Full wwPDB X-ray Structure Validation Report ⓘ

Aug 18, 2026 – 10:26 pm BST

PDB ID	:	1QJS / pdb_00001qjs
Title	:	mammalian blood serum haemopexin glycosylated-native protein and in complex with its ligand haem
Authors	:	Paoli, M.; Baker, H.M.; Morgan, W.T.; Smith, A.; Baker, E.N.
Deposited on	:	1999-07-01
Resolution	:	2.90 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 ⓘ 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 ⓘ) were used in the production of this report:

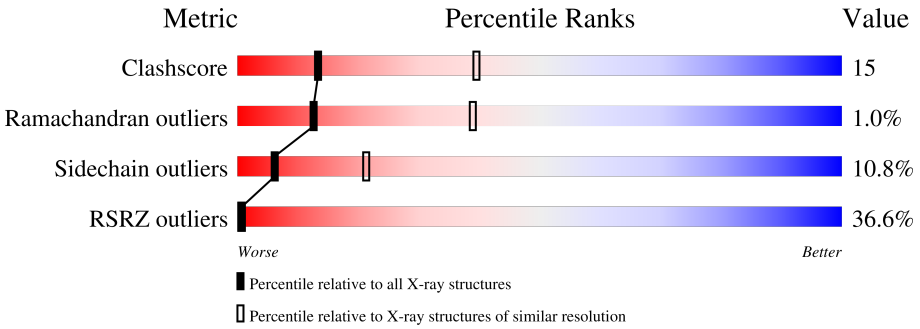
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	460	21% 52% 27% 8% • 11%
1	B	460	44% 50% 29% 9% • 11%

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
2	HEM	B	500	-	-	X	-
3	PO4	B	501	-	-	X	-

2 Entry composition

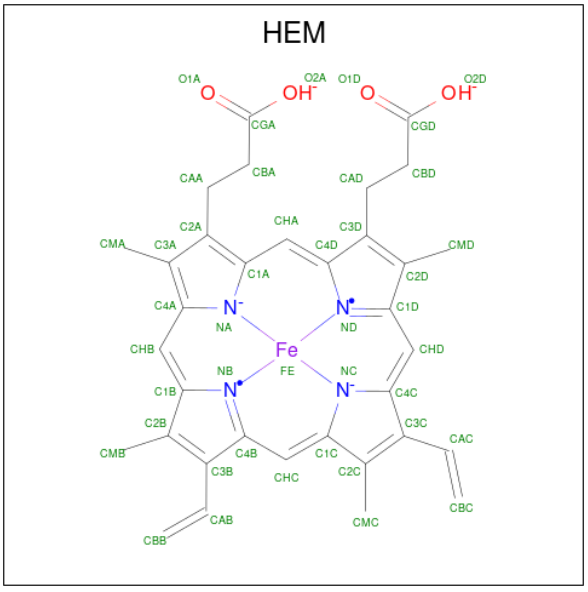
There are 5 unique types of molecules in this entry. The entry contains 6686 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 HEMOPEXIN.

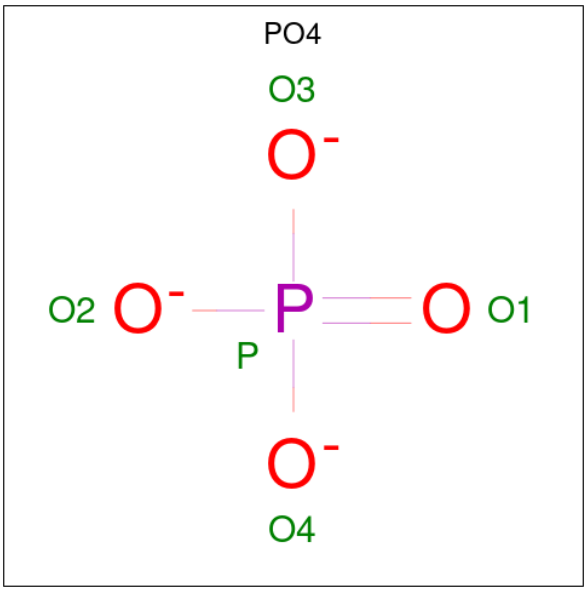
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3289	2102	579	592	16			
1	B	408	Total	C	N	O	S	0	0	0
			3289	2102	579	592	16			

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



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

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Cl 2 2	0	0
4	B	2	Total Cl 2 2	0	0

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

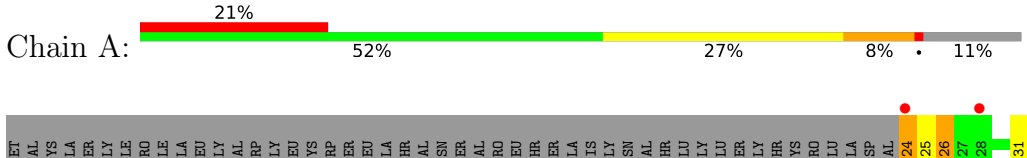
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	4	Total Na 4 4	0	0
5	B	4	Total Na 4 4	0	0

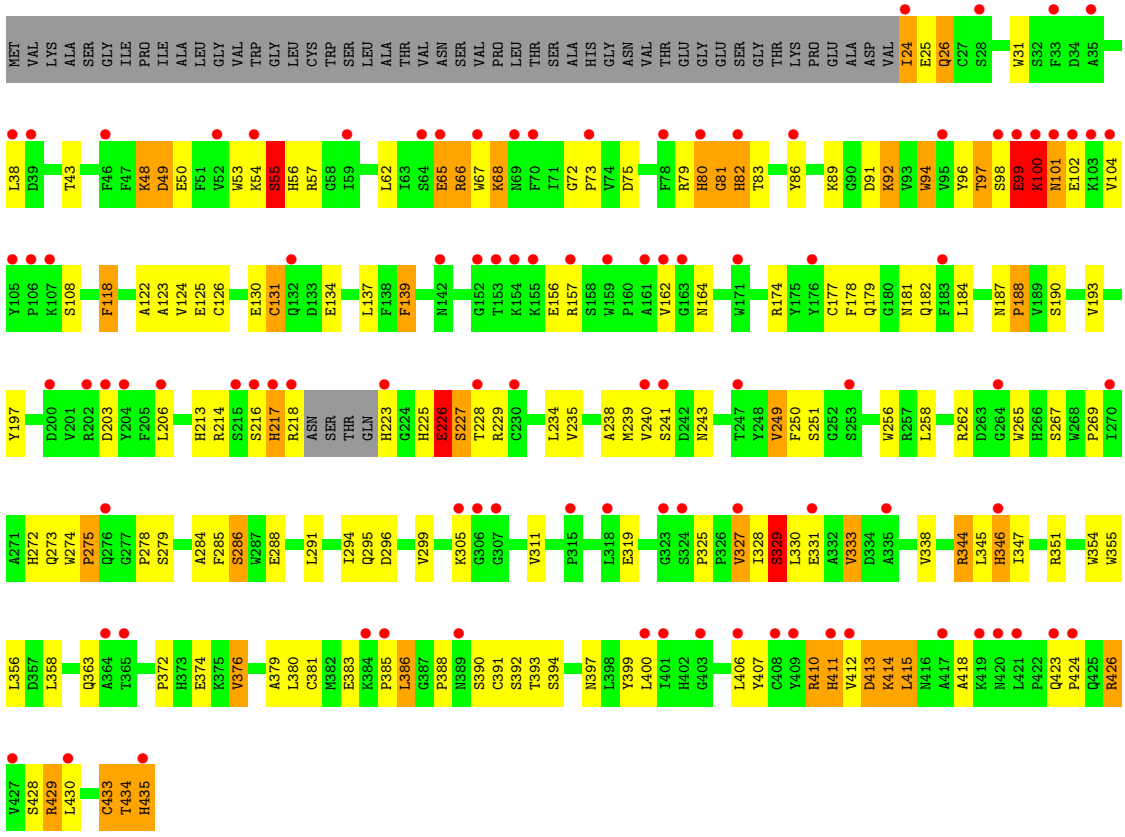
3 Residue-property plots (i)

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: HEMOPEXIN

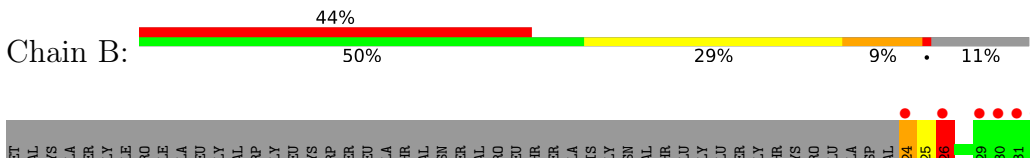
Chain A:

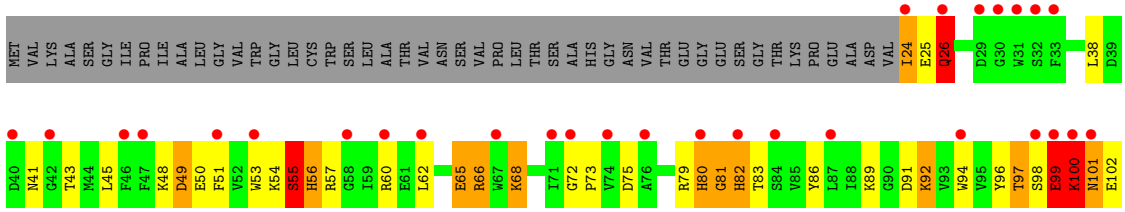


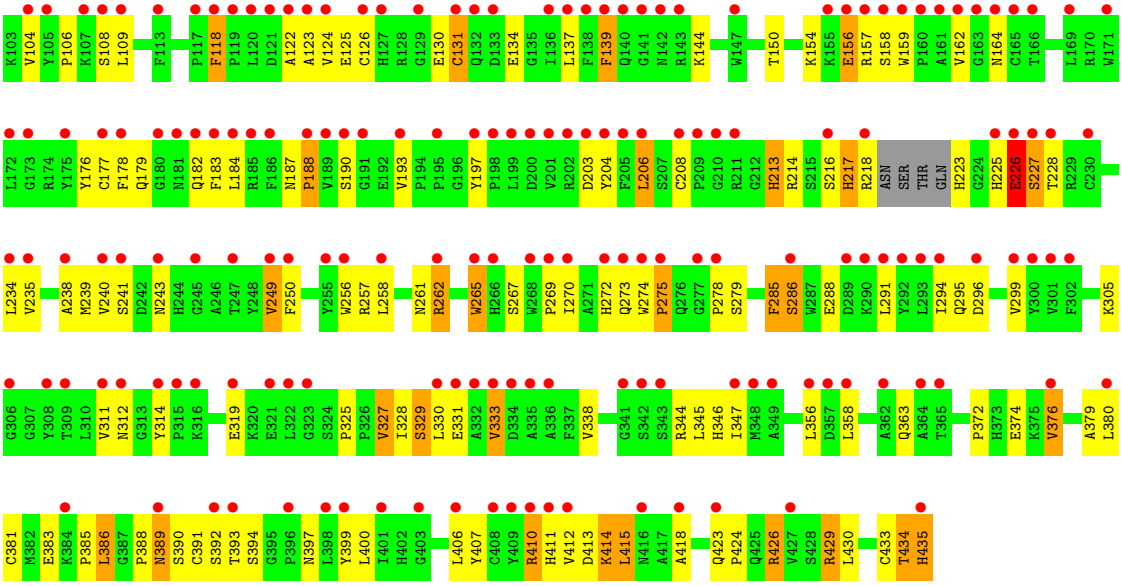


• Molecule 1: HEMOPEXIN

Chain B:






