Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2024 – 12:38 am GMT

PDB ID	:	5JHX
Title	:	Crystal Structure of Fungal MagKatG2 at pH 3.0
Authors	:	Gasselhuber, B.; Obinger, C.; Carpena, X.
Deposited on	:	2016-04-21
Resolution	:	1.40 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:

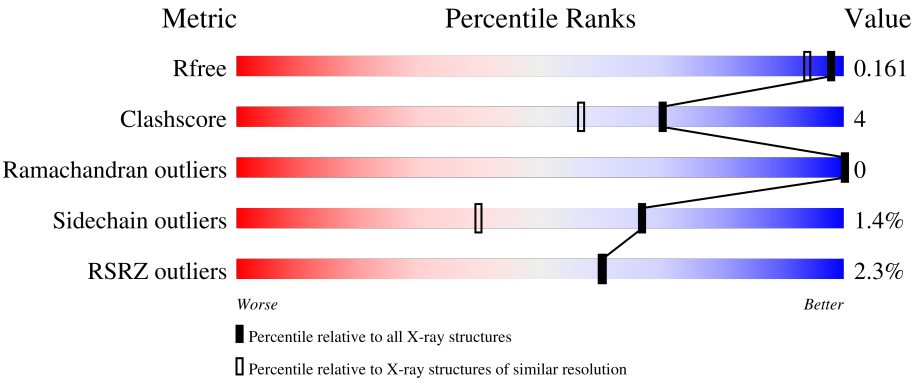
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	764	2% 81% 13%
1	B	764	3% 83% 12%

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	FLC	A	802[B]	-	X	-	-
3	FLC	B	1501[A]	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13405 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.

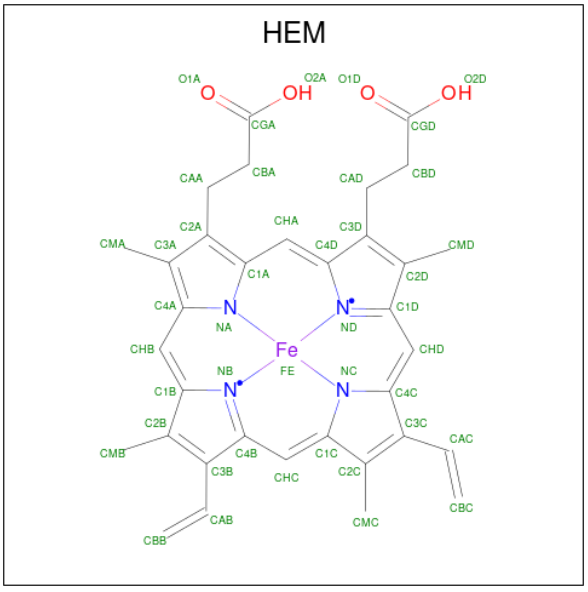
- Molecule 1 is a protein called Catalase-peroxidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	735	Total	C	N	O	S	0	15	0
			5726	3599	1003	1101	23			
1	B	734	Total	C	N	O	S	0	21	0
			5753	3623	1007	1101	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	initiating methionine	UNP A4QUT2
B	23	MET	-	initiating methionine	UNP A4QUT2

- 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		

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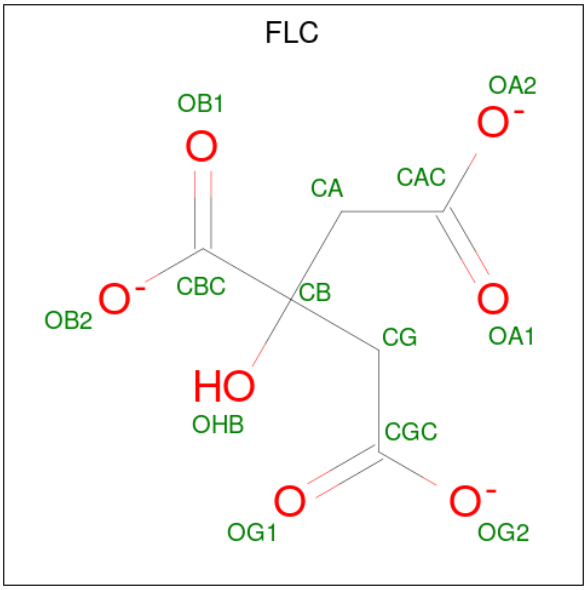
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			26	12	14		
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	1
			26	12	14		
3	B	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		

- Molecule 4 is water.

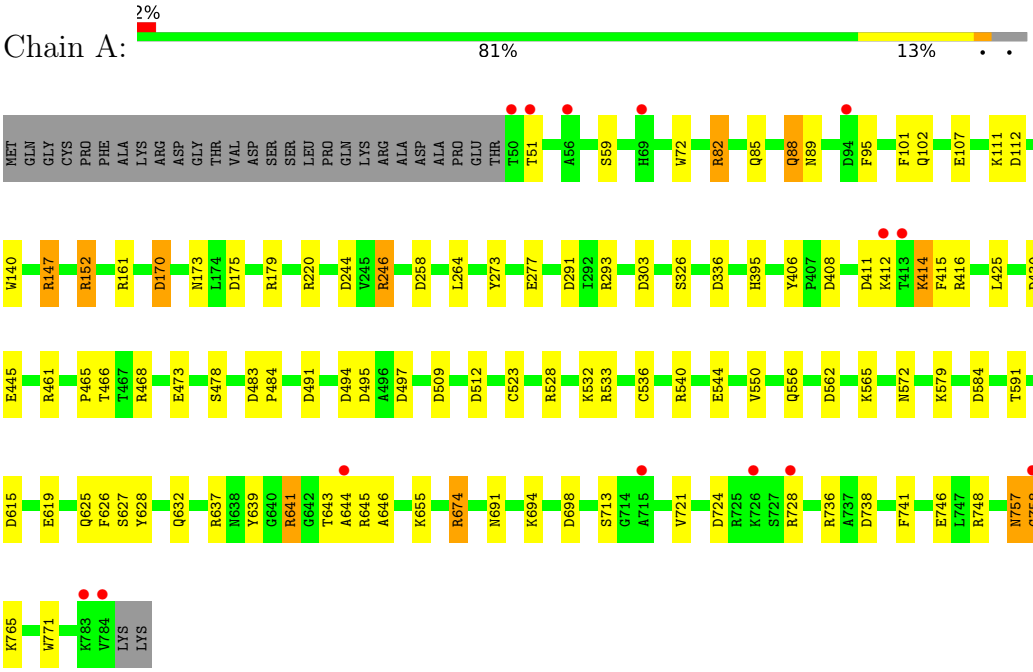
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	846	Total	O	0	0
			846	846		
4	B	903	Total	O	0	0
			903	903		

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.

