



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 06:09 PM EDT

PDB ID : 5SXS / pdb_00005sxs
Title : Crystal structure of catalase-peroxidase KatG with isonicotinic acid hydrazide and AMP bound
Authors : Loewen, P.C.
Deposited on : 2016-08-10
Resolution : 1.89 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

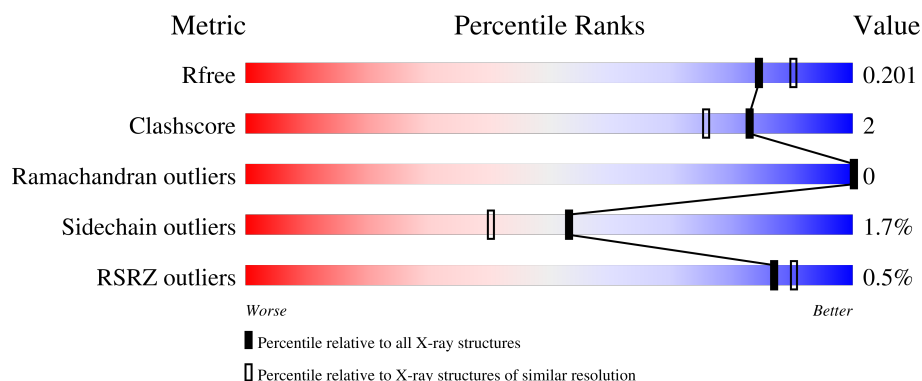
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	 90% 7% ..
1	B	728	 90% 6% ..

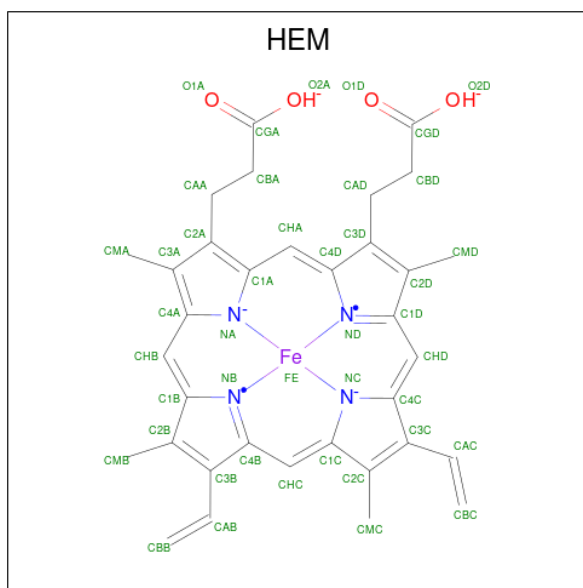
i

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total 5537	C 3497	N 988	O 1038	S 14	0	7	0
1	B	713	Total 5522	C 3489	N 982	O 1037	S 14	0	4	0

- 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 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

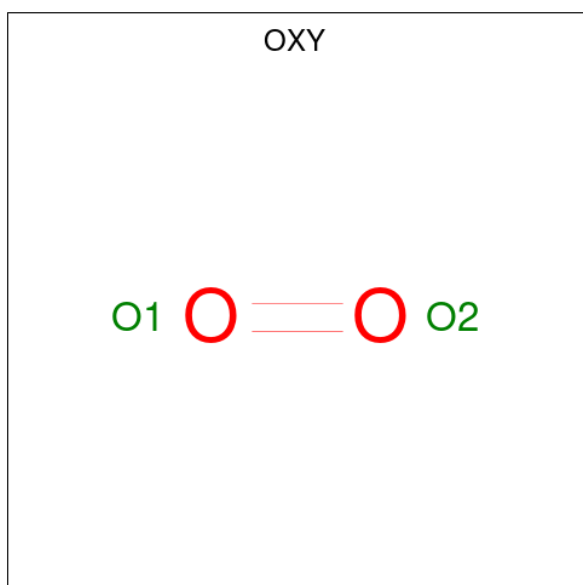
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

