
1	A	216	THR
1	A	236	GLN
1	A	266	ASP
1	A	279	GLU
1	A	293	MET
1	A	312	TYR
1	A	316	LEU
1	A	340	GLN
1	A	377	ASP
1	A	378	THR
1	A	392	TYR
1	A	419	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	459	ASN
1	B	40	LEU
1	B	135	LEU
1	B	174	LEU
1	B	182	ILE
1	B	196	LYS
1	B	208	ILE
1	B	209	PHE
1	B	210	GLN
1	B	234	GLN
1	B	260	ASP
1	B	266	ASP
1	B	287	TYR
1	B	312	TYR
1	B	337	LYS
1	B	392	TYR
1	B	461	ARG
1	B	464	SER
1	B	465	SER
1	B	466	GLN
1	B	467	SER
1	C	60	LYS
1	C	71	ILE
1	C	143	ARG
1	C	145	ILE
1	C	148	ARG
1	C	182	ILE
1	C	210	GLN
1	C	228	LYS
1	C	255	ASN
1	C	274	ARG
1	C	312	TYR
1	C	322	GLU
1	C	343	PHE
1	C	392	TYR
1	C	414	GLN
1	C	417	LEU
1	C	420	LYS
1	C	470	ASP
1	D	40	LEU
1	D	41	PRO
1	D	85	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	174	LEU
1	D	210	GLN
1	D	234	GLN
1	D	256	GLN
1	D	258	THR
1	D	279	GLU
1	D	312	TYR
1	D	392	TYR
1	D	418	ASN
1	D	419	GLU
1	D	466	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	210	GLN
1	A	412	ASN
1	A	414	GLN
1	A	458	GLN
1	B	48	GLN
1	B	255	ASN
1	B	414	GLN
1	B	418	ASN
1	C	150	GLN
1	C	167	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

4 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	2.33	16 (39%)	45,82,82	2.14	16 (35%)
2	HEM	C	500	1	41,50,50	2.23	15 (36%)	45,82,82	2.03	11 (24%)
2	HEM	D	500	1	41,50,50	2.32	16 (39%)	45,82,82	2.07	11 (24%)
2	HEM	B	500	1	41,50,50	2.27	16 (39%)	45,82,82	2.03	11 (24%)

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	-
2	HEM	D	500	1	-	2/12/54/54	-
2	HEM	B	500	1	-	2/12/54/54	-

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	HEM	C3C-CAC	-5.52	1.36	1.47
2	A	500	HEM	C1B-NB	-5.17	1.31	1.40
2	A	500	HEM	C1D-ND	-5.14	1.28	1.38
2	A	500	HEM	C3C-CAC	-5.11	1.37	1.47
2	B	500	HEM	C3C-CAC	-5.03	1.37	1.47
2	D	500	HEM	C1D-ND	-4.98	1.28	1.38
2	B	500	HEM	C1D-ND	-4.94	1.28	1.38
2	C	500	HEM	C1D-ND	-4.91	1.28	1.38
2	D	500	HEM	C1B-NB	-4.87	1.31	1.40
2	C	500	HEM	C3C-CAC	-4.83	1.37	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	C1B-NB	-4.72	1.32	1.40
2	C	500	HEM	C1B-NB	-4.41	1.32	1.40
2	B	500	HEM	C4D-ND	-4.04	1.33	1.40
2	C	500	HEM	C4D-ND	-4.02	1.33	1.40
2	A	500	HEM	C4B-NB	-3.93	1.30	1.38
2	B	500	HEM	C4B-NB	-3.87	1.30	1.38
2	A	500	HEM	CBB-CAB	3.80	1.49	1.30
2	D	500	HEM	CBB-CAB	3.79	1.49	1.30
2	B	500	HEM	CBB-CAB	3.77	1.49	1.30
2	C	500	HEM	CBB-CAB	3.75	1.48	1.30
2	C	500	HEM	C4B-NB	-3.66	1.31	1.38
2	D	500	HEM	C4D-ND	-3.61	1.34	1.40
2	D	500	HEM	C4B-NB	-3.57	1.31	1.38
2	A	500	HEM	C4D-ND	-3.52	1.34	1.40
2	D	500	HEM	CMA-C3A	3.24	1.58	1.51
2	A	500	HEM	O2A-CGA	-3.17	1.20	1.30
2	B	500	HEM	C4A-NA	-3.15	1.29	1.36
2	A	500	HEM	C4A-NA	-3.10	1.29	1.36
2	A	500	HEM	CMA-C3A	2.91	1.57	1.51
2	C	500	HEM	O2A-CGA	-2.91	1.20	1.30
2	B	500	HEM	O2A-CGA	-2.87	1.21	1.30
2	D	500	HEM	O2A-CGA	-2.83	1.21	1.30
2	D	500	HEM	C3B-C2B	2.80	1.43	1.37
2	C	500	HEM	CMA-C3A	2.79	1.57	1.51
2	D	500	HEM	C4A-NA	-2.76	1.30	1.36
2	C	500	HEM	C1D-C2D	-2.73	1.39	1.44
2	C	500	HEM	C4A-NA	-2.64	1.30	1.36
2	A	500	HEM	C4D-C3D	-2.61	1.40	1.45
2	B	500	HEM	CMA-C3A	2.57	1.57	1.51
2	C	500	HEM	C3B-C2B	2.48	1.42	1.37
2	D	500	HEM	C4D-C3D	-2.48	1.40	1.45
2	D	500	HEM	CAD-C3D	2.47	1.57	1.51
2	B	500	HEM	CAD-C3D	2.46	1.57	1.51
2	A	500	HEM	CAD-C3D	2.46	1.57	1.51
2	B	500	HEM	C1D-C2D	-2.45	1.39	1.44
2	A	500	HEM	C1D-C2D	-2.44	1.39	1.44
2	D	500	HEM	C1D-C2D	-2.41	1.39	1.44
2	A	500	HEM	C3B-C2B	2.34	1.42	1.37
2	A	500	HEM	C2C-C1C	-2.31	1.37	1.42
2	A	500	HEM	CBD-CGD	2.25	1.55	1.50
2	B	500	HEM	C4D-C3D	-2.24	1.41	1.45
2	B	500	HEM	CBD-CGD	2.22	1.55	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	HEM	CAD-C3D	2.20	1.57	1.51
2	B	500	HEM	C3B-C2B	2.18	1.41	1.37
2	D	500	HEM	CBD-CGD	2.15	1.55	1.50
2	C	500	HEM	C4D-C3D	-2.12	1.41	1.45
2	B	500	HEM	CHD-C1D	-2.09	1.35	1.41
2	C	500	HEM	CHD-C1D	-2.08	1.35	1.41
2	C	500	HEM	C2C-C1C	-2.06	1.37	1.42
2	D	500	HEM	CHD-C1D	-2.05	1.35	1.41
2	A	500	HEM	FE-NB	2.04	2.06	1.96
2	B	500	HEM	FE-ND	2.02	2.06	1.96
2	D	500	HEM	FE-ND	2.01	2.06	1.96