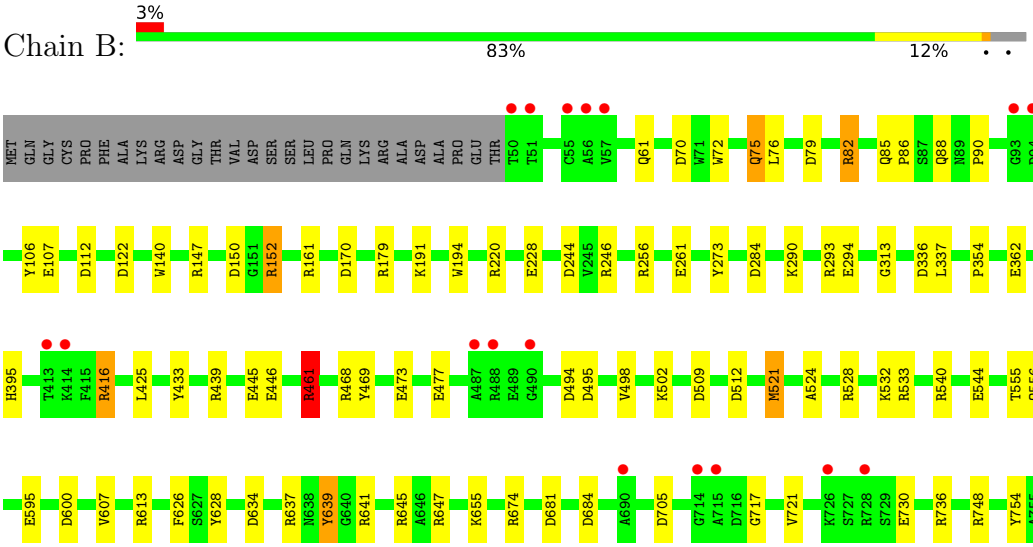
• Molecule 1: Catalase-peroxidase 2

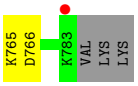
Chain A:



• Molecule 1: Catalase-peroxidase 2

Chain B:




K765
D766
K783
VAL
LYS
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	103.22Å 109.86Å 132.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.40 20.00 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-1.40) 99.9 (20.00-1.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.15 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.138 , 0.161 0.138 , 0.161	Depositor DCC
R_{free} test set	14720 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	13.4	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 41.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	13405	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, 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	1.35	26/5905 (0.4%)	1.44	85/8014 (1.1%)
1	B	1.36	27/5953 (0.5%)	1.38	76/8076 (0.9%)
All	All	1.35	53/11858 (0.4%)	1.41	161/16090 (1.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	758	GLY	N-CA	14.68	1.68	1.46
1	A	478	SER	CB-OG	-10.28	1.28	1.42
1	B	521	MET	SD-CE	-9.92	1.22	1.77
1	B	72	TRP	CZ3-CH2	-8.74	1.26	1.40
1	B	595	GLU	CD-OE1	8.55	1.35	1.25
1	B	639	TYR	CE1-CZ	-7.89	1.28	1.38
1	A	152	ARG	NE-CZ	-7.66	1.23	1.33
1	B	72	TRP	CD2-CE2	-7.42	1.32	1.41
1	A	72	TRP	CZ3-CH2	-7.09	1.28	1.40
1	A	72	TRP	CD2-CE2	-6.93	1.33	1.41
1	B	477	GLU	CD-OE2	6.86	1.33	1.25
1	A	544	GLU	CD-OE2	-6.76	1.18	1.25
1	B	101	PHE	CG-CD2	-6.70	1.28	1.38
1	A	432[A]	GLU	CD-OE1	6.67	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	432[B]	GLU	CD-OE1	6.67	1.32	1.25
1	B	445	GLU	CD-OE2	6.60	1.32	1.25
1	B	107	GLU	CD-OE1	-6.54	1.18	1.25
1	B	445	GLU	CD-OE1	6.52	1.32	1.25
1	A	550	VAL	CB-CG2	-6.51	1.39	1.52
1	A	644	ALA	C-O	6.50	1.35	1.23
1	A	277[A]	GLU	CD-OE2	6.44	1.32	1.25
1	A	277[B]	GLU	CD-OE2	6.44	1.32	1.25
1	A	758	GLY	CA-C	6.44	1.62	1.51
1	B	194	TRP	CZ3-CH2	-6.34	1.29	1.40
1	B	628	TYR	CG-CD2	-6.26	1.31	1.39
1	A	628	TYR	CE1-CZ	-6.23	1.30	1.38
1	A	628	TYR	CZ-OH	6.07	1.48	1.37
1	B	461[A]	ARG	C-O	6.06	1.34	1.23
1	B	461[B]	ARG	C-O	6.06	1.34	1.23
1	A	771	TRP	CZ3-CH2	-5.87	1.30	1.40
1	B	261	GLU	CD-OE1	5.83	1.32	1.25
1	A	619	GLU	CD-OE1	5.64	1.31	1.25
1	B	446	GLU	CD-OE1	-5.64	1.19	1.25
1	B	524	ALA	C-O	5.62	1.34	1.23
1	B	106	TYR	CE2-CZ	-5.56	1.31	1.38
1	A	639	TYR	CE1-CZ	-5.52	1.31	1.38
1	B	461[A]	ARG	CA-CB	-5.51	1.41	1.53
1	B	461[B]	ARG	CA-CB	-5.51	1.41	1.53
1	A	101	PHE	CG-CD2	-5.50	1.30	1.38
1	B	717	GLY	N-CA	5.46	1.54	1.46
1	A	326	SER	CA-CB	5.44	1.61	1.52
1	B	544	GLU	CD-OE2	-5.38	1.19	1.25
1	B	362	GLU	CD-OE2	-5.36	1.19	1.25
1	A	415	PHE	CG-CD2	5.33	1.46	1.38
1	A	89	ASN	N-CA	-5.26	1.35	1.46
1	B	607	VAL	N-CA	-5.25	1.35	1.46
1	A	491	ASP	CB-CG	5.24	1.62	1.51
1	A	761	GLU	CG-CD	-5.23	1.44	1.51
1	A	746	GLU	CD-OE1	-5.11	1.20	1.25
1	A	179	ARG	CZ-NH1	-5.10	1.26	1.33
1	B	313	GLY	N-CA	-5.06	1.38	1.46
1	B	90	PRO	N-CA	-5.06	1.38	1.47
1	B	294	GLU	CD-OE2	5.06	1.31	1.25

