Full wwPDB X-ray Structure Validation Report ⓘ

Jan 2, 2024 – 01:18 pm GMT

PDB ID	:	5JHY
Title	:	Crystal Structure of Fungal MagKatG2 at pH 5.5
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:

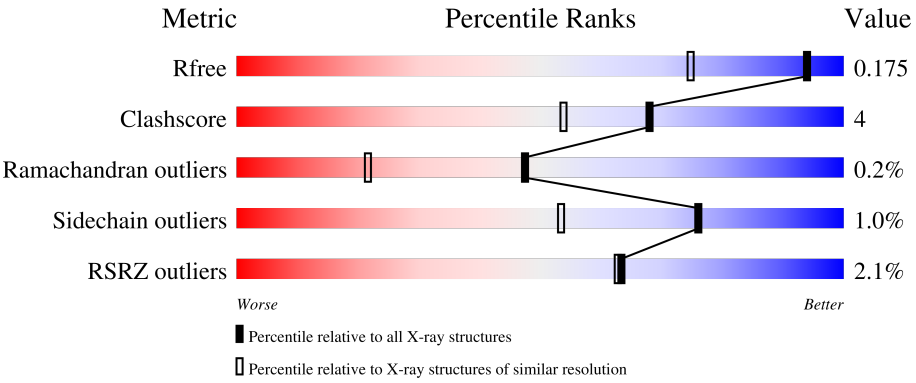
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
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% 85% 10%
1	B	764	2% 84% 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13350 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.

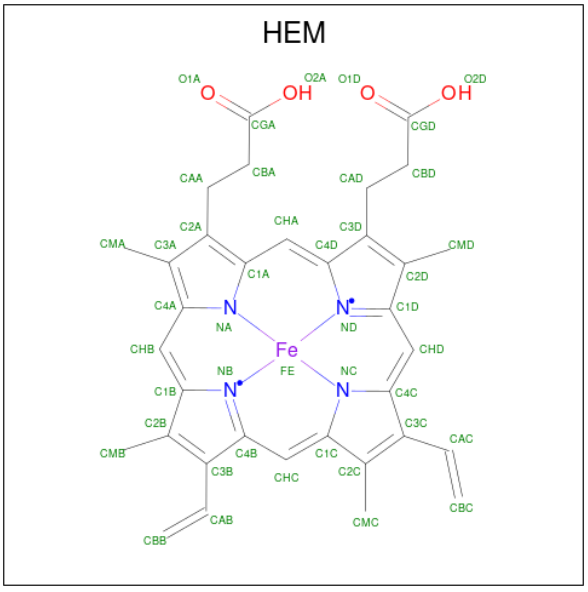
- Molecule 1 is a protein called Catalase-peroxidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	735	Total	C	N	O	S	4	15	0
			5722	3598	1002	1099	23			
1	B	734	Total	C	N	O	S	7	18	0
			5743	3608	1004	1108	23			

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 water.

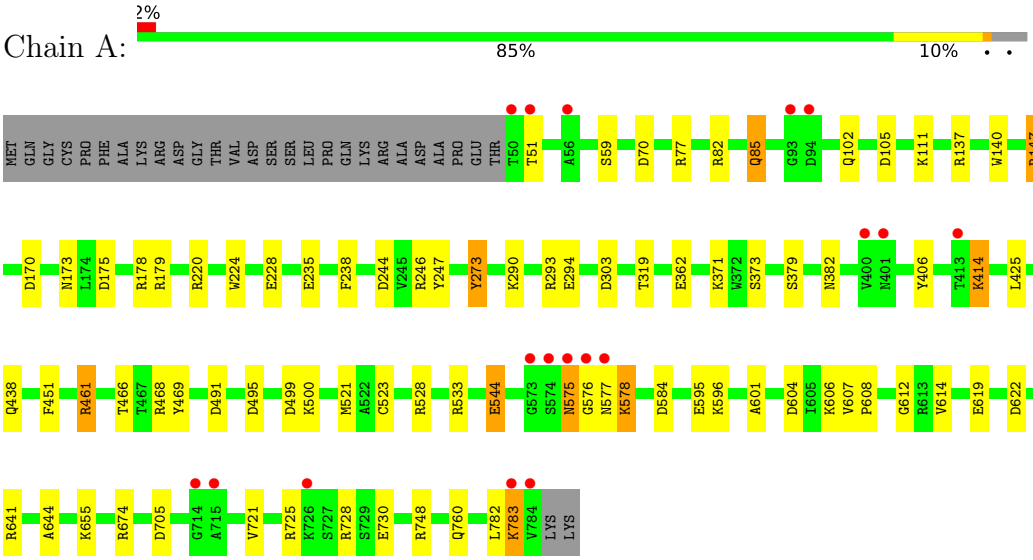
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	883	Total	O	0	0
			883	883		
3	B	916	Total	O	0	3
			916	916		

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.

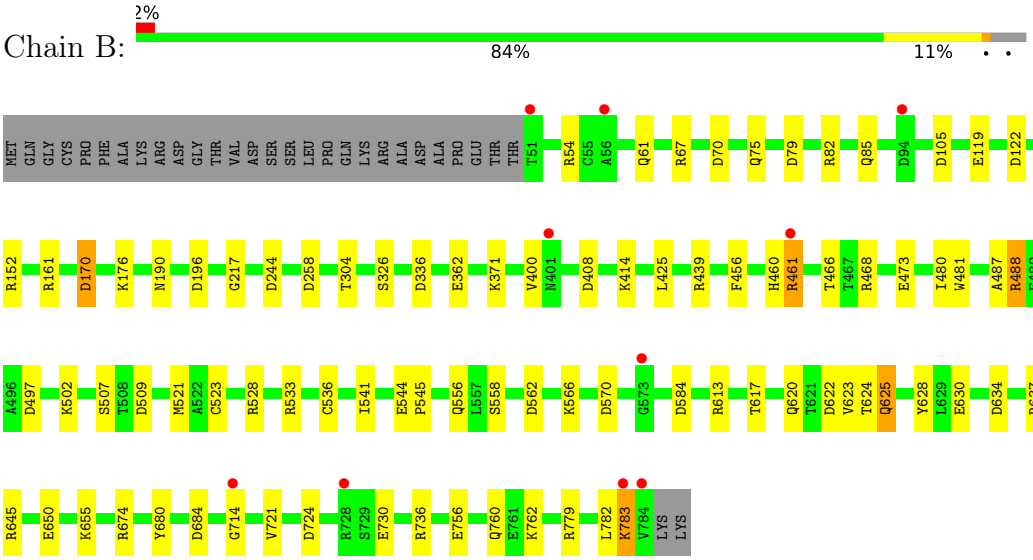
• Molecule 1: Catalase-peroxidase 2

Chain A:



• Molecule 1: Catalase-peroxidase 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	103.80Å 109.72Å 134.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.40 19.99 – 1.40	Depositor EDS
% Data completeness (in resolution range)	94.9 (20.00-1.40) 94.9 (19.99-1.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.151 , 0.176 0.151 , 0.175	Depositor DCC
R_{free} test set	14255 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	11.6	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	13350	wwPDB-VP
Average B, all atoms (Å^2)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: 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	1.31	30/5903 (0.5%)	1.31	47/8009 (0.6%)
1	B	1.34	30/5927 (0.5%)	1.41	68/8046 (0.8%)
All	All	1.33	60/11830 (0.5%)	1.36	115/16055 (0.7%)

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	1

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	461[A]	ARG	CZ-NH2	13.96	1.51	1.33
1	B	461[B]	ARG	CZ-NH2	13.96	1.51	1.33
1	B	461[C]	ARG	CZ-NH2	13.96	1.51	1.33
1	B	461[A]	ARG	CZ-NH1	-9.28	1.21	1.33
1	B	461[B]	ARG	CZ-NH1	-9.28	1.21	1.33
1	B	461[C]	ARG	CZ-NH1	-9.28	1.21	1.33
1	B	521	MET	SD-CE	-8.78	1.28	1.77
1	B	756	GLU	CD-OE2	8.18	1.34	1.25
1	B	119	GLU	CD-OE2	7.65	1.34	1.25
1	A	521	MET	SD-CE	-7.60	1.35	1.77
1	B	544	GLU	CD-OE2	-7.42	1.17	1.25
1	A	466[A]	THR	CB-CG2	-7.34	1.28	1.52
1	A	466[B]	THR	CB-CG2	-7.34	1.28	1.52
1	A	595	GLU	CD-OE1	-7.33	1.17	1.25
1	A	578	LYS	N-CA	-7.05	1.32	1.46
1	A	235	GLU	CD-OE2	6.83	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	294	GLU	CD-OE2	6.80	1.33	1.25
1	A	379	SER	CA-CB	-6.77	1.42	1.52
1	A	544	GLU	CD-OE1	6.63	1.32	1.25
1	B	507	SER	CB-OG	6.39	1.50	1.42
1	A	491	ASP	CB-CG	6.22	1.64	1.51
1	B	650	GLU	CD-OE1	-6.14	1.18	1.25
1	A	639	TYR	CE1-CZ	-6.10	1.30	1.38
1	A	382	ASN	CG-ND2	-6.04	1.17	1.32
1	A	373	SER	CB-OG	5.98	1.50	1.42
1	A	607	VAL	N-CA	-5.97	1.34	1.46
1	B	461[A]	ARG	CD-NE	5.96	1.56	1.46
1	B	461[B]	ARG	CD-NE	5.96	1.56	1.46
1	B	461[C]	ARG	CD-NE	5.96	1.56	1.46
1	B	628	TYR	CE1-CZ	-5.96	1.30	1.38
1	A	362	GLU	CD-OE2	-5.95	1.19	1.25
1	A	606	LYS	C-O	5.94	1.34	1.23
1	A	619	GLU	CD-OE1	5.77	1.31	1.25
1	A	432	GLU	CG-CD	5.65	1.60	1.51
1	A	179	ARG	CZ-NH1	-5.62	1.25	1.33
1	B	714	GLY	C-O	5.59	1.32	1.23
1	A	614	VAL	CB-CG2	-5.58	1.41	1.52
1	A	612	GLY	N-CA	5.49	1.54	1.46
1	B	119	GLU	CG-CD	5.49	1.60	1.51
1	A	644	ALA	C-O	5.45	1.33	1.23
1	B	628	TYR	CZ-OH	5.43	1.47	1.37
1	A	639	TYR	CZ-OH	5.43	1.47	1.37
1	A	224	TRP	CD2-CE2	5.41	1.47	1.41
1	B	466[A]	THR	CA-C	5.41	1.67	1.52
1	B	466[B]	THR	CA-C	5.41	1.67	1.52
1	B	624	THR	C-O	5.38	1.33	1.23
1	A	608	PRO	C-O	-5.36	1.12	1.23
1	B	760	GLN	CG-CD	5.35	1.63	1.51
1	B	558	SER	CB-OG	-5.30	1.35	1.42
1	B	326	SER	CB-OG	-5.29	1.35	1.42
1	A	85	GLN	CG-CD	5.28	1.63	1.51
1	B	783	LYS	CA-C	5.26	1.66	1.52
1	A	362	GLU	CD-OE1	5.25	1.31	1.25
1	B	119	GLU	CD-OE1	5.17	1.31	1.25
1	A	238	PHE	CG-CD2	5.13	1.46	1.38
1	B	362	GLU	CB-CG	-5.12	1.42	1.52
1	A	247	TYR	CG-CD1	5.09	1.45	1.39
1	B	630	GLU	CD-OE2	-5.08	1.20	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	481	TRP	CG-CD1	-5.05	1.29	1.36
1	A	273	TYR	CE2-CZ	-5.00	1.32	1.38

