



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:58 PM UTC

PDB ID : 5JHY / pdb_00005jhy
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

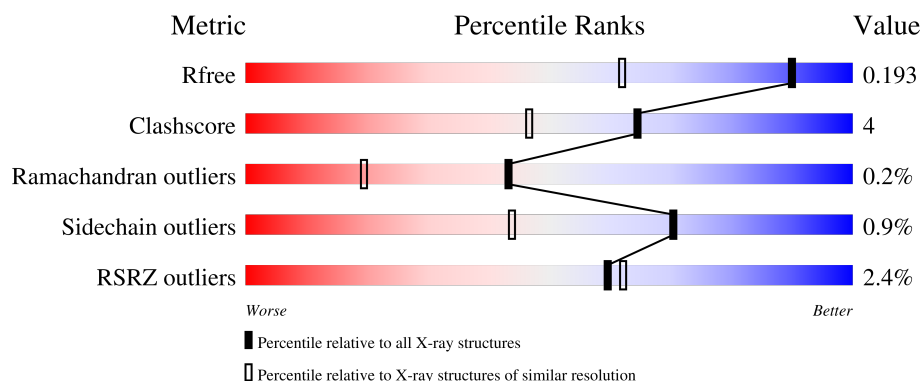
1 Overall quality at a glance

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}	180053	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (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 $\leq 5\%$. 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% 87% 8% • •

2 Entry composition [i](#)

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.

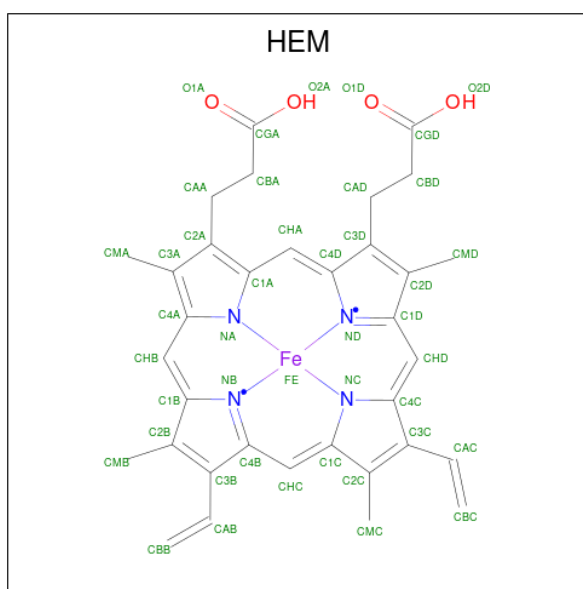
- Molecule 1 is a protein called Catalase-peroxidase 2.

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 (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		

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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		

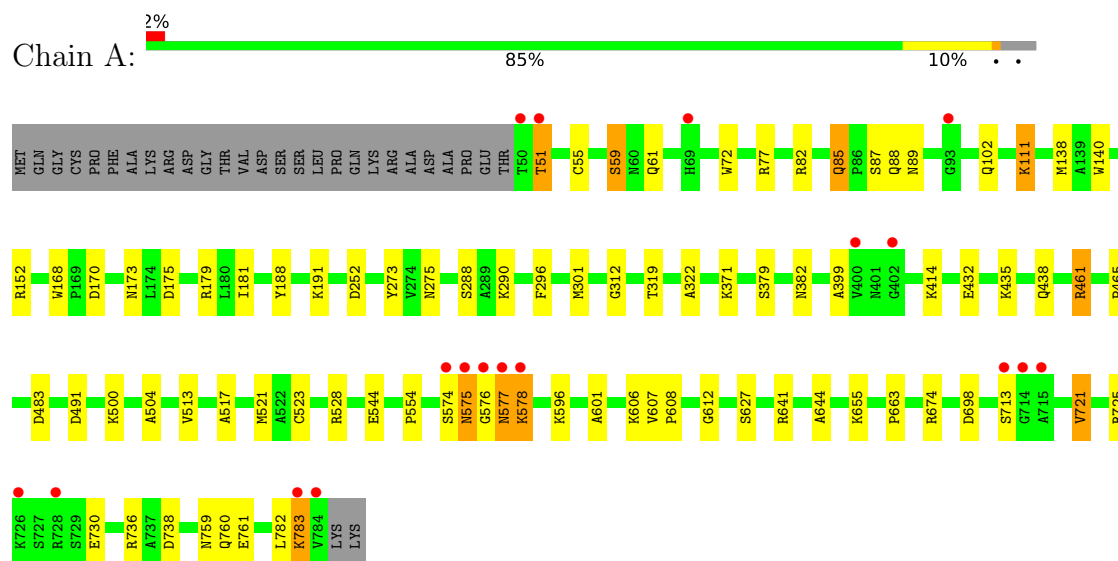
- Molecule 3 is water.

