



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:45 PM UTC

PDB ID : 5SX0 / pdb_00005sx0
Title : Crystal structure of an oxoferryl species of catalase-peroxidase KatG at pH7.5
Authors : Loewen, P.C.
Deposited on : 2016-08-09
Resolution : 2.00 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

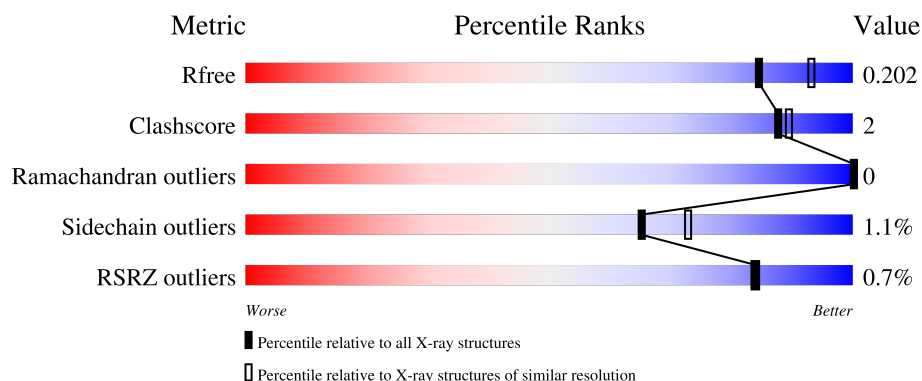
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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.

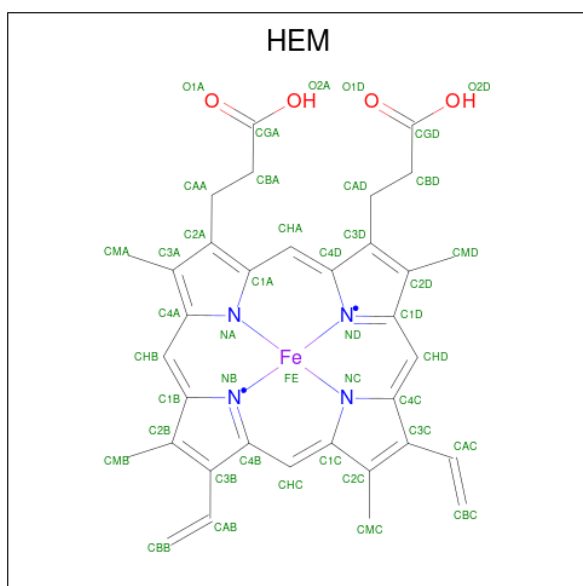
Mol	Chain	Length	Quality of chain
1	A	728	% 91% 7% .
2	B	728	% 90% 8% .

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 2 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	713	Total	C	N	O	S	0	2	0
			5514	3483	981	1036	14			

- $$\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4).$$

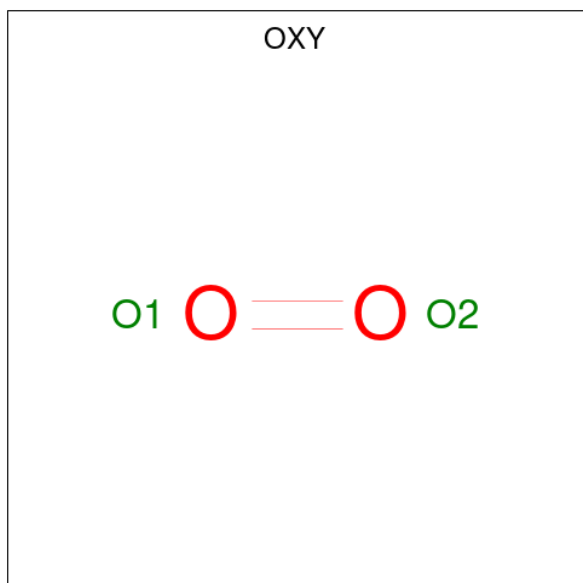


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		

- Molecule 5 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).

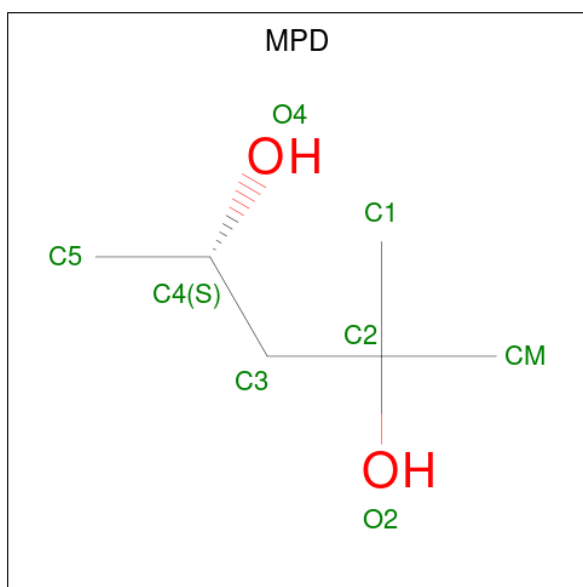


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			2	2		
5	A	1	Total	O	0	0
			2	2		
5	B	1	Total	O	0	0
			2	2		

- Molecule 6 is OXYGEN ATOM (CCD ID: O) (formula: O).

