Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2023 – 06:27 PM EDT

PDB ID	:	2PG5
Title	:	Crystal Structure of Human Microsomal P450 2A6 N297Q
Authors	:	Sansen, S.; Hsu, M.H.; Stout, C.D.; Johnson, E.F.
Deposited on	:	2007-04-06
Resolution	:	1.95 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:

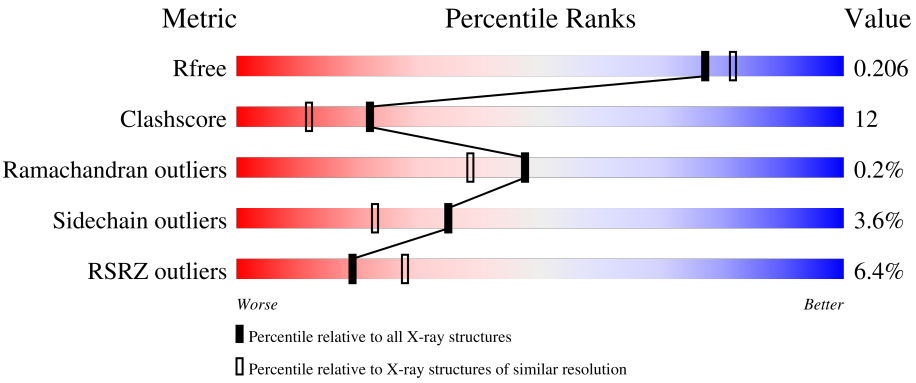
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	5% 78% 17%
1	B	476	7% 71% 24%
1	C	476	4% 78% 18%
1	D	476	9% 74% 21%

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	EDO	D	501	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 15846 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
			3752	2409	648	677	18			
1	B	464	Total	C	N	O	S	0	0	0
			3758	2413	650	677	18			
1	C	463	Total	C	N	O	S	0	0	0
			3748	2407	647	676	18			
1	D	464	Total	C	N	O	S	0	0	0
			3752	2409	648	677	18			

There are 48 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	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
B	495	HIS	-	expression tag	UNP P11509

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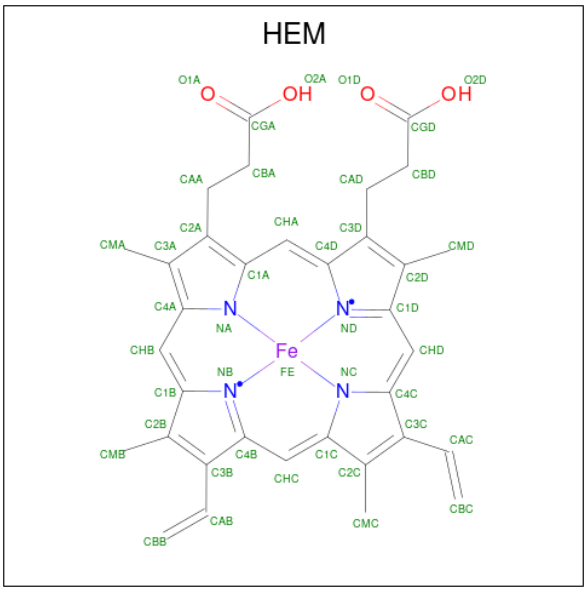
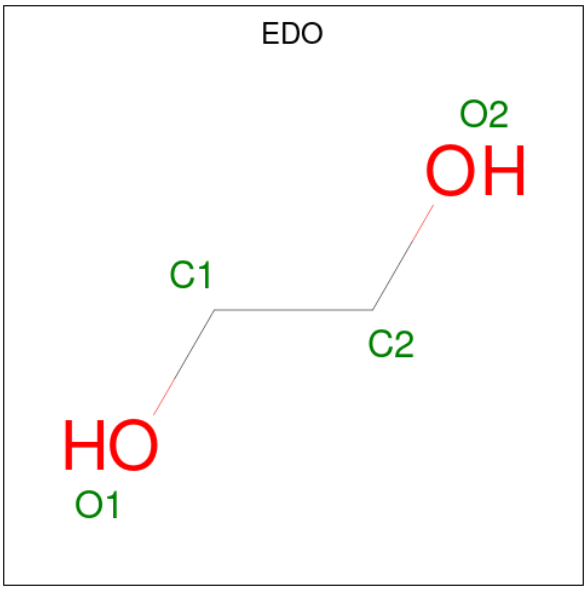
Chain	Residue	Modelled	Actual	Comment	Reference
B	496	HIS	-	expression tag	UNP P11509
B	497	HIS	-	expression tag	UNP P11509
B	498	HIS	-	expression tag	UNP P11509
C	23	MET	-	cloning artifact	UNP P11509
C	24	ALA	-	cloning artifact	UNP P11509
C	25	LYS	-	cloning artifact	UNP P11509
C	26	LYS	-	cloning artifact	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	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	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 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 4 is water.

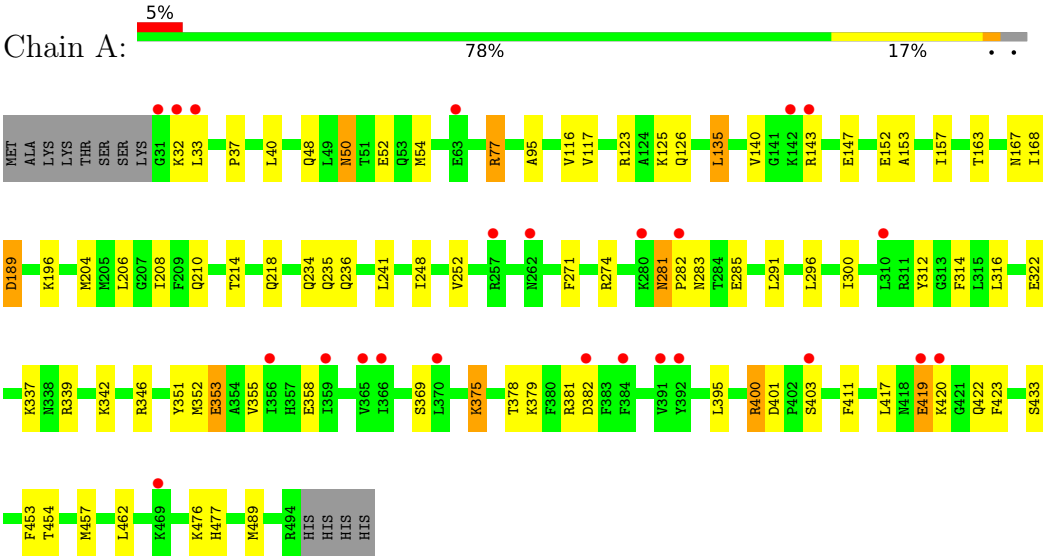
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	158	Total O 158 158	0	0
4	B	134	Total O 134 134	0	0
4	C	201	Total O 201 201	0	0
4	D	155	Total O 155 155	0	0

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.

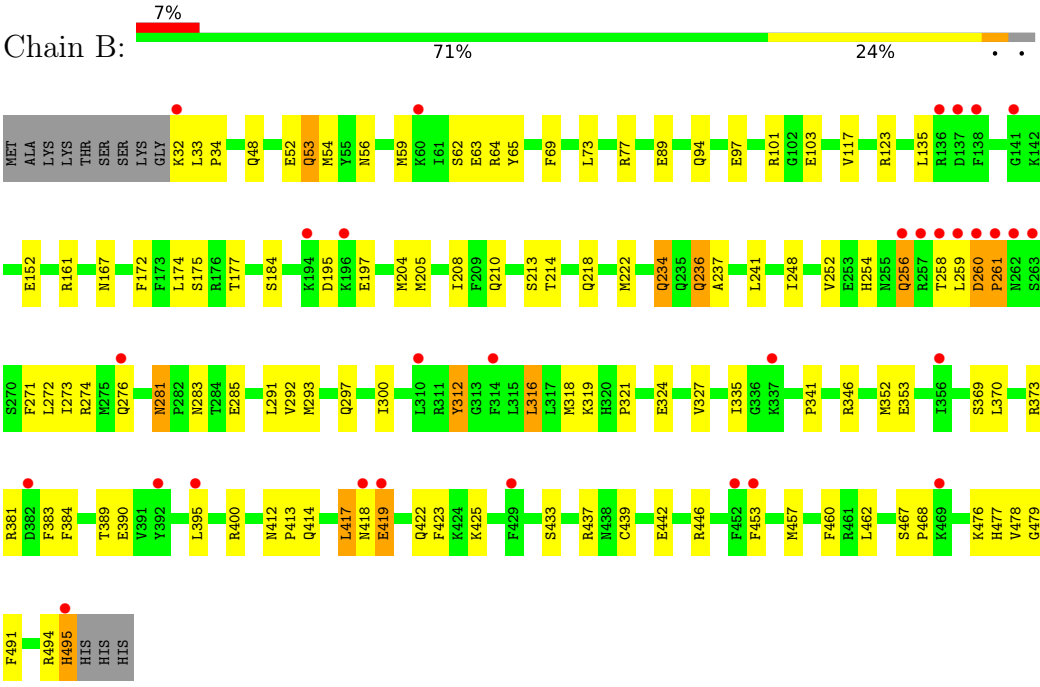
• Molecule 1: Cytochrome P450 2A6

Chain A:



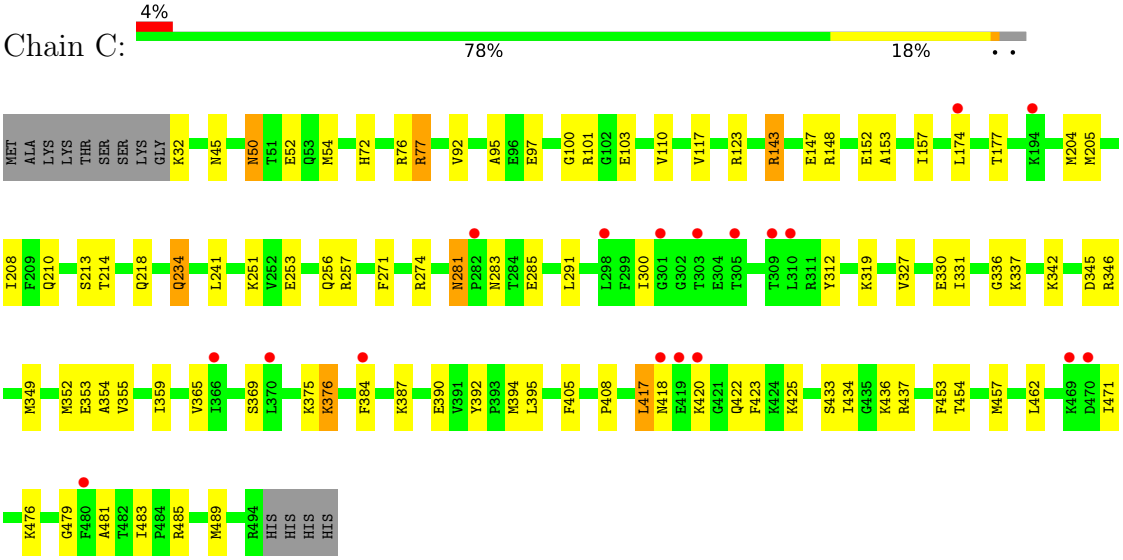
• Molecule 1: Cytochrome P450 2A6

Chain B:



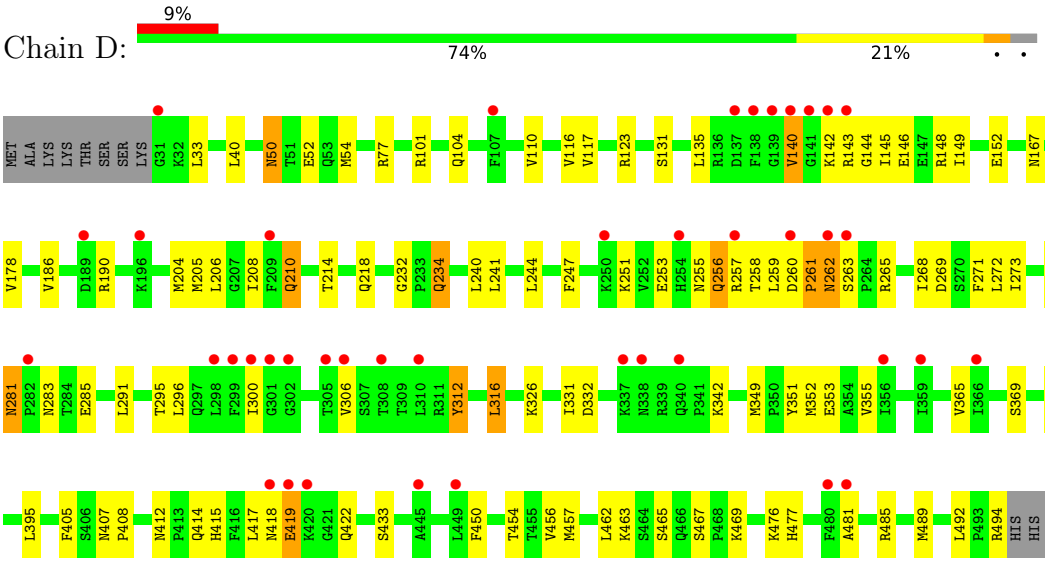
• Molecule 1: Cytochrome P450 2A6

Chain C:



• Molecule 1: Cytochrome P450 2A6

Chain D:



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 157.97Å 103.74Å 90.00° 92.23° 90.00°	Depositor
Resolution (Å)	35.00 – 1.95 29.38 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (35.00-1.95) 98.8 (29.38-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.53 (at 1.95Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.215 , 0.239 0.208 , 0.206	Depositor DCC
R_{free} test set	8204 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	31.3	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 47.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	15846	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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, EDO

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	0.39	0/3843	0.60	1/5176 (0.0%)
1	B	0.40	0/3850	0.63	0/5186
1	C	0.39	0/3839	0.61	0/5171
1	D	0.40	0/3843	0.61	1/5176 (0.0%)
All	All	0.39	0/15375	0.61	2/20709 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	104	GLN	N-CA-C	-5.54	96.04	111.00
1	A	417	LEU	CA-CB-CG	5.24	127.36	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	3752	0	3736	73	0
1	B	3758	0	3740	101	0
1	C	3748	0	3733	83	0
1	D	3752	0	3736	99	0
2	A	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	43	0	30	4	0
2	C	43	0	30	4	0
2	D	43	0	30	3	0
3	A	4	0	6	0	0
3	B	4	0	6	0	0
3	C	4	0	6	0	0
3	D	4	0	6	0	0
4	A	158	0	0	5	0
4	B	134	0	0	4	1
4	C	201	0	0	4	1
4	D	155	0	0	2	0
All	All	15846	0	15089	356	1

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 12.