All (115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	461[A]	ARG	NE-CZ-NH1	-21.91	109.34	120.30
1	B	461[B]	ARG	NE-CZ-NH1	-21.91	109.34	120.30
1	B	461[C]	ARG	NE-CZ-NH1	-21.91	109.34	120.30
1	A	82	ARG	NE-CZ-NH1	-18.87	110.87	120.30
1	B	461[A]	ARG	NE-CZ-NH2	15.43	128.01	120.30
1	B	461[B]	ARG	NE-CZ-NH2	15.43	128.01	120.30
1	B	461[C]	ARG	NE-CZ-NH2	15.43	128.01	120.30
1	A	82	ARG	NE-CZ-NH2	15.05	127.82	120.30
1	A	528	ARG	NE-CZ-NH2	-12.03	114.29	120.30
1	A	244	ASP	CB-CG-OD1	11.71	128.84	118.30
1	B	152[A]	ARG	NE-CZ-NH1	-10.76	114.92	120.30
1	B	152[B]	ARG	NE-CZ-NH1	-10.76	114.92	120.30
1	A	293	ARG	NE-CZ-NH1	10.04	125.32	120.30
1	A	637	ARG	NE-CZ-NH2	-9.70	115.45	120.30
1	A	499	ASP	CB-CG-OD2	-9.29	109.94	118.30
1	B	584	ASP	CB-CG-OD2	-9.26	109.97	118.30
1	B	152[A]	ARG	NE-CZ-NH2	9.21	124.91	120.30
1	B	152[B]	ARG	NE-CZ-NH2	9.21	124.91	120.30
1	B	495	ASP	CB-CG-OD2	-9.04	110.16	118.30
1	A	468	ARG	NE-CZ-NH1	9.03	124.81	120.30
1	B	736	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	B	122	ASP	CB-CG-OD1	8.85	126.26	118.30
1	A	105	ASP	CB-CG-OD1	8.82	126.24	118.30
1	B	634	ASP	CB-CG-OD2	8.61	126.05	118.30
1	B	684	ASP	CB-CG-OD1	8.48	125.93	118.30
1	A	461	ARG	NE-CZ-NH1	-8.28	116.16	120.30
1	B	67	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	A	77	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	B	684	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	A	622	ASP	CB-CG-OD2	-8.00	111.10	118.30
1	A	244	ASP	CB-CG-OD2	-7.81	111.27	118.30
1	A	406	TYR	CB-CG-CD2	7.78	125.67	121.00
1	A	137	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	A	533	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	B	497	ASP	CB-CG-OD2	-7.57	111.49	118.30
1	B	425	LEU	CB-CG-CD2	7.47	123.71	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	674	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	B	258	ASP	CB-CG-OD1	7.45	125.00	118.30
1	A	491	ASP	CB-CG-OD2	-7.45	111.60	118.30
1	B	439	ARG	NE-CZ-NH1	-7.41	116.59	120.30
1	A	246	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	B	613	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	B	521	MET	CG-SD-CE	7.29	111.87	100.20
1	A	246	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	A	499	ASP	CB-CG-OD1	7.29	124.86	118.30
1	B	468	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	B	756	GLU	OE1-CD-OE2	7.19	131.93	123.30
1	B	82	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	B	82	ARG	NE-CZ-NH2	7.08	123.84	120.30
1	B	147	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	B	79	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	A	584	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	B	634	ASP	OD1-CG-OD2	-6.86	110.27	123.30
1	A	70	ASP	CB-CG-OD1	6.81	124.43	118.30
1	A	303	ASP	CB-CG-OD2	-6.77	112.20	118.30
1	B	639	TYR	CB-CG-CD2	-6.68	116.99	121.00
1	B	336	ASP	CB-CG-OD1	6.68	124.31	118.30
1	A	469	TYR	CB-CG-CD1	6.64	124.99	121.00
1	B	161	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	B	170[A]	ASP	CB-CG-OD1	6.60	124.24	118.30
1	B	170[B]	ASP	CB-CG-OD1	6.60	124.24	118.30
1	B	497	ASP	CB-CG-OD1	6.57	124.21	118.30
1	A	705	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	705	ASP	CB-CG-OD2	-6.54	112.41	118.30
1	A	468	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	B	70	ASP	CB-CG-OD2	6.38	124.05	118.30
1	B	628	TYR	CE1-CZ-CE2	6.38	130.01	119.80
1	A	179	ARG	NE-CZ-NH1	-6.38	117.11	120.30
1	B	628	TYR	CZ-CE2-CD2	-6.27	114.16	119.80
1	B	408	ASP	CB-CG-OD1	6.26	123.94	118.30
1	A	220	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	604	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	B	625[A]	GLN	CA-CB-CG	6.10	126.82	113.40
1	B	625[B]	GLN	CA-CB-CG	6.10	126.82	113.40
1	B	54	ARG	NE-CZ-NH2	-6.09	117.25	120.30
1	B	637	ARG	NE-CZ-NH2	-6.07	117.27	120.30
1	A	178	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	B	634	ASP	CB-CG-OD1	5.96	123.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	724	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	A	161	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	B	502	LYS	CD-CE-NZ	-5.90	98.13	111.70
1	A	595	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	B	196	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	B	509	ASP	CB-CG-OD1	5.80	123.52	118.30
1	B	613	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	B	680	TYR	CB-CG-CD2	-5.61	117.64	121.00
1	B	783	LYS	N-CA-C	5.59	126.11	111.00
1	B	161	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	A	147	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	105	ASP	CB-CG-OD1	5.56	123.31	118.30
1	A	425	LEU	CB-CG-CD2	5.55	120.44	111.00
1	A	362	GLU	CG-CD-OE1	5.46	129.21	118.30
1	A	495	ASP	CB-CG-OD1	5.44	123.19	118.30
1	B	244	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	468	ARG	CD-NE-CZ	5.37	131.12	123.60
1	A	430	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	748	ARG	NE-CZ-NH1	-5.35	117.63	120.30
1	B	528	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	B	362	GLU	CG-CD-OE1	5.30	128.90	118.30
1	B	628	TYR	CD1-CE1-CZ	-5.27	115.06	119.80
1	A	228	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	A	466[A]	THR	CA-CB-CG2	5.24	119.74	112.40
1	A	466[B]	THR	CA-CB-CG2	5.24	119.74	112.40
1	B	466[A]	THR	N-CA-CB	-5.23	100.36	110.30
1	B	466[B]	THR	N-CA-CB	-5.23	100.36	110.30
1	B	495	ASP	CB-CG-OD1	5.23	123.01	118.30
1	B	473	GLU	OE1-CD-OE2	-5.23	117.03	123.30
1	B	650	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	A	491	ASP	CB-CG-OD1	5.17	122.96	118.30
1	B	147	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	A	178	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	451	PHE	CB-CG-CD1	5.15	124.41	120.80
1	B	562	ASP	CB-CG-OD2	-5.07	113.73	118.30
1	A	152[A]	ARG	NE-CZ-NH1	-5.07	117.77	120.30
1	A	152[B]	ARG	NE-CZ-NH1	-5.07	117.77	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	674	ARG	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	5722	0	5549	49	0
1	B	5743	0	5556	38	0
2	A	43	0	30	1	0
2	B	43	0	30	0	0
3	A	883	0	0	25	1
3	B	916	0	0	15	1
All	All	13350	0	11165	85	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 4.