All (161) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	540	ARG	NE-CZ-NH2	-18.34	111.13	120.30
1	B	82	ARG	NE-CZ-NH2	15.89	128.25	120.30
1	A	494	ASP	CB-CG-OD1	13.87	130.78	118.30
1	B	82	ARG	NE-CZ-NH1	-13.00	113.80	120.30
1	B	533	ARG	NE-CZ-NH1	12.07	126.33	120.30
1	B	152	ARG	NE-CZ-NH1	-12.00	114.30	120.30
1	A	244	ASP	CB-CG-OD1	11.49	128.64	118.30
1	A	528	ARG	NE-CZ-NH2	-10.43	115.09	120.30
1	A	82	ARG	NE-CZ-NH2	10.28	125.44	120.30
1	B	613	ARG	NE-CZ-NH2	-10.24	115.18	120.30
1	A	533	ARG	NE-CZ-NH1	10.22	125.41	120.30
1	A	246	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	B	641	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	A	674	ARG	NE-CZ-NH1	9.67	125.13	120.30
1	A	736	ARG	NE-CZ-NH1	9.51	125.05	120.30
1	B	494	ASP	CB-CG-OD1	9.51	126.86	118.30
1	B	512	ASP	CB-CG-OD1	9.45	126.81	118.30
1	B	509	ASP	CB-CG-OD1	9.33	126.70	118.30
1	B	244	ASP	CB-CG-OD1	9.32	126.69	118.30
1	A	430	ASP	CB-CG-OD1	9.24	126.61	118.30
1	A	179	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	B	674	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	A	579	LYS	CD-CE-NZ	9.06	132.54	111.70
1	B	228	GLU	OE1-CD-OE2	-9.02	112.48	123.30
1	A	637	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	A	461	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	A	628	TYR	CD1-CE1-CZ	-8.69	111.98	119.80
1	A	757	ASN	C-N-CA	-8.59	104.27	122.30
1	A	626	PHE	CB-CG-CD1	-8.58	114.80	120.80
1	A	82	ARG	NE-CZ-NH1	-8.53	116.03	120.30
1	B	416	ARG	CG-CD-NE	-8.48	93.99	111.80
1	B	684	ASP	CB-CG-OD1	8.48	125.93	118.30
1	A	152	ARG	NE-CZ-NH1	-8.38	116.11	120.30
1	A	757	ASN	O-C-N	-8.29	109.11	123.20
1	B	107	GLU	OE1-CD-OE2	8.19	133.13	123.30
1	A	137	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	B	284	ASP	CB-CG-OD1	8.17	125.65	118.30
1	B	674	ARG	NE-CZ-NH1	7.96	124.28	120.30
1	A	468	ARG	NE-CZ-NH2	-7.95	116.33	120.30
1	B	336	ASP	CB-CG-OD1	7.92	125.43	118.30
1	B	528	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	A	116	LEU	CB-CG-CD2	-7.67	97.95	111.00
1	B	584	ASP	CB-CG-OD2	-7.64	111.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	645	ARG	NE-CZ-NH1	-7.61	116.50	120.30
1	A	88	GLN	O-C-N	-7.60	110.55	122.70
1	A	147	ARG	NE-CZ-NH1	7.58	124.09	120.30
1	A	291	ASP	CB-CG-OD2	-7.57	111.49	118.30
1	B	112	ASP	CB-CG-OD1	7.42	124.98	118.30
1	A	220	ARG	NE-CZ-NH1	7.41	124.01	120.30
1	A	533	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	A	540	ARG	NH1-CZ-NH2	7.30	127.43	119.40
1	A	161	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	B	246	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	B	469	TYR	CB-CG-CD1	7.19	125.31	121.00
1	B	641	ARG	NE-CZ-NH2	-7.16	116.72	120.30
1	A	497	ASP	CB-CG-OD2	-7.15	111.86	118.30
1	B	628	TYR	CD1-CE1-CZ	-7.13	113.38	119.80
1	B	647	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	A	293	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	B	425	LEU	CB-CG-CD2	7.01	122.92	111.00
1	A	613	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	B	293	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	584	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	A	291	ASP	CB-CG-OD1	6.96	124.56	118.30
1	A	674	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	A	738	ASP	CB-CG-OD1	-6.87	112.12	118.30
1	A	628	TYR	CE1-CZ-CE2	6.86	130.78	119.80
1	B	161	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	A	724	ASP	CB-CG-OD1	6.85	124.46	118.30
1	B	244	ASP	CB-CG-OD2	-6.83	112.15	118.30
1	B	540	ARG	NE-CZ-NH1	-6.81	116.89	120.30
1	B	161	ARG	NE-CZ-NH1	6.73	123.67	120.30
1	B	433	TYR	CB-CG-CD1	6.71	125.03	121.00
1	A	619	GLU	OE1-CD-OE2	-6.69	115.27	123.30
1	B	79	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	B	705	ASP	CB-CG-OD2	-6.68	112.29	118.30
1	A	220	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	B	468	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	A	724	ASP	CB-CG-OD2	-6.54	112.42	118.30
1	B	337	LEU	CB-CG-CD2	6.45	121.96	111.00
1	A	433	TYR	CB-CG-CD1	6.43	124.86	121.00
1	A	512	ASP	CB-CG-OD1	6.41	124.07	118.30
1	A	494	ASP	OD1-CG-OD2	-6.37	111.19	123.30
1	B	256	ARG	NE-CZ-NH1	-6.37	117.12	120.30
1	A	88	GLN	CB-CA-C	6.32	123.05	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	430	ASP	OD1-CG-OD2	-6.31	111.31	123.30
1	B	532	LYS	CA-CB-CG	-6.30	99.55	113.40
1	B	246	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	B	72	TRP	CD1-CG-CD2	-6.17	101.36	106.30
1	A	465	PRO	N-CA-CB	-6.10	95.89	102.60
1	B	220	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	B	613	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	72	TRP	CD1-CG-CD2	-6.00	101.50	106.30
1	B	494	ASP	OD1-CG-OD2	-5.97	111.95	123.30
1	A	509	ASP	CB-CG-OD1	5.96	123.66	118.30
1	B	528	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	A	619	GLU	CG-CD-OE1	5.89	130.09	118.30
1	A	179	ARG	NH1-CZ-NH2	5.88	125.87	119.40
1	B	754	TYR	CB-CG-CD2	5.87	124.52	121.00
1	B	294	GLU	OE1-CD-OE2	-5.86	116.26	123.30
1	B	600	ASP	CB-CG-OD1	5.86	123.58	118.30
1	A	757	ASN	CA-C-N	5.84	127.89	116.20
1	A	147	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	A	748	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	A	277[A]	GLU	CG-CD-OE1	-5.78	106.75	118.30
1	A	277[B]	GLU	CG-CD-OE1	-5.78	106.75	118.30
1	A	741	PHE	CB-CG-CD1	5.77	124.84	120.80
1	B	736	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	736	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	B	681	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	626	PHE	CB-CG-CD1	5.71	124.80	120.80
1	B	70	ASP	O-C-N	-5.70	113.59	122.70
1	A	645	ARG	NH1-CZ-NH2	5.67	125.64	119.40
1	B	736	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	425	LEU	CB-CG-CD1	5.66	120.61	111.00
1	A	637	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	A	532	LYS	CA-CB-CG	-5.64	100.98	113.40
1	A	473	GLU	OE1-CD-OE2	-5.63	116.55	123.30
1	B	502	LYS	CD-CE-NZ	-5.61	98.80	111.70
1	A	532	LYS	CD-CE-NZ	5.61	124.60	111.70
1	B	290	LYS	CD-CE-NZ	-5.61	98.80	111.70
1	B	336	ASP	OD1-CG-OD2	-5.55	112.75	123.30
1	B	473	GLU	OE1-CD-OE2	-5.51	116.69	123.30
1	A	258	ASP	CB-CG-OD2	5.48	123.23	118.30
1	A	303	ASP	CB-CG-OD1	5.47	123.22	118.30
1	B	628	TYR	CZ-CE2-CD2	-5.40	114.94	119.80
1	A	277[A]	GLU	OE1-CD-OE2	5.39	129.77	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	277[B]	GLU	OE1-CD-OE2	5.39	129.77	123.30
1	B	555[A]	THR	CA-CB-CG2	-5.39	104.85	112.40
1	B	555[B]	THR	CA-CB-CG2	-5.39	104.85	112.40
1	A	748	ARG	NE-CZ-NH1	-5.35	117.62	120.30
1	A	584	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	439	ARG	NE-CZ-NH1	-5.33	117.64	120.30
1	A	698	ASP	CB-CG-OD1	5.33	123.09	118.30
1	A	336	ASP	CB-CG-OD2	5.32	123.08	118.30
1	B	72	TRP	CG-CD2-CE3	-5.31	129.12	133.90
1	B	684	ASP	OD1-CG-OD2	-5.31	113.20	123.30
1	B	498	VAL	O-C-N	-5.28	114.25	122.70
1	A	615	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	B	72	TRP	CH2-CZ2-CE2	-5.28	112.12	117.40
1	A	111	LYS	CD-CE-NZ	5.26	123.81	111.70
1	A	495	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	408	ASP	CB-CG-OD1	5.26	123.03	118.30
1	B	122	ASP	CB-CG-OD1	5.24	123.02	118.30
1	B	495	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	406	TYR	CD1-CE1-CZ	5.21	124.49	119.80
1	B	150	ASP	CB-CG-OD1	5.17	122.96	118.30
1	A	416	ARG	NE-CZ-NH2	5.17	122.88	120.30
1	A	112	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	562	ASP	CB-CG-OD2	-5.14	113.67	118.30
1	B	600	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	B	641	ARG	CD-NE-CZ	5.11	130.76	123.60
1	B	461[A]	ARG	CA-C-O	-5.11	109.38	120.10
1	B	461[B]	ARG	CA-C-O	-5.11	109.38	120.10
1	B	766	ASP	CB-CG-OD1	5.09	122.89	118.30
1	A	107	GLU	OE1-CD-OE2	5.08	129.39	123.30
1	A	95	PHE	CB-CG-CD1	-5.07	117.25	120.80
1	B	637	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	170	ASP	CB-CG-OD1	5.04	122.84	118.30
1	B	748	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	B	179	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	572	ASN	Mainchain
1	A	674	ARG	Sidechain
1	B	461[A]	ARG	Mainchain