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

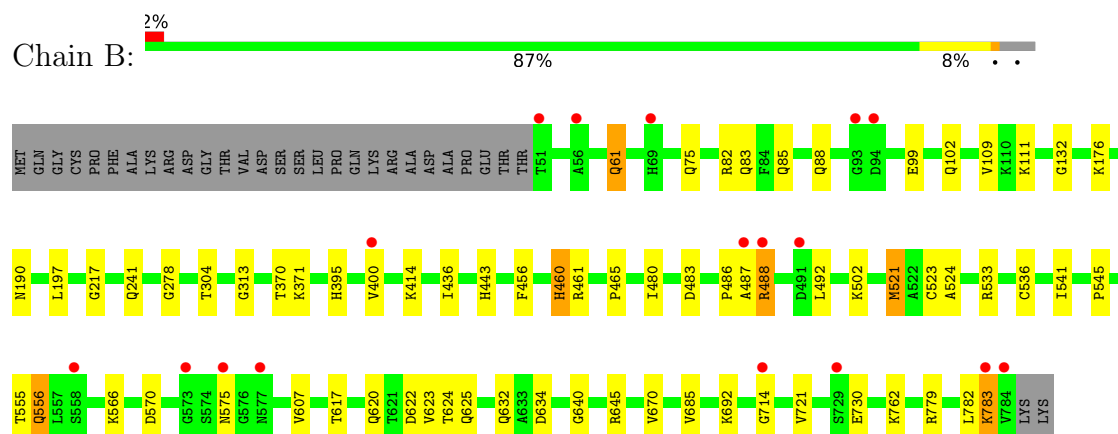
3 Residue-property plots [i](#)

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



• Molecule 1: Catalase-peroxidase 2



4 Data and refinement statistics

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 20.00 – 1.40	Depositor EDS
% Data completeness (in resolution range)	94.9 (20.00-1.40) 94.9 (20.00-1.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.48 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.151 , 0.176 (Not available) , 0.193	Depositor DCC
R_{free} test set	14255 reflections (4.76%)	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 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	1.64	37/5903 (0.6%)	1.39	23/8009 (0.3%)
1	B	1.58	34/5927 (0.6%)	1.36	12/8046 (0.1%)
All	All	1.61	71/11830 (0.6%)	1.38	35/16055 (0.2%)