All (85) 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:140:TRP:CH2	1:A:273:TYR:HE2	0.86	1.52
1:A:140:TRP:HH2	1:A:273:TYR:CE2	0.83	1.51
1:B:461[C]:ARG:O	1:B:461[C]:ARG:HG2	1.40	1.18
1:A:140:TRP:CH2	1:A:273:TYR:CE2	1.74	1.15
1:A:523[A]:CYS:SG	3:A:2152:HOH:O	1.91	1.10
1:A:577:ASN:O	1:A:578:LYS:HG3	1.59	1.02
1:A:140:TRP:CZ3	1:A:273:TYR:HE2	1.85	0.92
1:B:570[A]:ASP:OD1	3:B:1602:HOH:O	1.88	0.91
1:A:577:ASN:O	1:A:578:LYS:CG	2.22	0.86
1:B:762:LYS:NZ	3:B:1603:HOH:O	2.08	0.86
1:A:140:TRP:CH2	1:A:273:TYR:CD2	2.63	0.86
1:A:152[A]:ARG:NH2	3:A:1603:HOH:O	1.91	0.85
1:A:461:ARG:NE	3:A:1602:HOH:O	1.80	0.85
1:A:641[B]:ARG:NH1	3:A:1605:HOH:O	2.08	0.85
1:A:725:ARG:NH1	3:A:1607:HOH:O	2.11	0.84
1:A:140:TRP:HH2	1:A:273:TYR:CD2	1.86	0.83
1:B:304[B]:THR:HG22	3:B:1665:HOH:O	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:566:LYS:HD2	3:B:1602:HOH:O	1.79	0.81
1:B:141:HIS:NE2	3:B:1605:HOH:O	2.15	0.80
1:B:461[B]:ARG:CG	1:B:461[B]:ARG:HH21	1.96	0.79
1:B:217:GLY:H	1:B:460:HIS:HE1	1.32	0.76
1:A:577:ASN:C	1:A:578:LYS:HG3	2.05	0.76
1:B:461[C]:ARG:O	1:B:461[C]:ARG:CG	2.22	0.74
1:A:500:LYS:NZ	1:A:575:ASN:HD21	1.86	0.74
1:A:140:TRP:CZ2	1:A:273:TYR:CE2	2.72	0.73
1:B:461[B]:ARG:HH21	1:B:461[B]:ARG:HG3	1.54	0.72
1:A:140:TRP:CH2	1:A:273:TYR:CZ	2.69	0.70
1:A:500:LYS:HZ2	1:A:575:ASN:HD21	1.40	0.69
1:A:432:GLU:OE1	3:A:1606:HOH:O	2.09	0.69
1:B:622:ASP:HB3	1:B:625[B]:GLN:HG2	1.75	0.68
1:B:480:ILE:O	1:B:625[B]:GLN:NE2	2.27	0.68
1:B:523[C]:CYS:HG	1:B:536:CYS:HG	1.42	0.68
1:A:730[B]:GLU:HG2	3:A:1616:HOH:O	1.93	0.67
1:B:217:GLY:H	1:B:460:HIS:CE1	2.13	0.67
1:A:152[A]:ARG:NH1	3:A:1603:HOH:O	2.27	0.67
1:A:85:GLN:HG3	1:B:85[A]:GLN:OE1	1.95	0.67
1:B:190:ASN:OD1	3:B:1604:HOH:O	2.13	0.67
1:A:140:TRP:CZ3	1:A:273:TYR:CE2	2.69	0.66
1:B:371:LYS:HG3	3:B:1938:HOH:O	1.95	0.66
1:B:304[B]:THR:CG2	3:B:1665:HOH:O	2.42	0.65
1:B:779:ARG:O	1:B:783:LYS:HA	1.97	0.65
1:A:641[A]:ARG:NH2	3:A:1613:HOH:O	2.30	0.64
1:A:371:LYS:HG3	3:A:2055:HOH:O	1.99	0.63
1:A:721:VAL:HG13	1:A:730[A]:GLU:HG3	1.80	0.63
1:B:721:VAL:HG13	1:B:730[A]:GLU:HG3	1.82	0.62
1:A:730[B]:GLU:CG	3:A:1616:HOH:O	2.50	0.58
1:B:75:GLN:NE2	3:B:1611:HOH:O	2.37	0.58
1:A:438[A]:GLN:OE1	3:A:1608:HOH:O	2.17	0.58
1:B:414:LYS:HG2	3:B:2056:HOH:O	2.03	0.58
1:B:461[B]:ARG:HG3	1:B:461[B]:ARG:NH2	2.20	0.57
1:A:152[A]:ARG:CZ	3:A:1603:HOH:O	2.38	0.56
1:B:545:PRO:HB3	1:B:623[A]:VAL:HG13	1.86	0.56
1:A:601:ALA:O	1:A:760[A]:GLN:NE2	2.38	0.56
1:A:596[A]:LYS:NZ	3:A:1617:HOH:O	2.38	0.54
1:B:456:PHE:O	1:B:460:HIS:HD2	1.92	0.51
1:A:371:LYS:CD	3:A:2170:HOH:O	2.58	0.51
1:B:721:VAL:CG1	1:B:730[A]:GLU:HG3	2.40	0.50
1:A:414:LYS:HG2	3:A:1761:HOH:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:THR:HG23	3:A:2141:HOH:O	2.12	0.50
1:A:140:TRP:CZ2	1:A:273:TYR:CD2	2.98	0.50
1:A:575:ASN:ND2	3:A:1619:HOH:O	2.45	0.49
1:A:111[B]:LYS:HG2	3:A:2397:HOH:O	2.13	0.49
1:A:111[B]:LYS:HD2	3:A:1622:HOH:O	2.13	0.48
1:A:461:ARG:CG	3:A:1602:HOH:O	2.62	0.48
1:B:461[B]:ARG:HD2	3:B:1893[B]:HOH:O	2.14	0.47
1:A:140:TRP:HZ3	1:A:273:TYR:HH	1.62	0.47
1:A:290[A]:LYS:HE3	3:A:2307:HOH:O	2.15	0.46
1:A:371:LYS:CE	3:A:2170:HOH:O	2.63	0.46
1:A:577:ASN:O	1:A:578:LYS:HG2	2.08	0.46
1:B:461[B]:ARG:HH21	1:B:461[B]:ARG:HG2	1.79	0.46
1:A:371:LYS:HE2	3:A:2055:HOH:O	2.16	0.46
1:B:487[B]:ALA:O	1:B:488[B]:ARG:CB	2.64	0.45
1:A:544:GLU:OE1	3:A:1609:HOH:O	2.21	0.44
1:B:533:ARG:NH2	1:B:625[A]:GLN:HG3	2.33	0.44
1:B:176:LYS:CE	3:B:2031:HOH:O	2.66	0.44
1:A:173:ASN:HA	1:A:175:ASP:OD1	2.18	0.43
1:A:782:LEU:O	1:A:783:LYS:CB	2.66	0.43
1:B:523[B]:CYS:SG	1:B:541:ILE:HG21	2.59	0.43
1:B:617:THR:OG1	1:B:620:GLN:HG3	2.19	0.42
1:B:556:GLN:CG	3:B:2242:HOH:O	2.67	0.42
1:A:59:SER:HA	1:B:645:ARG:O	2.21	0.41
1:B:782:LEU:N	1:B:783:LYS:HA	2.35	0.41
1:A:319:THR:HG22	2:A:1500:HEM:CAA	2.51	0.41
1:B:400:VAL:HG22	3:B:1695:HOH:O	2.21	0.41
1:B:566:LYS:CE	3:B:1602:HOH:O	2.69	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)
3:A:2084:HOH:O	3:B:2049:HOH:O[2_554]	2.03	0.17