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	HEM	C4B-CHC-C1C	7.09	131.91	122.56
2	D	500	HEM	C4B-CHC-C1C	6.78	131.51	122.56
2	B	500	HEM	C4B-CHC-C1C	6.63	131.31	122.56
2	C	500	HEM	C4B-CHC-C1C	6.50	131.13	122.56
2	C	500	HEM	C4C-CHD-C1D	6.42	131.03	122.56
2	A	500	HEM	C4C-CHD-C1D	5.78	130.19	122.56
2	B	500	HEM	C4C-CHD-C1D	5.73	130.12	122.56
2	D	500	HEM	C4C-CHD-C1D	5.29	129.54	122.56
2	D	500	HEM	CHB-C1B-NB	-4.10	119.31	124.38
2	A	500	HEM	C4B-C3B-C2B	-3.77	104.12	107.11
2	D	500	HEM	C4B-C3B-C2B	-3.54	104.31	107.11
2	D	500	HEM	C1B-NB-C4B	3.52	108.70	105.07
2	B	500	HEM	C2C-C3C-C4C	-3.33	104.58	106.90
2	B	500	HEM	CHB-C1B-NB	-3.27	120.34	124.38
2	C	500	HEM	C4B-C3B-C2B	-3.27	104.52	107.11
2	B	500	HEM	C4B-C3B-C2B	-3.26	104.53	107.11
2	C	500	HEM	C2C-C3C-C4C	-3.25	104.63	106.90
2	A	500	HEM	C2C-C3C-C4C	-3.19	104.67	106.90
2	A	500	HEM	C4D-ND-C1D	3.18	108.36	105.07
2	D	500	HEM	C2C-C3C-C4C	-3.18	104.68	106.90
2	B	500	HEM	C1B-NB-C4B	3.17	108.35	105.07
2	D	500	HEM	C4D-ND-C1D	3.13	108.30	105.07
2	B	500	HEM	C4D-ND-C1D	3.10	108.27	105.07
2	A	500	HEM	CHB-C1B-NB	-3.07	120.59	124.38
2	A	500	HEM	C3B-C2B-C1B	-3.05	104.23	106.49
2	C	500	HEM	C1B-NB-C4B	3.04	108.22	105.07
2	C	500	HEM	C4D-ND-C1D	3.03	108.20	105.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	HEM	C1B-NB-C4B	2.81	107.97	105.07
2	B	500	HEM	C3B-C2B-C1B	-2.78	104.42	106.49
2	C	500	HEM	C3B-C2B-C1B	-2.75	104.44	106.49
2	D	500	HEM	C3B-C2B-C1B	-2.73	104.46	106.49
2	A	500	HEM	CMA-C3A-C4A	-2.44	124.72	128.46
2	D	500	HEM	O2A-CGA-CBA	2.41	121.77	114.03
2	A	500	HEM	CAD-CBD-CGD	2.38	118.73	113.60
2	A	500	HEM	O2A-CGA-CBA	2.30	121.41	114.03
2	A	500	HEM	C4D-C3D-C2D	-2.21	103.68	106.90
2	B	500	HEM	C4D-C3D-C2D	-2.19	103.70	106.90
2	C	500	HEM	CBA-CAA-C2A	2.16	116.31	112.62
2	D	500	HEM	C4D-C3D-C2D	-2.14	103.78	106.90
2	C	500	HEM	CHB-C1B-NB	-2.11	121.78	124.38
2	B	500	HEM	O2A-CGA-CBA	2.06	120.64	114.03
2	C	500	HEM	C4D-C3D-C2D	-2.06	103.90	106.90
2	A	500	HEM	CMA-C3A-C2A	2.05	128.81	124.94
2	D	500	HEM	CMA-C3A-C4A	-2.05	125.32	128.46
2	C	500	HEM	O2A-CGA-CBA	2.04	120.58	114.03
2	A	500	HEM	O2A-CGA-O1A	-2.04	118.22	123.30
2	A	500	HEM	CAD-C3D-C4D	2.03	128.21	124.66
2	A	500	HEM	CBA-CAA-C2A	2.02	116.06	112.62
2	B	500	HEM	CMA-C3A-C4A	-2.01	125.38	128.46