K103 V104 Y105 P106 K107 S108 L109 F113 P117 F118 P119 L120 D121 A122 A123 V124 E125 C126 H127 R128 G129 E130 C131 Q132 D133 E134 G135 I136 L137 F138 F139 Q140 G141 N142 R143 K144 W147 T150 K154 K155 E156 R157 S158 W159 P160 A161 V162 G163 N164 C165 T166 L169 R170 W171
L172 G173 R174 Y175 Y176 C177 F178 Q179 G180 N181 Q182 F183 L184 R185 F186 N187 P188 V189 S190 G191 E192 V193 P194 P195 G196 Y197 P198 L199 D200 V201 R202 D203 Y204 F205 L206 S207 C208 P209 G210 R211 G212 H213 R214 S215 S216 H217 R218 ASN SER THR GLN H223 G224 H225 E226 S227 T228 R229 C230
L234 V235 A238 M239 V240 S241 D242 N243 H244 G245 A246 T247 Y248 V249 F250 Y255 W256 R257 L258 N261 R262 W265 H266 S267 W268 P269 I270 A271 H272 Q273 W274 P275 Q276 G277 P278 S279 F285 S286 W287 E288 D289 K290 L291 Y292 L293 I294 Q295 D296 V299 Y300 V301 F302 K305
G306 G307 Y308 T309 L310 V311 N312 G313 Y314 P315 K316 E319 K320 E321 L322 G323 S324 P325 P326 V327 I328 S329 L330 E331 A332 V333 D334 A335 A336 F337 V338 G341 S342 S343 R344 L345 H346 I347 M348 A349 L356 D357 L358 A362 Q363 A364 T365 P372 H373 E374 K375 V376 A379 L380
C381 M382 E383 K384 P385 L386 G387 P388 N389 S390 C391 S392 T393 S394 G395 P396 N397 L398 Y399 L400 I401 H402 G403 L406 Y407 C408 Y409 R410 H411 V412 D413 K414 L415 N416 A417 A418 Q423 P424 Q425 R426 V427 S428 R429 L430 C433 T434 H435

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	103.90Å 69.90Å 151.81Å 90.00° 108.16° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.96	Depositor EDS
% Data completeness (in resolution range)	97.5 (20.00-2.90) 95.9 (20.00-2.96)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 2.98Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.255 , 0.312 0.360 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	59.9	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 11.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.77	EDS
Total number of atoms	6686	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 4.39% 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: CL, NA, PO4, 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	0.88	7/3400 (0.2%)	1.79	100/4624 (2.2%)
1	B	0.87	6/3400 (0.2%)	1.71	112/4624 (2.4%)
All	All	0.88	13/6800 (0.2%)	1.75	212/9248 (2.3%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	435	HIS	N-CA	-20.21	1.07	1.46
1	A	434	THR	C-N	-14.40	1.13	1.33
1	B	434	THR	CA-C	-14.15	1.30	1.53
1	B	435	HIS	N-CA	-10.57	1.26	1.46
1	B	434	THR	C-N	-9.45	1.20	1.33
1	B	433	CYS	C-N	-6.39	1.22	1.34
1	A	433	CYS	CA-C	-6.05	1.46	1.53
1	B	99	GLU	N-CA	-5.45	1.39	1.46
1	A	99	GLU	N-CA	-5.43	1.39	1.46
1	A	94	TRP	NE1-CE2	-5.27	1.31	1.37
1	A	434	THR	C-O	-5.19	1.17	1.24
1	A	97	THR	C-N	-5.11	1.25	1.33
1	B	97	THR	C-N	-5.05	1.25	1.33