All (356) 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:C:418:ASN:HD22	1:C:422:GLN:HB2	1.14	1.11
1:B:234:GLN:H	1:B:234:GLN:HE21	1.02	0.97
1:C:45:ASN:HD22	1:C:72:HIS:H	1.02	0.95
1:A:54:MET:HG3	1:A:218:GLN:HE21	1.32	0.91
1:C:234:GLN:H	1:C:234:GLN:HE21	1.12	0.91
1:C:375:LYS:HB3	1:C:376:LYS:HE2	1.53	0.90
1:D:259:LEU:HD11	1:D:273:ILE:HD11	1.54	0.90
1:D:142:LYS:HG3	1:D:144:GLY:H	1.38	0.89
1:B:236:GLN:HG2	4:B:619:HOH:O	1.73	0.88
1:B:205:MET:HE2	1:B:300:ILE:HA	1.56	0.88
1:C:32:LYS:HB3	1:C:384:PHE:HB3	1.54	0.87
1:C:77:ARG:HH11	1:C:77:ARG:HG2	1.39	0.87
1:B:54:MET:HG3	1:B:218:GLN:HE21	1.43	0.84
1:B:234:GLN:H	1:B:234:GLN:NE2	1.75	0.84
1:A:32:LYS:HD2	1:A:33:LEU:H	1.42	0.84
1:D:54:MET:HG3	1:D:218:GLN:HE21	1.44	0.83
1:C:97:GLU:HG3	4:C:562:HOH:O	1.80	0.81
1:C:45:ASN:HD22	1:C:72:HIS:N	1.81	0.78
1:A:143:ARG:O	1:A:147:GLU:HG2	1.85	0.77
1:A:419:GLU:HA	1:A:419:GLU:OE1	1.84	0.76
1:C:143:ARG:NE	1:C:147:GLU:HG3	2.00	0.76
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:186:VAL:HG11	1:D:295:THR:HG23	1.65	0.76
1:B:234:GLN:HE21	1:B:234:GLN:N	1.83	0.76
1:C:418:ASN:HB2	1:C:422:GLN:H	1.49	0.76
1:B:64:ARG:HG2	1:B:64:ARG:HH11	1.50	0.76
1:C:32:LYS:HE2	1:C:384:PHE:HB2	1.68	0.75
1:B:161:ARG:HG3	1:B:161:ARG:HH11	1.51	0.75
1:B:318:MET:HE1	1:B:489:MET:HB2	1.69	0.75
1:D:101:ARG:HD3	1:D:117:VAL:O	1.87	0.75
1:A:339:ARG:NH1	1:A:342:LYS:HZ3	1.86	0.74
1:C:418:ASN:ND2	1:C:422:GLN:HB2	1.98	0.73
1:D:457:MET:HE1	1:D:462:LEU:HD21	1.73	0.71
1:B:32:LYS:HG2	1:B:384:PHE:HB2	1.72	0.70
1:C:234:GLN:H	1:C:234:GLN:NE2	1.90	0.69
1:C:123:ARG:HA	1:C:285:GLU:HG3	1.75	0.69
1:D:261:PRO:HA	1:D:273:ILE:HD12	1.75	0.69
1:A:337:LYS:HD2	1:A:337:LYS:N	2.09	0.68
1:D:256:GLN:HE22	1:D:272:LEU:CD2	2.06	0.68
1:D:208:ILE:HD11	1:D:240:LEU:HB2	1.76	0.68
1:B:423:PHE:HE1	1:B:425:LYS:HG2	1.59	0.67
1:B:210:GLN:HE21	1:B:477:HIS:HD2	1.39	0.67
1:B:33:LEU:HD12	1:B:34:PRO:HD2	1.76	0.66
1:D:352:MET:HE3	1:D:454:THR:HG22	1.76	0.66
1:C:205:MET:HE2	1:C:300:ILE:HG12	1.77	0.65
1:D:50:ASN:ND2	1:D:52:GLU:H	1.93	0.65
1:D:50:ASN:HD22	1:D:50:ASN:C	1.99	0.65
1:D:167:ASN:HD21	1:D:465:SER:HB3	1.62	0.64
1:C:392:TYR:HB3	1:C:394:MET:CE	2.27	0.64
1:A:339:ARG:NH1	1:A:342:LYS:NZ	2.45	0.64
1:C:423:PHE:HE1	1:C:425:LYS:HG2	1.62	0.64
1:C:418:ASN:HB3	1:C:420:LYS:H	1.63	0.64
1:B:77:ARG:HH12	1:B:389:THR:HG23	1.62	0.64
1:C:45:ASN:ND2	1:C:72:HIS:H	1.86	0.63
1:D:256:GLN:HE22	1:D:272:LEU:HD22	1.62	0.63
1:D:419:GLU:H	1:D:419:GLU:CD	2.01	0.63
1:A:353:GLU:HG2	1:A:423:PHE:CD2	2.34	0.63
1:C:392:TYR:HB3	1:C:394:MET:HE1	1.78	0.63
1:D:256:GLN:HA	1:D:256:GLN:HE21	1.62	0.63
1:A:420:LYS:HG3	1:A:422:GLN:NE2	2.12	0.63
1:B:77:ARG:HG2	1:B:77:ARG:HH11	1.62	0.63
1:B:204:MET:O	1:B:208:ILE:HG13	1.98	0.63
1:B:259:LEU:HD21	1:B:273:ILE:HD13	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:GLN:HE21	1:B:477:HIS:CD2	2.17	0.62
1:A:420:LYS:CG	1:A:422:GLN:HE21	2.13	0.62
1:D:253:GLU:HG2	1:D:257:ARG:HH21	1.64	0.62
1:B:101:ARG:HD3	1:B:117:VAL:O	2.00	0.61
1:B:254:HIS:O	1:B:258:THR:HG22	2.00	0.61
1:C:54:MET:HG3	1:C:218:GLN:HE21	1.66	0.61
1:D:372:ARG:NH2	4:D:570:HOH:O	2.32	0.61
1:B:33:LEU:HD12	1:B:34:PRO:CD	2.31	0.61
1:B:346:ARG:HD2	1:B:353:GLU:OE2	2.01	0.61
1:D:247:PHE:O	1:D:251:LYS:HG2	2.00	0.61
1:C:257:ARG:HH11	1:C:257:ARG:HG2	1.65	0.60
1:D:205:MET:HE2	1:D:300:ILE:HA	1.82	0.60
1:B:101:ARG:NH2	1:B:370:LEU:HB3	2.17	0.60
1:A:123:ARG:HA	1:A:285:GLU:HG3	1.83	0.60
1:C:375:LYS:CB	1:C:376:LYS:HE2	2.29	0.60
1:A:188:GLY:O	1:A:189:ASP:HB3	2.00	0.60
1:D:204:MET:O	1:D:208:ILE:HG12	2.02	0.60
1:C:205:MET:HE2	1:C:300:ILE:CG1	2.31	0.59
1:A:476:LYS:HE2	1:A:477:HIS:NE2	2.18	0.59
1:A:77:ARG:HG2	1:A:77:ARG:NH1	2.15	0.59
1:B:148:ARG:HH11	1:B:184:SER:HB3	1.67	0.59
1:D:281:ASN:ND2	1:D:283:ASN:H	2.01	0.59
1:A:346:ARG:HD2	1:A:353:GLU:OE1	2.02	0.59
1:C:77:ARG:HG2	1:C:77:ARG:NH1	2.10	0.59
1:C:50:ASN:C	1:C:50:ASN:HD22	2.06	0.58
1:A:339:ARG:CZ	1:A:342:LYS:HZ3	2.16	0.58
1:C:50:ASN:ND2	1:C:52:GLU:H	2.01	0.58
1:C:234:GLN:HE21	1:C:234:GLN:N	1.93	0.58
1:C:210:GLN:NE2	4:C:617:HOH:O	2.37	0.58
1:D:456:VAL:HG12	1:D:457:MET:CE	2.33	0.58
1:B:73:LEU:HA	1:B:222:MET:HE3	1.85	0.58
1:B:423:PHE:CE1	1:B:425:LYS:HG2	2.38	0.57
1:D:117:VAL:HG22	2:D:500:HEM:HAD1	1.85	0.57
1:B:318:MET:HE3	1:B:462:LEU:HB3	1.87	0.57
1:A:281:ASN:C	1:A:281:ASN:HD22	2.08	0.57
1:D:186:VAL:CG1	1:D:295:THR:HG23	2.33	0.57
1:D:456:VAL:HG12	1:D:457:MET:HE3	1.86	0.56
1:C:253:GLU:HA	1:C:256:GLN:HE21	1.69	0.56
1:A:37:PRO:HB2	1:A:48:GLN:NE2	2.20	0.56
1:C:152:GLU:HG3	1:C:177:THR:HG23	1.87	0.56
1:B:205:MET:HE2	1:B:300:ILE:CA	2.32	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:SER:HB2	1:A:395:LEU:HG	1.88	0.56
1:B:281:ASN:C	1:B:281:ASN:HD22	2.09	0.56
1:D:206:LEU:HD12	4:D:647:HOH:O	2.06	0.56
1:C:103:GLU:HG2	1:C:390:GLU:OE2	2.05	0.56
1:D:261:PRO:HA	1:D:273:ILE:CD1	2.35	0.55
1:B:53:GLN:OE1	1:B:56:ASN:N	2.19	0.55
1:D:269:ASP:O	1:D:273:ILE:HG12	2.07	0.55
1:A:339:ARG:CZ	1:A:342:LYS:NZ	2.70	0.55
1:D:418:ASN:HD22	1:D:422:GLN:HB2	1.70	0.55
1:B:161:ARG:HG3	1:B:161:ARG:NH1	2.16	0.55
1:D:331:ILE:HG12	1:D:349:MET:HE3	1.89	0.54
1:A:135:LEU:HG	1:A:140:VAL:HG21	1.90	0.54
1:C:433:SER:HB3	2:C:500:HEM:HBA1	1.90	0.54
1:B:143:ARG:O	1:B:147:GLU:HG3	2.08	0.54
1:A:117:VAL:HG22	2:A:500:HEM:HAD1	1.90	0.54
1:D:101:ARG:CD	1:D:117:VAL:O	2.56	0.54
1:C:117:VAL:HG22	2:C:500:HEM:HAD1	1.89	0.54
1:A:400:ARG:HB2	1:A:400:ARG:HH11	1.72	0.53
1:B:494:ARG:O	1:B:495:HIS:HB2	2.08	0.53
1:C:32:LYS:HE2	1:C:384:PHE:CB	2.38	0.53
1:D:50:ASN:HD22	1:D:52:GLU:H	1.54	0.53
1:D:412:ASN:HD21	1:D:414:GLN:HB2	1.72	0.53
1:A:50:ASN:ND2	1:A:52:GLU:H	2.07	0.53
1:C:369:SER:HB2	1:C:395:LEU:HG	1.89	0.53
1:B:379:LYS:HD3	1:B:383:PHE:O	2.09	0.53
1:D:407:ASN:H	1:D:415:HIS:HE1	1.55	0.53
1:A:433:SER:HB3	2:A:500:HEM:HBA1	1.91	0.52
1:B:64:ARG:HG2	1:B:64:ARG:NH1	2.22	0.52
1:B:269:ASP:O	1:B:273:ILE:HG12	2.10	0.52
1:B:369:SER:HB2	1:B:395:LEU:HG	1.91	0.52
1:B:489:MET:HE1	1:B:491:PHE:CZ	2.44	0.52
1:C:346:ARG:HG2	1:C:353:GLU:OE1	2.10	0.52
1:D:110:VAL:HG11	1:D:241:LEU:HD22	1.92	0.52
1:B:293:MET:O	1:B:297:GLN:HG3	2.09	0.52
1:D:450:PHE:O	1:D:454:THR:HG23	2.09	0.52
1:B:261:PRO:HA	1:B:273:ILE:HD12	1.92	0.52
1:D:131:SER:O	1:D:135:LEU:HD13	2.10	0.51
1:D:271:PHE:HB3	1:D:291:LEU:HD13	1.92	0.51
1:D:271:PHE:CG	1:D:291:LEU:HD13	2.45	0.51
1:B:433:SER:HB3	2:B:500:HEM:HBA1	1.93	0.51
1:A:196:LYS:HG3	4:A:613:HOH:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:ARG:HA	1:B:285:GLU:HG3	1.92	0.51
1:B:161:ARG:HG2	1:B:460:PHE:HZ	1.76	0.51
1:D:123:ARG:HA	1:D:285:GLU:HG3	1.93	0.51
1:D:433:SER:HB3	2:D:500:HEM:HBA1	1.93	0.51
1:B:281:ASN:ND2	1:B:283:ASN:H	2.08	0.51
1:C:210:GLN:HA	1:C:483:ILE:CD1	2.40	0.51
1:A:420:LYS:CG	1:A:422:GLN:NE2	2.73	0.51
1:B:442:GLU:O	1:B:446:ARG:HG2	2.10	0.51
1:B:53:GLN:HE21	1:B:478:VAL:HB	1.75	0.51
1:B:412:ASN:OD1	1:B:414:GLN:HB2	2.11	0.51
1:B:32:LYS:HG2	1:B:384:PHE:CB	2.40	0.51
1:D:256:GLN:HB3	1:D:257:ARG:NH1	2.26	0.51
1:D:467:SER:OG	1:D:469:LYS:HG2	2.11	0.50
1:B:62:SER:HB3	1:B:69:PHE:CE2	2.46	0.50
1:A:271:PHE:CD2	1:A:291:LEU:HB2	2.47	0.50
1:B:418:ASN:HD22	1:B:422:GLN:HB2	1.76	0.50
1:B:259:LEU:HD11	1:B:273:ILE:HD11	1.92	0.50
1:D:276:GLN:O	1:D:279:GLU:HB2	2.12	0.50
1:A:33:LEU:HD21	1:A:77:ARG:NH1	2.26	0.50
1:D:142:LYS:O	1:D:145:ILE:HG22	2.11	0.50
1:B:318:MET:CE	1:B:489:MET:HB2	2.39	0.50
1:C:418:ASN:HB2	1:C:422:GLN:N	2.23	0.50
1:B:327:VAL:HG13	1:B:352:MET:HE2	1.94	0.49
1:D:232:GLY:HA3	1:D:234:GLN:HE22	1.77	0.49
1:B:258:THR:HG23	1:B:265:ARG:HH22	1.78	0.49
1:A:208:ILE:HD13	1:A:241:LEU:HD23	1.94	0.49
1:D:253:GLU:CG	1:D:257:ARG:HH21	2.26	0.49
1:A:208:ILE:HD13	1:A:241:LEU:CD2	2.43	0.49
1:C:281:ASN:ND2	1:C:283:ASN:H	2.11	0.49
1:B:261:PRO:HA	1:B:273:ILE:CD1	2.43	0.49
1:D:351:TYR:O	1:D:355:VAL:HG23	2.13	0.49
1:A:32:LYS:HD2	1:A:33:LEU:N	2.19	0.48
1:C:110:VAL:HG11	1:C:241:LEU:HD22	1.94	0.48