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	500	HEM	CAD-CBD-CGD-O1D
2	B	500	HEM	CAA-CBA-CGA-O2A
2	C	500	HEM	CAD-CBD-CGD-O2D
2	B	500	HEM	CAA-CBA-CGA-O1A
2	C	500	HEM	CAA-CBA-CGA-O2A
2	D	500	HEM	CAA-CBA-CGA-O2A
2	C	500	HEM	CAA-CBA-CGA-O1A
2	D	500	HEM	CAA-CBA-CGA-O1A
2	A	500	HEM	CAA-CBA-CGA-O2A
2	A	500	HEM	CAA-CBA-CGA-O1A

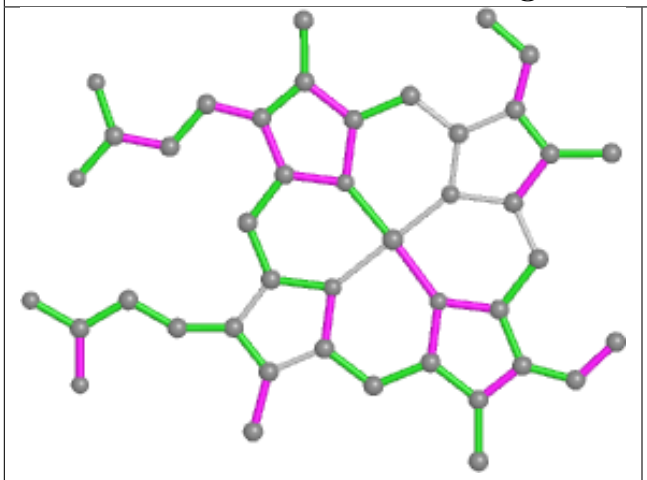
There are no ring outliers.

3 monomers are involved in 5 short contacts:

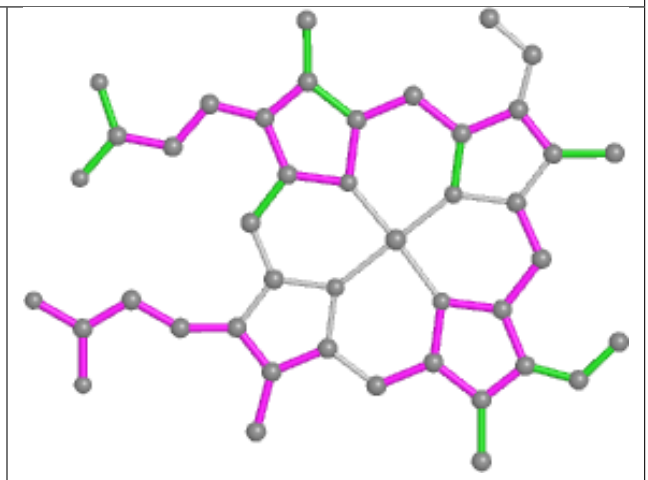
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	HEM	2	0
2	D	500	HEM	2	0
2	B	500	HEM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