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

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

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



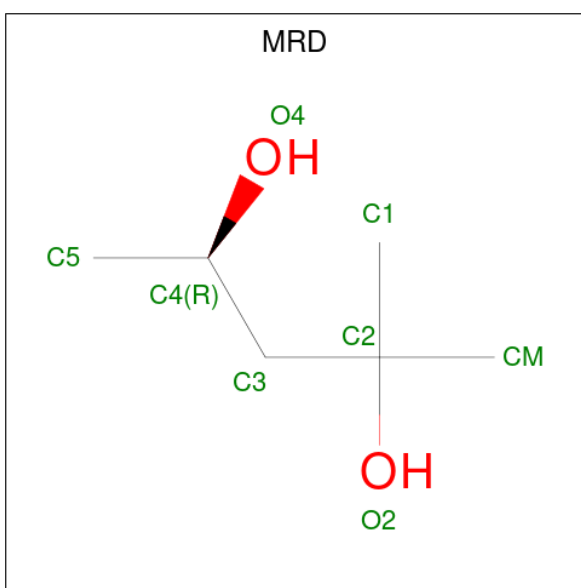
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 2 2	0	0
5	A	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



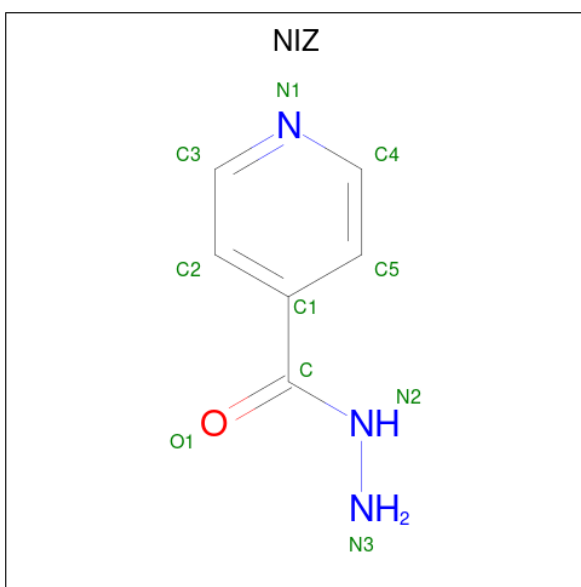
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: C₆H₁₄O₂).



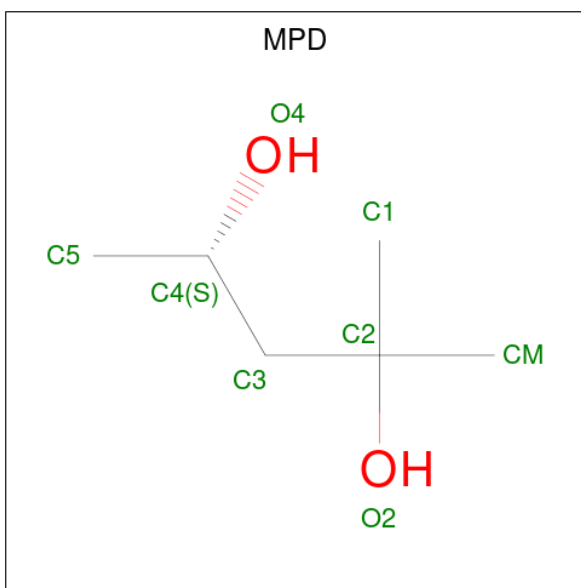
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is pyridine-4-carbohydrazide (CCD ID: NIZ) (formula: C₆H₇N₃O).



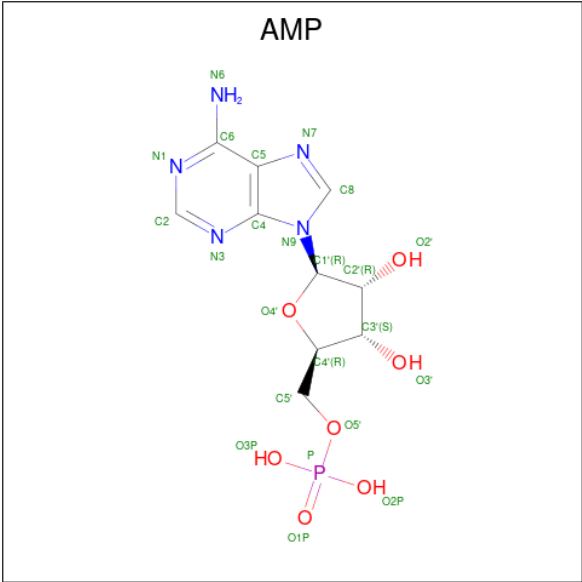
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	C	N	O	0	0
			10	6	3	1		