1:D:253:GLU:HG2	1:D:257:ARG:NH2	2.28	0.48
1:B:281:ASN:C	1:B:281:ASN:ND2	2.66	0.48
1:A:281:ASN:ND2	1:A:283:ASN:H	2.11	0.48
1:D:405:PHE:O	1:D:408:PRO:HD3	2.13	0.48
1:A:419:GLU:OE1	1:A:419:GLU:CA	2.58	0.48
1:B:89:GLU:CD	1:B:381:ARG:HH21	2.16	0.48
1:D:210:GLN:O	1:D:214:THR:HG23	2.13	0.48
1:B:413:PRO:O	1:B:417:LEU:HD22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:ARG:NH2	1:C:103:GLU:HG3	2.28	0.48
1:B:476:LYS:HE3	1:B:477:HIS:CD2	2.49	0.48
1:D:259:LEU:HD12	1:D:260:ASP:H	1.78	0.47
1:D:463:LYS:HD3	1:D:492:LEU:HD11	1.95	0.47
1:C:355:VAL:O	1:C:359:ILE:HG13	2.14	0.47
1:D:260:ASP:O	1:D:262:ASN:N	2.47	0.47
1:D:418:ASN:ND2	1:D:422:GLN:HB2	2.29	0.47
1:B:259:LEU:HD12	1:B:260:ASP:H	1.79	0.47
1:B:97:GLU:OE1	1:B:378:THR:HG23	2.14	0.47
1:B:101:ARG:CD	1:B:117:VAL:O	2.63	0.47
1:D:268:ILE:O	1:D:272:LEU:HG	2.14	0.47
1:B:77:ARG:HH11	1:B:77:ARG:CG	2.28	0.47
1:B:210:GLN:O	1:B:214:THR:HG23	2.15	0.47
1:B:400:ARG:NE	4:B:546:HOH:O	2.47	0.47
1:C:336:GLY:O	1:C:337:LYS:HG2	2.14	0.47
1:C:423:PHE:CE1	1:C:425:LYS:HG2	2.46	0.47
1:A:50:ASN:C	1:A:50:ASN:HD22	2.17	0.47
1:A:95:ALA:HB1	1:A:436:LYS:HG2	1.97	0.47
1:D:259:LEU:HD12	1:D:260:ASP:N	2.30	0.47
1:B:152:GLU:HG3	1:B:177:THR:HG23	1.96	0.46
1:A:381:ARG:O	1:A:382:ASP:HB2	2.15	0.46
1:B:248:ILE:HG22	1:B:292:VAL:HG13	1.96	0.46
1:B:327:VAL:HG13	1:B:352:MET:CE	2.45	0.46
1:C:153:ALA:O	1:C:157:ILE:HG12	2.15	0.46
1:D:33:LEU:HD11	1:D:77:ARG:NH1	2.30	0.46
1:C:204:MET:O	1:C:208:ILE:HG13	2.15	0.46
1:A:375:LYS:HE2	4:A:606:HOH:O	2.14	0.46
1:D:259:LEU:HD11	1:D:273:ILE:CD1	2.36	0.46
1:D:457:MET:CE	1:D:462:LEU:HD21	2.45	0.46
1:D:462:LEU:HD22	1:D:489:MET:HE1	1.98	0.46
1:D:312:TYR:O	1:D:316:LEU:HD22	2.16	0.46
1:C:50:ASN:HD22	1:C:52:GLU:H	1.64	0.46
1:B:335:ILE:HD13	1:B:341:PRO:HG3	1.99	0.45
1:C:271:PHE:CD2	1:C:291:LEU:HB2	2.50	0.45
1:D:253:GLU:CG	1:D:257:ARG:NH2	2.80	0.45
1:B:94:GLN:NE2	4:B:623:HOH:O	2.48	0.45
1:B:271:PHE:CG	1:B:291:LEU:HD13	2.51	0.45
1:D:281:ASN:C	1:D:281:ASN:HD22	2.20	0.45
1:D:326:LYS:HD2	1:D:351:TYR:CZ	2.52	0.45
1:A:314:PHE:CE2	1:A:457:MET:HE3	2.52	0.45
1:B:248:ILE:CG2	1:B:292:VAL:HG13	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:LEU:O	1:B:276:GLN:HG3	2.16	0.45
1:A:449:LEU:O	1:A:453:PHE:HB2	2.16	0.45
1:D:369:SER:HB2	1:D:395:LEU:HG	1.98	0.45
1:A:116:VAL:HG13	1:A:117:VAL:N	2.31	0.45
1:D:208:ILE:HD12	1:D:241:LEU:HG	1.97	0.45
1:C:281:ASN:C	1:C:281:ASN:HD22	2.20	0.45
1:D:376:LYS:O	1:D:377:ASP:C	2.55	0.45
1:C:103:GLU:HG2	1:C:390:GLU:CD	2.37	0.45
1:D:271:PHE:CB	1:D:291:LEU:HD13	2.46	0.45
1:D:152:GLU:HG3	1:D:177:THR:HG23	1.99	0.44
1:C:92:VAL:HG23	1:C:434:ILE:HD12	1.99	0.44
1:C:95:ALA:HB1	1:C:436:LYS:HD3	1.99	0.44
1:B:172:PHE:HA	1:B:175:SER:OG	2.16	0.44
1:B:324:GLU:HG3	1:B:457:MET:CE	2.47	0.44
1:C:210:GLN:O	1:C:214:THR:HG23	2.18	0.44
1:C:375:LYS:HD2	1:C:375:LYS:HA	1.81	0.44
1:A:332:ASP:OD1	1:A:337:LYS:HE3	2.18	0.44
1:B:195:ASP:OD1	1:B:195:ASP:C	2.56	0.44
1:C:392:TYR:HB3	1:C:394:MET:HE3	1.99	0.44
1:C:437:ARG:HE	2:C:500:HEM:CGD	2.31	0.44
1:D:50:ASN:ND2	1:D:50:ASN:C	2.66	0.44
1:D:234:GLN:NE2	1:D:234:GLN:H	2.15	0.44
1:A:433:SER:CB	2:A:500:HEM:HBA1	2.48	0.44
1:B:208:ILE:HD13	1:B:241:LEU:CD2	2.47	0.44
1:B:489:MET:HE1	1:B:491:PHE:CE2	2.52	0.44
1:C:352:MET:HE3	1:C:454:THR:HG22	2.00	0.44
1:C:405:PHE:O	1:C:408:PRO:HD3	2.17	0.44
1:D:259:LEU:HD21	1:D:273:ILE:HD13	1.99	0.44
1:D:433:SER:CB	2:D:500:HEM:HBA1	2.46	0.44
1:C:76:ARG:CZ	1:C:103:GLU:HG3	2.47	0.44
1:C:100:GLY:HA2	1:C:375:LYS:HE2	1.98	0.44
1:C:462:LEU:HD22	1:C:489:MET:HE1	2.00	0.44
1:A:420:LYS:HB2	1:A:422:GLN:HE21	1.83	0.44
1:A:125:LYS:HD2	4:A:530:HOH:O	2.18	0.44
1:A:358:GLU:HG3	1:A:411:PHE:CD1	2.53	0.43
1:A:378:THR:HG22	1:A:379:LYS:N	2.33	0.43
1:A:204:MET:O	1:A:208:ILE:HG13	2.19	0.43
1:C:453:PHE:O	1:C:457:MET:HG2	2.17	0.43
1:D:365:VAL:O	1:D:481:ALA:HA	2.18	0.43
1:A:210:GLN:O	1:A:214:THR:HG23	2.18	0.43
1:C:365:VAL:O	1:C:481:ALA:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:GLN:NE2	1:B:478:VAL:HB	2.33	0.43
1:B:64:ARG:HH11	1:B:64:ARG:CG	2.25	0.43
1:B:103:GLU:HG2	1:B:390:GLU:OE2	2.19	0.43
1:C:354:ALA:HB2	1:C:417:LEU:HD13	1.99	0.43
1:D:273:ILE:O	1:D:276:GLN:HB2	2.18	0.43
1:D:476:LYS:HB2	1:D:485:ARG:HA	2.00	0.43
1:A:271:PHE:HB3	1:A:291:LEU:HD13	1.99	0.43
1:D:457:MET:HE2	1:D:457:MET:HA	2.00	0.43
1:B:318:MET:HE3	1:B:489:MET:HE3	1.99	0.43
1:D:143:ARG:HA	1:D:146:GLU:HB3	2.01	0.43
1:D:210:GLN:HE21	1:D:477:HIS:HD2	1.67	0.43
1:A:351:TYR:O	1:A:355:VAL:HG23	2.19	0.43
1:B:370:LEU:HD12	1:B:480:PHE:HE1	1.83	0.43
1:D:419:GLU:CD	1:D:419:GLU:N	2.69	0.43
1:D:178:VAL:HG11	1:D:306:VAL:HB	2.00	0.43
1:D:244:LEU:HB3	1:D:296:LEU:HD11	2.01	0.43
1:D:369:SER:HB2	1:D:395:LEU:CD1	2.49	0.43
1:A:352:MET:HE3	1:A:454:THR:HA	2.01	0.43
1:D:258:THR:OG1	1:D:265:ARG:NH1	2.42	0.43
1:A:281:ASN:HD22	1:A:282:PRO:N	2.17	0.42
1:B:64:ARG:HD3	1:B:65:TYR:CE2	2.53	0.42
1:B:419:GLU:CD	1:B:419:GLU:H	2.21	0.42
1:B:319:LYS:C	1:B:321:PRO:HD3	2.40	0.42
1:C:52:GLU:O	1:C:52:GLU:HG2	2.19	0.42
1:A:457:MET:HE1	1:A:462:LEU:HD21	2.01	0.42
1:A:314:PHE:HE2	1:A:457:MET:CE	2.32	0.42
1:B:97:GLU:HG3	4:B:533:HOH:O	2.19	0.42
1:C:143:ARG:HD3	1:C:143:ARG:O	2.18	0.42
1:C:213:SER:HA	1:C:479:GLY:HA3	2.02	0.42
1:D:476:LYS:HE2	1:D:477:HIS:NE2	2.34	0.42
1:C:50:ASN:C	1:C:50:ASN:ND2	2.73	0.42
1:D:148:ARG:NH2	1:D:190:ARG:HB3	2.34	0.42
1:A:153:ALA:O	1:A:157:ILE:HG12	2.20	0.42
1:A:457:MET:CE	1:A:462:LEU:HD21	2.49	0.42
1:B:195:ASP:OD1	1:B:197:GLU:N	2.53	0.42
1:C:143:ARG:HD3	1:C:143:ARG:C	2.40	0.42
1:D:116:VAL:HG13	1:D:117:VAL:N	2.35	0.42
1:C:101:ARG:CD	1:C:117:VAL:O	2.68	0.42
1:C:327:VAL:O	1:C:331:ILE:HG13	2.19	0.42
1:A:206:LEU:HD12	4:A:592:HOH:O	2.18	0.42
1:B:161:ARG:HG2	1:B:460:PHE:CZ	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:GLN:HG3	1:B:237:ALA:N	2.33	0.42
1:C:257:ARG:HG2	1:C:257:ARG:NH1	2.32	0.42
1:A:126:GLN:NE2	4:A:571:HOH:O	2.52	0.41
1:A:152:GLU:HG3	1:A:177:THR:HG23	2.02	0.41
1:A:234:GLN:HG2	1:A:235:GLN:N	2.34	0.41
1:D:210:GLN:HE21	1:D:477:HIS:CD2	2.38	0.41
1:B:59:MET:O	1:B:63:GLU:HG3	2.20	0.41
1:B:400:ARG:NH1	1:B:400:ARG:HG3	2.34	0.41
1:A:50:ASN:ND2	1:A:50:ASN:C	2.74	0.41
1:B:312:TYR:O	1:B:316:LEU:HD22	2.20	0.41
1:D:148:ARG:HH21	1:D:190:ARG:HB3	1.84	0.41
1:A:281:ASN:C	1:A:281:ASN:ND2	2.71	0.41
1:A:322:GLU:OE2	1:A:322:GLU:N	2.34	0.41
1:D:255:ASN:HA	1:D:265:ARG:HH22	1.85	0.41
1:A:401:ASP:OD2	1:A:403:SER:HB3	2.20	0.41
1:C:476:LYS:HB2	1:C:485:ARG:HA	2.02	0.41
1:A:248:ILE:O	1:A:252:VAL:HG23	2.21	0.41
1:B:467:SER:O	1:B:468:PRO:C	2.59	0.41
1:D:140:VAL:HA	1:D:145:ILE:HG21	2.02	0.41
1:D:145:ILE:O	1:D:149:ILE:HG13	2.21	0.41
1:D:412:ASN:ND2	1:D:414:GLN:HB2	2.33	0.41
1:B:439:CYS:HB2	2:B:500:HEM:NA	2.34	0.41
1:C:210:GLN:HA	1:C:483:ILE:HD12	2.03	0.41
1:C:375:LYS:O	1:C:387:LYS:HG3	2.20	0.41
1:D:342:LYS:HB2	1:D:342:LYS:HE3	1.85	0.41
1:A:296:LEU:HD11	1:A:300:ILE:HD11	2.03	0.41
1:B:77:ARG:CG	1:B:77:ARG:NH1	2.84	0.41
1:B:213:SER:HA	1:B:479:GLY:HA3	2.03	0.41
1:B:252:VAL:O	1:B:256:GLN:HG3	2.21	0.41
1:B:453:PHE:O	1:B:457:MET:HG2	2.21	0.41
1:C:101:ARG:HD2	1:C:117:VAL:O	2.20	0.41
1:C:330:GLU:OE1	1:C:349:MET:HB3	2.21	0.41
1:D:281:ASN:ND2	1:D:281:ASN:C	2.73	0.41
1:A:462:LEU:HD22	1:A:489:MET:HE1	2.01	0.41
1:C:210:GLN:HG2	4:C:676:HOH:O	2.21	0.41
1:C:319:LYS:HD3	1:C:471:ILE:HB	2.03	0.41
1:A:274:ARG:HA	1:A:274:ARG:HD2	1.77	0.40
1:C:375:LYS:CE	4:C:585:HOH:O	2.68	0.40
1:C:342:LYS:HG2	1:C:345:ASP:OD2	2.20	0.40
1:A:163:THR:HG21	1:A:168:ILE:HD13	2.02	0.40
1:A:326:LYS:HB2	1:A:351:TYR:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:LYS:CB	1:A:422:GLN:HE21	2.35	0.40
1:C:433:SER:CB	2:C:500:HEM:HBA1	2.51	0.40
1:D:208:ILE:CD1	1:D:240:LEU:HB2	2.48	0.40
1:D:332:ASP:CG	1:D:494:ARG:HH22	2.23	0.40
1:B:433:SER:CB	2:B:500:HEM:HBA1	2.51	0.40
1:B:437:ARG:HE	2:B:500:HEM:CGD	2.34	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:609:HOH:O	4:C:671:HOH:O[1_554]	2.14	0.06