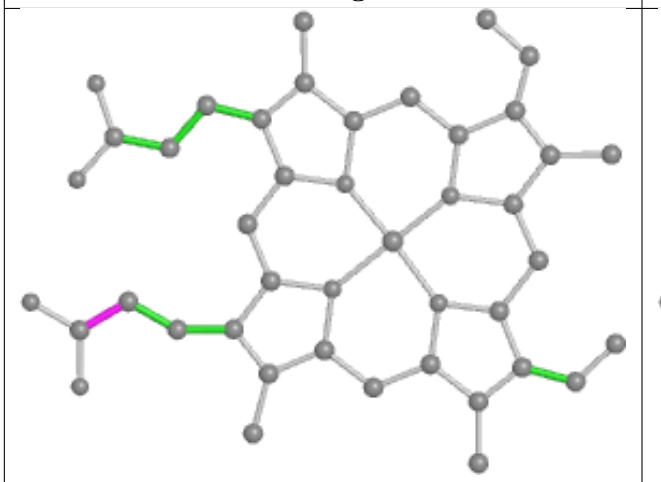
Ligand HEM A 500



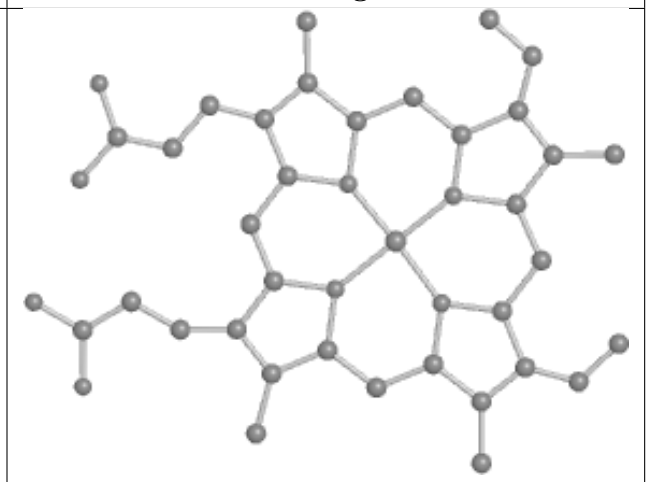
Bond lengths



Bond angles

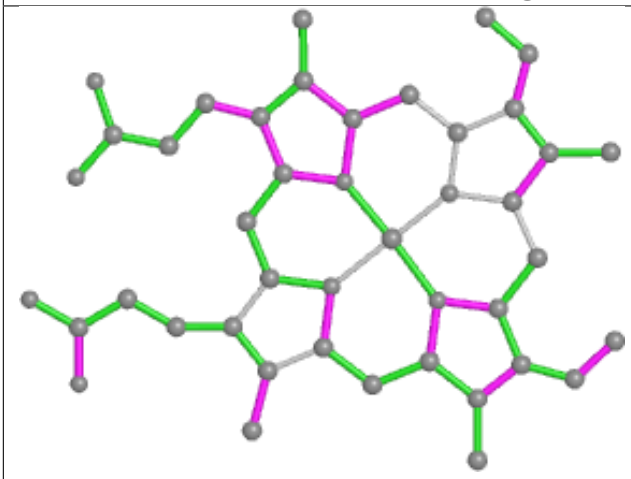


Torsions

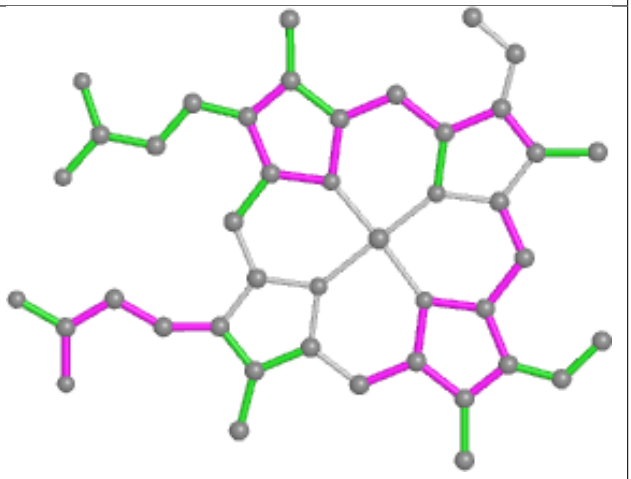


Rings

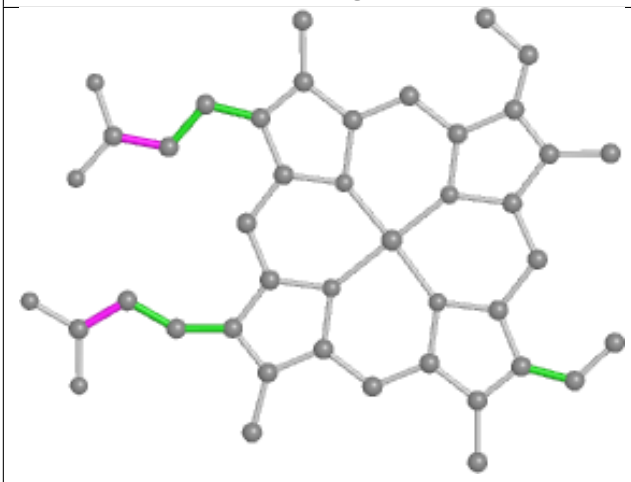
Ligand HEM C 500



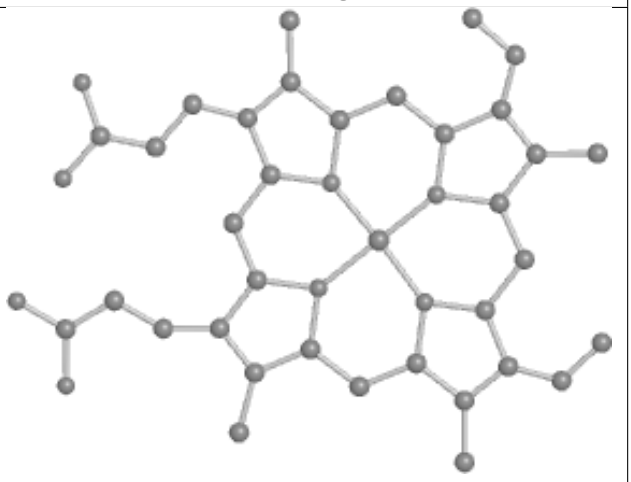
Bond lengths



Bond angles

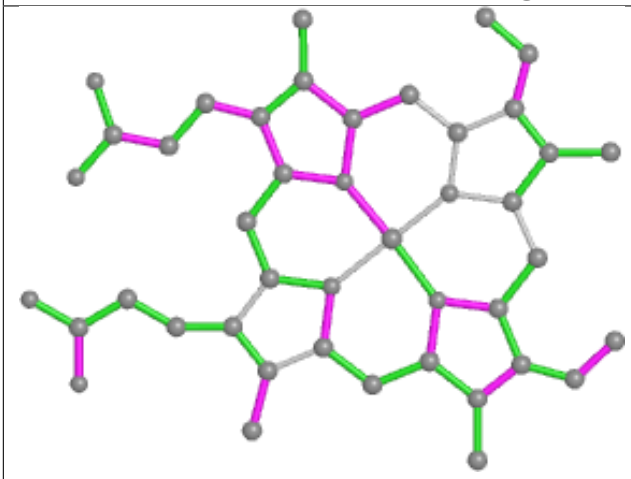


Torsions

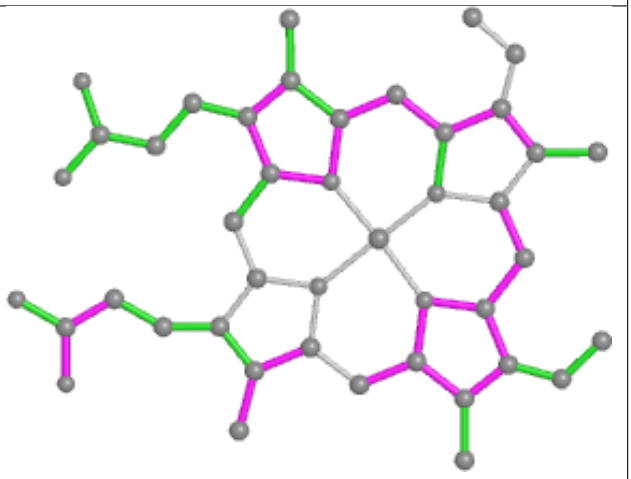


Rings

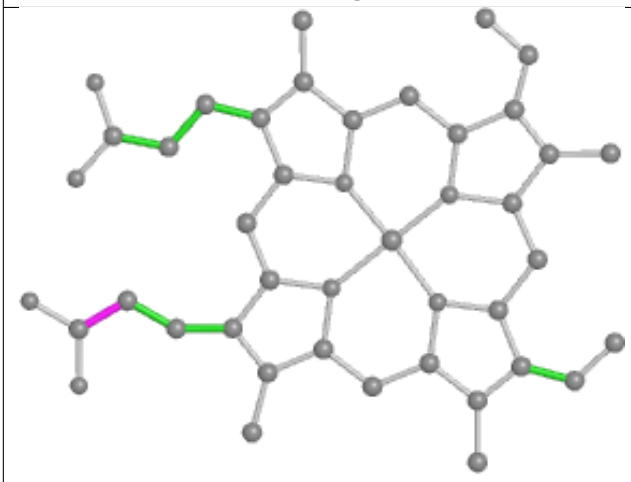
Ligand HEM D 500