- Molecule 9 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



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

- Molecule 10 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

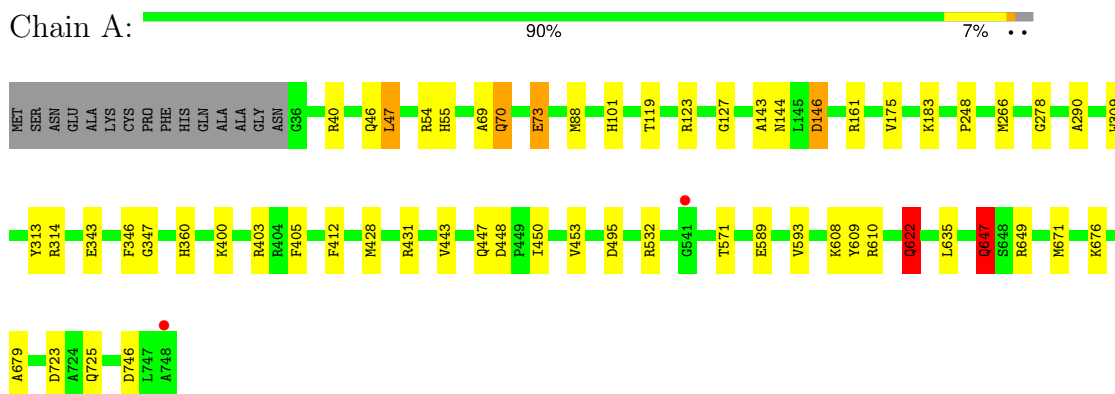
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	651	Total	O	0	0
			651	651		
11	B	709	Total	O	0	0
			709	709		

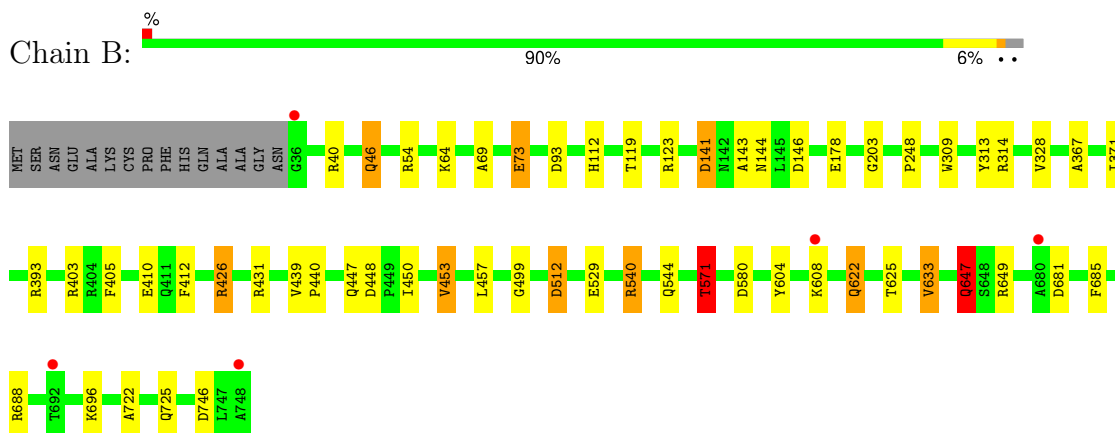
3 Residue-property plots [i](#)