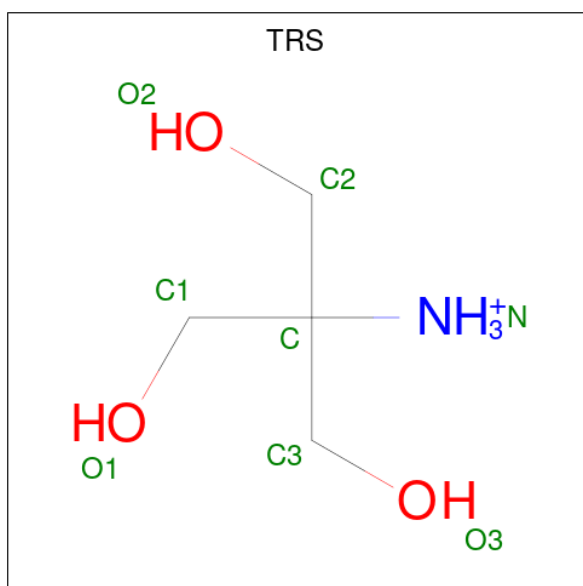
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		
6	B	1	Total	O	0	0
			1	1		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			8	6	2		
7	A	1	Total	C	O	0	0
			8	6	2		
7	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			8	4	1	3		
8	B	1	Total	C	N	O	0	0
			8	4	1	3		

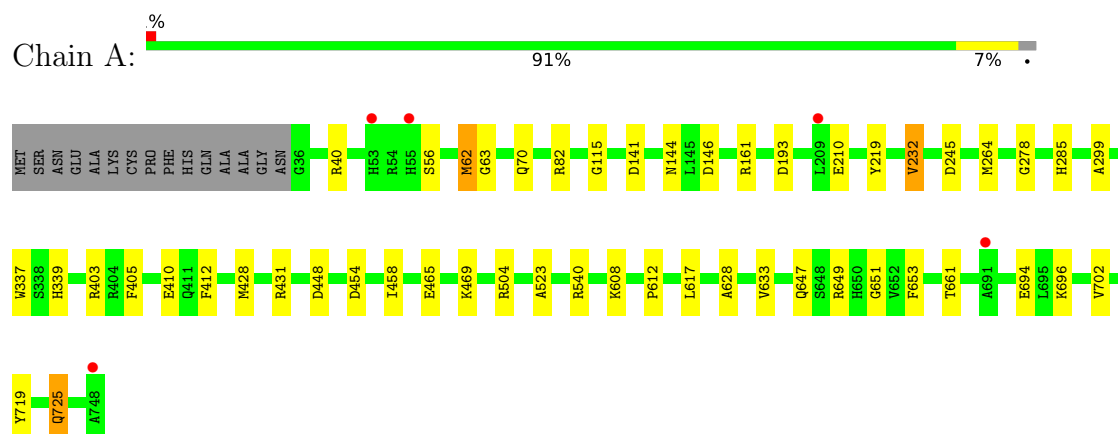
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	606	Total	O	0	0
			606	606		
9	B	619	Total	O	0	0
			619	619		

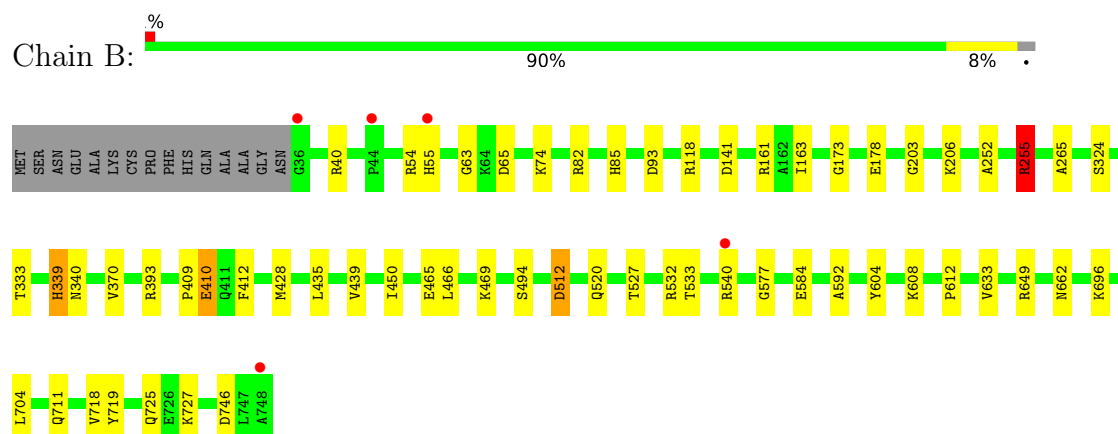
3 Residue-property plots [i](#)

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



- Molecule 2: Catalase-peroxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.36Å 114.89Å 174.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (20.00-2.00) 97.9 (20.00-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.159 , 0.194 0.170 , 0.202	Depositor DCC
R_{free} test set	13331 reflections (9.77%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12401	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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: O, HEM, NA, OXY, MHO, TRS, MPD

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	1.45	22/5671 (0.4%)	1.13	4/7709 (0.1%)
2	B	1.51	27/5662 (0.5%)	1.18	10/7698 (0.1%)
All	All	1.48	49/11333 (0.4%)	1.16	14/15407 (0.1%)