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 (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	521	MET	SD-CE	-20.35	1.28	1.79
1	A	521	MET	SD-CE	-17.71	1.35	1.79
1	B	241	GLN	CA-C	-12.61	1.46	1.53
1	A	578	LYS	N-CA	-12.03	1.32	1.46
1	A	608	PRO	C-O	-10.46	1.12	1.23
1	A	607	VAL	N-CA	-9.88	1.34	1.46
1	A	606	LYS	C-O	8.91	1.34	1.24
1	A	644	ALA	C-O	8.35	1.33	1.24
1	B	624	THR	C-O	8.15	1.33	1.24
1	B	607	VAL	N-CA	-8.00	1.40	1.46
1	B	241	GLN	N-CA	7.75	1.51	1.46
1	A	87	SER	N-CA	7.67	1.55	1.46
1	B	61	GLN	CA-C	-7.66	1.43	1.52
1	A	382	ASN	CG-ND2	-7.38	1.17	1.33
1	B	88	GLN	N-CA	-6.93	1.36	1.46
1	A	72	TRP	C-N	6.90	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	379	SER	CA-CB	-6.81	1.42	1.53
1	B	632	GLN	CA-C	6.58	1.61	1.52
1	B	783	LYS	CA-C	6.51	1.66	1.52
1	B	109	VAL	CA-CB	6.50	1.62	1.54
1	A	89	ASN	N-CA	-6.49	1.36	1.46
1	A	759	ASN	C-O	6.49	1.32	1.24
1	A	759	ASN	N-CA	6.47	1.53	1.46
1	B	99	GLU	C-O	-6.31	1.16	1.24
1	B	483	ASP	C-O	6.23	1.26	1.23
1	B	502	LYS	C-O	6.14	1.31	1.24
1	A	483	ASP	CA-CB	6.11	1.56	1.52
1	B	575	ASN	C-O	-6.06	1.16	1.23
1	B	556	GLN	N-CA	-6.05	1.39	1.46
1	A	301	MET	CA-C	-5.97	1.45	1.52
1	B	83	GLN	N-CA	5.97	1.53	1.45
1	B	524	ALA	C-O	5.93	1.30	1.24
1	A	399	ALA	CA-C	-5.91	1.45	1.52
1	B	465	PRO	CA-CB	5.87	1.62	1.53
1	A	312	GLY	C-O	5.82	1.30	1.23
1	B	278	GLY	N-CA	5.81	1.52	1.44
1	A	612	GLY	N-CA	5.78	1.54	1.45
1	A	61	GLN	CA-C	-5.76	1.45	1.52
1	B	714	GLY	C-O	5.73	1.32	1.23
1	A	252	ASP	CG-OD2	-5.72	1.14	1.25
1	B	640	GLY	C-O	-5.70	1.16	1.24
1	A	738	ASP	CG-OD2	5.63	1.36	1.25
1	A	191	LYS	N-CA	5.59	1.53	1.46
1	B	685	VAL	CA-C	5.56	1.58	1.52
1	B	670	VAL	N-CA	-5.53	1.40	1.46
1	A	168	TRP	CA-C	-5.50	1.47	1.53
1	A	85	GLN	CD-OE1	5.49	1.33	1.23
1	B	395	HIS	CA-C	5.38	1.59	1.52
1	A	513	VAL	N-CA	-5.36	1.40	1.46
1	B	313	GLY	C-O	5.34	1.30	1.23
1	B	692	LYS	C-O	5.32	1.30	1.23
1	A	59	SER	N-CA	5.31	1.52	1.46
1	A	77	ARG	CZ-NH2	-5.30	1.26	1.33
1	A	55	CYS	CA-CB	5.27	1.61	1.53
1	A	721	VAL	CA-CB	5.26	1.61	1.54
1	B	102	GLN	N-CA	5.25	1.53	1.46
1	A	504	ALA	CA-C	5.21	1.59	1.52
1	A	288	SER	CA-C	5.18	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	465	PRO	N-CA	-5.13	1.40	1.47
1	A	483	ASP	C-O	5.13	1.26	1.23
1	B	241	GLN	CD-NE2	-5.13	1.22	1.33
1	A	698	ASP	C-N	-5.11	1.27	1.33
1	A	491	ASP	CB-CG	5.10	1.64	1.52
1	B	555	THR	C-N	-5.09	1.27	1.33
1	B	436	ILE	N-CA	5.08	1.52	1.46
1	B	370	THR	CA-C	-5.08	1.46	1.52
1	A	296	PHE	C-O	5.07	1.30	1.24
1	B	197	LEU	CA-C	-5.04	1.46	1.52
1	B	486	PRO	CA-CB	-5.03	1.45	1.53
1	B	443	HIS	N-CA	5.03	1.52	1.46
1	A	179	ARG	CZ-NH1	-5.00	1.25	1.32