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 1: 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	100.44Å 114.17Å 174.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.89 20.00 – 1.89	Depositor EDS
% Data completeness (in resolution range)	90.1 (20.00-1.89) 90.0 (20.00-1.89)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.162 , 0.193 0.172 , 0.201	Depositor DCC
R_{free} test set	7143 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12576	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: NIZ, AMP, MRD, PO4, NA, HEM, CL, OXY, 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	1.44	27/5707 (0.5%)	1.18	15/7758 (0.2%)
1	B	1.48	22/5678 (0.4%)	1.18	14/7720 (0.2%)
All	All	1.46	49/11385 (0.4%)	1.18	29/15478 (0.2%)

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	448	ASP	C-O	12.22	1.29	1.23
1	A	347	GLY	C-O	-9.04	1.13	1.24
1	B	448	ASP	C-O	8.76	1.28	1.23
1	A	248	PRO	CA-C	-7.16	1.47	1.53
1	B	746	ASP	C-O	-7.15	1.14	1.24
1	A	343	GLU	CD-OE1	7.01	1.38	1.25
1	B	722	ALA	C-O	-6.92	1.15	1.24
1	B	685	PHE	CA-C	-6.89	1.44	1.52
1	A	622[A]	GLN	CA-C	6.84	1.61	1.52
1	A	622[B]	GLN	CA-C	6.84	1.61	1.52
1	A	647	GLN	CA-C	6.67	1.62	1.53
1	A	671	MET	CA-C	6.59	1.61	1.52
1	B	647	GLN	CA-C	6.55	1.62	1.53
1	A	571	THR	N-CA	-6.39	1.38	1.46
1	B	512	ASP	CG-OD2	6.34	1.37	1.25
1	A	266	MET	C-O	-5.99	1.16	1.24
1	B	203	GLY	C-O	5.96	1.28	1.23
1	B	440	PRO	N-CA	-5.93	1.40	1.47
1	B	529	GLU	CG-CD	5.89	1.66	1.52
1	B	248	PRO	CA-C	-5.86	1.48	1.53
1	B	328	VAL	C-O	5.79	1.29	1.24
1	B	499	GLY	C-O	5.72	1.29	1.23
1	B	453	VAL	C-O	-5.67	1.17	1.24
1	B	439	VAL	C-O	-5.66	1.17	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	453	VAL	C-O	-5.58	1.17	1.24
1	A	47	LEU	CB-CG	-5.54	1.42	1.53
1	A	746	ASP	C-O	-5.51	1.17	1.24
1	A	635	LEU	C-O	-5.46	1.17	1.24
1	A	679	ALA	N-CA	5.43	1.52	1.46
1	B	367	ALA	C-O	-5.39	1.17	1.23
1	A	428	MET	CG-SD	-5.36	1.67	1.80
1	A	589	GLU	C-O	-5.34	1.18	1.24
1	A	443	VAL	CA-C	-5.30	1.46	1.52
1	A	725	GLN	CD-OE1	5.29	1.33	1.23
1	A	175	VAL	CA-C	5.25	1.60	1.52
1	A	532	ARG	NE-CZ	-5.23	1.27	1.33
1	A	723	ASP	C-O	-5.18	1.17	1.24
1	B	580	ASP	C-O	-5.18	1.17	1.24
1	B	681	ASP	CA-C	5.16	1.58	1.52
1	A	278	GLY	C-O	5.15	1.30	1.23
1	B	604	TYR	N-CA	-5.14	1.39	1.46
1	A	676	LYS	CA-C	-5.13	1.47	1.52
1	B	426	ARG	CZ-NH2	5.11	1.40	1.33
1	A	495	ASP	N-CA	5.08	1.52	1.46
1	A	146	ASP	N-CA	-5.04	1.40	1.46
1	A	46	GLN	CG-CD	5.03	1.64	1.52
1	B	119	THR	CB-CG2	-5.02	1.35	1.52
1	B	633[A]	VAL	C-O	5.02	1.30	1.24
1	B	633[B]	VAL	C-O	5.02	1.30	1.24