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	577	GLY	C-O	-8.38	1.13	1.24
1	A	628	ALA	N-CA	-7.29	1.39	1.46
2	B	63	GLY	N-CA	7.28	1.54	1.45
2	B	439	VAL	C-O	-7.17	1.15	1.24
2	B	746	ASP	C-O	-7.15	1.15	1.24
1	A	725	GLN	CD-OE1	7.08	1.37	1.23
2	B	612	PRO	CA-C	6.62	1.60	1.52
2	B	604	TYR	N-CA	-6.36	1.38	1.46
2	B	370	VAL	C-O	-6.32	1.17	1.24
2	B	163	ILE	C-O	6.16	1.30	1.24
2	B	265	ALA	CA-C	-6.04	1.44	1.52
2	B	340	ASN	C-O	5.90	1.31	1.24
1	A	299	ALA	C-O	-5.80	1.16	1.24
1	A	285	HIS	C-O	5.77	1.30	1.24
2	B	466	LEU	C-O	-5.74	1.17	1.24
1	A	454	ASP	N-CA	5.71	1.53	1.46
2	B	494	SER	CA-C	5.67	1.60	1.52
1	A	63	GLY	N-CA	5.63	1.54	1.45
1	A	82	ARG	CZ-NH2	-5.53	1.26	1.33
2	B	450	ILE	C-O	-5.52	1.17	1.23
1	A	410	GLU	C-O	-5.46	1.17	1.24
2	B	527	THR	C-O	-5.44	1.17	1.24
2	B	592	ALA	CA-C	-5.44	1.45	1.52
1	A	232	VAL	C-O	5.40	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	333	THR	CA-C	5.40	1.58	1.52
1	A	694	GLU	CA-C	5.38	1.59	1.52
2	B	512	ASP	C-O	-5.38	1.16	1.23
1	A	245	ASP	C-O	-5.38	1.16	1.23
1	A	431	ARG	CD-NE	5.33	1.53	1.46
2	B	85	HIS	N-CA	5.32	1.52	1.46
1	A	458	ILE	CA-CB	-5.31	1.49	1.54
2	B	206	LYS	CA-C	-5.29	1.45	1.52
2	B	255	ARG	CA-C	5.28	1.59	1.52
2	B	584	GLU	C-O	-5.26	1.17	1.24
2	B	82	ARG	CZ-NH2	-5.24	1.26	1.33
2	B	252	ALA	CA-C	5.20	1.59	1.52
2	B	203	GLY	C-O	5.19	1.27	1.23
1	A	428	MET	CG-SD	-5.17	1.67	1.80
2	B	339	HIS	C-O	5.17	1.30	1.24
2	B	118	ARG	C-O	5.16	1.29	1.24
1	A	210	GLU	C-O	5.11	1.30	1.23
1	A	278	GLY	C-O	5.11	1.29	1.23
1	A	337	TRP	C-O	-5.09	1.17	1.23
1	A	523	ALA	C-O	-5.07	1.18	1.24
1	A	612	PRO	CA-C	5.06	1.58	1.52
1	A	193	ASP	C-O	5.04	1.30	1.23
1	A	448	ASP	CA-CB	5.04	1.57	1.52
2	B	412	PHE	C-O	5.04	1.29	1.24
1	A	56	SER	N-CA	5.03	1.52	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ARG	NE-CZ-NH2	-7.97	112.03	119.20
2	B	161	ARG	NE-CZ-NH1	7.71	129.21	121.50
1	A	161	ARG	NE-CZ-NH1	6.72	128.22	121.50
2	B	161	ARG	NE-CZ-NH2	-6.04	113.77	119.20
2	B	93	ASP	N-CA-C	5.80	118.38	111.71
2	B	428	MET	CA-CB-CG	-5.61	102.87	114.10
2	B	65	ASP	N-CA-C	5.46	119.21	112.54
2	B	393	ARG	NE-CZ-NH2	-5.40	114.34	119.20
2	B	533	THR	N-CA-C	-5.32	105.48	111.28
2	B	173	GLY	N-CA-C	5.31	119.07	112.64
2	B	435	LEU	N-CA-C	5.25	118.30	109.95
1	A	70	GLN	CA-CB-CG	5.15	124.41	114.10
1	A	428	MET	CA-CB-CG	-5.14	103.83	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	450	ILE	CA-CB-CG1	-5.13	101.68	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5526	0	5346	18	0
2	B	5514	0	5330	22	0
3	A	43	0	30	0	0
3	B	43	0	30	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	0	0	0
5	B	2	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	16	0	28	4	0
7	B	8	0	14	2	0
8	A	8	0	12	0	0
8	B	8	0	12	0	0
9	A	606	0	0	5	1
9	B	619	0	0	8	1
All	All	12401	0	10802	43	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 2.