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	82	ARG	NE-CZ-NH1	-10.63	110.87	121.50
1	A	82	ARG	NE-CZ-NH2	9.58	127.82	119.20
1	A	574	SER	N-CA-C	7.86	124.41	112.54
1	A	88	GLN	CA-C-O	7.49	128.69	119.11
1	A	188	TYR	CA-C-O	6.99	127.49	119.18
1	A	607	VAL	CA-C-N	-6.83	112.61	119.99
1	A	607	VAL	C-N-CA	-6.83	112.61	119.99
1	B	607	VAL	CA-C-N	-6.77	113.33	120.03
1	B	607	VAL	C-N-CA	-6.77	113.33	120.03
1	A	627	SER	N-CA-C	-6.29	104.48	111.71
1	A	89	ASN	CA-C-N	6.18	125.81	119.56
1	A	89	ASN	C-N-CA	6.18	125.81	119.56
1	B	524	ALA	CA-C-O	-6.05	114.47	120.70
1	A	275	ASN	CA-C-O	6.04	123.79	119.32
1	A	713	SER	N-CA-C	-5.96	105.00	112.93
1	A	517	ALA	O-C-N	5.81	128.06	122.07
1	A	578	LYS	CB-CA-C	5.72	119.55	109.89
1	B	241	GLN	O-C-N	-5.62	117.25	121.47
1	A	578	LYS	CA-CB-CG	-5.52	103.06	114.10
1	B	492	LEU	N-CA-C	5.51	117.69	109.59
1	A	578	LYS	CA-C-O	5.47	126.82	120.14
1	A	528	ARG	NE-CZ-NH2	-5.46	114.29	119.20
1	A	736	ARG	O-C-N	-5.45	116.34	122.12
1	B	132	GLY	N-CA-C	5.41	119.19	112.64
1	A	663	PRO	CB-CA-C	5.40	117.51	110.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	783	LYS	N-CA-C	5.39	126.11	111.00
1	B	61	GLN	CB-CG-CD	5.34	121.69	112.60
1	A	461	ARG	NE-CZ-NH1	-5.34	116.16	121.50
1	B	634	ASP	OD1-CG-OD2	-5.26	110.27	122.90
1	A	577	ASN	N-CA-C	5.20	116.49	109.11
1	A	322	ALA	N-CA-C	5.18	119.31	112.89
1	B	82	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	A	577	ASN	O-C-N	5.11	128.98	122.65
1	B	465	PRO	N-CA-CB	-5.09	98.61	103.39
1	B	460	HIS	CB-CG-ND1	5.07	130.31	122.70

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	52	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	26	1
3	B	916	0	0	14	1
All	All	13350	0	11165	88	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 (88) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:566:LYS:HD2	3:B:1602:HOH:O	1.79	0.81
1:A:577:ASN:C	1:A:578:LYS:HG3	2.05	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: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:577:ASN:C	1:A:578:LYS:CG	2.69	0.64
1:A:641[A]:ARG:NH2	3:A:1613:HOH:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:521:MET:HA	1:B:521:MET:HE2	2.00	0.44
1:A:138:MET:HE1	1:A:181:ILE:HD13	2.00	0.43
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:761:GLU:CD	3:A:1612:HOH:O	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	36	16
1	B	753/764 (99%)	736 (98%)	15 (2%)	2 (0%)	36	16
All	All	1502/1528 (98%)	1466 (98%)	32 (2%)	4 (0%)	43	16

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 ⓘ

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%)	584 (98%)	9 (2%)	57	26
1	B	596/606 (98%)	594 (100%)	2 (0%)	86	70
All	All	1189/1212 (98%)	1178 (99%)	11 (1%)	70	44

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	A	102	GLN
1	A	111[A]	LYS
1	A	111[B]	LYS
1	A	170	ASP
1	A	435	LYS
1	A	554	PRO
1	A	575	ASN
1	A	655	LYS
1	B	61	GLN
1	B	111	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	102	GLN
1	A	190	ASN
1	A	356	GLN
1	A	401	ASN
1	A	546	GLN
1	A	575	ASN
1	A	577	ASN
1	A	625	GLN
1	A	691	ASN
1	A	707	ASN
1	B	102	GLN

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Mol	Chain	Res	Type
1	B	121	GLN
1	B	190	ASN
1	B	356	GLN
1	B	460	HIS
1	B	707	ASN
1	B	759	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	A	1500	1	50,50,50	1.40	5 (10%)	67,82,82	1.25	6 (8%)
2	HEM	B	1500	1	50,50,50	1.56	10 (20%)	67,82,82	1.66	18 (26%)

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	1500	1	-	3/14/54/54	-
2	HEM	B	1500	1	-	4/14/54/54	-