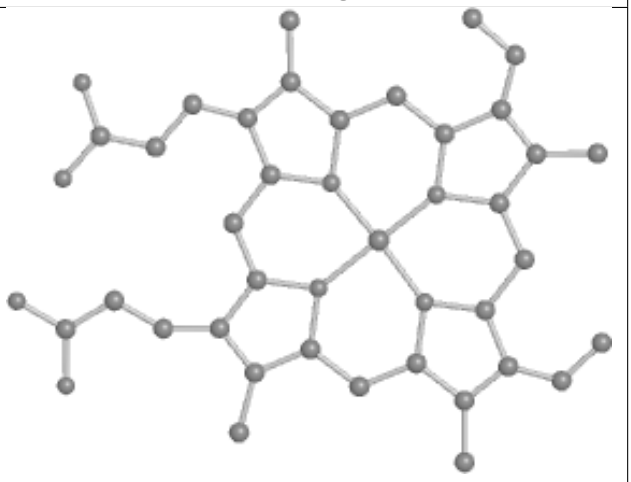
Bond lengths



Bond angles

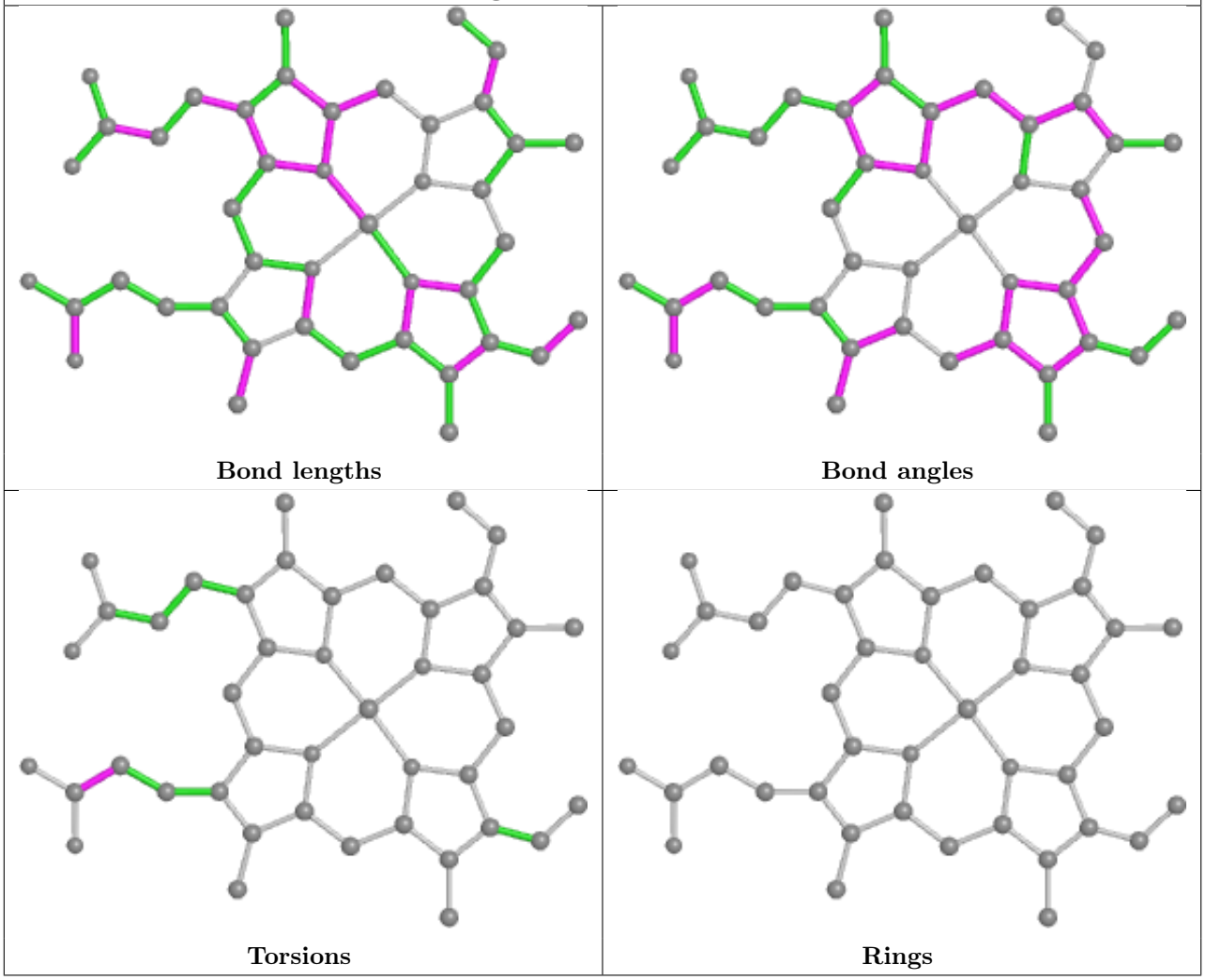


Torsions



Rings

Ligand HEM B 500



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	464/476 (97%)	-0.22	2 (0%)	92	91	21, 48, 81, 107	1 (0%)
1	B	464/476 (97%)	-0.11	5 (1%)	80	75	24, 53, 86, 136	0
1	C	464/476 (97%)	-0.22	2 (0%)	92	91	22, 49, 81, 120	0
1	D	464/476 (97%)	-0.15	4 (0%)	84	80	23, 50, 79, 134	0
All	All	1856/1904 (97%)	-0.17	13 (0%)	87	84	21, 50, 82, 136	1 (0%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	338	ASN	4.0