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	434	THR	O-C-N	39.80	170.66	123.30
1	A	433	CYS	CA-C-N	-16.60	99.59	122.99
1	A	433	CYS	C-N-CA	-16.60	99.59	122.99
1	A	434	THR	CA-C-N	13.26	145.57	121.70
1	A	434	THR	C-N-CA	13.26	145.57	121.70
1	B	434	THR	CA-C-N	-12.58	99.06	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	434	THR	C-N-CA	-12.58	99.06	121.70
1	A	130	GLU	N-CA-C	-11.55	95.68	111.96
1	A	386	LEU	N-CA-C	-11.19	90.29	108.52
1	B	433	CYS	CA-C-N	-11.17	106.04	123.24
1	B	433	CYS	C-N-CA	-11.17	106.04	123.24
1	B	130	GLU	N-CA-C	-11.13	96.27	111.96
1	B	386	LEU	N-CA-C	-11.12	90.29	108.41
1	B	213	HIS	CA-C-O	10.53	129.93	119.08
1	A	213	HIS	CA-C-O	10.29	129.68	119.08
1	B	434	THR	CB-CA-C	-9.12	99.04	112.09
1	A	227	SER	CA-CB-OG	8.84	128.78	111.10
1	B	338	VAL	N-CA-C	-8.46	95.17	107.78
1	B	433	CYS	O-C-N	-8.37	111.46	122.59
1	A	179	GLN	N-CA-C	-8.25	96.91	108.54
1	B	179	GLN	N-CA-C	-8.15	97.05	108.54
1	A	104	VAL	N-CA-C	7.95	120.55	108.71
1	A	162	VAL	N-CA-C	-7.94	99.33	109.58
1	B	104	VAL	N-CA-C	7.93	120.53	108.71
1	B	193	VAL	CA-C-N	7.87	125.41	119.66
1	B	193	VAL	C-N-CA	7.87	125.41	119.66
1	A	286	SER	CA-CB-OG	7.75	126.59	111.10
1	B	376	VAL	CA-C-O	-7.74	113.08	121.28
1	B	38	LEU	O-C-N	-7.73	113.18	123.23
1	A	193	VAL	CA-C-N	7.72	125.30	119.66
1	A	193	VAL	C-N-CA	7.72	125.30	119.66
1	A	38	LEU	O-C-N	-7.72	113.41	123.21
1	A	131	CYS	N-CA-C	-7.69	99.44	110.59
1	A	376	VAL	CA-C-O	-7.67	113.15	121.28
1	B	227	SER	CA-CB-OG	7.59	126.28	111.10
1	B	345	LEU	O-C-N	-7.57	114.18	123.04
1	B	162	VAL	N-CA-C	-7.54	99.85	109.58
1	A	275	PRO	N-CA-C	7.51	127.95	112.47
1	B	126	CYS	CA-CB-SG	-7.48	97.19	114.40
1	B	275	PRO	N-CA-C	7.46	127.84	112.47
1	A	65	GLU	CB-CG-CD	7.42	125.22	112.60
1	A	126	CYS	CA-CB-SG	-7.40	97.39	114.40
1	A	345	LEU	O-C-N	-7.38	114.41	123.04
1	B	131	CYS	O-C-N	-7.33	114.11	122.68
1	B	363	GLN	N-CA-C	-7.29	104.41	112.72
1	B	131	CYS	N-CA-C	-7.29	100.02	110.59
1	B	435	HIS	CA-CB-CG	-7.25	106.55	113.80
1	A	358	LEU	CA-C-O	7.22	128.26	119.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	311	VAL	O-C-N	-7.16	114.91	122.57
1	A	295	GLN	CA-C-O	7.11	127.78	120.24
1	A	413	ASP	O-C-N	-7.07	113.57	122.27
1	B	65	GLU	CB-CG-CD	7.07	124.61	112.60
1	A	363	GLN	N-CA-C	-7.04	104.69	112.72
1	B	79	ARG	O-C-N	-7.01	114.02	123.14
1	B	225	HIS	N-CA-C	-6.99	99.16	110.20
1	B	414	LYS	N-CA-C	-6.95	104.28	112.89
1	B	325	PRO	O-C-N	-6.94	118.12	121.31
1	A	423	GLN	CA-C-N	6.90	127.07	120.31
1	A	423	GLN	C-N-CA	6.90	127.07	120.31
1	A	311	VAL	O-C-N	-6.88	115.20	122.57
1	B	188	PRO	N-CA-C	6.87	122.77	113.84
1	A	414	LYS	N-CA-C	-6.84	104.41	112.89
1	A	225	HIS	N-CA-C	-6.80	99.46	110.20
1	A	79	ARG	O-C-N	-6.77	114.06	123.34
1	A	130	GLU	CB-CG-CD	6.76	124.09	112.60
1	B	413	ASP	O-C-N	-6.71	114.02	122.27
1	B	286	SER	CA-CB-OG	6.65	124.40	111.10
1	B	388	PRO	N-CA-C	6.64	122.76	113.53
1	A	203	ASP	O-C-N	6.64	129.13	122.10
1	B	295	GLN	N-CA-C	-6.62	97.48	108.34
1	B	75	ASP	N-CA-C	-6.60	103.91	112.68
1	B	325	PRO	N-CA-C	-6.59	104.14	110.47
1	B	203	ASP	CA-C-O	6.59	126.06	118.55
1	B	358	LEU	CA-C-O	6.58	127.47	119.31
1	A	374	GLU	N-CA-C	-6.55	105.82	113.88
1	B	26	GLN	OE1-CD-NE2	-6.53	116.07	122.60
1	B	423	GLN	CA-C-N	6.53	126.71	120.31
1	B	423	GLN	C-N-CA	6.53	126.71	120.31
1	A	188	PRO	N-CA-C	6.50	122.28	113.84
1	A	118	PHE	O-C-N	-6.48	116.92	121.65
1	A	388	PRO	N-CA-C	6.47	122.53	113.53
1	B	81	GLY	N-CA-C	-6.42	106.27	115.64
1	A	325	PRO	O-C-N	-6.41	118.36	121.31
1	B	295	GLN	CA-C-O	6.39	127.01	120.24
1	A	156	GLU	CB-CG-CD	6.38	123.45	112.60
1	A	372	PRO	N-CA-C	6.38	121.32	114.68
1	A	251	SER	CA-C-O	6.37	127.44	119.98
1	B	213	HIS	CG-CD2-NE2	6.34	113.54	107.20
1	A	81	GLY	N-CA-C	-6.32	106.41	115.64
1	A	295	GLN	N-CA-C	-6.32	97.97	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	235	VAL	CA-C-O	-6.27	113.86	120.57
1	B	68	LYS	N-CA-C	6.26	119.30	110.23
1	A	338	VAL	N-CA-C	-6.25	96.37	107.18
1	A	241	SER	N-CA-C	-6.24	97.40	108.13
1	A	325	PRO	N-CA-C	-6.19	104.53	110.47
1	A	187	ASN	CA-C-O	-6.17	114.71	119.46
1	A	346	HIS	N-CA-C	-6.16	98.48	108.52
1	B	278	PRO	N-CA-C	6.15	119.83	111.22
1	A	381	CYS	CA-CB-SG	-6.13	100.31	114.40
1	B	187	ASN	CA-C-O	-6.10	114.81	119.32
1	A	80	HIS	CA-C-O	6.08	127.07	120.32
1	B	372	PRO	N-CA-C	6.03	120.95	114.68
1	B	241	SER	N-CA-C	-6.00	97.81	108.13
1	B	256	TRP	O-C-N	-6.00	116.25	123.27
1	A	278	PRO	N-CA-C	5.99	119.61	111.22
1	A	391	CYS	O-C-N	-5.95	113.58	122.39
1	B	346	HIS	N-CA-C	-5.95	98.82	108.52
1	B	393	THR	O-C-N	-5.95	115.17	122.19
1	B	156	GLU	CB-CG-CD	5.95	122.71	112.60
1	B	383	GLU	CB-CG-CD	5.93	122.68	112.60
1	B	391	CYS	O-C-N	-5.93	113.62	122.39
1	A	134	GLU	N-CA-C	-5.92	100.34	109.76
1	B	330	LEU	N-CA-C	5.92	118.84	109.96
1	A	239	MET	O-C-N	-5.91	116.65	123.33
1	B	130	GLU	CB-CG-CD	5.91	122.65	112.60
1	A	92	LYS	N-CA-C	5.90	119.16	109.72
1	A	31	TRP	O-C-N	-5.88	116.09	122.79
1	B	239	MET	O-C-N	-5.85	116.72	123.33
1	B	235	VAL	CA-C-O	-5.84	114.32	120.57
1	B	226	GLU	CB-CG-CD	5.84	122.53	112.60
1	B	424	PRO	N-CA-C	5.84	120.44	111.57
1	A	68	LYS	N-CA-C	5.81	118.66	110.23
1	A	383	GLU	CB-CG-CD	5.80	122.47	112.60
1	B	92	LYS	N-CA-C	5.80	119.00	109.72
1	B	124	VAL	O-C-N	-5.76	116.97	123.20
1	A	131	CYS	O-C-N	-5.75	115.96	122.68
1	B	374	GLU	N-CA-C	-5.74	106.81	113.88
1	B	418	ALA	N-CA-C	5.74	118.57	109.96
1	B	265	TRP	O-C-N	5.73	130.28	123.24
1	B	80	HIS	CA-C-O	5.70	126.65	120.32
1	B	109	LEU	N-CA-C	-5.70	105.07	111.28
1	A	226	GLU	CB-CG-CD	5.69	122.27	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	208	CYS	CA-CB-SG	-5.68	101.32	114.40
1	B	270	ILE	N-CA-C	-5.68	104.99	110.72
1	B	381	CYS	CA-CB-SG	-5.67	101.35	114.40
1	A	434	THR	CA-C-O	5.67	126.49	120.36
1	B	197	TYR	CA-C-O	-5.67	115.03	120.64
1	B	190	SER	N-CA-C	5.67	120.32	112.90
1	B	206	LEU	CA-C-O	5.65	126.80	120.70
1	B	319	GLU	O-C-N	5.64	128.59	122.11
1	A	124	VAL	O-C-N	-5.63	117.12	123.20
1	A	424	PRO	N-CA-C	5.60	120.08	111.57
1	A	319	GLU	O-C-N	5.59	128.53	122.11
1	B	49	ASP	CB-CA-C	-5.58	110.12	116.54
1	B	314	TYR	N-CA-C	5.58	117.64	110.39
1	B	383	GLU	N-CA-C	5.57	118.54	111.69
1	B	118	PHE	O-C-N	-5.57	117.59	121.65
1	B	134	GLU	N-CA-C	-5.54	100.95	109.76
1	A	190	SER	N-CA-C	5.54	120.15	112.90
1	A	48	LYS	CA-C-O	5.53	126.73	119.98
1	A	203	ASP	CA-C-O	5.53	124.86	118.55
1	B	389	ASN	N-CA-C	5.53	118.72	110.14
1	A	256	TRP	O-C-N	-5.52	116.81	123.27
1	B	213	HIS	CE1-NE2-CD2	-5.51	103.49	109.00
1	A	75	ASP	N-CA-C	-5.51	105.35	112.68
1	B	126	CYS	O-C-N	-5.51	116.82	123.27
1	A	383	GLU	O-C-N	-5.50	115.08	122.23
1	A	330	LEU	N-CA-C	5.49	118.49	109.76
1	A	86	TYR	O-C-N	-5.48	116.97	123.22
1	A	125	GLU	CB-CG-CD	5.48	121.92	112.60
1	A	418	ALA	N-CA-C	5.48	118.18	109.96
1	A	284	ALA	CA-C-O	5.47	126.88	120.75
1	A	67	TRP	CA-C-O	5.47	126.61	120.92
1	A	229	ARG	O-C-N	-5.46	116.34	122.12
1	B	164	ASN	N-CA-C	-5.45	98.35	107.99
1	B	178	PHE	O-C-N	-5.44	116.68	123.04
1	A	429	ARG	N-CA-C	-5.43	105.26	111.07
1	B	68	LYS	O-C-N	-5.43	116.19	122.87
1	A	351	ARG	N-CA-C	-5.43	106.85	112.93
1	B	273	GLN	CB-CG-CD	5.42	121.82	112.60
1	A	178	PHE	O-C-N	-5.42	116.70	123.04
1	B	429	ARG	N-CA-C	-5.41	105.28	111.07
1	A	415	LEU	N-CA-C	-5.37	105.34	111.14
1	A	393	THR	O-C-N	-5.36	115.87	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	319	GLU	CA-C-O	5.36	126.92	120.92
1	A	319	GLU	CA-C-O	5.34	126.90	120.92
1	B	159	TRP	CA-C-N	5.32	124.83	119.19
1	B	159	TRP	C-N-CA	5.32	124.83	119.19
1	B	262	ARG	N-CA-C	-5.30	105.55	112.23
1	A	182	GLN	N-CA-C	5.27	117.87	109.81
1	B	261	ASN	O-C-N	-5.26	115.59	122.59
1	A	164	ASN	N-CA-C	-5.25	98.70	107.99
1	A	285	PHE	CA-C-O	-5.24	115.82	121.38
1	B	100	LYS	CB-CA-C	5.24	116.24	109.80
1	A	100	LYS	CB-CA-C	5.23	116.23	109.80
1	B	415	LEU	N-CA-C	-5.22	105.50	111.14
1	A	329	SER	N-CA-C	-5.22	98.89	108.02
1	B	125	GLU	CB-CG-CD	5.21	121.46	112.60
1	B	285	PHE	CA-C-O	-5.20	115.87	121.38
1	A	139	PHE	O-C-N	-5.19	117.25	123.27
1	A	49	ASP	CB-CA-C	-5.19	110.57	116.54
1	A	249	VAL	N-CA-C	-5.18	98.58	109.34
1	B	150	THR	CA-C-O	5.17	126.22	120.90
1	A	273	GLN	CB-CG-CD	5.16	121.37	112.60
1	B	319	GLU	CB-CG-CD	5.16	121.36	112.60
1	A	181	ASN	CA-C-O	5.15	125.72	119.38
1	B	249	VAL	N-CA-C	-5.15	98.62	109.34
1	A	288	GLU	CB-CA-C	-5.15	110.66	116.63
1	B	144	LYS	N-CA-C	5.15	118.14	109.95
1	B	101	ASN	CA-CB-CG	5.14	117.74	112.60
1	A	197	TYR	CA-C-O	-5.13	115.56	120.64
1	A	99	GLU	N-CA-CB	-5.12	101.84	110.49
1	B	139	PHE	O-C-N	-5.12	117.33	123.27
1	B	257	ARG	N-CA-C	-5.12	102.12	110.20
1	B	99	GLU	N-CA-CB	-5.11	101.86	110.49
1	A	101	ASN	CA-CB-CG	5.10	117.70	112.60
1	A	49	ASP	N-CA-C	5.09	116.05	108.31
1	B	182	GLN	N-CA-C	5.09	117.59	109.81
1	B	435	HIS	CB-CA-C	-5.09	100.44	110.10
1	B	288	GLU	CB-CA-C	-5.07	110.75	116.63
1	B	86	TYR	O-C-N	-5.04	117.48	123.22
1	B	49	ASP	N-CA-C	5.03	115.96	108.31

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	3289	0	3120	97	0
1	B	3289	0	3121	113	12
2	A	43	0	30	7	0
2	B	43	0	30	24	0
3	A	5	0	0	1	0
3	B	5	0	0	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
All	All	6686	0	6301	192	12

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 15.