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1500	HEM	FE-NB	4.09	2.07	1.94
2	A	1500	HEM	FE-NB	4.07	2.07	1.94
2	A	1500	HEM	FE-NC	3.95	2.08	1.95
2	B	1500	HEM	FE-NC	3.64	2.07	1.95
2	B	1500	HEM	C1D-C2D	3.59	1.51	1.44
2	A	1500	HEM	CHC-C1C	3.25	1.44	1.38
2	A	1500	HEM	C1C-C2C	-3.14	1.39	1.45
2	B	1500	HEM	FE-ND	2.99	2.04	1.94
2	A	1500	HEM	FE-NA	2.92	2.04	1.95
2	B	1500	HEM	O2D-CGD	-2.67	1.22	1.30
2	B	1500	HEM	CHB-C4A	2.41	1.44	1.39
2	B	1500	HEM	C3B-C4B	2.41	1.49	1.44
2	B	1500	HEM	CHC-C4B	-2.22	1.34	1.39
2	B	1500	HEM	C3B-C2B	2.09	1.41	1.37
2	B	1500	HEM	C1A-NA	2.09	1.43	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1500	HEM	CHA-C4D-ND	-4.87	118.34	124.37
2	A	1500	HEM	C3B-C4B-NB	-3.39	107.03	109.47
2	A	1500	HEM	CAA-CBA-CGA	-3.28	104.96	113.67
2	B	1500	HEM	C4A-C3A-C2A	-3.28	103.06	106.82
2	B	1500	HEM	C3A-C4A-NA	3.19	115.25	110.14
2	B	1500	HEM	C3D-C4D-ND	2.97	113.43	110.17
2	B	1500	HEM	C1B-NB-C4B	2.88	108.61	105.21
2	A	1500	HEM	C4A-C3A-C2A	-2.83	103.57	106.82
2	B	1500	HEM	CMB-C2B-C1B	2.79	129.40	125.03
2	B	1500	HEM	CHB-C1B-NB	2.49	127.45	124.37
2	B	1500	HEM	O2D-CGD-O1D	2.44	129.62	123.33
2	B	1500	HEM	C4B-C3B-C2B	-2.43	105.05	107.28
2	B	1500	HEM	C4A-NA-C1A	-2.30	102.08	105.82
2	B	1500	HEM	C1A-CHA-C4D	2.26	131.56	126.25
2	A	1500	HEM	CMD-C2D-C1D	2.22	128.50	125.03
2	B	1500	HEM	O1D-CGD-CBD	-2.18	116.17	123.09
2	B	1500	HEM	CMA-C3A-C4A	2.16	128.70	125.42
2	B	1500	HEM	C3B-C4B-NB	-2.14	107.93	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	HEM	C1B-NB-C4B	2.14	107.74	105.21
2	B	1500	HEM	CHD-C1D-ND	2.09	126.67	124.42
2	B	1500	HEM	CAA-CBA-CGA	-2.08	108.14	113.67
2	B	1500	HEM	CMB-C2B-C3B	-2.02	123.53	128.43
2	B	1500	HEM	O1A-CGA-CBA	-2.02	116.68	123.09
2	A	1500	HEM	C4B-C3B-C2B	2.01	109.12	107.28

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-O2A
2	A	1500	HEM	CAA-CBA-CGA-O1A
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

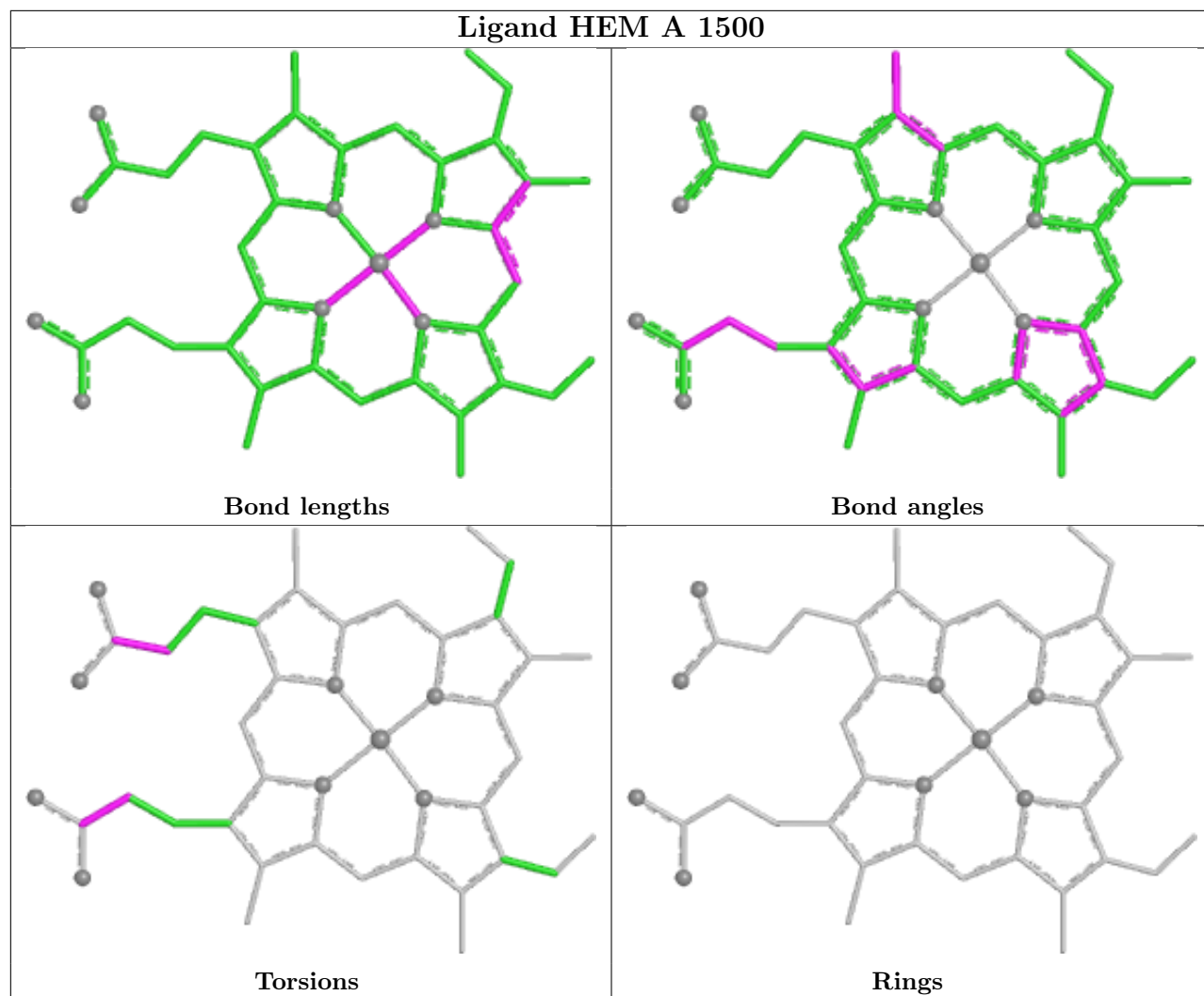
There are no ring outliers.