All (43) 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)
7:A:807:MPD:H53	7:A:807:MPD:H11	1.69	0.74
2:B:55:HIS:NE2	9:B:1904:HOH:O	2.22	0.73
2:B:512:ASP:OD1	9:B:1901:HOH:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:178:GLU:OE1	9:B:1902:HOH:O	2.12	0.68
1:A:647:GLN:HG2	9:A:1221:HOH:O	1.93	0.67
2:B:540:ARG:HA	2:B:540:ARG:NH1	2.11	0.65
2:B:255:ARG:HD2	9:B:1925:HOH:O	1.96	0.65
2:B:711[A]:GLN:NE2	9:B:1903:HOH:O	2.20	0.62
1:A:696:LYS:HE2	9:A:989:HOH:O	2.00	0.61
2:B:696:LYS:HE2	9:B:1908:HOH:O	2.02	0.59
1:A:62:MHO:HE3	1:A:62:MHO:HA	1.85	0.57
2:B:54:ARG:HB3	2:B:55:HIS:CD2	2.42	0.54
1:A:62:MHO:HE1	9:A:1066:HOH:O	2.08	0.53
7:B:805:MPD:O4	7:B:805:MPD:H12	2.09	0.52
7:A:806:MPD:O4	7:A:806:MPD:CM	2.58	0.52
2:B:410:GLU:HB2	9:B:2326:HOH:O	2.10	0.52
2:B:465:GLU:HG2	2:B:469:LYS:HE2	1.92	0.51
1:A:339:HIS:HB2	9:A:1357:HOH:O	2.13	0.49
2:B:662:ASN:H	2:B:725:GLN:HE22	1.58	0.49
7:A:806:MPD:O4	7:A:806:MPD:HM2	2.13	0.48
2:B:633:VAL:CG2	2:B:719:TYR:CZ	2.96	0.48
1:A:62:MHO:CE	2:B:727:LYS:HE2	2.45	0.47
2:B:540:ARG:HA	2:B:540:ARG:CZ	2.44	0.47
1:A:504:ARG:HD2	9:A:965:HOH:O	2.15	0.46
2:B:540:ARG:HA	2:B:540:ARG:HH11	1.80	0.46
2:B:324:SER:O	7:B:805:MPD:H53	2.15	0.45
1:A:633:VAL:CG2	1:A:719:TYR:CZ	3.00	0.45
1:A:62:MHO:HE2	2:B:718:VAL:HG11	1.99	0.43
1:A:403[B]:ARG:HH11	1:A:403[B]:ARG:HD3	1.61	0.43
1:A:405:PHE:HB3	1:A:412:PHE:HB2	2.00	0.43
1:A:219:TYR:HH	1:A:232:VAL:HG12	1.83	0.43
2:B:339:HIS:CD2	2:B:409:PRO:HB3	2.53	0.43
1:A:661:THR:HA	1:A:725:GLN:HE22	1.84	0.42
2:B:633:VAL:HG22	2:B:719:TYR:CZ	2.55	0.42
1:A:617:LEU:HD22	1:A:702:VAL:HG13	2.02	0.42
7:A:807:MPD:H11	7:A:807:MPD:C5	2.43	0.42
1:A:115:GLY:O	1:A:264:MET:SD	2.78	0.41
1:A:144:ASN:HA	1:A:146:ASP:OD1	2.20	0.41
2:B:532:ARG:HD3	9:B:2383:HOH:O	2.20	0.41
2:B:520:GLN:O	2:B:520:GLN:HG2	2.17	0.41
1:A:651:GLY:HA2	1:A:653:PHE:CE2	2.55	0.40
2:B:704:LEU:HA	2:B:704:LEU:HD23	1.88	0.40
1:A:465:GLU:HG2	1:A:469:LYS:HE2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1091:HOH:O	9:B:2080:HOH:O[2_444]	2.15	0.05

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	714/728 (98%)	706 (99%)	8 (1%)	0	100	100
2	B	713/728 (98%)	704 (99%)	9 (1%)	0	100	100
All	All	1427/1456 (98%)	1410 (99%)	17 (1%)	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	553/560 (99%)	548 (99%)	5 (1%)	70	78
2	B	552/561 (98%)	545 (99%)	7 (1%)	61	68
All	All	1105/1121 (99%)	1093 (99%)	12 (1%)	65	73

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

Mol	Chain	Res	Type
1	A	40	ARG

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Mol	Chain	Res	Type
1	A	141	ASP
1	A	540	ARG
1	A	608	LYS
1	A	649	ARG
2	B	40	ARG
2	B	74	LYS
2	B	141	ASP
2	B	255	ARG
2	B	410	GLU
2	B	608	LYS
2	B	649	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	70	GLN
1	A	336	GLN
1	A	725	GLN
1	A	737	ASN
2	B	55	HIS
2	B	336	GLN
2	B	339	HIS
2	B	650	HIS
2	B	725	GLN
2	B	737	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](#)

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	MHO	A	62	1	6,8,9	2.54	3 (50%)	3,9,11	5.34	2 (66%)

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
1	MHO	A	62	1	-	2/6/7/9	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	62	MHO	OD1-SD	3.91	1.62	1.50
1	A	62	MHO	CE-SD	-3.65	1.60	1.77
1	A	62	MHO	CG-SD	-2.67	1.68	1.80

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	MHO	CE-SD-CG	8.21	117.99	97.45
1	A	62	MHO	OD1-SD-CE	4.15	122.58	106.69

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	62	MHO	CB-CG-SD-OD1
1	A	62	MHO	CA-CB-CG-SD

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	62	MHO	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEM	A	801	6,1	50,50,50	1.55	7 (14%)	67,82,82	1.71	17 (25%)
5	OXY	A	803	-	1,1,1	0.08	0	-		
5	OXY	A	804	-	1,1,1	0.01	0	-		
7	MPD	B	805	-	7,7,7	0.35	0	9,10,10	1.23	0
8	TRS	A	808	-	7,7,7	1.38	2 (28%)	9,9,9	2.55	3 (33%)
7	MPD	A	807	-	7,7,7	0.60	0	9,10,10	1.35	2 (22%)
3	HEM	B	801	6,2	50,50,50	1.78	15 (30%)	67,82,82	1.67	17 (25%)
5	OXY	B	803	-	1,1,1	0.10	0	-		
8	TRS	B	806	-	7,7,7	1.70	1 (14%)	9,9,9	1.46	2 (22%)
7	MPD	A	806	-	7,7,7	0.93	0	9,10,10	1.38	1 (11%)