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	GLN	N-CA-C	-7.78	100.84	110.41
1	A	343	GLU	OE1-CD-OE2	7.51	140.93	122.90
1	B	571	THR	CB-CA-C	-7.49	97.39	109.75
1	B	54	ARG	CG-CD-NE	-7.26	96.03	112.00
1	B	93	ASP	N-CA-C	6.96	119.71	111.71
1	B	529	GLU	CB-CG-CD	6.45	123.56	112.60
1	B	46	GLN	N-CA-C	-6.09	102.92	110.41
1	A	448	ASP	CA-C-N	-6.03	114.06	120.03
1	A	448	ASP	C-N-CA	-6.03	114.06	120.03
1	A	127	GLY	N-CA-C	5.86	121.11	114.67
1	B	393	ARG	NE-CZ-NH2	-5.82	113.96	119.20
1	B	448	ASP	CA-C-N	-5.74	114.35	120.03
1	B	448	ASP	C-N-CA	-5.74	114.35	120.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	73	GLU	CB-CA-C	-5.61	100.25	110.63
1	A	54	ARG	CG-CD-NE	-5.58	99.72	112.00
1	A	47	LEU	N-CA-CB	-5.52	101.90	110.29
1	A	55	HIS	CB-CA-C	5.51	119.93	111.39
1	B	371	ILE	CA-C-N	-5.46	114.96	120.31
1	B	371	ILE	C-N-CA	-5.46	114.96	120.31
1	A	450	ILE	CB-CA-C	-5.41	104.88	110.13
1	A	70	GLN	CA-CB-CG	5.37	124.83	114.10
1	A	343	GLU	CG-CD-OE2	-5.30	106.21	118.40
1	A	73	GLU	CB-CA-C	-5.24	100.94	110.63
1	B	450	ILE	CB-CA-C	-5.23	104.72	110.52
1	A	46	GLN	CB-CG-CD	5.13	121.32	112.60
1	B	571	THR	N-CA-CB	5.10	118.74	110.43
1	B	46	GLN	N-CA-CB	5.07	117.33	110.38
1	A	609	TYR	CA-C-N	5.03	127.33	120.54
1	A	609	TYR	C-N-CA	5.03	127.33	120.54