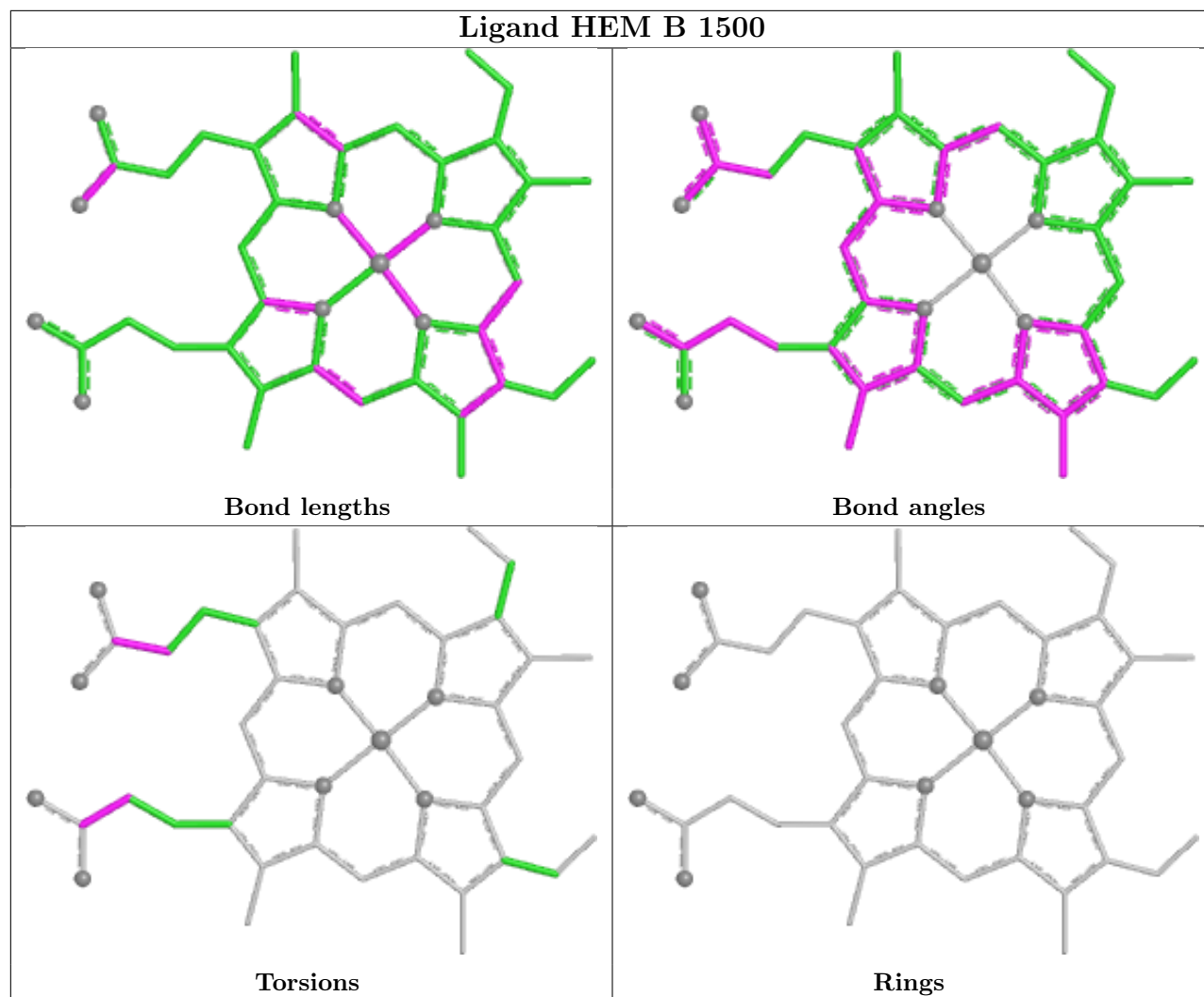
1 monomer is involved in 1 short contact:

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 than 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 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, 95th 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%)	-0.24	18 (2%) 59 62	5, 12, 27, 54	16 (2%)
1	B	734/764 (96%)	-0.32	17 (2%) 61 63	4, 12, 24, 47	21 (2%)
All	All	1469/1528 (96%)	-0.28	35 (2%) 59 62	4, 12, 26, 54	37 (2%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	784	VAL	7.7
1	A	50	THR	6.7
1	B	783	LYS	5.6
1	B	51	THR	4.7
1	A	576	GLY	4.5
1	A	577	ASN	4.3
1	A	400	VAL	4.1
1	A	575	ASN	3.2
1	A	715	ALA	3.1
1	B	56	ALA	3.1
1	A	783	LYS	3.0
1	A	714	GLY	2.9
1	A	784	VAL	2.9
1	B	69	HIS	2.8
1	B	714	GLY	2.7
1	B	94	ASP	2.7
1	B	558	SER	2.7
1	B	487[A]	ALA	2.6
1	A	574	SER	2.6
1	A	51	THR	2.5
1	A	402	GLY	2.4
1	B	573	GLY	2.4
1	A	69	HIS	2.4
1	A	713	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	488[A]	ARG	2.3
1	A	726	LYS	2.2
1	B	400	VAL	2.2
1	B	491	ASP	2.2
1	B	93	GLY	2.2
1	B	575	ASN	2.2
1	B	577	ASN	2.1
1	A	578	LYS	2.1
1	A	93	GLY	2.1
1	A	728	ARG	2.0
1	B	729	SER	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](#)

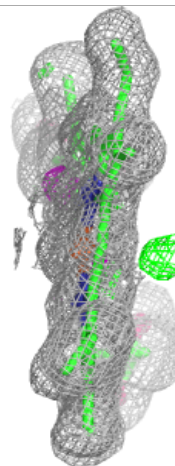
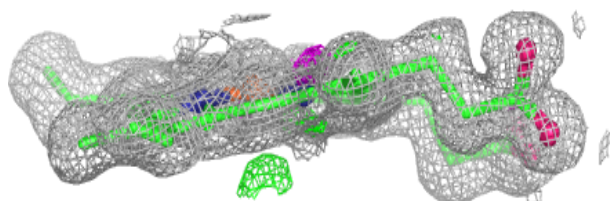
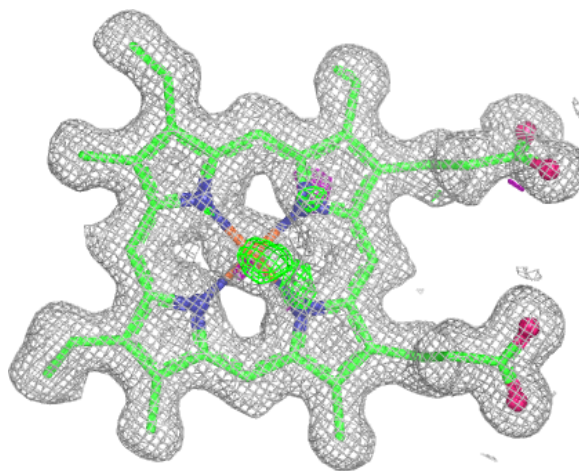
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