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Mol	Chain	Res	Type	Group
1	B	756	GLU	Sidechain

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	5726	0	5543	44	0
1	B	5753	0	5613	33	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	A	39	0	15	3	0
3	B	52	0	20	6	0
4	A	846	0	0	23	0
4	B	903	0	0	17	0
All	All	13405	0	11251	81	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (81) 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:758:GLY:CA	1:A:758:GLY:N	1.68	1.53
1:A:523[A]:CYS:SG	4:A:1436:HOH:O	1.92	1.26
1:B:556:GLN:HG3	4:B:2173:HOH:O	1.56	1.03
1:A:757:ASN:O	1:A:758:GLY:HA3	1.71	0.90
1:A:757:ASN:C	1:A:758:GLY:CA	2.42	0.87
1:A:757:ASN:O	1:A:758:GLY:CA	2.24	0.84
1:B:152:ARG:NH2	4:B:1601:HOH:O	2.01	0.81
3:B:1501[A]:FLC:CGC	3:B:1501[A]:FLC:OA1	2.30	0.79
1:B:761:GLU:HG2	1:B:765:LYS:HE3	1.64	0.78
1:B:461[B]:ARG:HB2	4:B:2255:HOH:O	1.87	0.74
1:A:85:GLN:HG3	1:B:85[A]:GLN:OE1	1.86	0.74
1:A:395[A]:HIS:HB2	4:A:971:HOH:O	1.91	0.70
3:B:1501[A]:FLC:OA1	3:B:1501[A]:FLC:CG	2.40	0.69
1:A:625[A]:GLN:NE2	4:A:904:HOH:O	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641[B]:ARG:NH2	4:A:905:HOH:O	2.27	0.67
1:B:371[B]:LYS:HD2	4:B:2328:HOH:O	1.93	0.66
1:B:371[A]:LYS:HE3	4:B:1993:HOH:O	1.97	0.65
1:B:152:ARG:NH1	4:B:1601:HOH:O	2.28	0.65
1:B:730:GLU:OE2	4:B:1602:HOH:O	2.13	0.65
1:B:152:ARG:CZ	4:B:1601:HOH:O	2.41	0.64
1:A:523[C]:CYS:HG	1:A:536:CYS:HG	1.44	0.64
1:A:641[B]:ARG:CZ	4:A:917:HOH:O	2.45	0.64
1:A:632[B]:GLN:HE22	1:A:643:THR:HG23	1.63	0.63
1:B:556:GLN:CG	4:B:2173:HOH:O	2.29	0.63
1:B:371[A]:LYS:HG3	4:B:1993:HOH:O	1.99	0.62
1:B:102[B]:GLN:OE1	4:B:1603:HOH:O	2.16	0.61
1:A:625[B]:GLN:NE2	4:A:908:HOH:O	2.33	0.61
3:B:1501[A]:FLC:CGC	3:B:1501[A]:FLC:CAC	2.81	0.58
1:B:461[B]:ARG:HG2	4:B:2255:HOH:O	2.03	0.58
1:A:765:LYS:HG3	4:A:1202:HOH:O	2.02	0.57
1:B:721:VAL:HG13	1:B:730:GLU:HG3	1.85	0.57
1:B:75:GLN:HE21	1:B:76:LEU:H	1.53	0.56
1:B:461[B]:ARG:CB	4:B:2255:HOH:O	2.52	0.56
1:A:140:TRP:HZ3	1:A:273:TYR:HH	1.53	0.55
3:A:802[A]:FLC:OG2	3:A:802[A]:FLC:CBC	2.54	0.55
3:A:802[B]:FLC:OG2	3:A:802[B]:FLC:HA2	2.07	0.54
3:B:1501[A]:FLC:CAC	3:B:1501[A]:FLC:OG1	2.57	0.53
1:A:760:GLN:HB2	4:A:1511:HOH:O	2.08	0.53
1:A:88:GLN:OE1	1:B:82:ARG:HG2	2.09	0.53
1:A:641[B]:ARG:NH2	4:A:917:HOH:O	2.42	0.52
1:B:191[B]:LYS:HD2	4:B:2044:HOH:O	2.08	0.52
1:A:82:ARG:HG2	1:B:88[B]:GLN:OE1	2.10	0.52
1:A:591:THR:HG23	1:A:607:VAL:HG12	1.93	0.51
1:B:521:MET:HA	1:B:521:MET:HE2	1.91	0.51
3:A:802[B]:FLC:OG2	3:A:802[B]:FLC:CA	2.58	0.51
1:A:627[A]:SER:OG	4:A:901:HOH:O	2.20	0.49
1:A:556:GLN:HG3	4:A:1554:HOH:O	2.12	0.49
1:B:85[B]:GLN:HB3	1:B:86:PRO:HD2	1.94	0.49
1:A:641[A]:ARG:NH1	4:A:909:HOH:O	2.34	0.48
1:B:395[B]:HIS:HB2	4:B:1743:HOH:O	2.11	0.48
1:A:395[A]:HIS:CB	4:A:971:HOH:O	2.53	0.48
1:A:565:LYS:HE3	4:A:911:HOH:O	2.14	0.47
1:B:103:SER:OG	1:B:191[A]:LYS:HD3	2.14	0.47
1:B:140:TRP:HZ3	1:B:273:TYR:HH	1.57	0.47
1:A:264:LEU:CD1	4:A:926:HOH:O	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:ALA:HB1	1:B:61[A]:GLN:HG3	1.96	0.47
1:A:565:LYS:NZ	4:A:911:HOH:O	2.36	0.46
1:A:691:ASN:HB3	1:A:694:LYS:HD2	1.97	0.46
1:A:59:SER:HA	1:B:645:ARG:O	2.16	0.46
1:A:523[C]:CYS:SG	1:A:536:CYS:SG	3.00	0.46
1:A:625[A]:GLN:OE1	4:A:902:HOH:O	2.21	0.46
1:A:646:ALA:CB	1:B:61[A]:GLN:HG3	2.46	0.46
1:B:371[A]:LYS:CD	4:B:1609:HOH:O	2.63	0.46
1:A:173:ASN:HA	1:A:175:ASP:OD1	2.16	0.45
1:A:246:ARG:NH2	4:A:926:HOH:O	2.49	0.44
1:B:634[A]:ASP:HB3	1:B:639:TYR:HB3	1.98	0.44
1:B:761:GLU:CG	1:B:765:LYS:HE3	2.41	0.44
1:A:411:ASP:OD2	1:A:414:LYS:HD2	2.18	0.44
1:A:116:LEU:C	1:A:116:LEU:HD23	2.37	0.44
1:A:565:LYS:CE	4:A:911:HOH:O	2.66	0.43
1:A:641[B]:ARG:NH2	4:A:923:HOH:O	2.46	0.43
1:A:152:ARG:NH2	4:A:907:HOH:O	2.31	0.42
1:B:387:LEU:HD11	1:B:395[B]:HIS:HB3	2.01	0.42
1:A:641[B]:ARG:CZ	4:A:905:HOH:O	2.64	0.41
1:A:483:ASP:N	1:A:484:PRO:HD3	2.34	0.41
3:B:1501[A]:FLC:OG1	3:B:1501[A]:FLC:CA	2.67	0.41
1:A:466[B]:THR:HG22	4:A:1206:HOH:O	2.21	0.41
3:B:1501[A]:FLC:OA1	3:B:1501[A]:FLC:HG1	2.19	0.41
1:A:713:SER:HB3	1:A:721[A]:VAL:HG23	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	749/764 (98%)	733 (98%)	16 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	754/764 (99%)	736 (98%)	18 (2%)	0	100	100
All	All	1503/1528 (98%)	1469 (98%)	34 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	594/606 (98%)	582 (98%)	12 (2%)	55	23
1	B	600/606 (99%)	594 (99%)	6 (1%)	76	53
All	All	1194/1212 (98%)	1176 (98%)	18 (2%)	67	37