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%)	730 (98%)	17 (2%)	2 (0%)	41 18
1	B	753/764 (99%)	736 (98%)	15 (2%)	2 (0%)	41 18
All	All	1502/1528 (98%)	1466 (98%)	32 (2%)	4 (0%)	47 18

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	783	LYS
1	B	488[A]	ARG
1	B	488[B]	ARG
1	A	576	GLY

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	593/606 (98%)	586 (99%)	7 (1%)	71 47
1	B	596/606 (98%)	591 (99%)	5 (1%)	81 62
All	All	1189/1212 (98%)	1177 (99%)	12 (1%)	76 53

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	147	ARG
1	A	170	ASP
1	A	414	LYS
1	A	575	ASN
1	A	655	LYS
1	A	728	ARG
1	B	61	GLN

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Mol	Chain	Res	Type
1	B	147	ARG
1	B	170[A]	ASP
1	B	170[B]	ASP
1	B	655	LYS

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	102	GLN
1	A	355	ASN
1	A	401	ASN
1	A	575	ASN
1	A	577	ASN
1	A	707	ASN
1	B	61	GLN
1	B	190	ASN
1	B	241	GLN
1	B	460	HIS
1	B	556	GLN

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

2 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	B	1500	1	41,50,50	1.44	8 (19%)	45,82,82	2.15	14 (31%)
2	HEM	A	1500	1	41,50,50	1.07	2 (4%)	45,82,82	1.73	10 (22%)

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	B	1500	1	-	4/12/54/54	-
2	HEM	A	1500	1	-	3/12/54/54	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1500	HEM	C1D-C2D	3.74	1.51	1.44
2	B	1500	HEM	C1A-NA	3.59	1.43	1.36
2	B	1500	HEM	O2D-CGD	-2.60	1.22	1.30
2	B	1500	HEM	CHC-C4B	-2.39	1.34	1.41
2	B	1500	HEM	C3B-C4B	2.36	1.49	1.44
2	A	1500	HEM	CHB-C1B	2.32	1.40	1.35
2	B	1500	HEM	FE-NB	2.15	2.07	1.96
2	A	1500	HEM	FE-NB	2.14	2.07	1.96
2	B	1500	HEM	CHA-C4D	2.10	1.40	1.35
2	B	1500	HEM	C3B-C2B	2.04	1.41	1.37

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1500	HEM	C4A-C3A-C2A	-5.66	103.06	107.00
2	B	1500	HEM	C4B-CHC-C1C	5.45	129.75	122.56
2	A	1500	HEM	C4A-C3A-C2A	-4.92	103.57	107.00
2	B	1500	HEM	CHA-C4D-ND	-4.89	118.34	124.38
2	B	1500	HEM	C1B-NB-C4B	3.43	108.61	105.07
2	A	1500	HEM	C4B-CHC-C1C	3.43	127.08	122.56
2	A	1500	HEM	CMC-C2C-C3C	3.28	130.81	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1500	HEM	CAA-CBA-CGA	-3.14	104.96	113.76
2	A	1500	HEM	CBA-CAA-C2A	3.14	117.98	112.62
2	B	1500	HEM	C4C-CHD-C1D	3.11	126.67	122.56
2	B	1500	HEM	C3D-C4D-ND	2.93	113.43	110.17
2	B	1500	HEM	CMB-C2B-C1B	2.86	129.40	125.04
2	B	1500	HEM	CBA-CAA-C2A	2.78	117.36	112.62
2	B	1500	HEM	C4B-C3B-C2B	-2.60	105.05	107.11
2	A	1500	HEM	C1B-NB-C4B	2.58	107.74	105.07
2	B	1500	HEM	O2D-CGD-O1D	2.53	129.62	123.30
2	A	1500	HEM	C4B-C3B-C2B	2.53	109.12	107.11
2	B	1500	HEM	CHB-C1B-NB	2.48	127.45	124.38
2	A	1500	HEM	CMA-C3A-C2A	2.45	129.56	124.94
2	A	1500	HEM	C4C-CHD-C1D	2.43	125.76	122.56
2	A	1500	HEM	CMD-C2D-C1D	2.27	128.50	125.04
2	B	1500	HEM	O1D-CGD-CBD	-2.15	116.17	123.08
2	B	1500	HEM	CHD-C1D-ND	2.06	126.67	124.43
2	B	1500	HEM	CAA-CBA-CGA	-2.00	108.14	113.76