1	C	31	GLY	3.5
1	D	143	ARG	3.1
1	A	305	THR	2.4
1	B	305	THR	2.4
1	D	307	SER	2.3
1	D	310	LEU	2.2
1	B	378	THR	2.2
1	B	495	HIS	2.2
1	A	309	THR	2.1
1	B	138	PHE	2.1
1	D	283	ASN	2.1
1	B	143	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

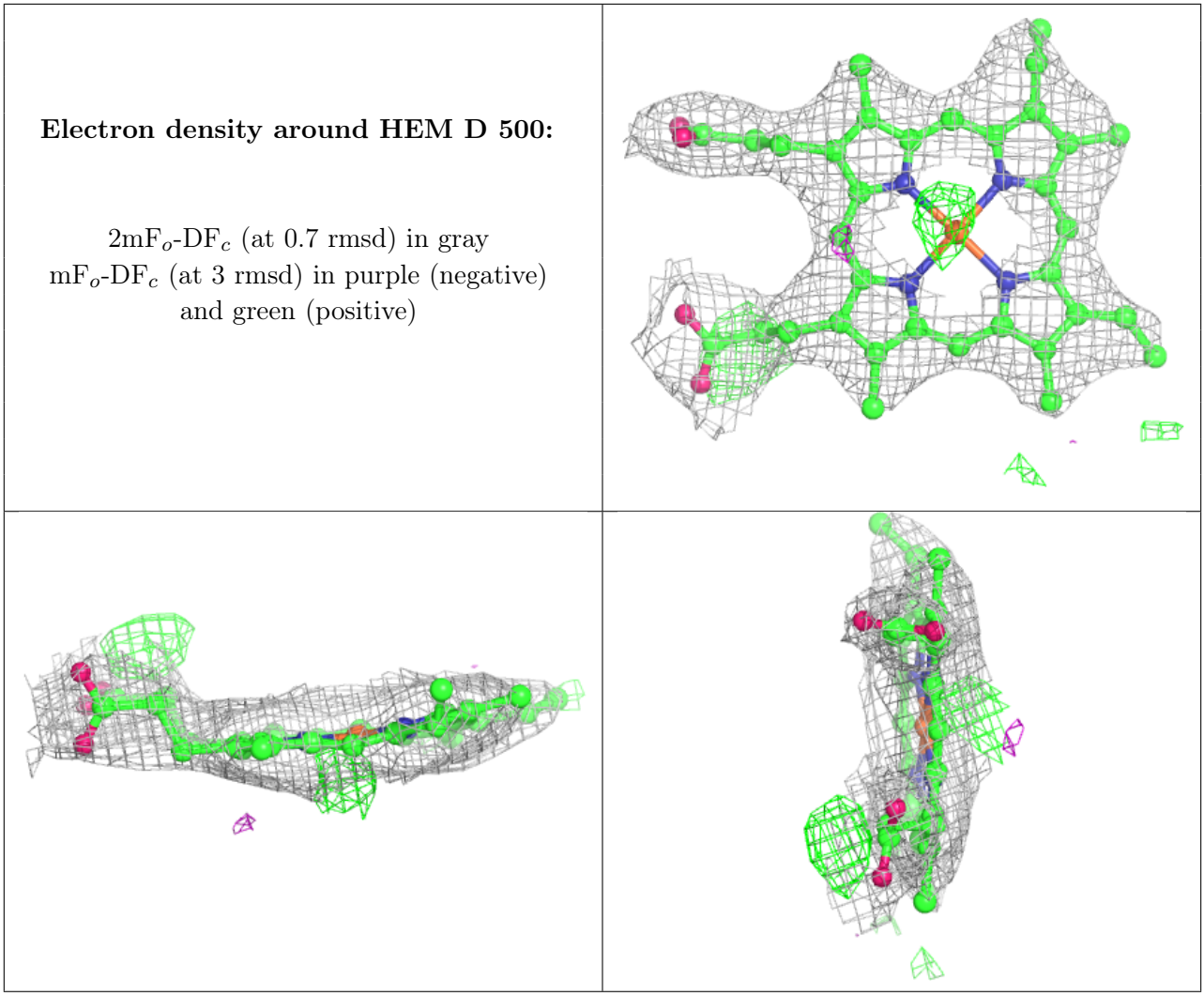
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	D	500	43/43	0.95	0.23	48,48,48,48	0
2	HEM	B	500	43/43	0.96	0.27	48,48,48,48	0
2	HEM	A	500	43/43	0.96	0.26	48,48,48,48	0
2	HEM	C	500	43/43	0.97	0.24	48,48,48,48	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.