All (192) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:THR:HG23	1:A:435:HIS:CB	1.24	1.65
1:A:434:THR:CG2	1:A:435:HIS:HB3	1.54	1.37
1:A:434:THR:CG2	1:A:435:HIS:CB	2.04	1.30
1:A:411:HIS:CE1	1:B:100:LYS:NZ	2.04	1.25
1:A:411:HIS:HE1	1:B:100:LYS:NZ	1.39	1.15
1:B:99:GLU:HB3	1:B:100:LYS:HE2	1.34	1.10
1:A:99:GLU:HB3	1:A:100:LYS:HE2	1.34	1.09
1:A:413:ASP:OD2	1:B:99:GLU:OE2	1.69	1.09
1:A:411:HIS:CE1	1:B:100:LYS:HZ3	1.71	1.06
1:B:434:THR:O	1:B:434:THR:HG23	1.50	1.04
1:A:411:HIS:NE2	1:B:99:GLU:OE1	1.91	1.03
1:A:434:THR:HG23	1:A:435:HIS:HB2	1.05	1.03
1:A:380:LEU:HA	3:A:501:PO4:O2	1.58	1.01
1:A:434:THR:HG23	1:A:435:HIS:HB3	1.00	0.99
1:B:380:LEU:HA	3:B:501:PO4:O2	1.67	0.94
1:A:434:THR:HG22	1:A:435:HIS:HB3	1.52	0.90
1:A:434:THR:CG2	1:A:435:HIS:HB2	1.87	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:HIS:HD2	2:B:500:HEM:C1D	1.90	0.89
1:A:411:HIS:HE1	1:B:100:LYS:HZ2	1.05	0.88
1:A:385:PRO:HB3	1:A:390:SER:HB3	1.55	0.88
1:A:411:HIS:CE1	1:B:100:LYS:HZ2	1.79	0.87
1:B:204:TYR:HB3	2:B:500:HEM:C3A	2.10	0.87
1:B:214:ARG:HD2	2:B:500:HEM:C2C	2.10	0.86
1:B:213:HIS:CD2	2:B:500:HEM:C1D	2.65	0.85
1:B:434:THR:O	1:B:434:THR:CG2	2.17	0.83
1:B:385:PRO:HB3	1:B:390:SER:HB3	1.59	0.82
1:B:380:LEU:HD23	1:B:386:LEU:HD22	1.62	0.80
1:A:413:ASP:CG	1:B:99:GLU:OE2	2.26	0.78
1:B:213:HIS:HD2	2:B:500:HEM:ND	1.80	0.78
1:A:411:HIS:HE1	1:B:100:LYS:CE	1.96	0.78
1:B:213:HIS:HD2	2:B:500:HEM:C4D	2.02	0.78
1:A:411:HIS:CE1	1:B:100:LYS:CD	2.68	0.77
1:A:380:LEU:HD23	1:A:386:LEU:HD22	1.65	0.77
1:B:100:LYS:O	1:B:102:GLU:N	2.18	0.77
1:A:100:LYS:O	1:A:102:GLU:N	2.18	0.75
1:B:41:ASN:HD22	1:B:262:ARG:HH21	1.33	0.74
1:A:411:HIS:CE1	1:B:100:LYS:CE	2.70	0.74
1:B:56:HIS:ND1	2:B:500:HEM:CBB	2.52	0.73
1:A:411:HIS:HE1	1:B:100:LYS:CD	2.03	0.72
1:B:94:TRP:HB3	1:B:96:TYR:CE2	2.25	0.71
1:B:214:ARG:HD2	2:B:500:HEM:C1C	2.26	0.71
1:B:213:HIS:CD2	2:B:500:HEM:C4D	2.79	0.71
1:A:411:HIS:CE1	1:B:99:GLU:OE1	2.45	0.69
1:A:94:TRP:HB3	1:A:96:TYR:CE2	2.27	0.68
1:A:82:HIS:CE1	1:A:262:ARG:HG2	2.28	0.68
1:A:413:ASP:HB2	1:B:99:GLU:OE2	1.94	0.68
1:B:183:PHE:HE2	2:B:500:HEM:CGA	2.07	0.68
1:A:413:ASP:HB2	1:B:99:GLU:CD	2.20	0.66
1:A:428:SER:HB2	1:A:433:CYS:HB2	1.75	0.66
1:B:41:ASN:HD22	1:B:262:ARG:NH2	1.93	0.66
1:B:204:TYR:CD1	2:B:500:HEM:C1A	2.85	0.66
1:A:410:ARG:HG3	1:A:414:LYS:HD2	1.79	0.65
1:B:410:ARG:HG3	1:B:414:LYS:HD2	1.80	0.64
1:A:226:GLU:HG2	1:A:267:SER:H	1.63	0.63
1:A:413:ASP:CB	1:B:99:GLU:OE2	2.46	0.63
2:B:500:HEM:HBB2	2:B:500:HEM:HMB2	1.81	0.62
1:B:226:GLU:HG2	1:B:267:SER:H	1.64	0.62
1:A:411:HIS:CE1	1:B:100:LYS:HD3	2.35	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:HIS:CE1	2:A:500:HEM:CBB	2.84	0.60
1:B:204:TYR:HB3	2:B:500:HEM:C2A	2.37	0.59
1:B:49:ASP:HA	1:B:73:PRO:HB3	1.85	0.58
1:A:49:ASP:HA	1:A:73:PRO:HB3	1.86	0.58
1:A:434:THR:CB	1:A:435:HIS:HB2	2.34	0.57
1:B:56:HIS:CE1	2:B:500:HEM:CBB	2.88	0.57
1:B:183:PHE:CE2	2:B:500:HEM:CGA	2.88	0.57
1:A:406:LEU:HD22	1:A:430:LEU:HD23	1.87	0.56
1:B:286:SER:HB3	1:B:291:LEU:HD23	1.86	0.56
1:A:238:ALA:HB3	1:A:250:PHE:HB2	1.87	0.56
1:B:434:THR:O	1:B:435:HIS:CB	2.39	0.56
1:A:413:ASP:CB	1:B:99:GLU:CD	2.79	0.56
1:A:91:ASP:HB3	1:A:118:PHE:CE2	2.41	0.56
1:B:72:GLY:HA3	1:B:89:LYS:NZ	2.21	0.56
1:B:91:ASP:HB3	1:B:118:PHE:CE2	2.40	0.55
1:B:238:ALA:HB3	1:B:250:PHE:HB2	1.88	0.55
1:A:428:SER:HB2	1:A:433:CYS:CB	2.35	0.55
1:A:123:ALA:HA	1:A:137:LEU:O	2.07	0.55
1:A:56:HIS:CE1	2:A:500:HEM:HBB1	2.42	0.55
1:B:72:GLY:HA3	1:B:89:LYS:HZ2	1.71	0.55
1:A:286:SER:HB3	1:A:291:LEU:HD23	1.88	0.54
1:A:327:VAL:HG23	1:A:328:ILE:HD12	1.88	0.54
1:A:269:PRO:HD2	1:A:272:HIS:CD2	2.43	0.54
1:A:82:HIS:NE2	1:A:262:ARG:HG2	2.21	0.54
2:A:500:HEM:HBB2	2:A:500:HEM:HMB2	1.89	0.54
1:B:183:PHE:HE2	2:B:500:HEM:O2A	1.91	0.54
1:B:410:ARG:CG	1:B:414:LYS:HD2	2.38	0.54
2:A:500:HEM:HMC2	2:A:500:HEM:HBC2	1.89	0.54
1:A:56:HIS:HE1	2:A:500:HEM:HBB1	1.74	0.53
1:A:410:ARG:CG	1:A:414:LYS:HD2	2.37	0.53
1:B:269:PRO:HD2	1:B:272:HIS:CD2	2.45	0.52
1:B:327:VAL:HG23	1:B:328:ILE:HD12	1.91	0.52
1:A:392:SER:HB3	1:A:410:ARG:HA	1.92	0.52
1:B:406:LEU:HD22	1:B:430:LEU:HD23	1.92	0.52
1:A:131:CYS:SG	1:A:188:PRO:HB2	2.51	0.51
1:B:123:ALA:HA	1:B:137:LEU:O	2.11	0.51
1:B:204:TYR:HD1	2:B:500:HEM:C1A	2.29	0.51
1:B:392:SER:HB3	1:B:410:ARG:HA	1.93	0.51
1:B:56:HIS:CD2	1:B:56:HIS:C	2.89	0.50
1:B:176:TYR:HE1	2:B:500:HEM:O2A	1.94	0.50
1:B:214:ARG:HD2	2:B:500:HEM:C3C	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:ILE:HG12	1:A:299:VAL:HG22	1.92	0.50
1:B:54:LYS:HZ1	1:B:66:ARG:HH21	1.59	0.50
1:B:328:ILE:HG22	1:B:329:SER:N	2.27	0.50
1:B:216:SER:O	1:B:217:HIS:ND1	2.45	0.49
1:A:48:LYS:HB3	1:A:53:TRP:CZ3	2.47	0.49
1:B:412:VAL:O	1:B:415:LEU:HB3	2.12	0.49
1:B:434:THR:O	1:B:435:HIS:HB2	2.12	0.49
1:A:410:ARG:HG3	1:A:414:LYS:CD	2.43	0.48
1:B:294:ILE:HG12	1:B:299:VAL:HG22	1.94	0.48
1:A:56:HIS:CD2	1:A:56:HIS:C	2.92	0.48
1:A:216:SER:O	1:A:217:HIS:ND1	2.46	0.48
1:B:390:SER:HB2	1:B:397:ASN:ND2	2.29	0.47
1:B:333:VAL:HG21	1:B:347:ILE:HD11	1.96	0.47
1:A:379:ALA:HB2	1:A:400:LEU:HD23	1.94	0.47
1:A:48:LYS:HB3	1:A:53:TRP:HZ3	1.79	0.47
1:A:328:ILE:HG22	1:A:329:SER:N	2.29	0.47
1:B:379:ALA:HB2	1:B:400:LEU:HD23	1.95	0.47
1:A:26:GLN:HE21	1:A:26:GLN:H	1.62	0.47
1:A:411:HIS:CD2	1:B:99:GLU:OE1	2.63	0.47
1:B:24:ILE:HG23	1:B:25:GLU:H	1.78	0.47
1:B:48:LYS:HB3	1:B:53:TRP:CZ3	2.49	0.47
1:B:94:TRP:NE1	1:B:106:PRO:HG3	2.31	0.46
1:A:411:HIS:NE2	1:B:100:LYS:HD3	2.30	0.46
1:A:412:VAL:O	1:A:415:LEU:HB3	2.15	0.46
1:A:333:VAL:HG21	1:A:347:ILE:HD11	1.97	0.46
1:B:26:GLN:HE21	1:B:26:GLN:H	1.62	0.46
1:B:243:ASN:H	1:B:243:ASN:ND2	2.14	0.46
1:B:410:ARG:HG3	1:B:414:LYS:CD	2.44	0.46
1:A:24:ILE:HG23	1:A:25:GLU:H	1.79	0.46
1:A:122:ALA:HB3	1:A:139:PHE:HB2	1.98	0.46
1:A:327:VAL:HG11	1:B:389:ASN:HB3	1.98	0.46
1:A:390:SER:HB2	1:A:397:ASN:ND2	2.30	0.46
1:B:214:ARG:HG3	2:B:500:HEM:CBC	2.45	0.46
1:A:54:LYS:HE3	1:A:66:ARG:HH21	1.81	0.46
1:A:62:LEU:O	1:A:65:GLU:HB3	2.16	0.46
1:A:414:LYS:HG3	1:B:100:LYS:HD2	1.98	0.46
1:A:26:GLN:H	1:A:26:GLN:NE2	2.13	0.46
1:B:50:GLU:O	1:B:62:LEU:HD12	2.16	0.45
1:A:243:ASN:ND2	1:A:243:ASN:H	2.14	0.45
1:B:100:LYS:HD3	1:B:100:LYS:HA	1.44	0.45
1:B:426:ARG:HB3	1:B:426:ARG:HH11	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:122:ALA:HB3	1:B:139:PHE:HB2	1.99	0.45
1:B:48:LYS:HB3	1:B:53:TRP:HZ3	1.81	0.45
1:B:131:CYS:SG	1:B:188:PRO:HB2	2.57	0.45
1:A:100:LYS:C	1:A:102:GLU:N	2.75	0.45
1:B:100:LYS:HE2	1:B:100:LYS:N	2.32	0.45
1:B:62:LEU:O	1:B:65:GLU:HB3	2.17	0.44
1:A:50:GLU:O	1:A:62:LEU:HD12	2.18	0.44
1:A:100:LYS:HE2	1:A:100:LYS:N	2.32	0.44
1:B:390:SER:HB2	1:B:397:ASN:HD21	1.82	0.44
1:A:399:TYR:HA	1:A:407:TYR:O	2.16	0.44
2:A:500:HEM:HHA	2:A:500:HEM:HBD2	1.99	0.44
1:B:214:ARG:CD	2:B:500:HEM:C3C	3.00	0.44
1:B:55:SER:OG	1:B:57:ARG:HB2	2.18	0.44
1:A:72:GLY:HA3	1:A:89:LYS:NZ	2.33	0.43
1:B:100:LYS:C	1:B:102:GLU:N	2.75	0.43
1:B:204:TYR:CD1	2:B:500:HEM:C2A	3.06	0.43
1:B:223:HIS:CD2	1:B:234:LEU:HD12	2.52	0.43
1:A:56:HIS:ND1	2:A:500:HEM:CBB	2.81	0.43
1:A:214:ARG:N	1:A:214:ARG:HD3	2.33	0.43
1:B:258:LEU:HD23	1:B:265:TRP:HZ3	1.82	0.43
1:A:55:SER:OG	1:A:57:ARG:HB2	2.19	0.43
1:B:26:GLN:H	1:B:26:GLN:NE2	2.15	0.43
1:B:214:ARG:N	1:B:214:ARG:HD3	2.33	0.43
1:A:174:ARG:HH22	1:A:272:HIS:CD2	2.37	0.43
1:A:81:GLY:C	1:A:83:THR:H	2.26	0.43
1:B:386:LEU:HG	1:B:430:LEU:HD22	2.01	0.43
1:B:399:TYR:HA	1:B:407:TYR:O	2.18	0.42
1:B:204:TYR:CD1	2:B:500:HEM:CHA	3.02	0.42
1:A:426:ARG:HH11	1:A:426:ARG:HB3	1.84	0.42
1:A:386:LEU:HG	1:A:430:LEU:HD22	2.01	0.42
1:A:54:LYS:CE	1:A:66:ARG:HH21	2.33	0.42
1:A:223:HIS:CD2	1:A:234:LEU:HD12	2.54	0.42
1:B:24:ILE:HG23	1:B:25:GLU:N	2.34	0.42
1:A:274:TRP:HA	1:A:275:PRO:HD2	1.86	0.42
1:B:386:LEU:HD12	1:B:386:LEU:HA	1.78	0.42
1:A:97:THR:C	1:A:99:GLU:H	2.28	0.42
1:A:99:GLU:HB3	1:A:100:LYS:CE	2.25	0.42
1:A:344:ARG:HG2	1:A:355:TRP:CE3	2.55	0.42
1:A:346:HIS:HA	1:A:354:TRP:O	2.20	0.42
1:B:81:GLY:C	1:B:83:THR:H	2.26	0.41
1:A:54:LYS:HZ1	1:A:66:ARG:HH21	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:LYS:HD3	1:A:100:LYS:HA	1.44	0.41
1:B:54:LYS:NZ	1:B:66:ARG:HH21	2.17	0.41
1:A:99:GLU:O	1:A:100:LYS:C	2.64	0.41
1:B:82:HIS:O	1:B:82:HIS:ND1	2.53	0.41
1:A:258:LEU:HD23	1:A:265:TRP:HZ3	1.85	0.41
1:B:94:TRP:CE2	1:B:106:PRO:HG3	2.55	0.41
1:B:213:HIS:CD2	2:B:500:HEM:CHD	3.03	0.41
1:B:285:PHE:HA	3:B:501:PO4:O4	2.20	0.41
1:B:99:GLU:O	1:B:100:LYS:C	2.64	0.41
1:B:274:TRP:HA	1:B:275:PRO:HD2	1.85	0.40
1:B:97:THR:C	1:B:99:GLU:H	2.28	0.40