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
3	HEM	A	801	6,1	-	3/14/54/54	-
7	MPD	B	805	-	-	3/5/5/5	-
8	TRS	A	808	-	-	1/9/9/9	-
7	MPD	A	807	-	-	1/5/5/5	-
3	HEM	B	801	6,2	-	2/14/54/54	-
8	TRS	B	806	-	-	2/9/9/9	-
7	MPD	A	806	-	-	3/5/5/5	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	HEM	FE-NC	4.84	2.11	1.95
3	B	801	HEM	FE-NC	4.14	2.08	1.95
3	A	801	HEM	C3C-C2C	3.62	1.44	1.37
3	B	801	HEM	C1B-NB	-3.60	1.34	1.40
3	B	801	HEM	C4B-NB	-3.59	1.31	1.38
3	B	801	HEM	C3B-C4B	3.55	1.51	1.44
3	A	801	HEM	FE-NB	3.43	2.05	1.94
3	A	801	HEM	C1B-NB	-3.32	1.34	1.40
3	B	801	HEM	FE-NB	3.18	2.04	1.94
3	A	801	HEM	C4D-ND	-3.10	1.34	1.40
3	A	801	HEM	FE-NA	3.09	2.05	1.95
3	B	801	HEM	C1C-C2C	-3.05	1.39	1.45
3	B	801	HEM	CBA-CGA	2.96	1.57	1.50
3	B	801	HEM	C1D-ND	-2.89	1.33	1.38
8	B	806	TRS	O1-C1	2.87	1.51	1.42
3	B	801	HEM	C1A-NA	-2.84	1.34	1.39
3	B	801	HEM	O1A-CGA	2.76	1.31	1.22
3	B	801	HEM	C1C-NC	-2.65	1.34	1.39
3	B	801	HEM	CAB-C3B	2.44	1.53	1.47
8	A	808	TRS	C2-C	2.44	1.59	1.53
3	B	801	HEM	C4D-ND	-2.24	1.36	1.40
3	B	801	HEM	C4C-NC	-2.23	1.35	1.39
8	A	808	TRS	C1-C	2.19	1.58	1.53
3	B	801	HEM	C2A-C3A	-2.01	1.33	1.38
3	A	801	HEM	O1A-CGA	2.01	1.28	1.22

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	808	TRS	O1-C1-C	5.25	125.51	110.88
3	A	801	HEM	C4B-C3B-C2B	-4.59	103.06	107.28
3	B	801	HEM	C4B-C3B-C2B	-4.23	103.39	107.28
3	A	801	HEM	C4C-NC-C1C	3.97	112.29	105.82
8	A	808	TRS	C3-C-N	-3.96	98.06	108.17
3	A	801	HEM	C3B-C2B-C1B	3.95	109.38	106.41
3	A	801	HEM	CHC-C1C-NC	3.40	128.15	124.45
3	B	801	HEM	CAA-CBA-CGA	-3.25	105.05	113.67
3	B	801	HEM	CBB-CAB-C3B	-3.13	111.89	127.53
3	B	801	HEM	C3D-C4D-ND	3.11	113.58	110.17
3	B	801	HEM	CHA-C4D-C3D	-3.03	119.64	125.23
3	A	801	HEM	CMC-C2C-C1C	-2.92	119.58	124.73
7	A	806	MPD	CM-C2-C3	2.91	122.76	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	HEM	CHD-C4C-NC	2.90	127.61	124.45
3	A	801	HEM	CAA-CBA-CGA	-2.90	105.97	113.67
3	B	801	HEM	C1B-NB-C4B	2.88	108.62	105.21
3	B	801	HEM	O2A-CGA-CBA	2.77	122.75	114.00
3	B	801	HEM	CHD-C1D-C2D	-2.74	120.70	125.03
3	A	801	HEM	C3D-C4D-ND	2.72	113.15	110.17
3	B	801	HEM	CAD-C3D-C4D	2.70	129.40	124.70
3	B	801	HEM	CHD-C1D-ND	2.69	127.31	124.42
8	B	806	TRS	O1-C1-C	2.68	118.34	110.88
3	A	801	HEM	CMD-C2D-C1D	2.56	129.03	125.03
8	A	808	TRS	C3-C-C1	2.51	117.35	110.66
7	A	807	MPD	O4-C4-C3	-2.48	101.47	111.35
3	B	801	HEM	C4C-NC-C1C	2.47	109.85	105.82
3	A	801	HEM	CMB-C2B-C1B	-2.42	121.26	125.03
3	A	801	HEM	CHB-C1B-NB	2.36	127.29	124.37
8	B	806	TRS	C1-C-N	2.31	114.07	108.17
3	A	801	HEM	CHA-C4D-C3D	-2.29	121.00	125.23
3	B	801	HEM	CMA-C3A-C2A	2.25	130.40	125.62
3	B	801	HEM	CHC-C1C-NC	-2.23	122.02	124.45
3	A	801	HEM	O2D-CGD-CBD	2.23	121.05	114.00
3	A	801	HEM	C1B-NB-C4B	2.21	107.83	105.21
3	B	801	HEM	CHC-C4B-NB	2.21	126.80	124.42
3	B	801	HEM	C4D-C3D-C2D	-2.15	103.77	106.89
3	A	801	HEM	C3B-C4B-NB	2.14	111.00	109.47
3	A	801	HEM	C2D-C1D-ND	2.14	112.38	109.90
3	A	801	HEM	CAD-C3D-C4D	2.03	128.24	124.70
3	A	801	HEM	CHC-C4B-NB	2.03	126.61	124.42
3	B	801	HEM	O1A-CGA-CBA	-2.03	116.67	123.09
7	A	807	MPD	O2-C2-CM	-2.00	101.75	107.99