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	A	102[A]	GLN
1	A	102[B]	GLN
1	A	147	ARG
1	A	170	ASP
1	A	412	LYS
1	A	414	LYS
1	A	445	GLU
1	A	641[A]	ARG
1	A	641[B]	ARG
1	A	655	LYS
1	A	728	ARG
1	B	75	GLN
1	B	147	ARG
1	B	170	ASP
1	B	354	PRO
1	B	416	ARG
1	B	655	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	443	HIS
1	A	556	GLN
1	A	707	ASN
1	B	548	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

9 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	HEM	A	801	4,1	41,50,50	1.25	4 (9%)	45,82,82	1.93	13 (28%)
3	FLC	A	803	-	12,12,12	1.05	1 (8%)	17,17,17	2.63	6 (35%)
2	HEM	B	1500	4,1	41,50,50	1.09	1 (2%)	45,82,82	1.71	8 (17%)
3	FLC	B	1502	-	12,12,12	1.64	3 (25%)	17,17,17	2.04	5 (29%)
3	FLC	A	802[A]	-	12,12,12	1.70	3 (25%)	17,17,17	2.00	3 (17%)
3	FLC	B	1501[A]	-	12,12,12	1.04	0	17,17,17	1.65	4 (23%)
3	FLC	B	1503	-	12,12,12	2.27	5 (41%)	17,17,17	3.46	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	FLC	A	802[B]	-	12,12,12	1.87	4 (33%)	17,17,17	4.02	12 (70%)
3	FLC	B	1501[B]	-	12,12,12	1.54	4 (33%)	17,17,17	1.56	3 (17%)

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	801	4,1	-	4/12/54/54	-
3	FLC	A	803	-	-	5/16/16/16	-
2	HEM	B	1500	4,1	-	3/12/54/54	-
3	FLC	B	1502	-	-	6/16/16/16	-
3	FLC	A	802[A]	-	-	1/16/16/16	-
3	FLC	B	1501[A]	-	-	6/16/16/16	-
3	FLC	B	1503	-	-	4/16/16/16	-
3	FLC	A	802[B]	-	-	7/16/16/16	-
3	FLC	B	1501[B]	-	-	0/16/16/16	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1503	FLC	CB-CBC	-4.89	1.48	1.53
3	A	802[B]	FLC	CB-CBC	4.05	1.57	1.53
3	B	1503	FLC	OHB-CB	3.69	1.50	1.43
3	A	802[A]	FLC	OB1-CBC	3.02	1.31	1.22
3	B	1502	FLC	CG-CB	2.84	1.57	1.53
2	A	801	HEM	C1A-NA	2.84	1.42	1.36
3	B	1503	FLC	OA2-CAC	-2.81	1.21	1.30
3	A	802[A]	FLC	CG-CB	2.78	1.57	1.53
3	A	802[B]	FLC	CA-CB	-2.76	1.50	1.53
3	A	802[B]	FLC	OB2-CBC	-2.43	1.21	1.30
3	A	802[A]	FLC	CB-CBC	2.42	1.55	1.53
3	B	1501[B]	FLC	CA-CB	2.40	1.56	1.53
3	B	1502	FLC	CA-CB	2.39	1.56	1.53
3	B	1503	FLC	OA1-CAC	2.36	1.30	1.22
2	A	801	HEM	C1B-NB	-2.27	1.36	1.40
2	B	1500	HEM	C3C-C2C	-2.26	1.37	1.40
2	A	801	HEM	CAA-C2A	-2.18	1.48	1.52
3	A	802[B]	FLC	CG-CB	-2.17	1.51	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1501[B]	FLC	CB-CBC	2.16	1.55	1.53
3	A	803	FLC	OA1-CAC	2.13	1.29	1.22
3	B	1502	FLC	OA1-CAC	2.11	1.29	1.22
2	A	801	HEM	FE-NB	2.10	2.07	1.96
3	B	1503	FLC	CG-CB	-2.08	1.51	1.53
3	B	1501[B]	FLC	OB1-CBC	2.05	1.28	1.22
3	B	1501[B]	FLC	OA2-CAC	-2.03	1.23	1.30