All (12) 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)
1:B:118:PHE:CZ	1:B:312:ASN:CG[4_556]	1.31	0.89
1:B:51:PHE:CE1	1:B:156:GLU:O[4_556]	1.44	0.76
1:B:118:PHE:CE1	1:B:312:ASN:ND2[4_556]	1.73	0.47
1:B:118:PHE:CZ	1:B:312:ASN:OD1[4_556]	1.80	0.40
1:B:118:PHE:CE2	1:B:312:ASN:CB[4_556]	1.88	0.32
1:B:118:PHE:CZ	1:B:312:ASN:CB[4_556]	1.92	0.28
1:B:118:PHE:CZ	1:B:312:ASN:ND2[4_556]	1.93	0.27
1:B:25:GLU:OE2	1:B:154:LYS:O[4_556]	1.98	0.22
1:B:118:PHE:CE1	1:B:312:ASN:CG[4_556]	2.11	0.09
1:B:51:PHE:CD1	1:B:156:GLU:O[4_556]	2.14	0.06
1:B:60:ARG:NH2	1:B:156:GLU:OE1[4_556]	2.16	0.04
1:B:62:LEU:CD1	1:B:158:SER:CB[4_556]	2.18	0.02

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	404/460 (88%)	370 (92%)	30 (7%)	4 (1%)	12	39
1	B	404/460 (88%)	369 (91%)	31 (8%)	4 (1%)	12	39
All	All	808/920 (88%)	739 (92%)	61 (8%)	8 (1%)	12	39

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	296	ASP
1	B	101	ASN
1	B	296	ASP
1	A	55	SER
1	B	55	SER
1	B	82	HIS
1	A	82	HIS

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	352/393 (90%)	315 (90%)	37 (10%)	6	22
1	B	352/393 (90%)	313 (89%)	39 (11%)	6	20
All	All	704/786 (90%)	628 (89%)	76 (11%)	6	21

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ILE
1	A	26	GLN
1	A	43	THR
1	A	55	SER
1	A	66	ARG
1	A	68	LYS
1	A	80	HIS
1	A	92	LYS

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Mol	Chain	Res	Type
1	A	98	SER
1	A	99	GLU
1	A	100	LYS
1	A	108	SER
1	A	157	ARG
1	A	177	CYS
1	A	184	LEU
1	A	206	LEU
1	A	217	HIS
1	A	218	ARG
1	A	226	GLU
1	A	227	SER
1	A	228	THR
1	A	240	VAL
1	A	249	VAL
1	A	279	SER
1	A	305	LYS
1	A	327	VAL
1	A	329	SER
1	A	331	GLU
1	A	333	VAL
1	A	344	ARG
1	A	356	LEU
1	A	376	VAL
1	A	394	SER
1	A	410	ARG
1	A	411	HIS
1	A	426	ARG
1	A	429	ARG
1	B	24	ILE
1	B	26	GLN
1	B	43	THR
1	B	45	LEU
1	B	55	SER
1	B	56	HIS
1	B	66	ARG
1	B	68	LYS
1	B	80	HIS
1	B	92	LYS
1	B	98	SER
1	B	99	GLU
1	B	100	LYS

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Mol	Chain	Res	Type
1	B	108	SER
1	B	157	ARG
1	B	177	CYS
1	B	184	LEU
1	B	206	LEU
1	B	217	HIS
1	B	218	ARG
1	B	226	GLU
1	B	227	SER
1	B	228	THR
1	B	240	VAL
1	B	249	VAL
1	B	279	SER
1	B	305	LYS
1	B	327	VAL
1	B	329	SER
1	B	331	GLU
1	B	333	VAL
1	B	344	ARG
1	B	356	LEU
1	B	376	VAL
1	B	394	SER
1	B	410	ARG
1	B	411	HIS
1	B	426	ARG
1	B	429	ARG

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	26	GLN
1	A	41	ASN
1	A	56	HIS
1	A	243	ASN
1	A	273	GLN
1	A	402	HIS
1	A	411	HIS
1	B	26	GLN
1	B	41	ASN
1	B	243	ASN
1	B	272	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	PO4	A	501	5	4,4,4	1.77	2 (50%)	6,6,6	1.55	1 (16%)
3	PO4	B	501	5	4,4,4	1.77	2 (50%)	6,6,6	1.55	1 (16%)
2	HEM	A	500	1	50,50,50	2.26	20 (40%)	66,82,82	1.09	4 (6%)
2	HEM	B	500	1	50,50,50	2.68	24 (48%)	66,82,82	2.31	24 (36%)