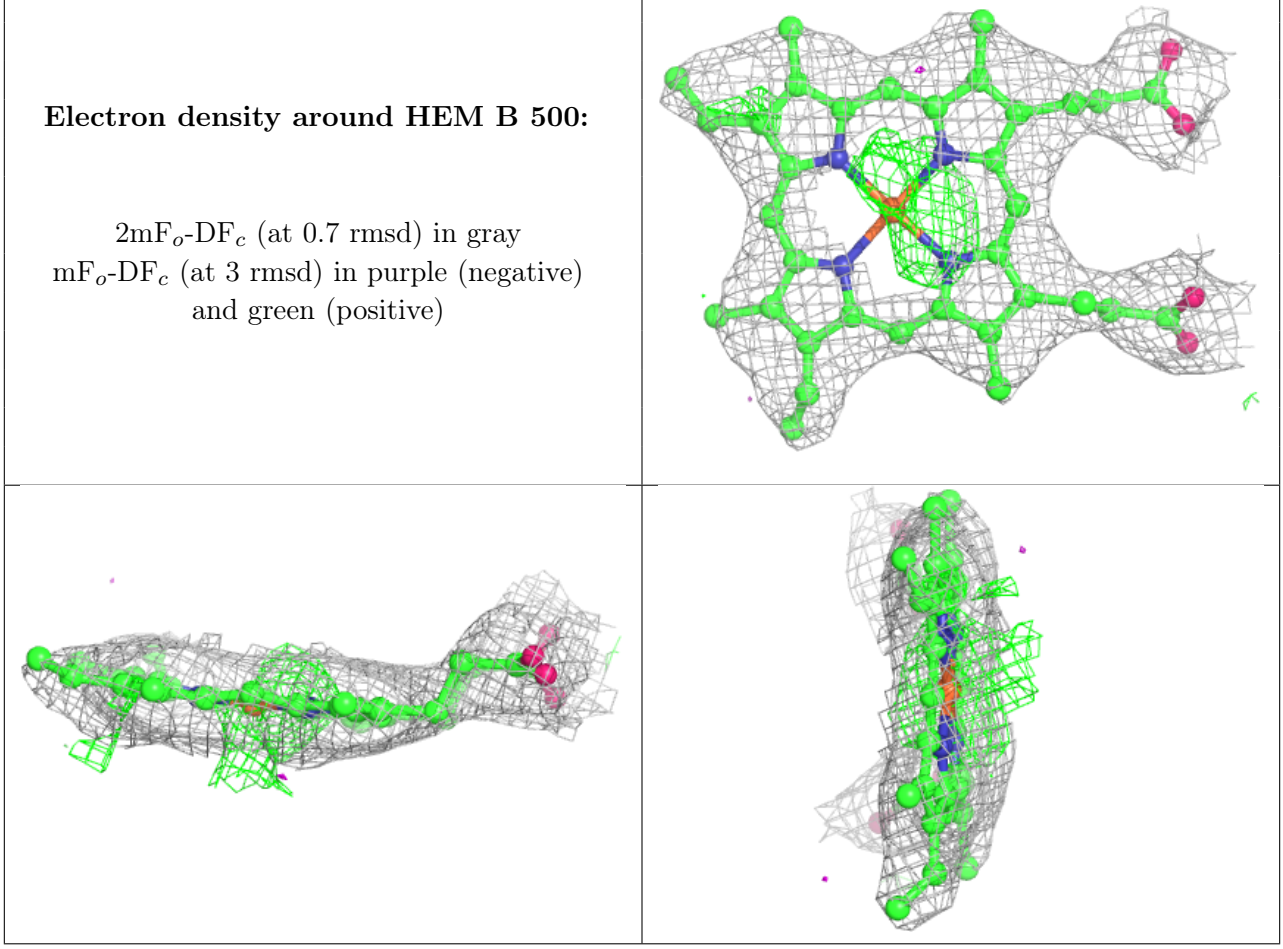
Electron density around HEM D 500:

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



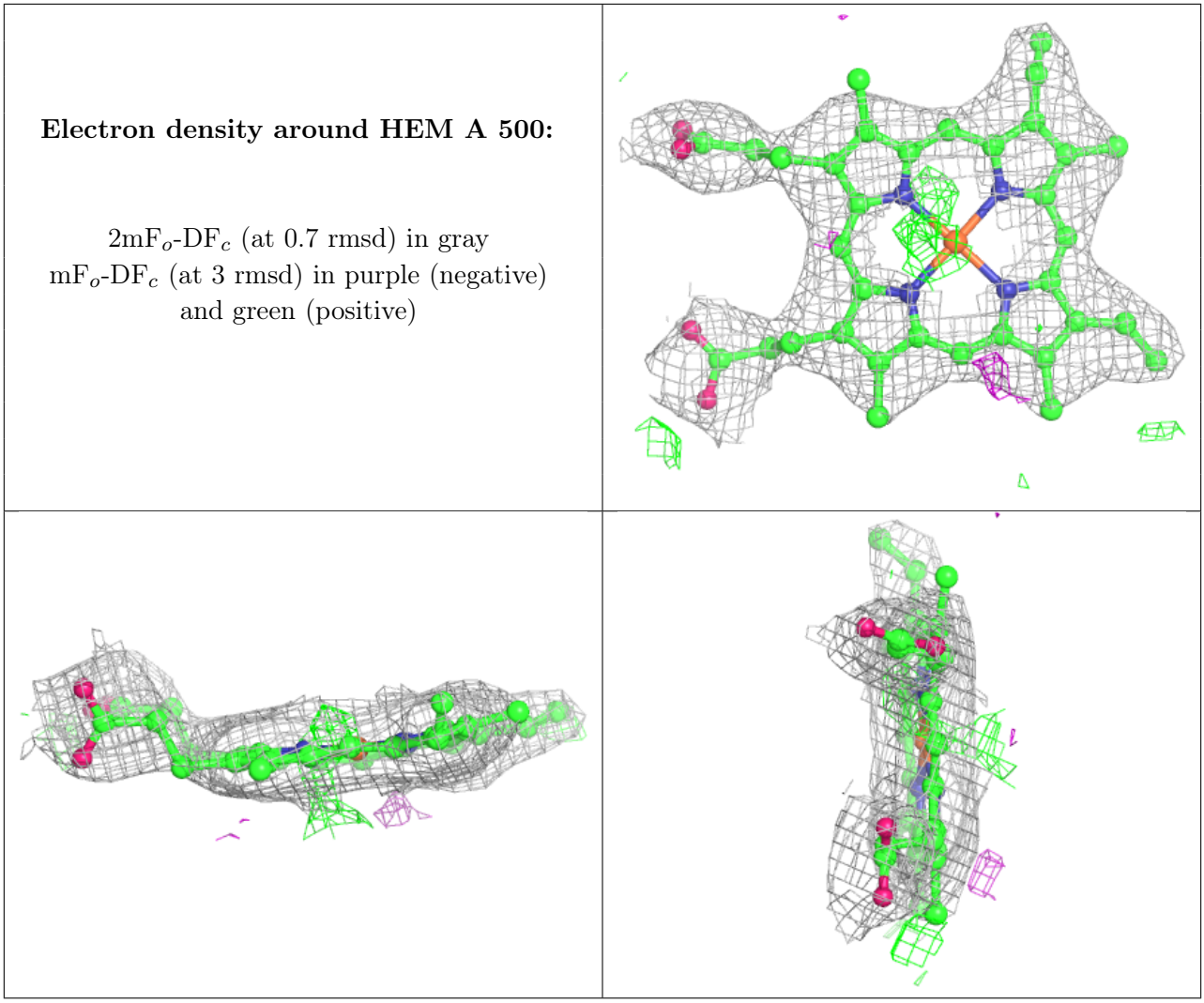
Electron density around HEM B 500:

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



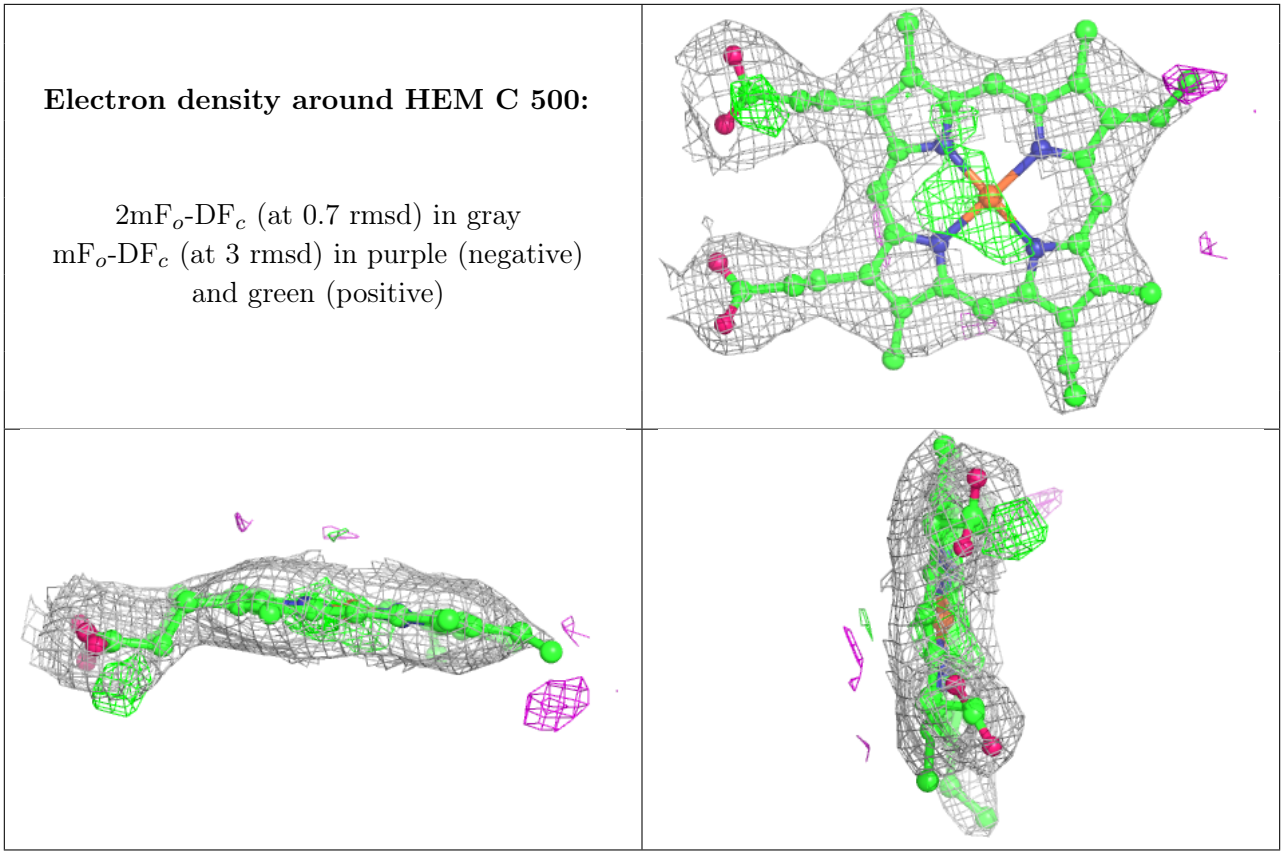
Electron density around HEM A 500:

$2mF_o$-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 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)



6.5 Other polymers

There are no such residues in this entry.