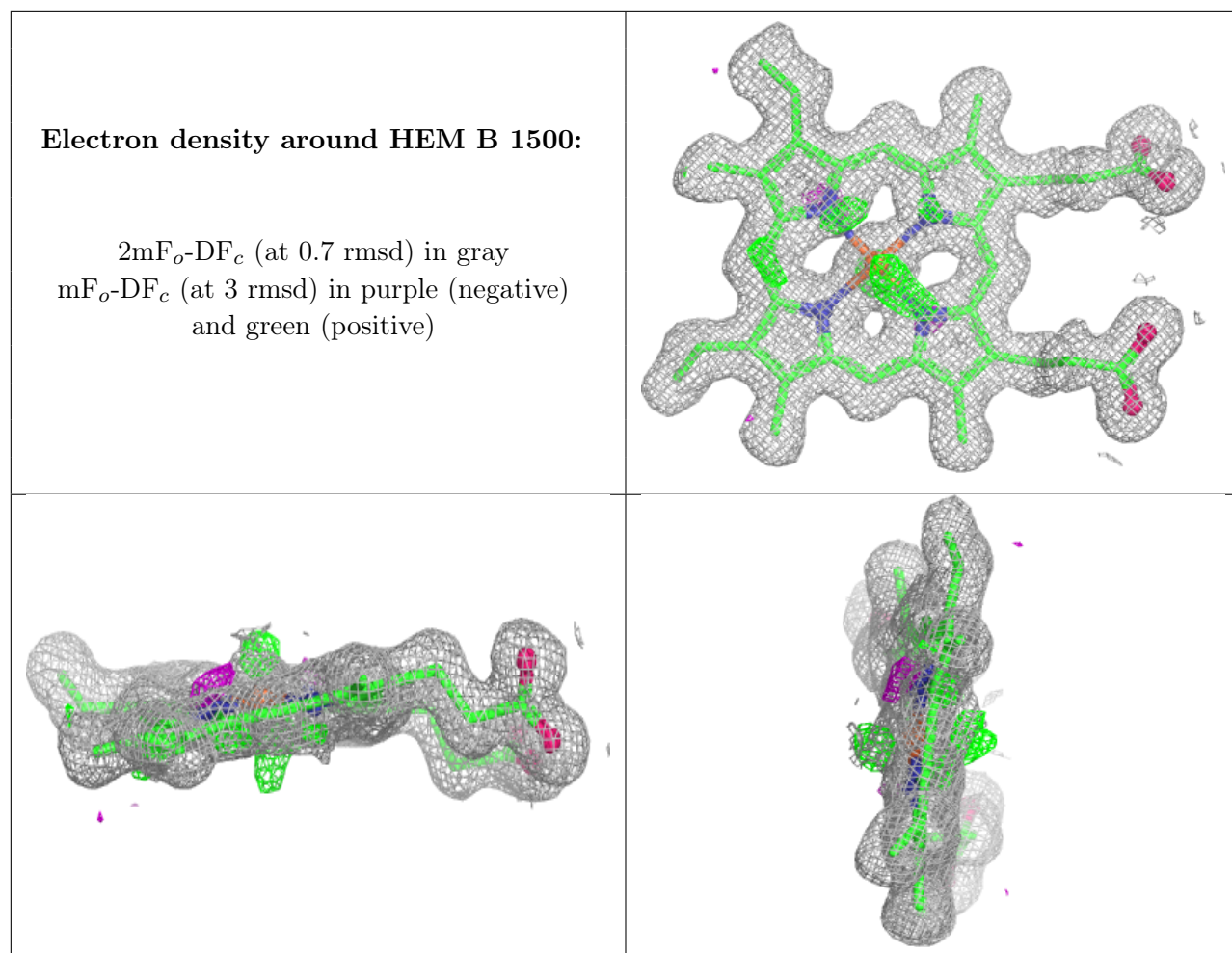
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	A	1500	43/43	0.99	0.04	7,8,9,10	0
2	HEM	B	1500	43/43	0.99	0.04	9,9,11,12	0

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)





6.5 Other polymers [i](#)

There are no such residues in this entry.