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	-	2/14/54/54	-
2	HEM	B	500	1	-	5/14/54/54	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	HEM	FE-ND	7.29	2.17	1.94
2	B	500	HEM	FE-NB	6.43	2.14	1.94
2	B	500	HEM	CBC-CAC	5.49	1.57	1.30
2	B	500	HEM	CHD-C4C	4.94	1.48	1.38
2	B	500	HEM	FE-NC	4.29	2.09	1.95
2	A	500	HEM	C4D-ND	-4.19	1.33	1.40
2	A	500	HEM	FE-ND	4.15	2.07	1.94
2	A	500	HEM	CAB-C3B	-4.08	1.36	1.47
2	A	500	HEM	C1A-NA	-4.02	1.32	1.39
2	B	500	HEM	C1A-NA	-3.99	1.32	1.39
2	B	500	HEM	C4A-C3A	-3.89	1.34	1.43
2	B	500	HEM	C4A-NA	-3.68	1.32	1.39
2	A	500	HEM	C3C-C4C	-3.64	1.39	1.46
2	A	500	HEM	C1C-NC	-3.57	1.32	1.39
2	A	500	HEM	CBC-CAC	3.57	1.48	1.30
2	A	500	HEM	FE-NC	3.56	2.07	1.95
2	A	500	HEM	C1C-C2C	-3.50	1.38	1.45
2	B	500	HEM	C1B-C2B	-3.50	1.37	1.44
2	B	500	HEM	C1A-C2A	-3.49	1.37	1.44
2	B	500	HEM	C3B-C4B	-3.40	1.38	1.44
2	B	500	HEM	CBB-CAB	3.34	1.46	1.30
2	A	500	HEM	FE-NB	3.28	2.05	1.94
2	A	500	HEM	C4C-NC	-3.28	1.33	1.39
2	B	500	HEM	FE-NA	3.27	2.06	1.95
2	A	500	HEM	C4A-NA	-3.16	1.33	1.39
2	A	500	HEM	C3B-C4B	-3.13	1.38	1.44
2	A	500	HEM	C1A-C2A	-3.05	1.38	1.44
2	B	500	HEM	C4B-NB	-2.98	1.32	1.38
2	B	500	HEM	CHD-C1D	2.92	1.45	1.39
2	A	500	HEM	C1B-NB	-2.82	1.35	1.40
2	A	500	HEM	C4D-C3D	-2.73	1.40	1.45
2	A	500	HEM	C1D-C2D	-2.71	1.39	1.44
2	B	500	HEM	CHA-C4D	2.60	1.43	1.38
2	B	500	HEM	C3C-C2C	2.58	1.42	1.37
2	A	500	HEM	C1D-ND	-2.44	1.33	1.38
2	A	500	HEM	CAC-C3C	-2.43	1.40	1.47
3	A	501	PO4	P-O2	-2.42	1.47	1.54
3	B	501	PO4	P-O2	-2.40	1.47	1.54
2	A	500	HEM	FE-NA	2.37	2.03	1.95
2	B	500	HEM	C1C-NC	-2.32	1.35	1.39
2	B	500	HEM	C1C-C2C	-2.30	1.40	1.45
2	B	500	HEM	CBA-CAA	2.20	1.59	1.52
2	B	500	HEM	C3B-C2B	2.18	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	PO4	P-O4	-2.16	1.48	1.54
3	B	501	PO4	P-O4	-2.15	1.48	1.54
2	B	500	HEM	O2A-CGA	-2.15	1.23	1.30
2	B	500	HEM	C1B-NB	-2.11	1.36	1.40
2	B	500	HEM	CHC-C1C	2.04	1.42	1.38

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	500	HEM	CHC-C1C-NC	5.62	130.52	124.44
2	B	500	HEM	C4C-NC-C1C	5.30	110.54	105.35
2	B	500	HEM	C3B-C2B-C1B	-4.70	103.00	106.49
2	B	500	HEM	CBD-CAD-C3D	4.67	125.61	112.63
2	B	500	HEM	CAD-CBD-CGD	4.56	123.42	113.60
2	B	500	HEM	CMD-C2D-C1D	4.04	131.20	125.04
2	B	500	HEM	CAD-C3D-C4D	3.91	131.49	124.66
2	B	500	HEM	CBA-CAA-C2A	3.75	123.05	112.63
2	B	500	HEM	C4B-C3B-C2B	-3.54	104.30	107.11
2	B	500	HEM	C2B-C1B-NB	3.44	113.92	109.84
2	B	500	HEM	C4D-C3D-C2D	-3.43	101.90	106.90
2	B	500	HEM	CHD-C4C-C3C	3.35	131.00	125.26
3	B	501	PO4	O4-P-O1	3.09	122.20	110.89
3	A	501	PO4	O4-P-O1	3.08	122.17	110.89
2	B	500	HEM	CHB-C4A-C3A	-3.02	118.72	127.24
2	B	500	HEM	CHB-C4A-NA	2.94	129.26	123.85
2	B	500	HEM	CHB-C1B-NB	-2.85	120.86	124.37
2	B	500	HEM	CMD-C2D-C3D	-2.81	118.49	126.12
2	B	500	HEM	C1B-NB-C4B	-2.76	102.22	105.07
2	B	500	HEM	CHC-C1C-C2C	-2.58	120.06	125.48
2	B	500	HEM	C1D-C2D-C3D	2.57	109.66	106.96
2	B	500	HEM	CMA-C3A-C2A	2.50	131.01	125.61
2	A	500	HEM	C4A-C3A-C2A	-2.42	104.00	106.83
2	B	500	HEM	CHA-C4D-ND	-2.39	121.42	124.37
2	B	500	HEM	C4A-C3A-C2A	-2.38	104.04	106.83
2	B	500	HEM	C4D-ND-C1D	-2.31	102.69	105.07
2	A	500	HEM	C4C-C3C-C2C	-2.25	104.90	106.75
2	A	500	HEM	C3D-C4D-ND	2.25	112.67	110.17
2	B	500	HEM	CMB-C2B-C1B	2.19	128.38	125.04
2	A	500	HEM	C4D-C3D-C2D	-2.05	103.92	106.90

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	500	HEM	C3D-CAD-CBD-CGD
2	B	500	HEM	C3A-C2A-CAA-CBA
2	B	500	HEM	C2D-C3D-CAD-CBD
2	B	500	HEM	C4D-C3D-CAD-CBD
2	B	500	HEM	C1A-C2A-CAA-CBA
2	A	500	HEM	CAD-CBD-CGD-O2D
2	A	500	HEM	CAD-CBD-CGD-O1D

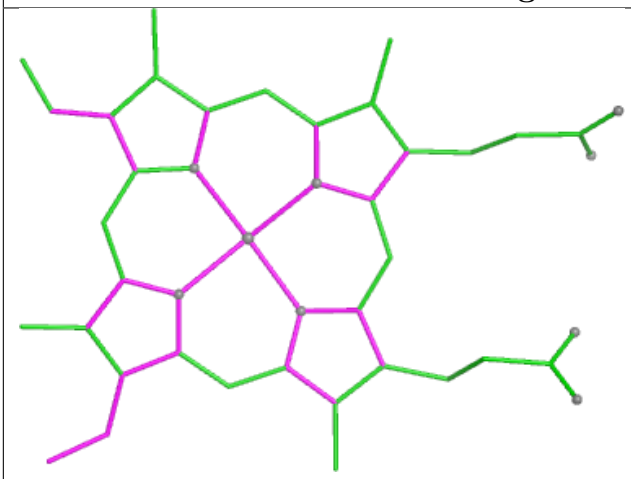
There are no ring outliers.

4 monomers are involved in 34 short contacts:

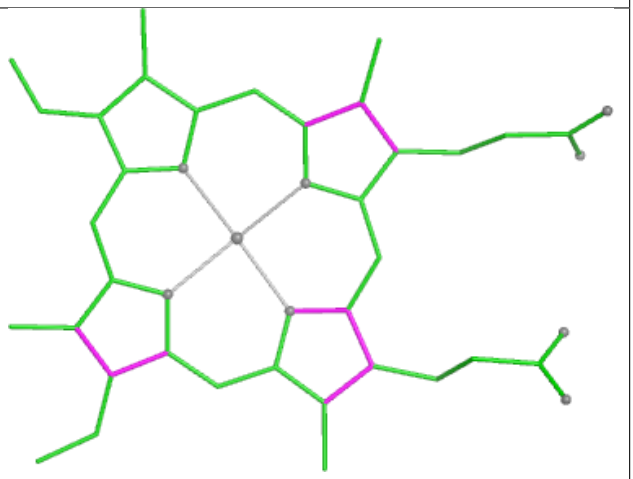
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	501	PO4	1	0
3	B	501	PO4	2	0
2	A	500	HEM	7	0
2	B	500	HEM	24	0

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.