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	806	MPD	O2-C2-C3-C4
7	A	806	MPD	CM-C2-C3-C4
7	B	805	MPD	C1-C2-C3-C4
7	B	805	MPD	O2-C2-C3-C4
7	A	807	MPD	O2-C2-C3-C4
7	A	806	MPD	C1-C2-C3-C4
8	B	806	TRS	C1-C-C3-O3
8	B	806	TRS	C2-C-C3-O3

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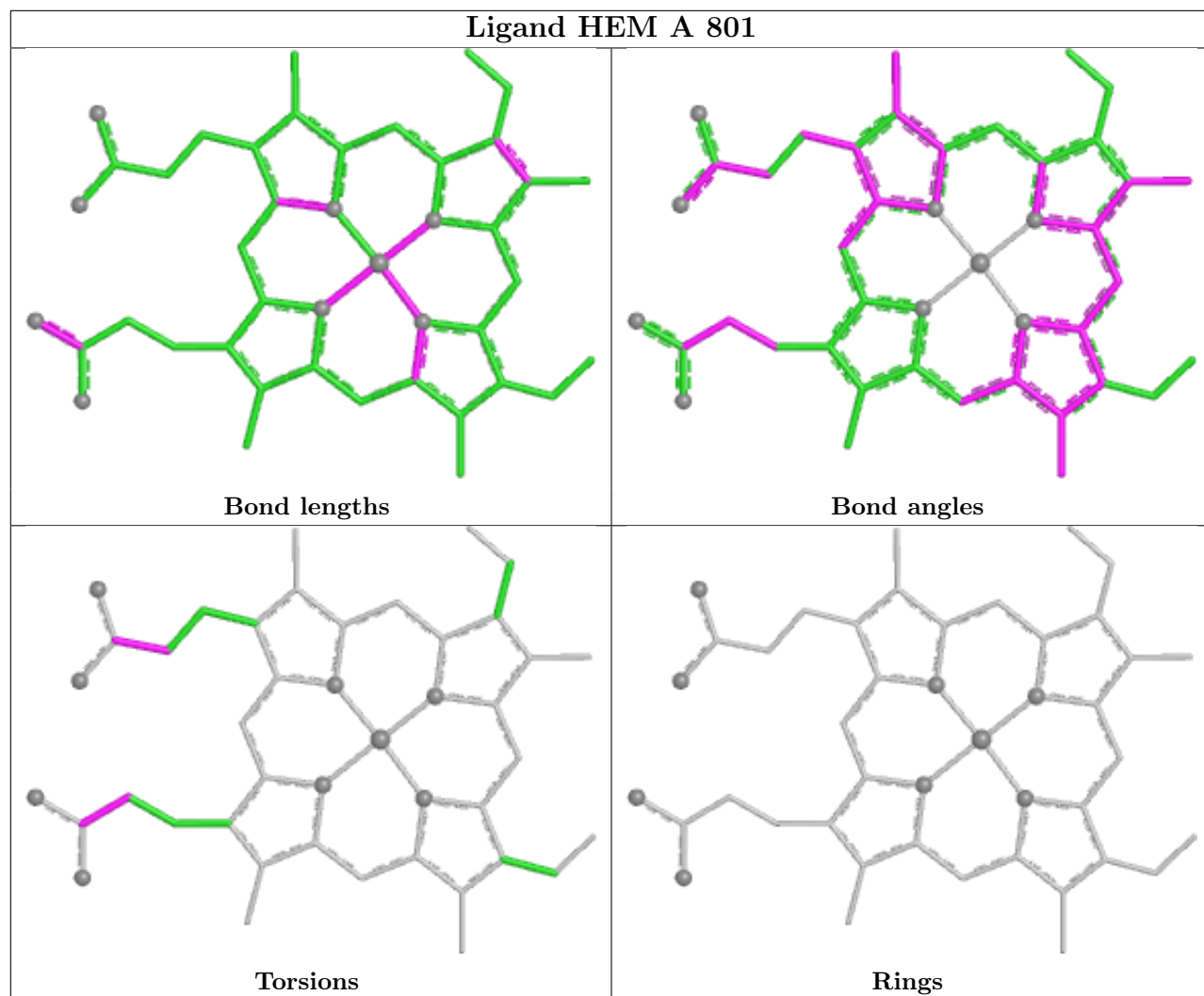
Mol	Chain	Res	Type	Atoms
3	A	801	HEM	CAA-CBA-CGA-O2A
3	A	801	HEM	CAA-CBA-CGA-O1A
3	B	801	HEM	CAA-CBA-CGA-O1A
3	B	801	HEM	CAA-CBA-CGA-O2A
8	A	808	TRS	C2-C-C3-O3
7	B	805	MPD	CM-C2-C3-C4
3	A	801	HEM	CAD-CBD-CGD-O2D