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%)	448 (97%)	14 (3%)	0	100	100
1	B	462/476 (97%)	445 (96%)	16 (4%)	1 (0%)	47	38
1	C	461/476 (97%)	448 (97%)	13 (3%)	0	100	100
1	D	462/476 (97%)	442 (96%)	18 (4%)	2 (0%)	34	22
All	All	1847/1904 (97%)	1783 (96%)	61 (3%)	3 (0%)	47	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	140	VAL
1	D	261	PRO
1	B	261	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	411/422 (97%)	397 (97%)	14 (3%)	37	25
1	B	412/422 (98%)	393 (95%)	19 (5%)	27	14
1	C	411/422 (97%)	399 (97%)	12 (3%)	42	31
1	D	411/422 (97%)	396 (96%)	15 (4%)	35	23
All	All	1645/1688 (98%)	1585 (96%)	60 (4%)	35	23

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	LEU
1	A	50	ASN
1	A	77	ARG
1	A	135	LEU
1	A	167	ASN
1	A	189	ASP
1	A	236	GLN
1	A	281	ASN
1	A	312	TYR
1	A	316	LEU
1	A	353	GLU
1	A	375	LYS
1	A	400	ARG
1	A	419	GLU
1	B	48	GLN
1	B	52	GLU
1	B	53	GLN
1	B	135	LEU
1	B	167	ASN
1	B	174	LEU
1	B	234	GLN
1	B	236	GLN
1	B	256	GLN
1	B	260	ASP

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Mol	Chain	Res	Type
1	B	274	ARG
1	B	281	ASN
1	B	312	TYR
1	B	316	LEU
1	B	373	ARG
1	B	379	LYS
1	B	417	LEU
1	B	419	GLU
1	B	495	HIS
1	C	50	ASN
1	C	77	ARG
1	C	143	ARG
1	C	148	ARG
1	C	174	LEU
1	C	234	GLN
1	C	251	LYS
1	C	274	ARG
1	C	281	ASN
1	C	312	TYR
1	C	376	LYS
1	C	417	LEU
1	D	40	LEU
1	D	50	ASN
1	D	174	LEU
1	D	210	GLN
1	D	234	GLN
1	D	256	GLN
1	D	262	ASN
1	D	263	SER
1	D	279	GLU
1	D	281	ASN
1	D	312	TYR
1	D	316	LEU
1	D	353	GLU
1	D	417	LEU
1	D	419	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	53	GLN

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Mol	Chain	Res	Type
1	A	56	ASN
1	A	126	GLN
1	A	218	GLN
1	A	276	GLN
1	A	281	ASN
1	A	283	ASN
1	A	320	HIS
1	A	422	GLN
1	B	48	GLN
1	B	50	ASN
1	B	56	ASN
1	B	94	GLN
1	B	126	GLN
1	B	210	GLN
1	B	218	GLN
1	B	234	GLN
1	B	281	ASN
1	B	328	HIS
1	B	418	ASN
1	B	422	GLN
1	B	477	HIS
1	C	45	ASN
1	C	50	ASN
1	C	53	GLN
1	C	56	ASN
1	C	94	GLN
1	C	126	GLN
1	C	167	ASN
1	C	210	GLN
1	C	218	GLN
1	C	234	GLN
1	C	256	GLN
1	C	281	ASN
1	C	414	GLN
1	C	418	ASN
1	D	50	ASN
1	D	53	GLN
1	D	56	ASN
1	D	94	GLN
1	D	167	ASN
1	D	210	GLN
1	D	218	GLN

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Mol	Chain	Res	Type
1	D	234	GLN
1	D	239	GLN
1	D	256	GLN
1	D	281	ASN
1	D	283	ASN
1	D	415	HIS
1	D	418	ASN
1	D	422	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	D	500	4,1	41,50,50	2.19	15 (36%)	45,82,82	1.96	9 (20%)
3	EDO	C	501	-	3,3,3	0.58	0	2,2,2	0.29	0
2	HEM	C	500	4,1	41,50,50	2.17	15 (36%)	45,82,82	2.04	9 (20%)
2	HEM	B	500	4,1	41,50,50	2.17	14 (34%)	45,82,82	1.97	9 (20%)
3	EDO	B	501	-	3,3,3	0.63	0	2,2,2	0.30	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEM	A	500	4,1	41,50,50	2.20	16 (39%)	45,82,82	1.99	9 (20%)
3	EDO	D	501	-	3,3,3	0.66	0	2,2,2	0.29	0
3	EDO	A	501	-	3,3,3	0.55	0	2,2,2	0.29	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	D	500	4,1	-	2/12/54/54	-
3	EDO	C	501	-	-	0/1/1/1	-
2	HEM	C	500	4,1	-	1/12/54/54	-
2	HEM	B	500	4,1	-	4/12/54/54	-
3	EDO	B	501	-	-	0/1/1/1	-
2	HEM	A	500	4,1	-	0/12/54/54	-
3	EDO	D	501	-	-	0/1/1/1	-
3	EDO	A	501	-	-	0/1/1/1	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	HEM	C3C-CAC	-5.42	1.36	1.47
2	D	500	HEM	C3C-CAC	-5.00	1.37	1.47
2	B	500	HEM	C3C-CAC	-4.93	1.37	1.47
2	C	500	HEM	C3C-CAC	-4.84	1.37	1.47
2	B	500	HEM	C1D-ND	-4.55	1.29	1.38
2	C	500	HEM	C1D-ND	-4.52	1.29	1.38
2	A	500	HEM	C1B-NB	-4.42	1.32	1.40
2	D	500	HEM	C1B-NB	-4.33	1.32	1.40
2	A	500	HEM	C1D-ND	-4.28	1.30	1.38
2	D	500	HEM	C1D-ND	-4.24	1.30	1.38
2	B	500	HEM	C1B-NB	-4.22	1.33	1.40
2	C	500	HEM	C4D-ND	-3.96	1.33	1.40
2	A	500	HEM	C4D-ND	-3.90	1.33	1.40
2	D	500	HEM	C4D-ND	-3.88	1.33	1.40
2	C	500	HEM	C1B-NB	-3.87	1.33	1.40
2	B	500	HEM	CBB-CAB	3.80	1.49	1.30
2	D	500	HEM	CBB-CAB	3.77	1.49	1.30
2	B	500	HEM	C4D-ND	-3.71	1.33	1.40
2	A	500	HEM	CBB-CAB	3.68	1.48	1.30
2	C	500	HEM	CBB-CAB	3.60	1.48	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	HEM	C4B-NB	-3.43	1.31	1.38
2	D	500	HEM	CMA-C3A	3.36	1.58	1.51
2	A	500	HEM	C4B-NB	-3.33	1.31	1.38
2	B	500	HEM	C4B-NB	-3.27	1.32	1.38
2	A	500	HEM	CMA-C3A	3.25	1.58	1.51
2	C	500	HEM	CMA-C3A	3.04	1.58	1.51
2	D	500	HEM	C4B-NB	-2.99	1.32	1.38
2	C	500	HEM	C3B-C2B	2.92	1.43	1.37
2	B	500	HEM	CMA-C3A	2.91	1.57	1.51
2	D	500	HEM	C3B-C2B	2.90	1.43	1.37
2	D	500	HEM	O2A-CGA	-2.67	1.21	1.30
2	B	500	HEM	O2A-CGA	-2.65	1.21	1.30
2	C	500	HEM	O2A-CGA	-2.59	1.22	1.30
2	D	500	HEM	C4D-C3D	-2.45	1.40	1.45
2	A	500	HEM	C3B-C2B	2.44	1.42	1.37
2	A	500	HEM	O2A-CGA	-2.40	1.22	1.30
2	B	500	HEM	FE-ND	2.40	2.08	1.96
2	D	500	HEM	CMC-C2C	2.35	1.57	1.51
2	B	500	HEM	C3B-C2B	2.31	1.42	1.37
2	A	500	HEM	FE-ND	2.30	2.08	1.96
2	C	500	HEM	CMC-C2C	2.29	1.57	1.51
2	D	500	HEM	C4A-NA	-2.27	1.31	1.36
2	C	500	HEM	FE-ND	2.26	2.08	1.96
2	D	500	HEM	FE-ND	2.26	2.08	1.96
2	C	500	HEM	C1D-C2D	-2.25	1.40	1.44
2	A	500	HEM	C4D-C3D	-2.24	1.41	1.45
2	A	500	HEM	C1D-C2D	-2.23	1.40	1.44
2	B	500	HEM	CAD-C3D	2.21	1.57	1.51
2	A	500	HEM	CMD-C2D	2.19	1.55	1.50
2	C	500	HEM	C4D-C3D	-2.16	1.41	1.45
2	B	500	HEM	CBD-CGD	2.16	1.55	1.50
2	B	500	HEM	CMC-C2C	2.15	1.56	1.51
2	C	500	HEM	C4A-NA	-2.14	1.31	1.36
2	A	500	HEM	C4A-NA	-2.12	1.31	1.36
2	A	500	HEM	CMC-C2C	2.10	1.56	1.51
2	B	500	HEM	C4D-C3D	-2.10	1.41	1.45
2	D	500	HEM	CMD-C2D	2.06	1.55	1.50
2	A	500	HEM	FE-NB	2.05	2.07	1.96
2	D	500	HEM	FE-NB	2.03	2.06	1.96
2	C	500	HEM	CAD-C3D	2.03	1.56	1.51

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	500	HEM	C4B-CHC-C1C	7.02	131.82	122.56
2	C	500	HEM	C4B-CHC-C1C	7.01	131.81	122.56
2	D	500	HEM	C4B-CHC-C1C	6.87	131.63	122.56
2	B	500	HEM	C4B-CHC-C1C	6.58	131.24	122.56
2	B	500	HEM	C4C-CHD-C1D	6.30	130.87	122.56
2	C	500	HEM	C4C-CHD-C1D	6.10	130.60	122.56
2	A	500	HEM	C4C-CHD-C1D	6.06	130.55	122.56
2	D	500	HEM	C4C-CHD-C1D	5.51	129.83	122.56
2	D	500	HEM	C2C-C3C-C4C	-3.51	104.45	106.90
2	C	500	HEM	C2C-C3C-C4C	-3.29	104.60	106.90
2	D	500	HEM	C4B-C3B-C2B	-3.19	104.58	107.11
2	B	500	HEM	C2C-C3C-C4C	-3.15	104.70	106.90
2	C	500	HEM	C4D-ND-C1D	3.10	108.27	105.07
2	A	500	HEM	C4B-C3B-C2B	-3.07	104.68	107.11
2	D	500	HEM	C4D-ND-C1D	3.06	108.23	105.07
2	B	500	HEM	C4B-C3B-C2B	-3.06	104.69	107.11
2	C	500	HEM	C1B-NB-C4B	3.05	108.22	105.07
2	C	500	HEM	C4B-C3B-C2B	-3.04	104.70	107.11
2	A	500	HEM	C4D-ND-C1D	2.95	108.12	105.07
2	B	500	HEM	C4D-ND-C1D	2.95	108.12	105.07
2	D	500	HEM	C1B-NB-C4B	2.91	108.08	105.07
2	A	500	HEM	C1B-NB-C4B	2.91	108.08	105.07
2	A	500	HEM	C2C-C3C-C4C	-2.85	104.91	106.90
2	A	500	HEM	C3B-C2B-C1B	-2.72	104.47	106.49
2	C	500	HEM	C3B-C2B-C1B	-2.72	104.47	106.49
2	B	500	HEM	C1B-NB-C4B	2.66	107.82	105.07
2	D	500	HEM	C3B-C2B-C1B	-2.64	104.53	106.49
2	A	500	HEM	O2A-CGA-CBA	2.62	122.45	114.03
2	B	500	HEM	C3B-C2B-C1B	-2.60	104.56	106.49
2	C	500	HEM	O2A-CGA-CBA	2.49	122.03	114.03
2	D	500	HEM	O2A-CGA-CBA	2.43	121.85	114.03
2	B	500	HEM	O2A-CGA-CBA	2.41	121.79	114.03
2	C	500	HEM	CAD-CBD-CGD	2.36	118.67	113.60
2	A	500	HEM	CHB-C1B-NB	-2.26	121.58	124.38
2	D	500	HEM	CHB-C1B-NB	-2.14	121.74	124.38
2	B	500	HEM	C4D-C3D-C2D	-2.02	103.96	106.90

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	HEM	CAA-CBA-CGA-O1A
2	D	500	HEM	CAA-CBA-CGA-O1A

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

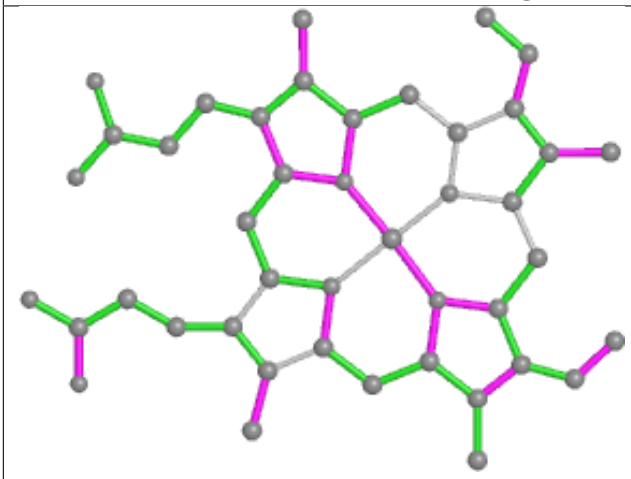
There are no ring outliers.