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1500	HEM	CAA-CBA-CGA-O2A
2	A	1500	HEM	CAA-CBA-CGA-O1A
2	A	1500	HEM	CAA-CBA-CGA-O2A
2	B	1500	HEM	CAA-CBA-CGA-O1A
2	A	1500	HEM	CAD-CBD-CGD-O2D
2	B	1500	HEM	CAD-CBD-CGD-O2D
2	B	1500	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

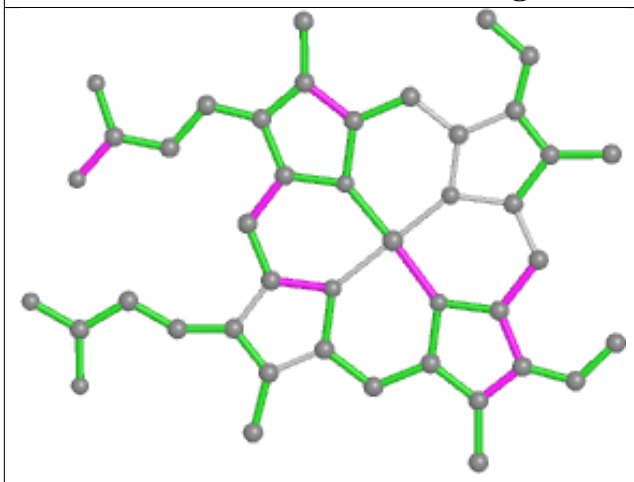
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1500	HEM	1	0

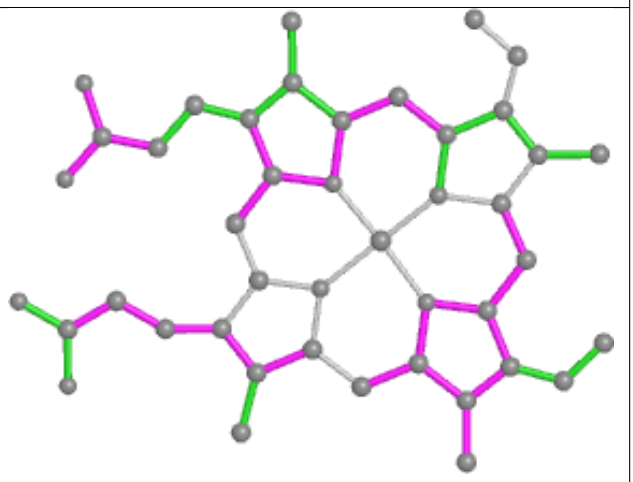
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