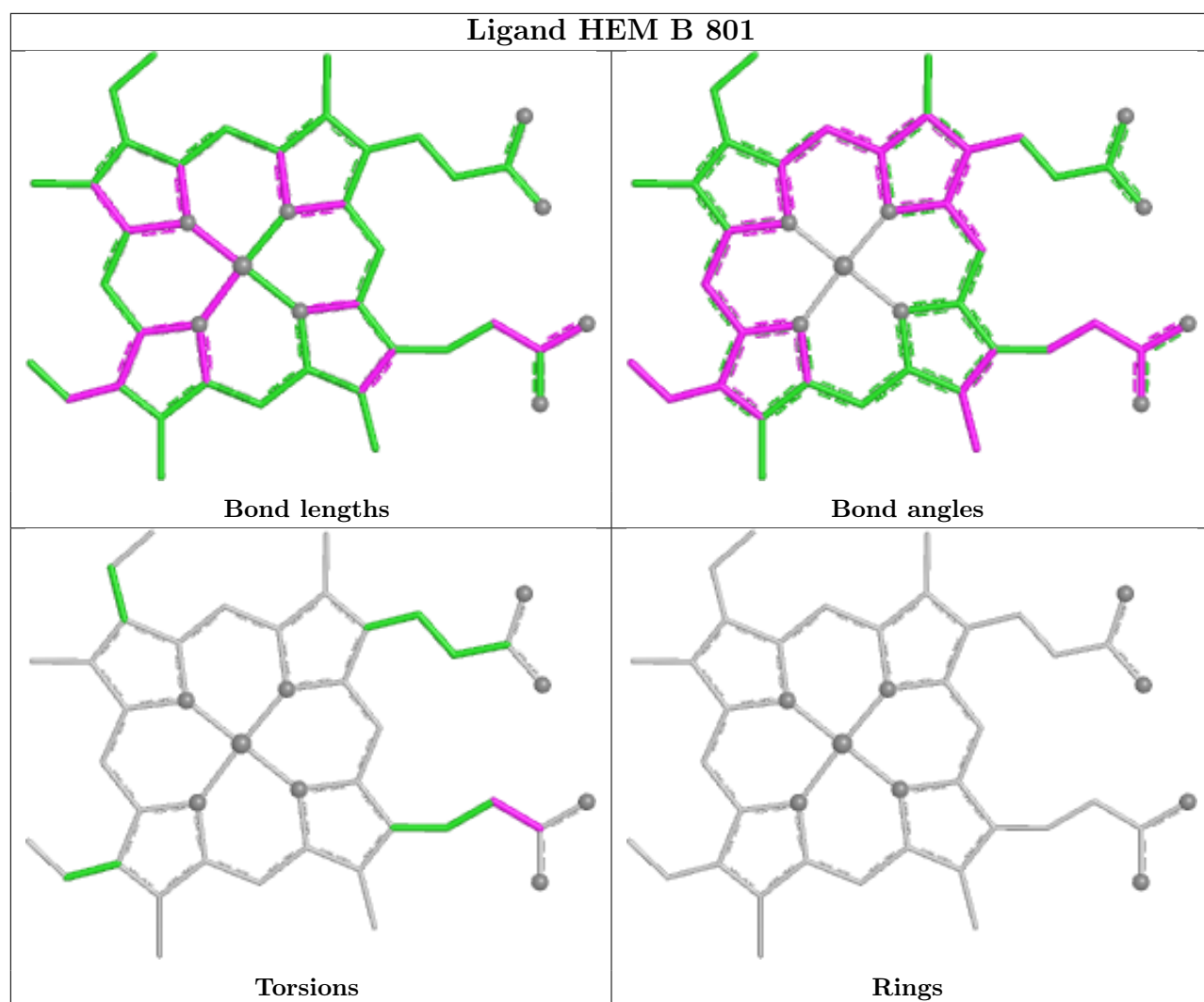
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	805	MPD	2	0
7	A	807	MPD	2	0
7	A	806	MPD	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 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.





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	712/728 (97%)	-0.42	5 (0%) 84 84	12, 26, 48, 78	4 (0%)
2	B	713/728 (97%)	-0.47	5 (0%) 84 84	13, 24, 45, 75	2 (0%)
All	All	1425/1456 (97%)	-0.45	10 (0%) 84 84	12, 25, 46, 78	6 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	55	HIS	3.3
2	B	36	GLY	3.0
2	B	748	ALA	2.8
1	A	748	ALA	2.5
2	B	44	PRO	2.5
2	B	55	HIS	2.3
1	A	691	ALA	2.1
1	A	53	HIS	2.0
1	A	209	LEU	2.0
2	B	540	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	MHO	A	62	9/10	0.95	0.10	27,31,42,57	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

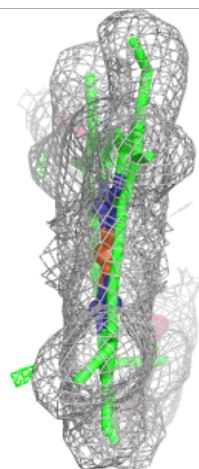
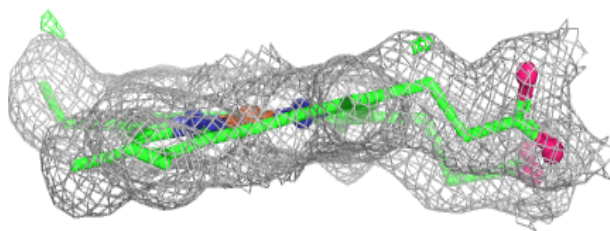
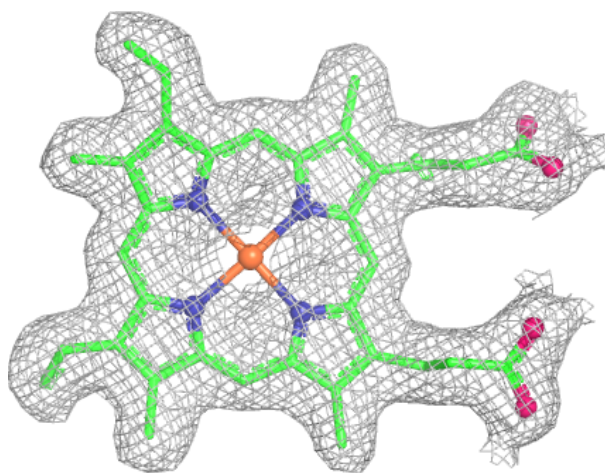
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