4 monomers are involved in 14 short contacts:

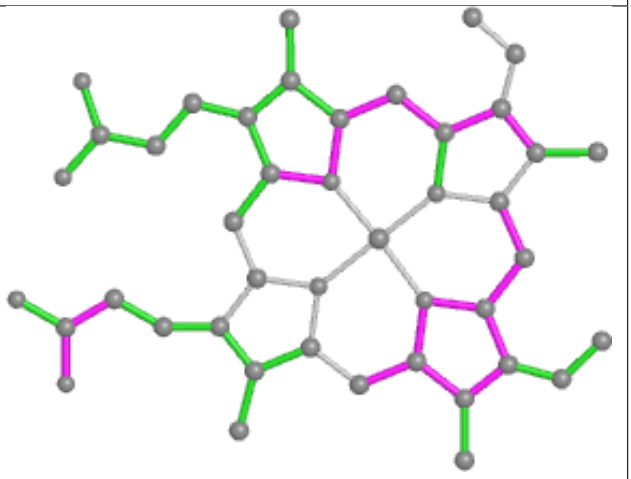
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500	HEM	3	0
2	C	500	HEM	4	0
2	B	500	HEM	4	0
2	A	500	HEM	3	0

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.

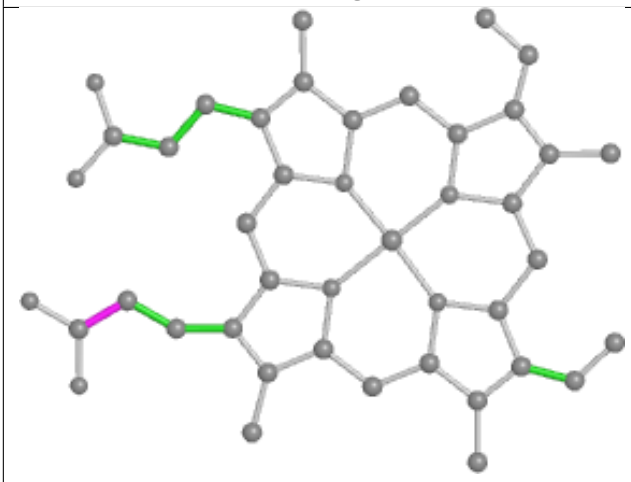
Ligand HEM D 500



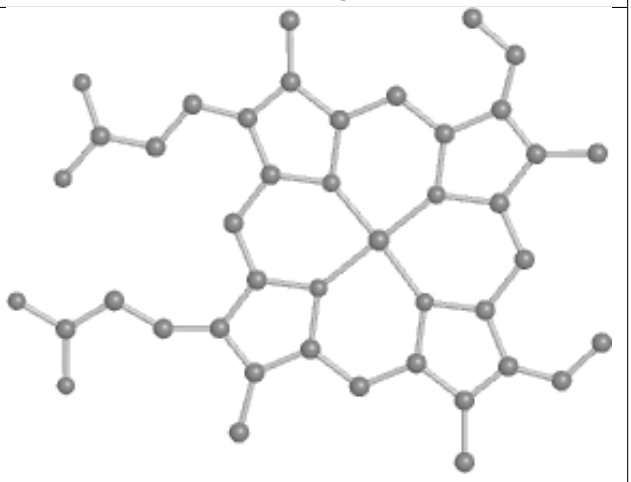
Bond lengths



Bond angles

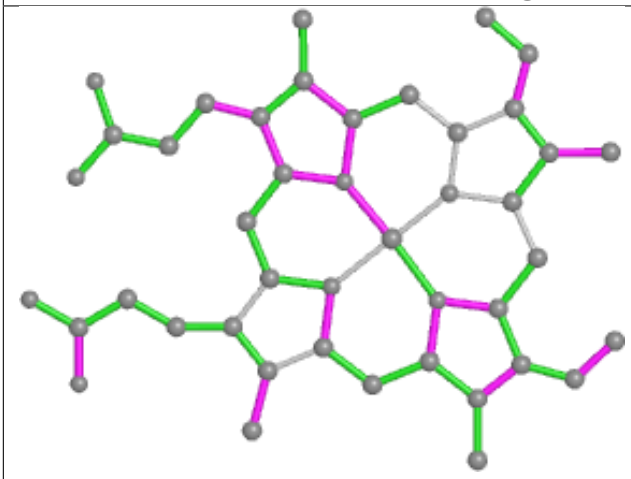


Torsions

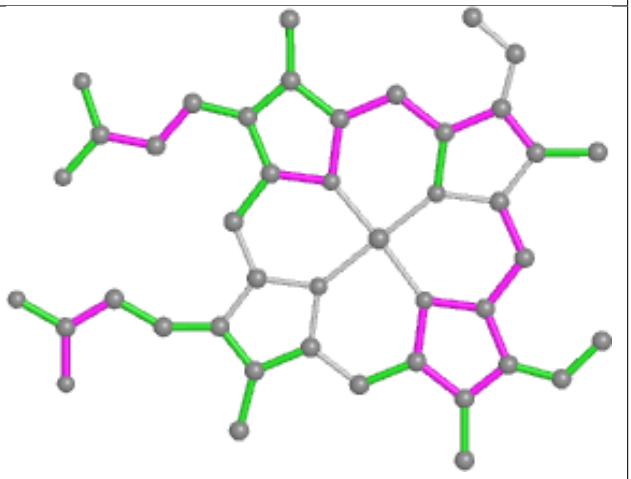


Rings

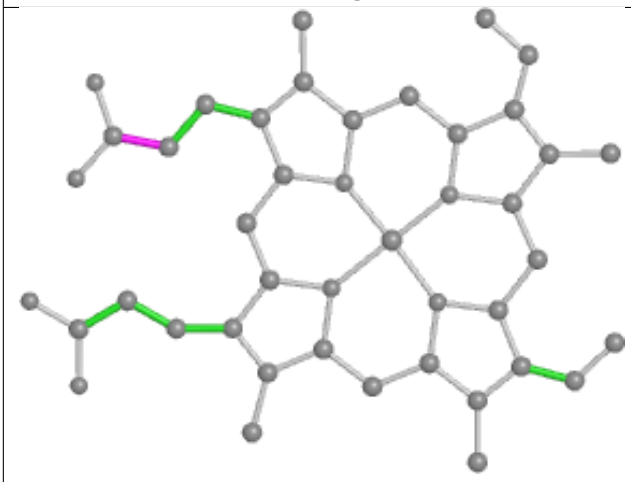
Ligand HEM C 500



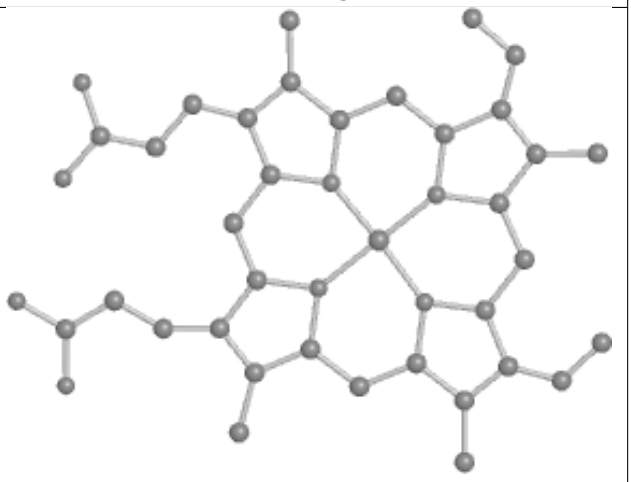
Bond lengths



Bond angles

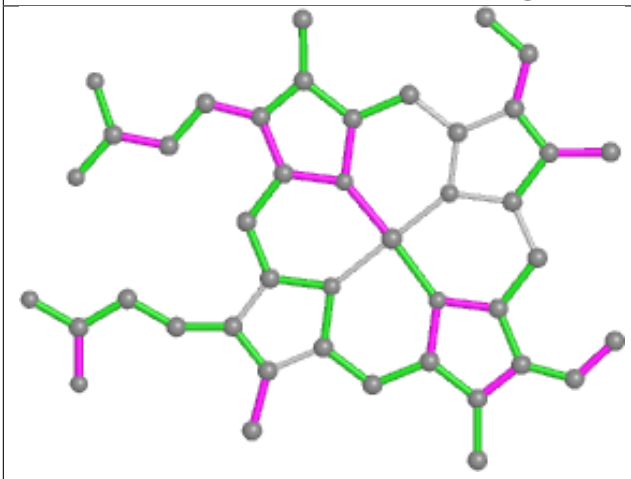


Torsions

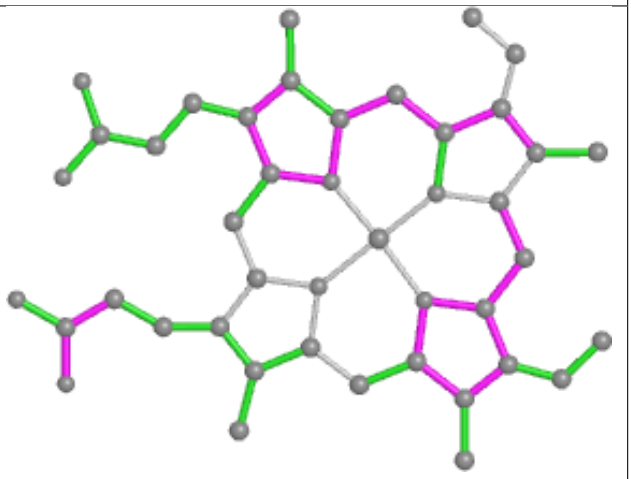


Rings

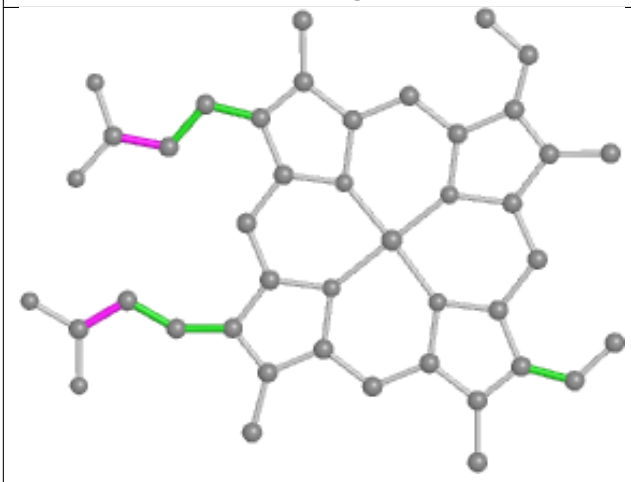
Ligand HEM B 500



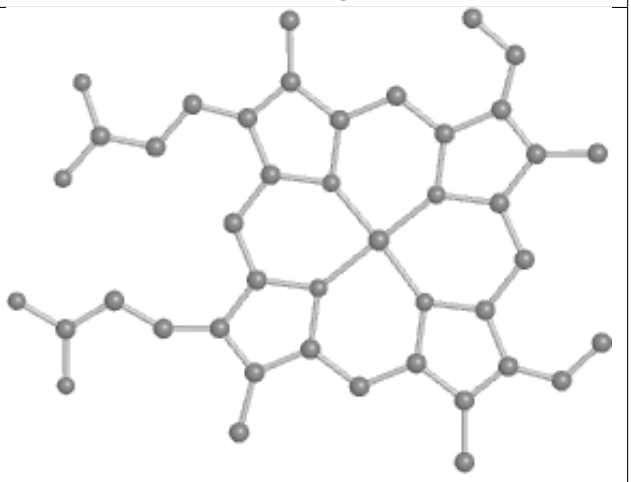
Bond lengths



Bond angles

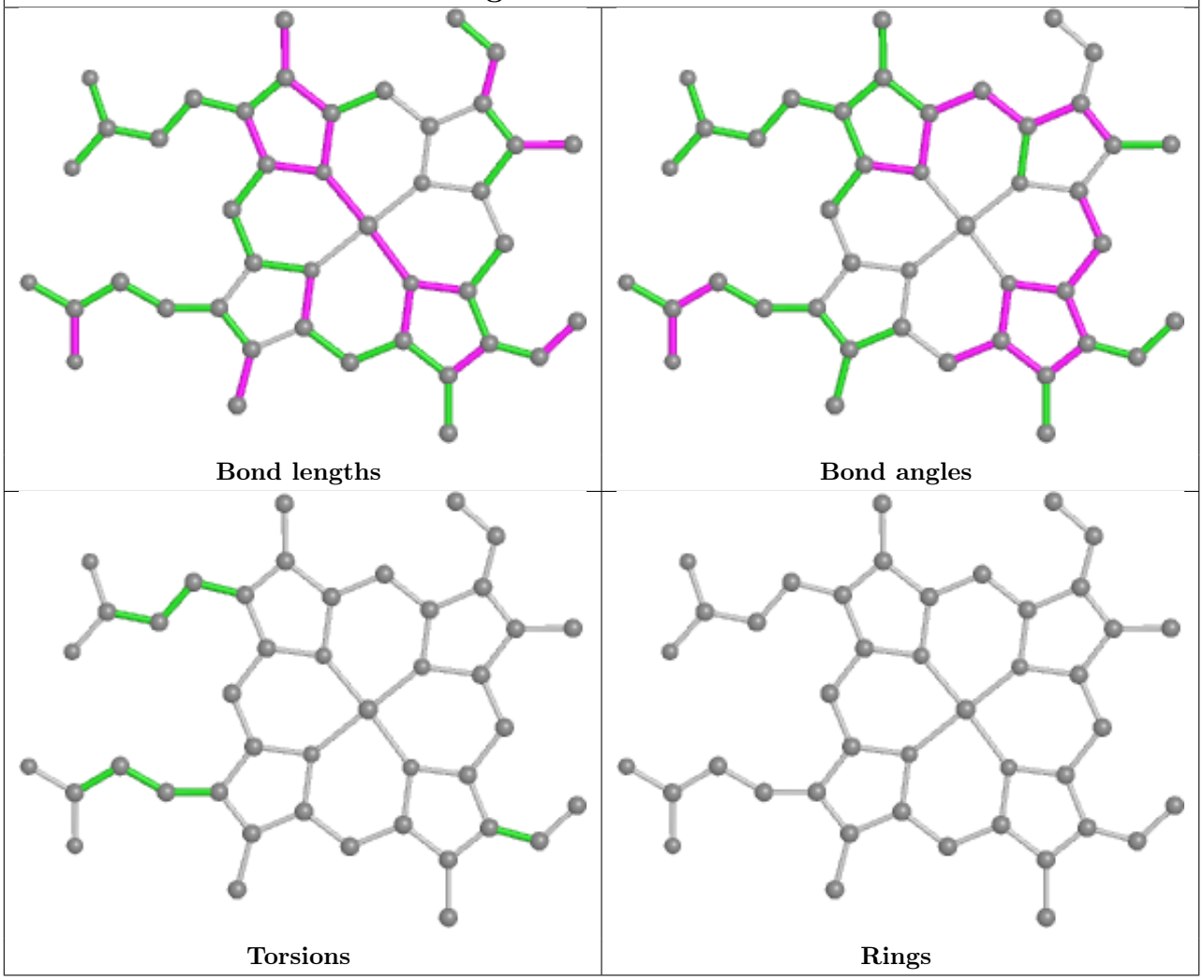


Torsions



Rings

Ligand HEM A 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%)	0.34	24 (5%)	27	37	23, 34, 44, 50	1 (0%)
1	B	464/476 (97%)	0.44	32 (6%)	16	25	26, 36, 45, 50	0
1	C	463/476 (97%)	0.28	18 (3%)	39	49	22, 33, 44, 50	0
1	D	464/476 (97%)	0.48	44 (9%)	8	13	23, 35, 47, 51	0
All	All	1855/1904 (97%)	0.39	118 (6%)	19	28	22, 34, 45, 51	1 (0%)

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	370	LEU	12.1
1	B	495	HIS	7.5
1	D	143	ARG	5.9
1	D	280	LYS	4.8
1	B	143	ARG	4.7
1	D	31	GLY	4.4
1	B	196	LYS	4.3
1	D	300	ILE	4.2
1	D	420	LYS	4.2
1	D	138	PHE	4.2
1	D	142	LYS	4.0
1	D	262	ASN	3.8
1	D	305	THR	3.8
1	A	280	LYS	3.6
1	B	259	LEU	3.6
1	C	282	PRO	3.6
1	A	356	ILE	3.5
1	D	301	GLY	3.4
1	D	263	SER	3.4
1	A	143	ARG	3.3
1	C	418	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	419	GLU	3.2
1	C	370	LEU	3.2
1	A	257	ARG	3.1
1	C	419	GLU	3.1
1	D	139	GLY	3.0
1	D	418	ASN	3.0
1	D	310	LEU	3.0
1	A	382	ASP	3.0
1	C	305	THR	3.0
1	B	419	GLU	3.0
1	C	298	LEU	2.9
1	D	209	PHE	2.9
1	D	480	PHE	2.8
1	C	310	LEU	2.8
1	D	445	ALA	2.8
1	A	359	ILE	2.8