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	802[B]	FLC	OHB-CB-CBC	12.10	125.86	108.86
3	B	1503	FLC	OHB-CB-CG	-9.43	87.34	109.40
3	A	803	FLC	OB1-CBC-CB	-8.09	110.79	122.25
2	B	1500	HEM	C4C-CHD-C1D	6.36	130.95	122.56
3	B	1503	FLC	CG-CB-CBC	6.14	123.31	110.11
3	A	802[A]	FLC	OB1-CBC-CB	5.95	130.69	122.25
3	A	802[B]	FLC	OHB-CB-CG	-5.71	96.05	109.40
3	B	1502	FLC	OB1-CBC-CB	-5.09	115.04	122.25
2	A	801	HEM	C4B-CHC-C1C	4.49	128.49	122.56
3	A	802[B]	FLC	OHB-CB-CA	-4.43	99.03	109.40
3	B	1503	FLC	OHB-CB-CA	-4.33	99.27	109.40
3	A	802[B]	FLC	OB1-CBC-CB	4.17	128.16	122.25
2	A	801	HEM	CAA-CBA-CGA	-4.16	102.10	113.76
3	A	803	FLC	OB2-CBC-CB	3.82	119.69	113.05
3	B	1501[A]	FLC	OB1-CBC-CB	-3.78	116.91	122.25
2	A	801	HEM	CHC-C4B-C3B	3.73	130.28	124.57
2	B	1500	HEM	CAA-CBA-CGA	-3.70	103.38	113.76
3	B	1503	FLC	OG1-CGC-CG	-3.54	112.60	122.94
2	A	801	HEM	CMC-C2C-C3C	3.50	131.22	124.68
3	B	1501[A]	FLC	OB2-CBC-CB	3.47	119.07	113.05
3	B	1502	FLC	OHB-CB-CA	-3.43	101.38	109.40
2	A	801	HEM	C4B-C3B-C2B	3.39	109.81	107.11
3	A	802[B]	FLC	CB-CG-CGC	-3.39	105.61	113.81
2	A	801	HEM	C1D-C2D-C3D	3.38	110.51	106.96
3	B	1501[B]	FLC	OA2-CAC-CA	3.36	125.13	114.35
2	A	801	HEM	C1B-NB-C4B	3.32	108.50	105.07
3	B	1503	FLC	OG2-CGC-CG	3.32	125.00	114.35
3	B	1503	FLC	CG-CB-CA	3.21	117.53	109.16
2	A	801	HEM	C2D-C1D-ND	-3.21	106.04	109.88
3	A	802[B]	FLC	CG-CB-CA	3.18	117.46	109.16
3	A	803	FLC	OG1-CGC-CG	-3.09	113.92	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1500	HEM	O1D-CGD-CBD	-3.07	113.20	123.08
3	B	1501[B]	FLC	OHB-CB-CG	-3.06	102.23	109.40
2	A	801	HEM	C4D-ND-C1D	3.03	108.20	105.07
2	B	1500	HEM	C2C-C3C-C4C	-3.02	104.79	106.90
2	B	1500	HEM	C4B-CHC-C1C	3.01	126.53	122.56
3	A	802[B]	FLC	OB2-CBC-OB1	-2.98	114.35	123.82
2	B	1500	HEM	C1B-NB-C4B	2.83	108.00	105.07
3	B	1502	FLC	CG-CB-CA	2.71	116.24	109.16
3	B	1501[B]	FLC	OA2-CAC-OA1	-2.71	116.56	123.30
3	A	802[A]	FLC	OB2-CBC-OB1	-2.70	115.22	123.82
3	B	1502	FLC	OB2-CBC-CB	2.63	117.62	113.05
3	A	802[A]	FLC	OHB-CB-CA	-2.54	103.47	109.40
3	B	1501[A]	FLC	CB-CG-CGC	2.51	119.90	113.81
3	B	1503	FLC	OB1-CBC-CB	2.50	125.80	122.25
3	A	802[B]	FLC	OB2-CBC-CB	2.50	117.39	113.05
2	A	801	HEM	CBA-CAA-C2A	2.42	116.75	112.62
2	B	1500	HEM	CMA-C3A-C4A	-2.42	124.75	128.46
3	B	1502	FLC	OG1-CGC-CG	-2.40	115.94	122.94
3	A	803	FLC	OG2-CGC-CG	2.35	121.89	114.35
2	B	1500	HEM	O2D-CGD-CBD	2.30	121.43	114.03
3	B	1501[A]	FLC	OHB-CB-CBC	-2.29	105.64	108.86
3	A	802[B]	FLC	OG1-CGC-CG	-2.26	116.34	122.94
3	A	802[B]	FLC	CB-CA-CAC	-2.25	108.37	113.81
2	A	801	HEM	CMA-C3A-C4A	-2.24	125.02	128.46
3	A	802[B]	FLC	OA1-CAC-CA	-2.22	116.44	122.94
3	A	803	FLC	OA1-CAC-CA	-2.19	116.55	122.94
2	A	801	HEM	C4C-CHD-C1D	2.19	125.44	122.56
2	A	801	HEM	CHD-C1D-ND	2.17	126.79	124.43
3	A	803	FLC	OHB-CB-CG	-2.14	104.39	109.40
3	A	802[B]	FLC	OG2-CGC-OG1	2.03	128.37	123.30

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802[B]	FLC	CG-CB-CBC-OB1
3	A	802[B]	FLC	CG-CB-CBC-OB2
3	A	802[B]	FLC	OHB-CB-CBC-OB1
3	A	802[B]	FLC	OHB-CB-CBC-OB2
3	A	803	FLC	CG-CB-CBC-OB1
3	A	803	FLC	CG-CB-CBC-OB2
3	A	803	FLC	OHB-CB-CBC-OB1

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Mol	Chain	Res	Type	Atoms
3	A	803	FLC	OHB-CB-CBC-OB2
3	B	1501[A]	FLC	CA-CB-CG-CGC
3	B	1501[A]	FLC	CBC-CB-CG-CGC
3	B	1502	FLC	CG-CB-CBC-OB1
3	B	1502	FLC	CG-CB-CBC-OB2
3	B	1502	FLC	OHB-CB-CBC-OB1
3	B	1502	FLC	OHB-CB-CBC-OB2
3	B	1503	FLC	CBC-CB-CG-CGC
3	B	1501[A]	FLC	OHB-CB-CG-CGC
3	B	1503	FLC	OHB-CB-CG-CGC
3	B	1501[A]	FLC	CAC-CA-CB-OHB
3	B	1503	FLC	CB-CG-CGC-OG1
3	B	1501[A]	FLC	CAC-CA-CB-CG
3	B	1503	FLC	CB-CG-CGC-OG2
3	B	1502	FLC	CA-CB-CBC-OB2
3	A	802[B]	FLC	OHB-CB-CG-CGC
3	A	803	FLC	CAC-CA-CB-OHB
3	B	1502	FLC	CAC-CA-CB-OHB
2	A	801	HEM	CAA-CBA-CGA-O2A
2	B	1500	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O1A
2	B	1500	HEM	CAA-CBA-CGA-O1A
3	B	1501[A]	FLC	CG-CB-CBC-OB2
3	A	802[A]	FLC	CB-CG-CGC-OG2
2	B	1500	HEM	CAD-CBD-CGD-O2D
3	A	802[B]	FLC	CB-CG-CGC-OG1
3	A	802[B]	FLC	CB-CG-CGC-OG2
2	A	801	HEM	CAD-CBD-CGD-O1D
2	A	801	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

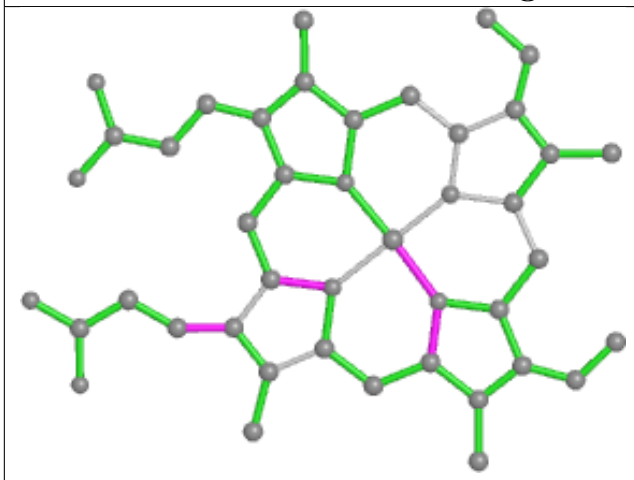
3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802[A]	FLC	1	0
3	B	1501[A]	FLC	6	0
3	A	802[B]	FLC	2	0

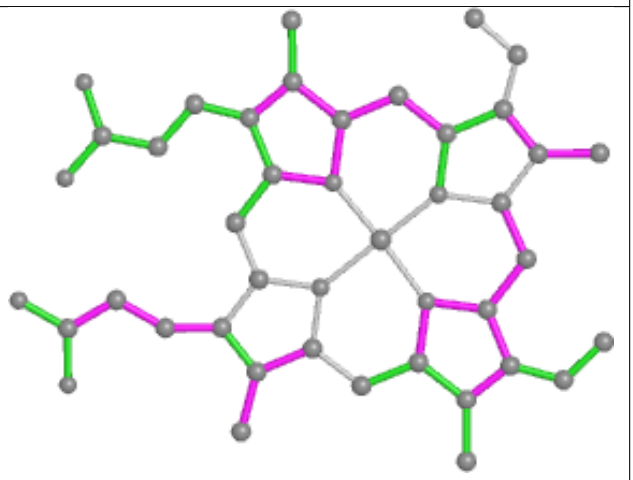
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