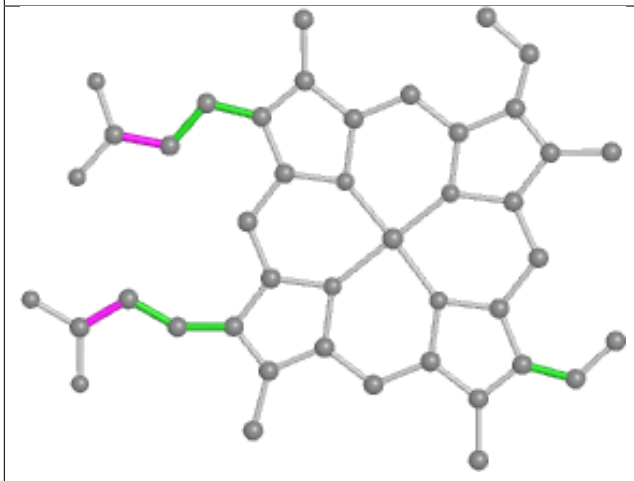
Ligand HEM B 1500



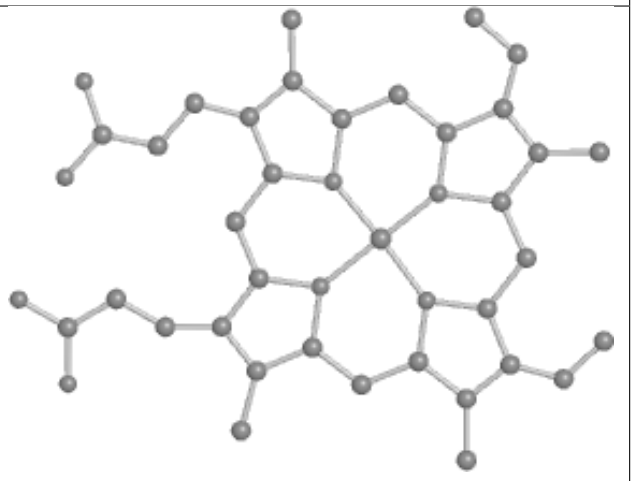
Bond lengths



Bond angles

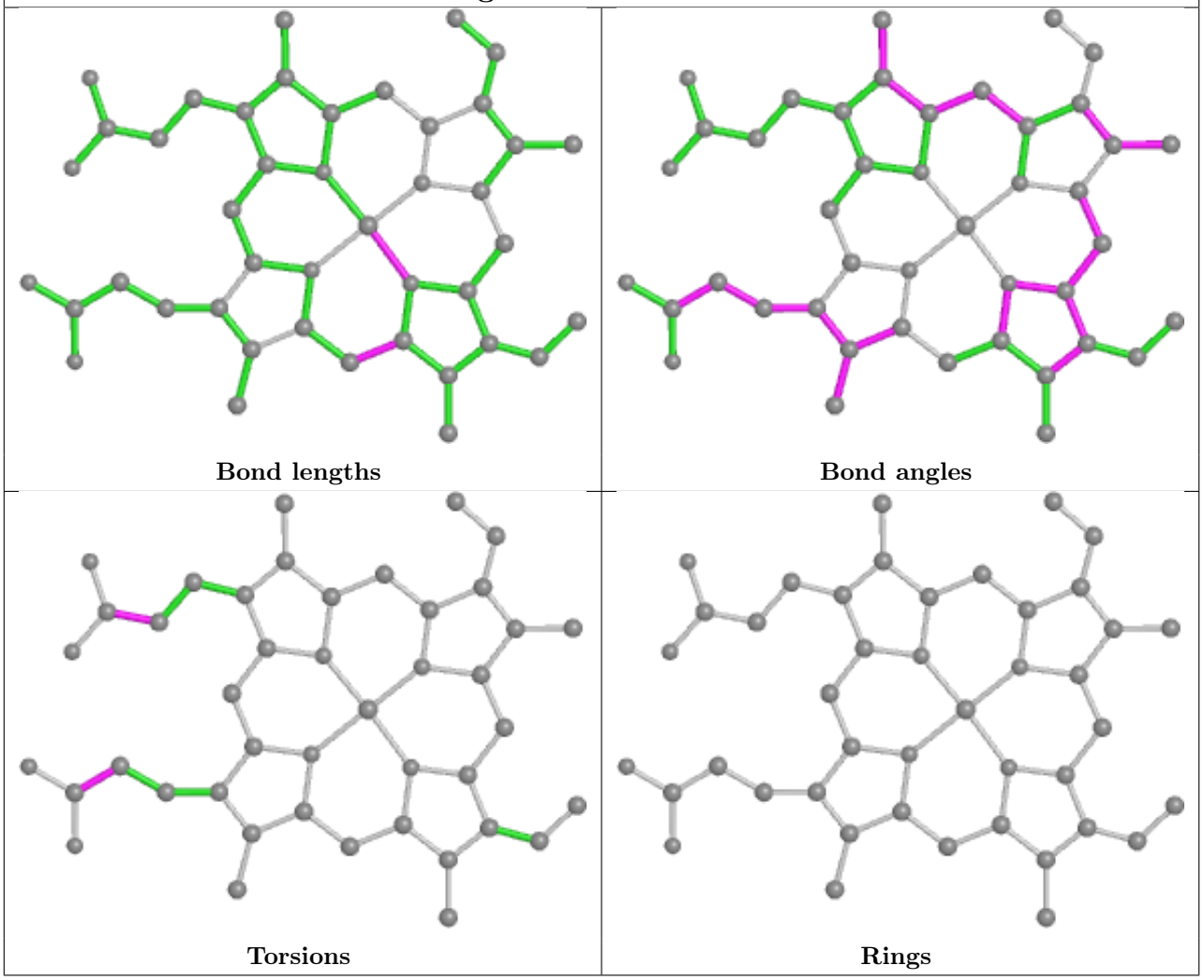


Torsions



Rings

Ligand HEM A 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%)	-0.33	18 (2%)	59	58	7, 12, 27, 54	2 (0%)
1	B	734/764 (96%)	-0.40	13 (1%)	68	68	7, 12, 25, 47	4 (0%)
All	All	1469/1528 (96%)	-0.36	31 (2%)	63	63	7, 12, 26, 54	6 (0%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	50	THR	10.6
1	B	784	VAL	7.7
1	A	715	ALA	5.6
1	A	400	VAL	4.2
1	B	783	LYS	4.2
1	A	784	VAL	3.9
1	B	51	THR	3.5
1	A	573	GLY	3.3
1	A	783	LYS	3.3
1	A	413	THR	3.2
1	A	51	THR	3.2
1	B	94	ASP	3.1
1	B	573	GLY	3.1
1	A	574	SER	3.0
1	A	577	ASN	2.9
1	B	728	ARG	2.9
1	B	490	GLY	2.8
1	A	726	LYS	2.7
1	A	714	GLY	2.7
1	A	93	GLY	2.6
1	B	401	ASN	2.4
1	B	461[A]	ARG	2.4
1	A	94	ASP	2.3
1	B	714	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	644	ALA	2.2
1	A	56	ALA	2.2
1	B	491	ASP	2.1
1	A	575	ASN	2.1
1	A	576	GLY	2.1
1	B	56	ALA	2.1
1	A	401	ASN	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)