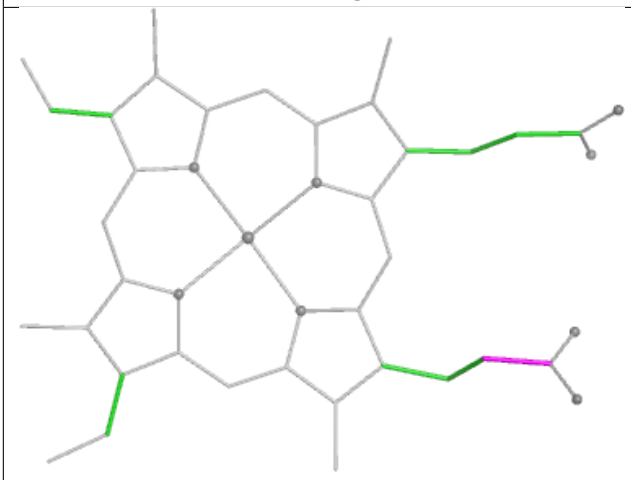
Ligand HEM A 500



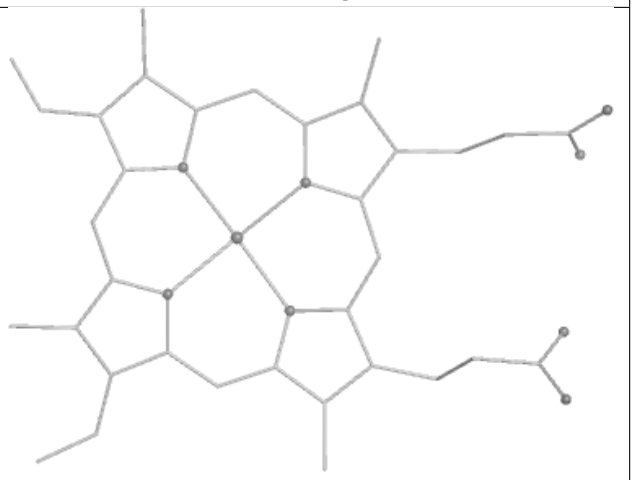
Bond lengths



Bond angles

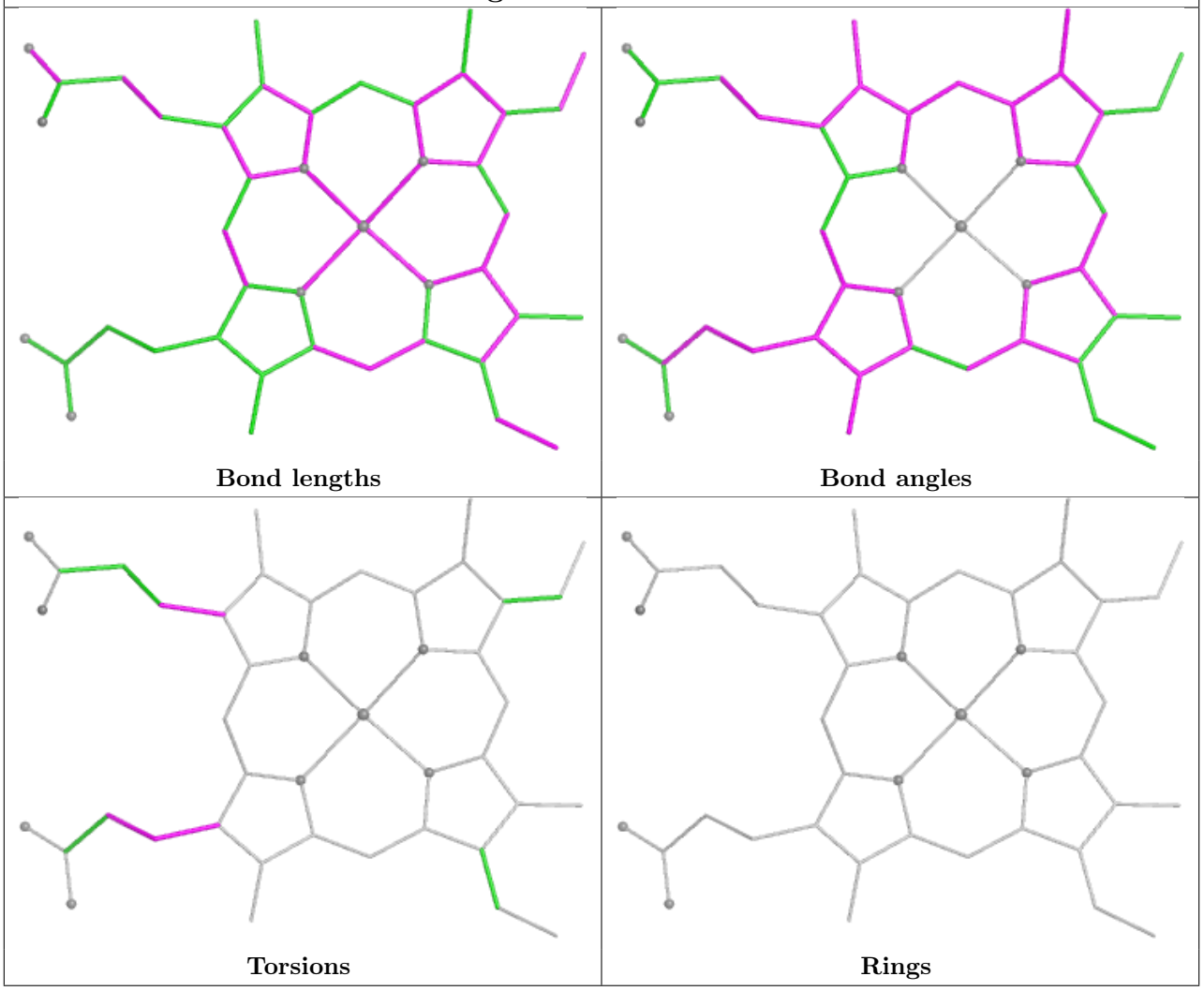


Torsions



Rings

Ligand HEM B 500



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	434:THR	C	435:HIS	N	1.20
1	A	434:THR	C	435:HIS	N	1.13

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	408/460 (88%)	1.36	97 (23%)	2 2	19, 39, 59, 70	0
1	B	408/460 (88%)	2.15	202 (49%)	0 0	18, 38, 59, 68	0
All	All	816/920 (88%)	1.76	299 (36%)	1 0	18, 38, 59, 70	0

All (299) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	341	GLY	7.1
1	B	30	GLY	6.3
1	B	101	ASN	6.2
1	B	186	PHE	6.2
1	B	180	GLY	6.1
1	B	349	ALA	5.7
1	B	32	SER	5.5
1	B	210	GLY	5.5
1	A	101	ASN	5.4
1	B	336	ALA	5.3
1	B	195	PRO	5.2
1	A	98	SER	4.9
1	B	335	ALA	4.9
1	B	188	PRO	4.8
1	B	141	GLY	4.7
1	B	119	PRO	4.6
1	B	189	VAL	4.6
1	B	51	PHE	4.5
1	B	183	PHE	4.4
1	B	226	GLU	4.3
1	B	184	LEU	4.3
1	B	193	VAL	4.3
1	B	159	TRP	4.3
1	A	216	SER	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	162	VAL	4.2
1	B	206	LEU	4.1
1	B	157	ARG	4.1
1	B	204	TYR	4.0
1	B	139	PHE	4.0
1	B	198	PRO	4.0
1	B	403	GLY	3.9
1	B	293	LEU	3.9
1	A	423	GLN	3.9
1	B	412	VAL	3.9
1	B	209	PRO	3.8
1	B	269	PRO	3.8
1	B	211	ARG	3.8
1	B	312	ASN	3.8
1	A	152	GLY	3.8
1	B	286	SER	3.8
1	A	162	VAL	3.8
1	A	203	ASP	3.7
1	B	24	ILE	3.7
1	B	216	SER	3.7
1	A	217	HIS	3.7
1	B	133	ASP	3.7
1	B	31	TRP	3.7
1	B	72	GLY	3.7
1	B	129	GLY	3.7
1	B	358	LEU	3.7
1	B	240	VAL	3.7
1	B	243	ASN	3.7
1	A	430	LEU	3.6
1	B	161	ALA	3.6
1	B	124	VAL	3.6
1	A	80	HIS	3.6
1	A	52	VAL	3.6
1	B	191	GLY	3.6
1	B	142	ASN	3.5
1	B	105	TYR	3.5
1	A	102	GLU	3.4
1	B	309	THR	3.4
1	B	181	ASN	3.4
1	B	60	ARG	3.4
1	B	289	ASP	3.4
1	A	315	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	176	TYR	3.4
1	A	65	GLU	3.4
1	B	200	ASP	3.4
1	B	262	ARG	3.3
1	B	190	SER	3.3
1	A	24	ILE	3.3
1	B	138	PHE	3.3
1	B	143	ARG	3.3
1	B	249	VAL	3.3
1	A	105	TYR	3.3
1	B	241	SER	3.3
1	B	118	PHE	3.2
1	B	228	THR	3.2
1	B	245	GLY	3.2
1	A	384	LYS	3.2
1	A	99	GLU	3.2
1	B	171	TRP	3.2
1	A	215	SER	3.2
1	B	158	SER	3.2
1	B	205	PHE	3.2
1	B	42	GLY	3.2
1	A	420	ASN	3.2
1	B	120	LEU	3.2
1	A	206	LEU	3.1
1	B	199	LEU	3.1
1	B	99	GLU	3.1
1	B	272	HIS	3.1
1	A	327	VAL	3.1
1	A	78	PHE	3.1
1	B	47	PHE	3.1
1	B	300	TYR	3.1
1	B	306	GLY	3.1
1	B	67	TRP	3.0
1	B	46	PHE	3.0
1	B	409	TYR	3.0
1	A	305	LYS	3.0
1	A	385	PRO	3.0
1	A	153	THR	3.0
1	B	156	GLU	3.0
1	B	256	TRP	3.0
1	B	169	LEU	3.0
1	A	324	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	203	ASP	3.0
1	B	202	ARG	2.9
1	B	132	GLN	2.9
1	B	29	ASP	2.9
1	B	247	THR	2.9
1	A	82	HIS	2.9
1	A	401	ILE	2.9
1	A	400	LEU	2.9
1	A	67	TRP	2.9
1	B	58	GLY	2.9
1	A	253	SER	2.9
1	B	165	CYS	2.9
1	B	126	CYS	2.9
1	B	408	CYS	2.9
1	B	273	GLN	2.8
1	B	315	PRO	2.8
1	A	331	GLU	2.8
1	B	250	PHE	2.8
1	B	160	PRO	2.8
1	B	401	ILE	2.8
1	A	228	THR	2.8
1	B	376	VAL	2.8
1	A	417	ALA	2.8
1	B	356	LEU	2.8
1	B	365	THR	2.8
1	B	343	SER	2.8
1	B	277	GLY	2.7
1	A	202	ARG	2.7
1	A	35	ALA	2.7
1	B	234	LEU	2.7
1	B	291	LEU	2.7
1	B	348	MET	2.7
1	B	40	ASP	2.7
1	B	121	ASP	2.7
1	B	342	SER	2.7
1	B	392	SER	2.7
1	A	33	PHE	2.7
1	A	38	LEU	2.7
1	A	161	ALA	2.7
1	B	322	LEU	2.7
1	B	332	ALA	2.7
1	B	155	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	302	PHE	2.7
1	B	127	HIS	2.7
1	B	147	TRP	2.7
1	B	314	TYR	2.7
1	B	275	PRO	2.7
1	B	74	VAL	2.7
1	B	330	LEU	2.7
1	B	301	VAL	2.6
1	B	418	ALA	2.6
1	B	411	HIS	2.6
1	A	365	THR	2.6
1	B	380	LEU	2.6
1	A	157	ARG	2.6
1	B	218	ARG	2.6
1	A	163	GLY	2.6
1	B	235	VAL	2.6
1	A	389	ASN	2.6
1	B	26	GLN	2.6
1	B	80	HIS	2.6
1	B	266	HIS	2.6
1	B	62	LEU	2.6
1	B	137	LEU	2.6
1	A	247	THR	2.6
1	B	201	VAL	2.6
1	B	178	PHE	2.6
1	B	225	HIS	2.5
1	B	230	CYS	2.5
1	B	410	ARG	2.5
1	A	171	TRP	2.5
1	A	406	LEU	2.5
1	B	109	LEU	2.5
1	B	268	TRP	2.5
1	B	427	VAL	2.5
1	B	334	ASP	2.5
1	B	84	SER	2.5
1	A	104	VAL	2.5
1	A	408	CYS	2.5
1	B	299	VAL	2.5
1	B	172	LEU	2.4
1	B	347	ILE	2.4
1	B	163	GLY	2.4
1	B	227	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	54	LYS	2.4
1	B	122	ALA	2.4
1	B	175	TYR	2.4
1	B	362	ALA	2.4
1	A	411	HIS	2.4
1	A	142	ASN	2.4
1	B	308	TYR	2.4
1	B	82	HIS	2.4
1	B	177	CYS	2.4
1	B	311	VAL	2.4
1	B	333	VAL	2.4
1	A	218	ARG	2.4
1	A	46	PHE	2.4
1	B	108	SER	2.4
1	B	265	TRP	2.4
1	B	274	TRP	2.4
1	B	292	TYR	2.4
1	A	435	HIS	2.4
1	A	155	LYS	2.4
1	B	208	CYS	2.4
1	B	319	GLU	2.4
1	B	331	GLU	2.4
1	B	399	TYR	2.4
1	A	223	HIS	2.4
1	B	294	ILE	2.4
1	B	278	PRO	2.4
1	B	396	PRO	2.4
1	A	39	ASP	2.3
1	B	76	ALA	2.3
1	B	423	GLN	2.3
1	B	87	LEU	2.3
1	A	100	LYS	2.3
1	B	357	ASP	2.3
1	A	154	LYS	2.3
1	B	117	PRO	2.3
1	B	323	GLY	2.3
1	B	185	ARG	2.3
1	B	255	TYR	2.3
1	A	183	PHE	2.3
1	A	421	LEU	2.3
1	A	230	CYS	2.3
1	B	136	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	103	LYS	2.2
1	A	132	GLN	2.2
1	A	403	GLY	2.2
1	A	70	PHE	2.2
1	B	182	GLN	2.2
1	B	296	ASP	2.2
1	A	159	TRP	2.2
1	A	412	VAL	2.2
1	A	64	SER	2.2
1	A	204	TYR	2.2
1	A	306	GLY	2.2
1	A	307	GLY	2.2
1	B	100	LYS	2.2
1	B	123	ALA	2.2
1	B	164	ASN	2.2
1	A	427	VAL	2.2
1	B	173	GLY	2.2
1	B	197	TYR	2.2
1	B	270	ILE	2.2
1	B	33	PHE	2.2
1	B	131	CYS	2.2
1	B	98	SER	2.2
1	B	406	LEU	2.2
1	B	140	GLN	2.1
1	A	95	VAL	2.1
1	A	200	ASP	2.1
1	B	384	LYS	2.1
1	B	393	THR	2.1
1	A	318	LEU	2.1
1	B	71	ILE	2.1
1	A	69	ASN	2.1
1	B	416	ASN	2.1
1	A	73	PRO	2.1
1	A	424	PRO	2.1
1	A	107	LYS	2.1
1	B	290	LYS	2.1
1	A	323	GLY	2.1
1	A	86	TYR	2.1
1	A	346	HIS	2.1
1	A	106	PRO	2.1
1	B	107	LYS	2.1
1	A	264	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	59	ILE	2.1
1	A	270	ILE	2.1
1	B	104	VAL	2.1
1	B	258	LEU	2.1
1	B	166	THR	2.1
1	B	53	TRP	2.1
1	B	94	TRP	2.1
1	B	364	ALA	2.1
1	B	321	GLU	2.1
1	A	409	TYR	2.1
1	A	419	LYS	2.0
1	B	435	HIS	2.0
1	B	389	ASN	2.0
1	A	335	ALA	2.0
1	A	364	ALA	2.0
1	A	28	SER	2.0
1	A	240	VAL	2.0
1	A	241	SER	2.0
1	A	276	GLN	2.0
1	B	398	LEU	2.0
1	B	113	PHE	2.0
1	B	238	ALA	2.0
1	B	316	LYS	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 oligosaccharides in this entry.