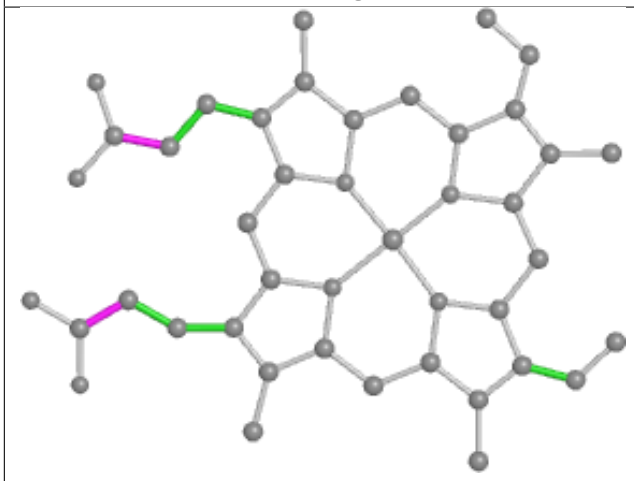
Ligand HEM A 801



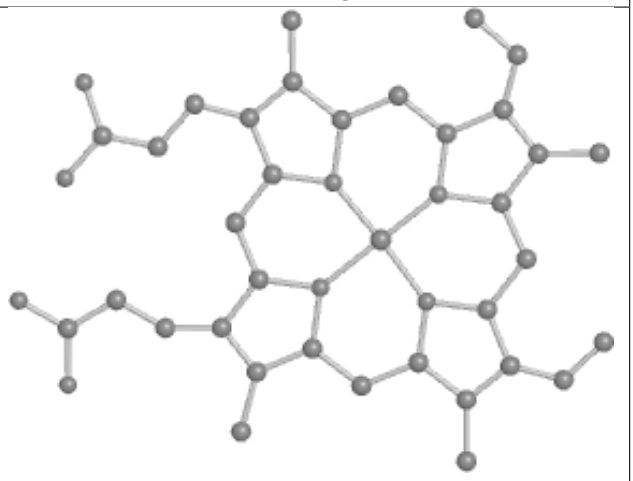
Bond lengths



Bond angles

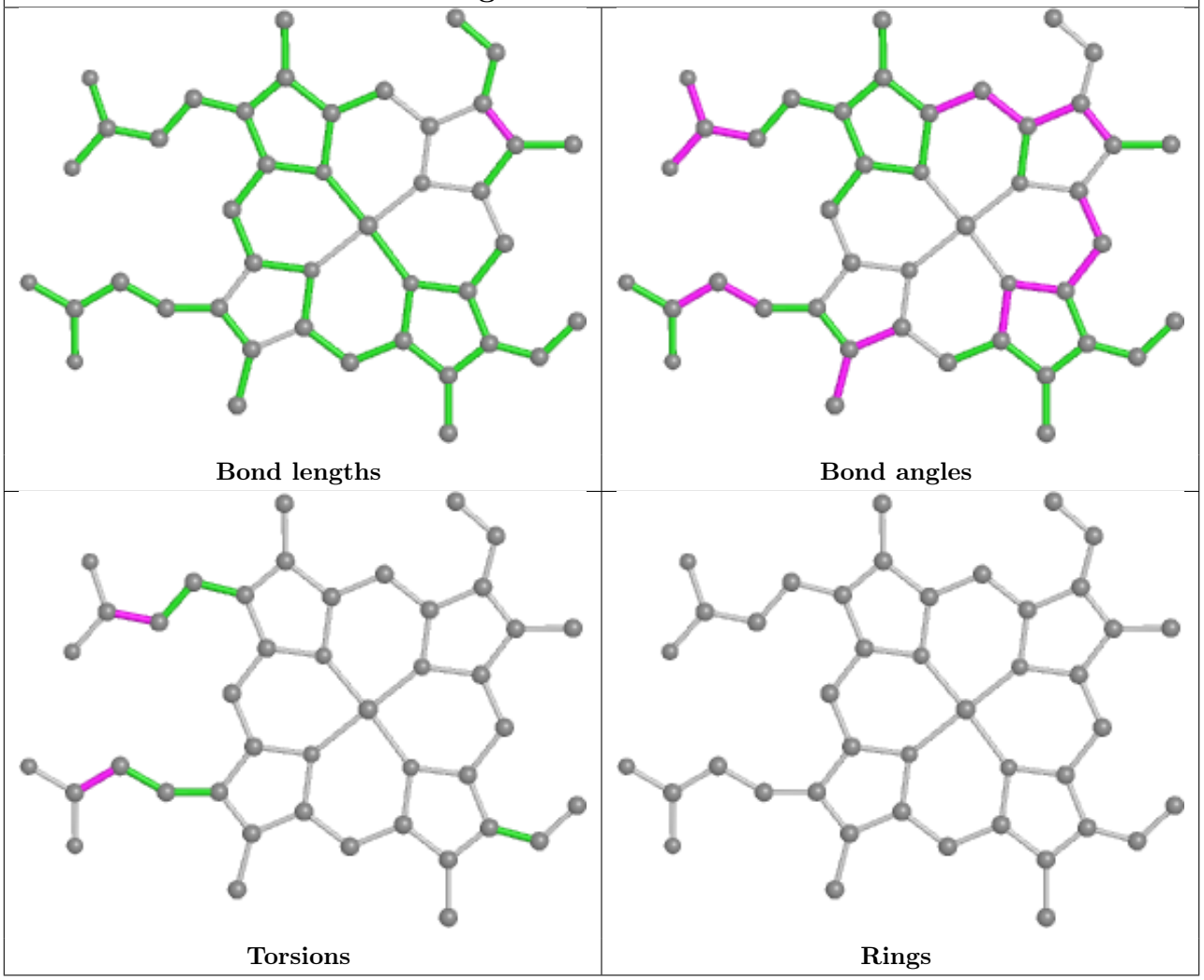


Torsions



Rings

Ligand HEM B 1500



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	735/764 (96%)	-0.23	14 (1%)	66	67	8, 14, 27, 81	0
1	B	734/764 (96%)	-0.24	20 (2%)	54	54	9, 14, 27, 59	0
All	All	1469/1528 (96%)	-0.23	34 (2%)	60	60	8, 14, 27, 81	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	50	THR	10.8
1	A	784	VAL	8.6
1	A	51	THR	5.4
1	B	50	THR	5.1
1	B	714	GLY	4.9
1	A	56	ALA	4.5
1	B	94	ASP	4.0
1	A	94	ASP	3.8
1	B	56	ALA	3.7
1	B	715	ALA	3.4
1	B	573	GLY	3.4
1	A	644	ALA	3.3
1	B	728	ARG	3.3
1	B	51	THR	3.3
1	B	490	GLY	3.3
1	B	726	LYS	3.2
1	B	413	THR	3.0
1	B	783	LYS	3.0
1	A	726	LYS	2.9
1	B	93	GLY	2.8
1	B	488	ARG	2.7
1	B	55	CYS	2.7
1	A	783	LYS	2.6
1	A	413	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	758	GLY	2.4
1	A	715	ALA	2.4
1	A	412	LYS	2.3
1	B	487	ALA	2.2
1	B	102[A]	GLN	2.2
1	A	69	HIS	2.2
1	B	414	LYS	2.1
1	B	690	ALA	2.1
1	A	728	ARG	2.0
1	B	57	VAL	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)