1	B	257	ARG	2.8
1	D	366	ILE	2.8
1	B	337	LYS	2.8
1	A	32	LYS	2.8
1	B	453	PHE	2.8
1	A	365	VAL	2.8
1	D	189	ASP	2.7
1	D	302	GLY	2.7
1	B	429	PHE	2.7
1	B	262	ASN	2.7
1	D	298	LEU	2.7
1	B	260	ASP	2.7
1	D	140	VAL	2.7
1	D	338	ASN	2.6
1	C	301	GLY	2.6
1	D	141	GLY	2.6
1	D	306	VAL	2.6
1	D	254	HIS	2.5
1	A	31	GLY	2.5
1	D	376	LYS	2.5
1	B	418	ASN	2.5
1	C	470	ASP	2.5
1	C	384	PHE	2.5
1	B	452	PHE	2.5
1	B	382	ASP	2.4
1	B	138	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	174	LEU	2.4
1	B	276	GLN	2.4
1	B	392	TYR	2.4
1	C	469	LYS	2.4
1	B	256	GLN	2.4
1	D	359	ILE	2.4
1	A	310	LEU	2.4
1	C	480	PHE	2.4
1	D	299	PHE	2.4
1	B	469	LYS	2.4
1	D	276	GLN	2.4
1	D	107	PHE	2.4
1	D	257	ARG	2.4
1	D	308	THR	2.4
1	A	262	ASN	2.4
1	D	196	LYS	2.4
1	D	337	LYS	2.3
1	D	137	ASP	2.3
1	B	194	LYS	2.3
1	A	469	LYS	2.3
1	B	32	LYS	2.3
1	A	366	ILE	2.3
1	B	356	ILE	2.3
1	D	356	ILE	2.3
1	D	449	LEU	2.3
1	B	137	ASP	2.3
1	C	303	THR	2.3
1	B	310	LEU	2.3
1	A	63	GLU	2.3
1	B	141	GLY	2.3
1	A	419	GLU	2.3
1	B	314	PHE	2.2
1	A	282	PRO	2.2
1	B	263	SER	2.2
1	D	260	ASP	2.2
1	C	309	THR	2.2
1	D	282	PRO	2.2
1	A	420	LYS	2.2
1	A	384	PHE	2.2
1	A	403	SER	2.1
1	B	136	ARG	2.1
1	B	258	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	194	LYS	2.1
1	A	391	VAL	2.1
1	A	33	LEU	2.1
1	C	420	LYS	2.1
1	A	392	TYR	2.1
1	C	366	ILE	2.1
1	D	250	LYS	2.1
1	A	142	LYS	2.0
1	D	481	ALA	2.0
1	B	261	PRO	2.0
1	B	395	LEU	2.0
1	B	60	LYS	2.0
1	D	340	GLN	2.0

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, 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.

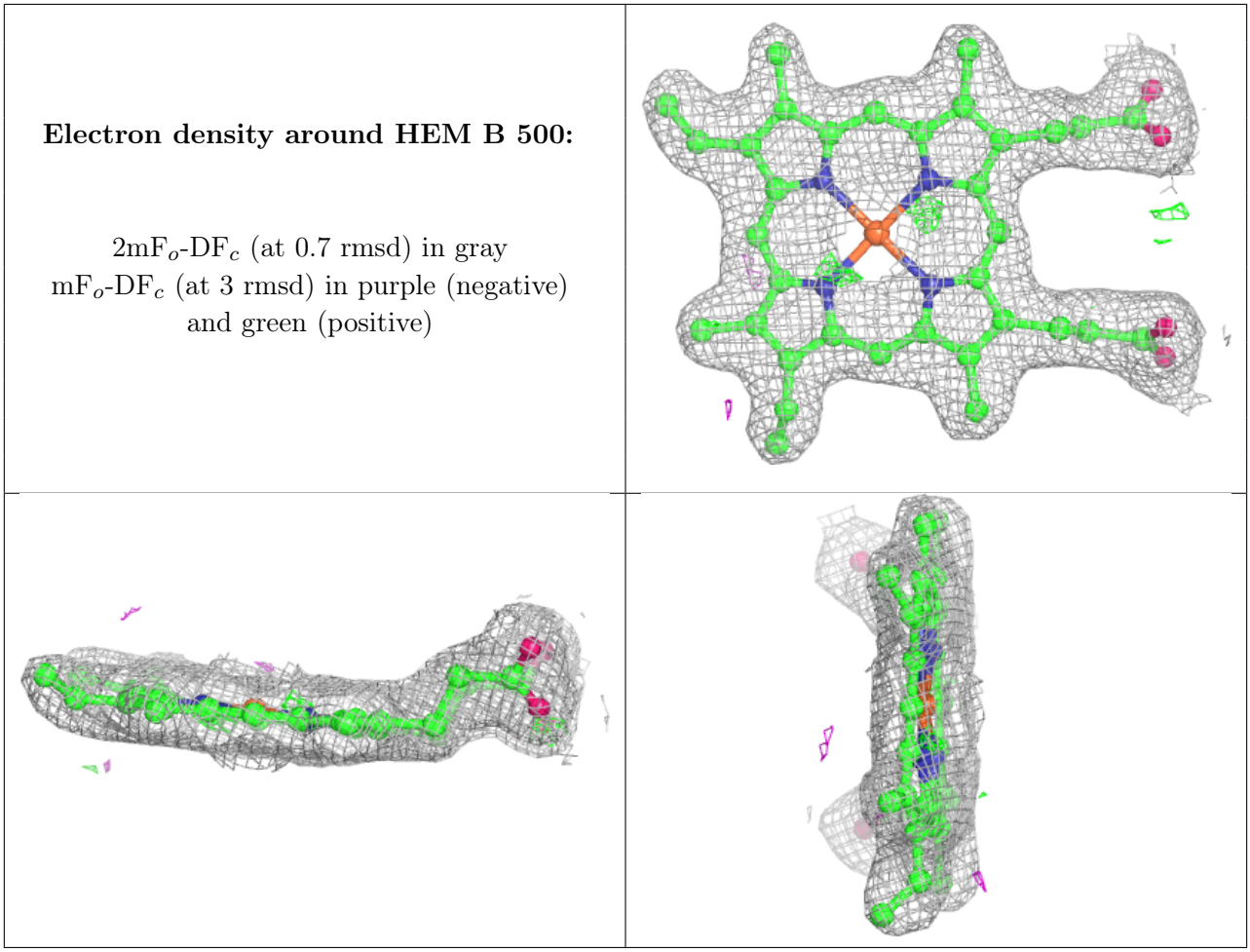
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	B	501	4/4	0.79	0.36	40,42,42,47	0
3	EDO	D	501	4/4	0.80	0.61	40,40,43,48	0
3	EDO	C	501	4/4	0.84	0.51	40,40,42,45	0
3	EDO	A	501	4/4	0.87	0.38	42,42,43,44	0
2	HEM	B	500	43/43	0.97	0.16	25,29,31,38	0
2	HEM	D	500	43/43	0.97	0.18	25,30,33,37	0
2	HEM	A	500	43/43	0.97	0.17	23,27,30,33	0
2	HEM	C	500	43/43	0.98	0.19	24,28,31,36	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.