6.4 Ligands (i)

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

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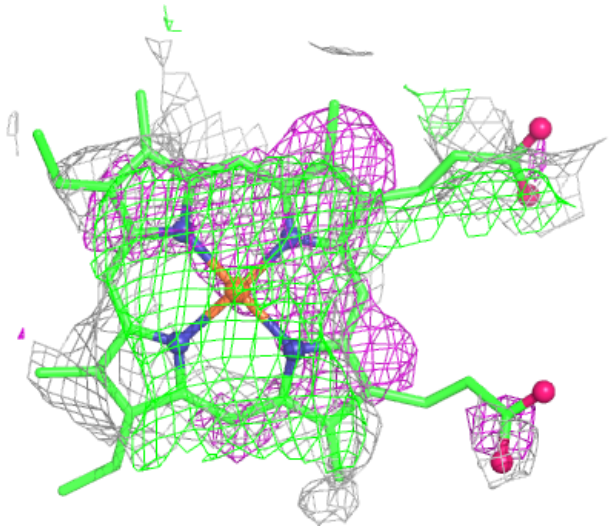
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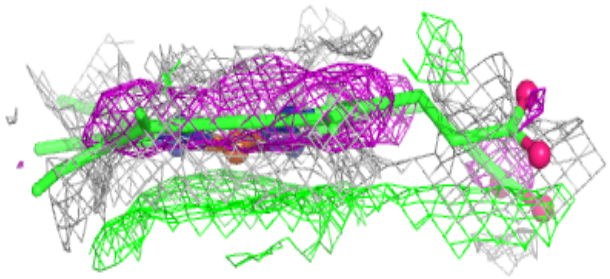
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	CL	B	511	1/1	0.36	0.28	26,26,26,26	0
5	NA	A	513	1/1	0.45	0.18	32,32,32,32	0
4	CL	B	521	1/1	0.58	0.12	20,20,20,20	0
2	HEM	B	500	43/43	0.63	0.22	14,30,39,40	0
4	CL	A	521	1/1	0.67	0.17	20,20,20,20	0
5	NA	A	512	1/1	0.70	0.20	33,33,33,33	0
5	NA	B	512	1/1	0.72	0.13	33,33,33,33	0
3	PO4	B	501	5/5	0.75	0.14	18,19,20,20	5
5	NA	B	522	1/1	0.78	0.10	26,26,26,26	0
5	NA	B	513	1/1	0.80	0.13	32,32,32,32	0
5	NA	A	522	1/1	0.80	0.14	26,26,26,26	0
4	CL	A	511	1/1	0.81	0.08	26,26,26,26	0
3	PO4	A	501	5/5	0.83	0.15	18,19,20,20	5
5	NA	A	523	1/1	0.87	0.13	27,27,27,27	0
5	NA	B	523	1/1	0.90	0.13	27,27,27,27	0
2	HEM	A	500	43/43	0.91	0.14	23,33,49,60	0

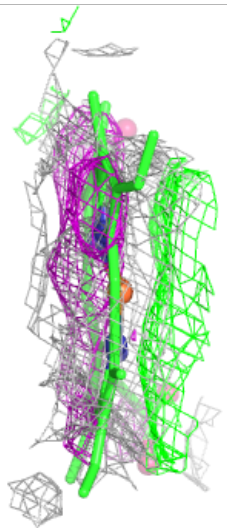
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

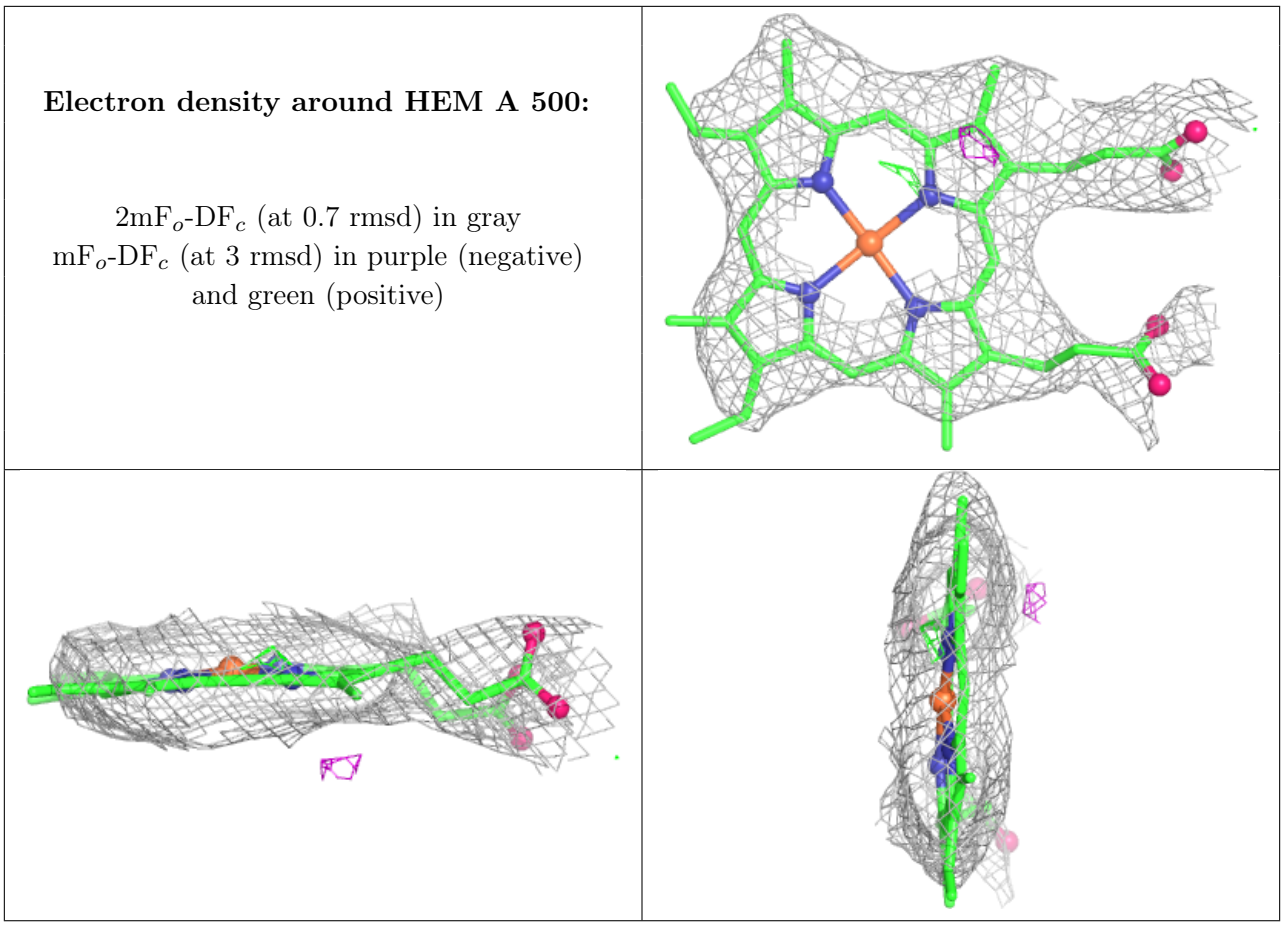






Electron density around HEM A 500:

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



6.5 Other polymers (i)

There are no such residues in this entry.