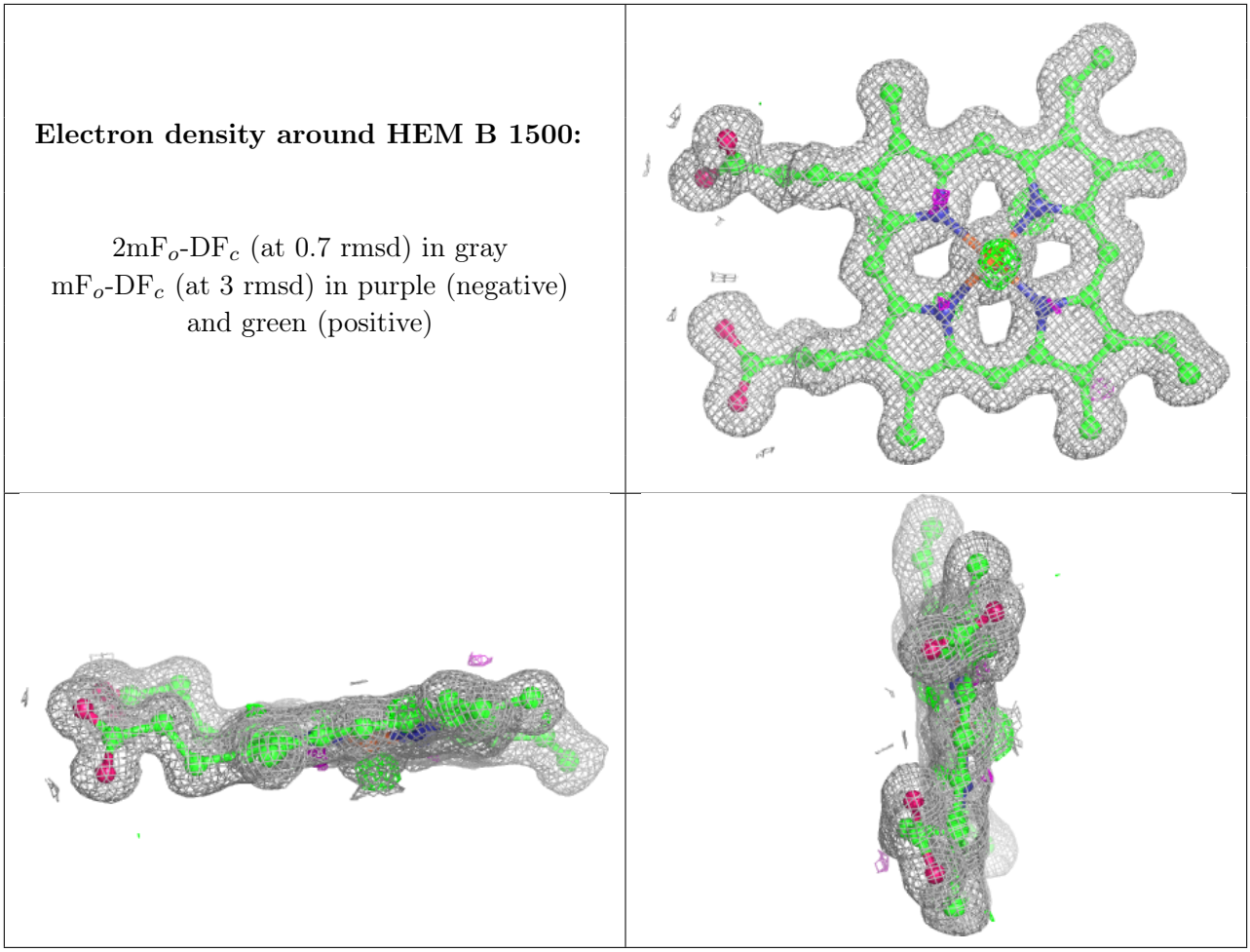
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	FLC	B	1502	13/13	0.83	0.20	17,25,36,40	13
3	FLC	A	802[B]	13/13	0.89	0.21	18,25,30,30	13
3	FLC	A	803	13/13	0.89	0.15	17,25,31,35	13
3	FLC	A	802[A]	13/13	0.89	0.21	12,18,28,29	13
3	FLC	B	1501[B]	13/13	0.90	0.23	15,20,27,28	13
3	FLC	B	1501[A]	13/13	0.90	0.23	17,37,52,57	13
3	FLC	B	1503	13/13	0.90	0.17	13,24,28,38	13
2	HEM	B	1500	43/43	0.99	0.06	9,10,11,13	0
2	HEM	A	801	43/43	0.99	0.06	8,10,11,12	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.

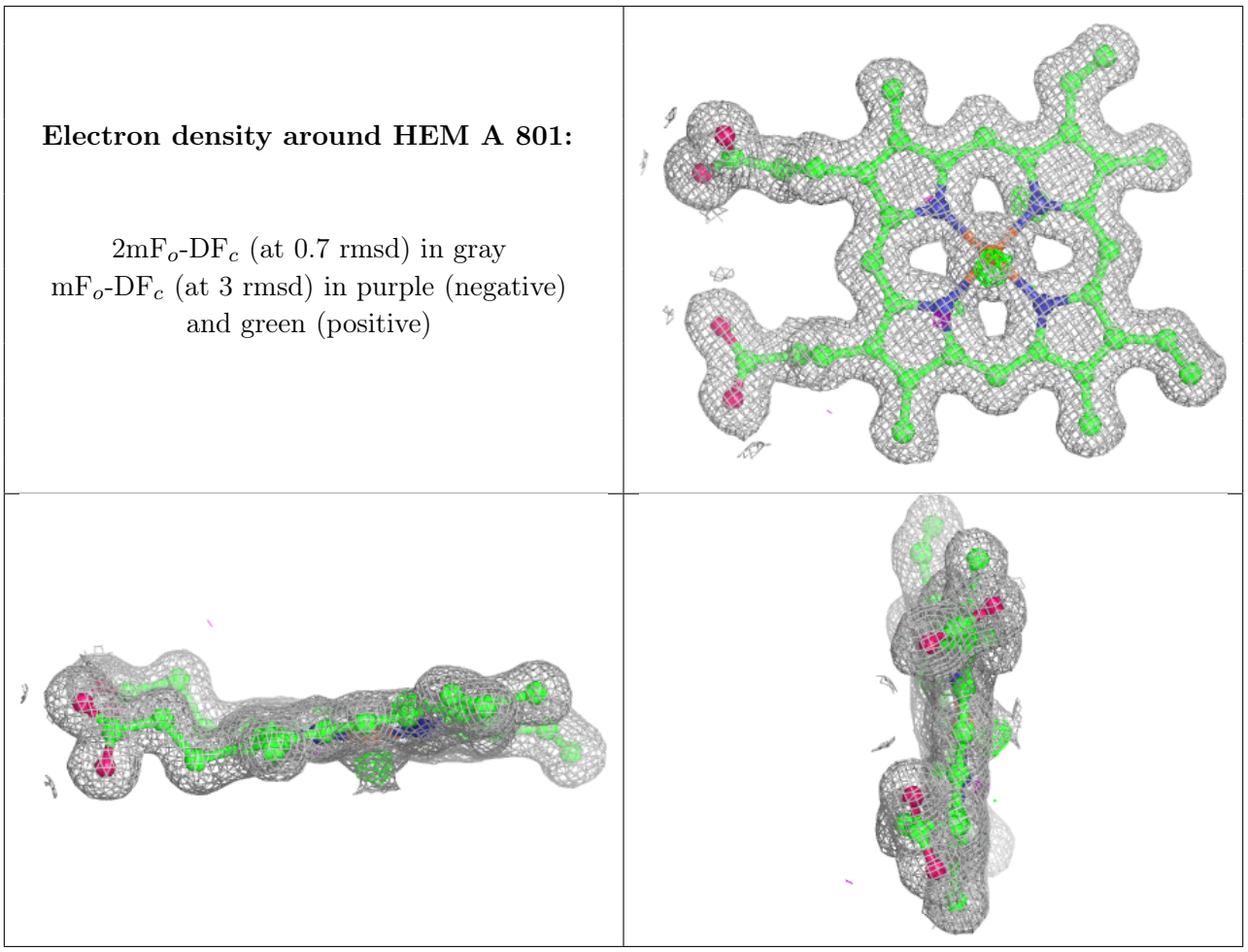
Electron density around HEM B 1500:

$2mF_o$-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 801:

$2mF_o$-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.