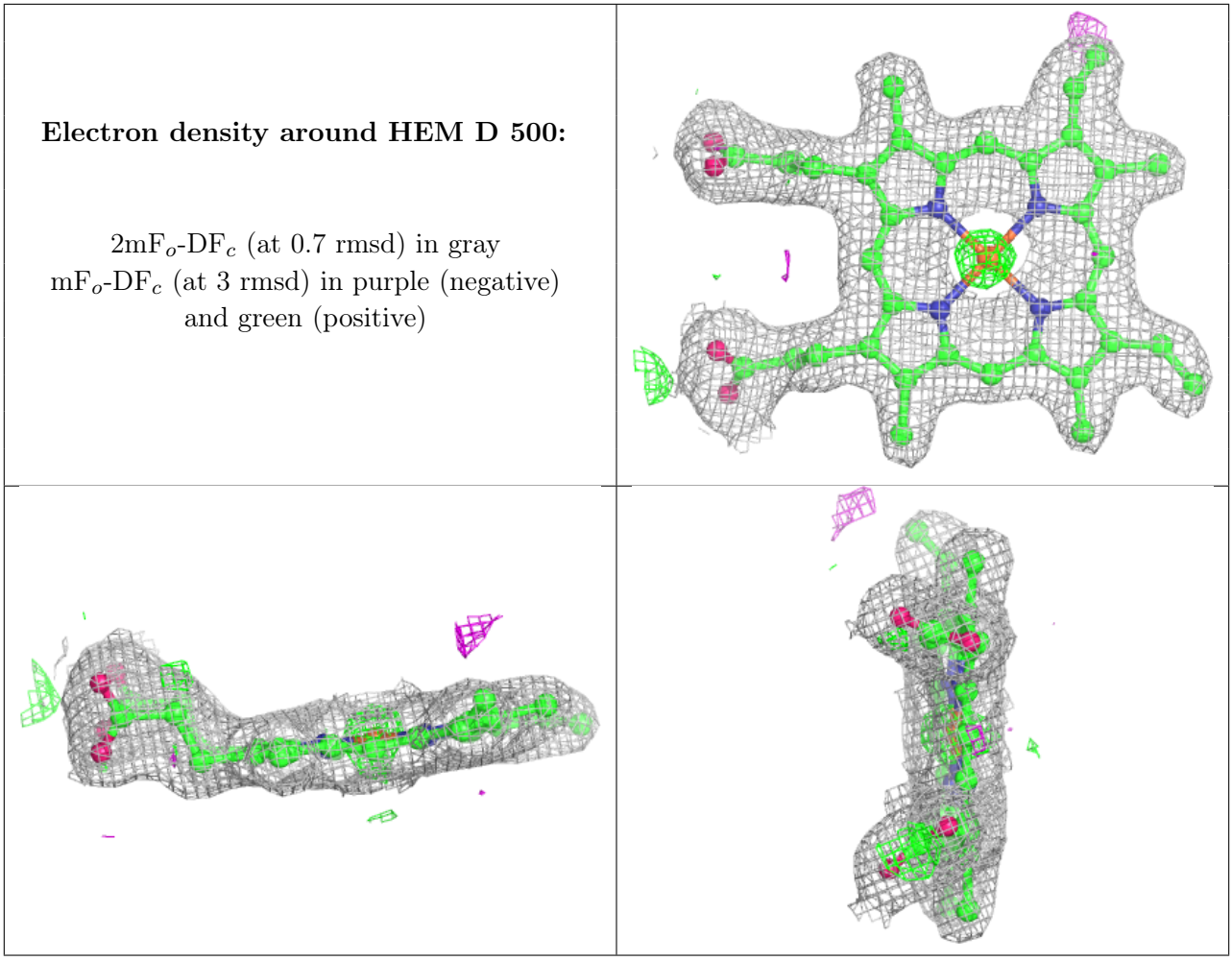
Electron density around HEM B 500:

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



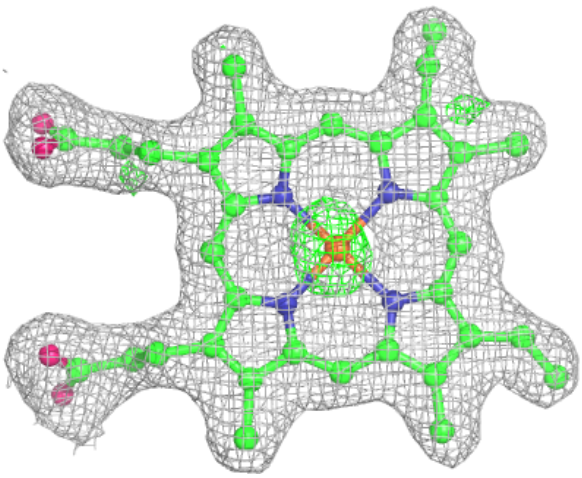
Electron density around HEM D 500:

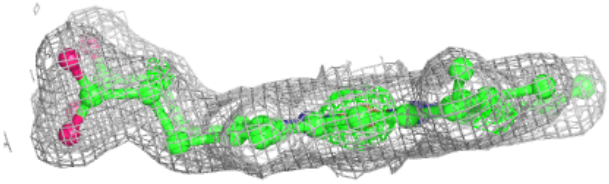
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

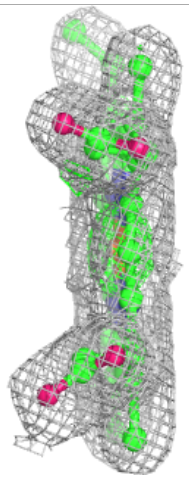


Electron density around HEM A 500:

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

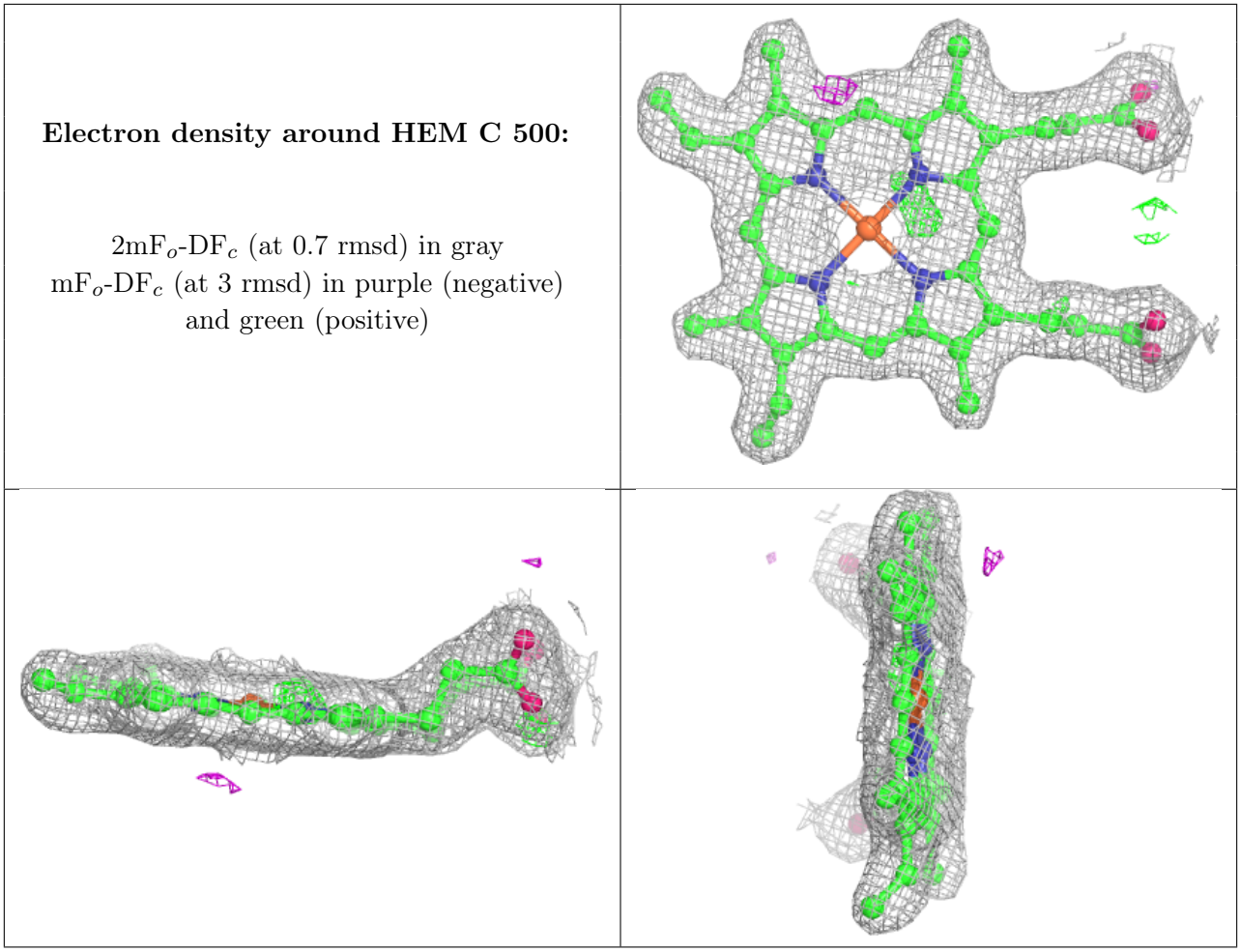






Electron density around HEM C 500:

$2mF_o$-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 (i)

There are no such residues in this entry.