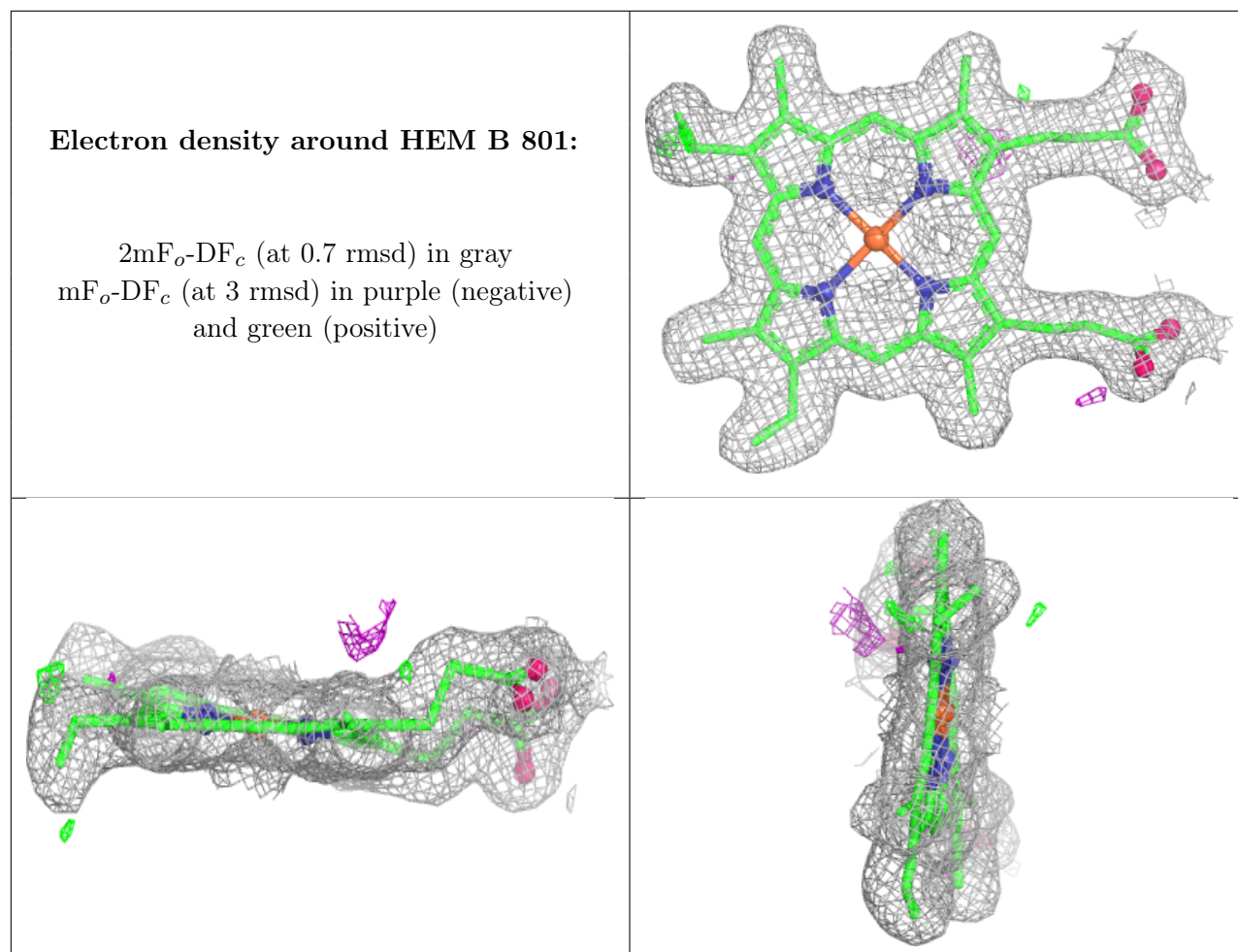
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MPD	A	806	8/8	0.83	0.18	52,61,67,69	0
7	MPD	A	807	8/8	0.86	0.14	50,52,55,59	0
7	MPD	B	805	8/8	0.88	0.14	45,50,55,56	0
5	OXY	B	803	2/2	0.91	0.29	39,39,39,41	0
5	OXY	A	804	2/2	0.91	0.11	48,48,48,51	0
8	TRS	A	808	8/8	0.92	0.12	35,39,46,47	0
8	TRS	B	806	8/8	0.92	0.13	28,35,37,38	0
5	OXY	A	803	2/2	0.95	0.16	35,35,35,46	0
4	NA	B	802	1/1	0.96	0.12	25,25,25,25	0
4	NA	A	802	1/1	0.98	0.10	24,24,24,24	0
3	HEM	A	801	43/43	0.99	0.05	19,22,25,26	0
6	O	A	805	1/1	0.99	0.06	27,27,27,27	0
6	O	B	804	1/1	0.99	0.04	22,22,22,22	0
3	HEM	B	801	43/43	0.99	0.05	19,20,22,23	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 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.