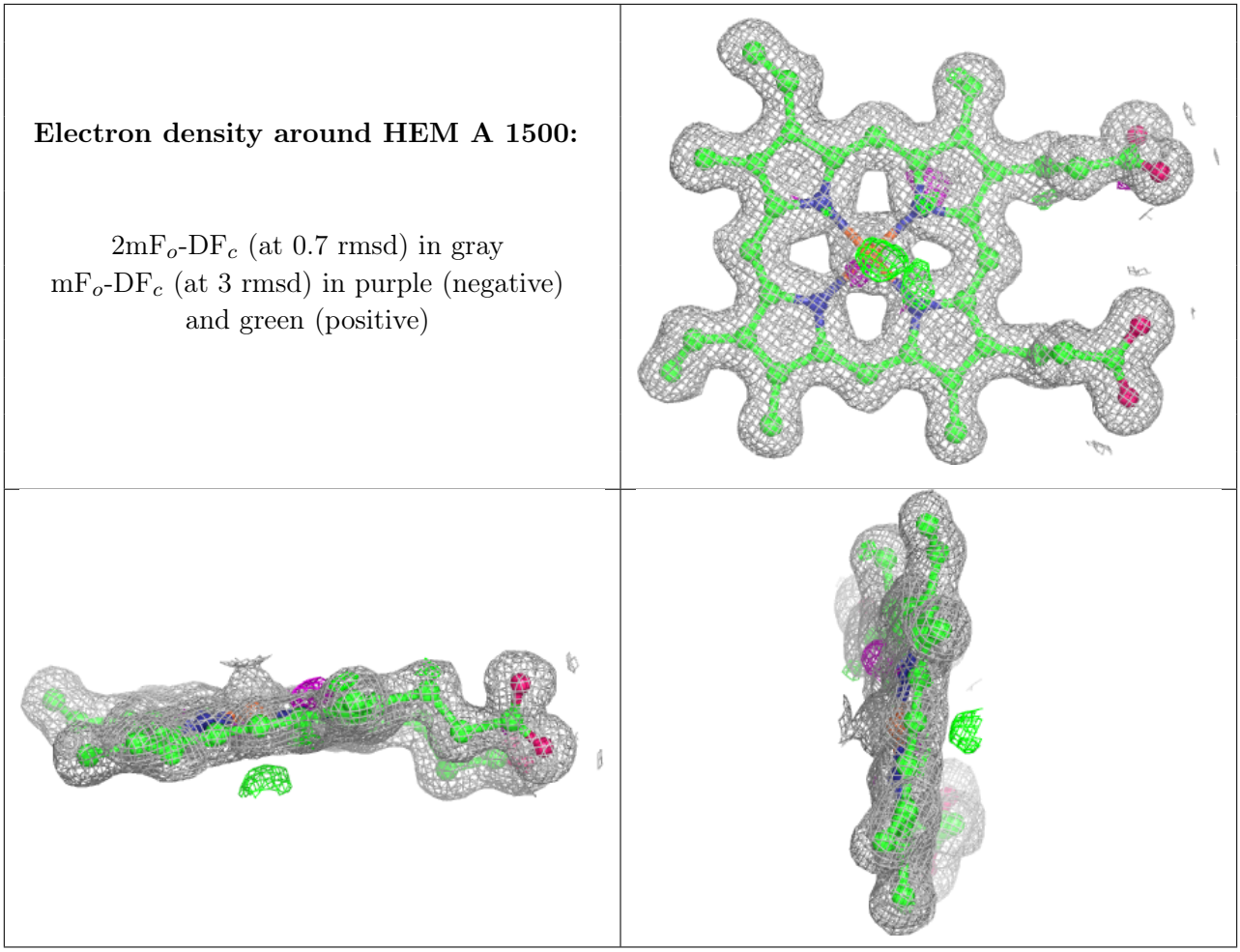
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	HEM	A	1500	43/43	0.99	0.06	7,8,9,10	0
2	HEM	B	1500	43/43	0.99	0.06	9,9,11,12	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.

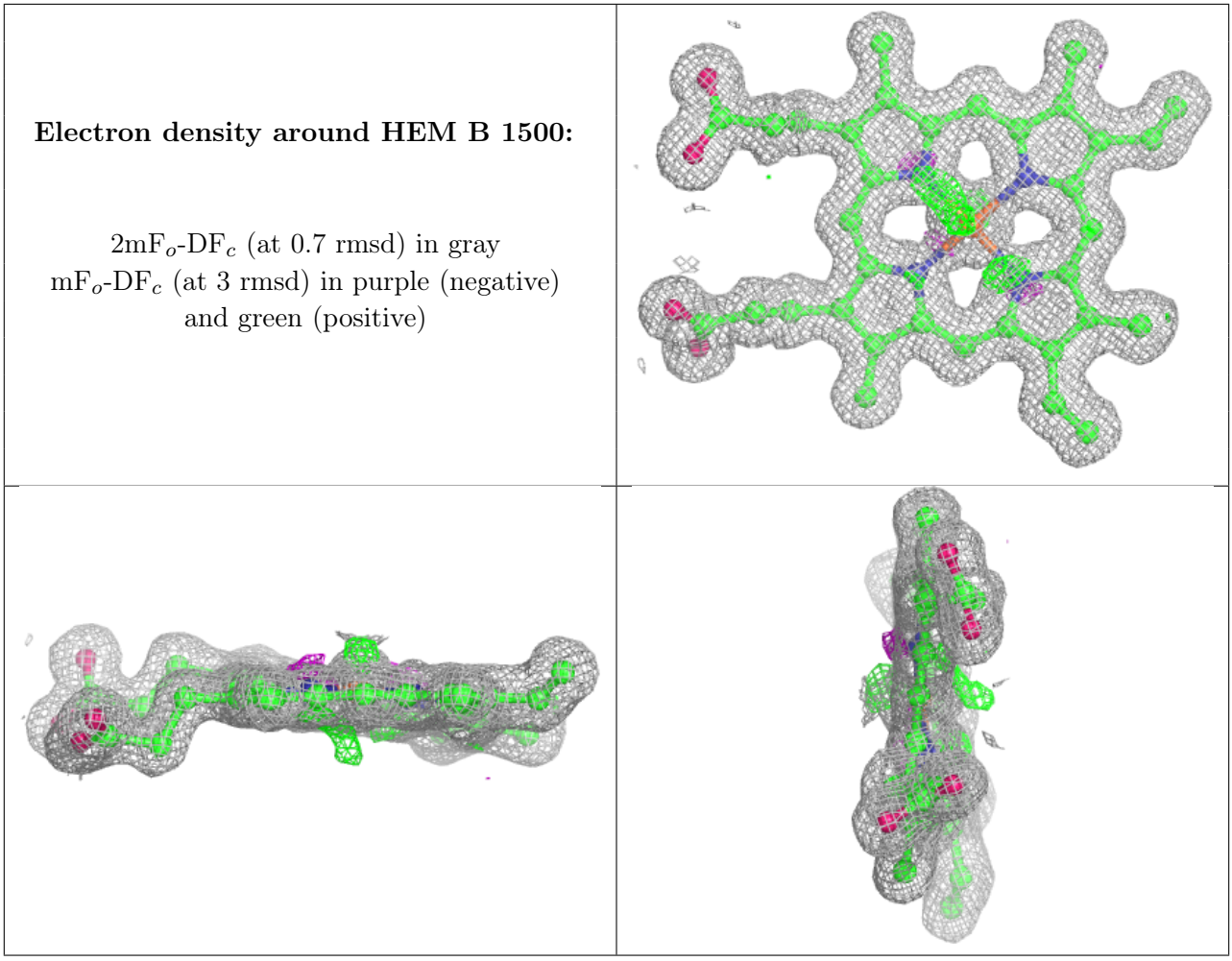
Electron density around HEM A 1500:

$2mF_o$-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 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)



6.5 Other polymers

There are no such residues in this entry.