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	5537	0	5360	21	0
1	B	5522	0	5343	28	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	A	1	0	0	0	0
3	B	1	0	0	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	4	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	8	0	14	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	10	0	7	2	0
9	B	8	0	14	2	0
10	B	23	0	12	0	0
11	A	651	0	0	7	1
11	B	709	0	0	12	1
All	All	12576	0	10810	53	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 (53) 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:161[B]:ARG:NH1	11:A:901:HOH:O	2.01	0.93
1:B:622[A]:GLN:NE2	8:B:806:NIZ:O1	2.04	0.91
1:A:161[B]:ARG:CZ	11:A:901:HOH:O	2.20	0.88
1:A:119[B]:THR:HG21	11:A:1066:HOH:O	1.74	0.87
7:A:807:MRD:H1C2	7:A:807:MRD:O4	1.76	0.84
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.64	0.79
1:B:571:THR:HG23	11:B:1118:HOH:O	1.86	0.74
9:B:807:MPD:O4	9:B:807:MPD:H11	1.89	0.73
7:A:807:MRD:O4	7:A:807:MRD:C1	2.31	0.73
1:B:178:GLU:OE1	11:B:901:HOH:O	2.06	0.72
1:B:571:THR:CG2	11:B:1118:HOH:O	2.37	0.72
1:B:512:ASP:OD1	11:B:902:HOH:O	2.08	0.71
1:B:540:ARG:NE	1:B:540:ARG:HA	2.05	0.71
1:B:540:ARG:HA	1:B:540:ARG:CZ	2.23	0.69
1:B:69:ALA:O	1:B:73:GLU:HG2	1.98	0.64
1:A:69:ALA:O	1:A:73:GLU:HG2	1.98	0.63
9:B:807:MPD:O4	9:B:807:MPD:C1	2.49	0.60
1:B:123:ARG:NH2	1:B:622[B]:GLN:OE1	2.36	0.58
1:A:119[B]:THR:CG2	1:A:593:VAL:HG11	2.34	0.56
1:A:290:ALA:HB1	7:A:807:MRD:H5C3	1.86	0.56
1:B:123:ARG:HH21	1:B:622[A]:GLN:HE21	1.56	0.54
1:B:696:LYS:HE2	11:B:967:HOH:O	2.08	0.54
1:A:144:ASN:HA	1:A:146:ASP:OD1	2.10	0.51
1:A:360:HIS:ND1	11:A:906:HOH:O	2.35	0.50
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.12	0.50
1:A:47:LEU:O	11:A:902:HOH:O	2.19	0.50
1:A:313:TYR:CE2	1:A:314:ARG:HD3	2.47	0.49
1:A:290:ALA:CB	7:A:807:MRD:H5C3	2.41	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:PHE:CE2	1:A:403[A]:ARG:NE	2.82	0.47
1:A:400:LYS:HE2	11:A:1466:HOH:O	2.15	0.46
1:B:313:TYR:CE2	1:B:314:ARG:HD3	2.50	0.46
1:B:405:PHE:HB3	1:B:412:PHE:HB2	1.97	0.46
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.15	0.46
1:B:725:GLN:NE2	11:B:931:HOH:O	2.49	0.46
1:A:123:ARG:HH21	1:A:622[A]:GLN:NE2	2.15	0.45
1:A:647:GLN:HG2	11:A:1112:HOH:O	2.15	0.45
1:B:571:THR:HG22	11:B:1118:HOH:O	2.09	0.45
1:B:410:GLU:HB2	11:B:1383:HOH:O	2.17	0.45
1:B:544:GLN:OE1	11:B:903:HOH:O	2.21	0.44
1:A:88:MET:HB3	1:A:101:HIS:CE1	2.53	0.44
1:A:143:ALA:HA	1:A:309:TRP:CH2	2.53	0.43
1:B:123:ARG:HH21	1:B:622[A]:GLN:NE2	2.17	0.43
1:B:403:ARG:NH1	11:B:938:HOH:O	2.51	0.43
1:A:346:PHE:CD2	1:A:403[A]:ARG:CZ	3.03	0.42
1:B:426:ARG:HA	1:B:426:ARG:HD2	1.90	0.42
1:B:453:VAL:HG11	1:B:457:LEU:HD21	2.00	0.42
1:A:405:PHE:HB3	1:A:412:PHE:HB2	1.99	0.42
1:B:625:THR:HG22	8:B:806:NIZ:H4	2.01	0.42
1:B:112:HIS:CE1	1:B:141:ASP:O	2.73	0.41
1:B:143:ALA:HA	1:B:309:TRP:CH2	2.55	0.41
1:A:431:ARG:HD2	1:A:447:GLN:OE1	2.20	0.41
1:B:647:GLN:HG2	11:B:1038:HOH:O	2.19	0.40
1:B:688:ARG:NE	11:B:905:HOH:O	2.38	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)
11:A:1166:HOH:O	11:B:979:HOH:O[2_444]	2.14	0.06

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	718/728 (99%)	708 (99%)	10 (1%)	0	100	100
1	B	715/728 (98%)	707 (99%)	8 (1%)	0	100	100
All	All	1433/1456 (98%)	1415 (99%)	18 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	557/561 (99%)	548 (98%)	9 (2%)	55	43
1	B	554/561 (99%)	541 (98%)	13 (2%)	44	29
All	All	1111/1122 (99%)	1089 (98%)	22 (2%)	53	33

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	70	GLN
1	A	183	LYS
1	A	608	LYS
1	A	610	ARG
1	A	622[A]	GLN
1	A	622[B]	GLN
1	A	647	GLN
1	A	649	ARG
1	B	40	ARG
1	B	46	GLN
1	B	64	LYS
1	B	141	ASP
1	B	540	ARG
1	B	571	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	608	LYS
1	B	622[A]	GLN
1	B	622[B]	GLN
1	B	633[A]	VAL
1	B	633[B]	VAL
1	B	647	GLN
1	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	227	ASN
1	A	247	ASN
1	A	737	ASN
1	B	39	ASN
1	B	46	GLN
1	B	520	GLN
1	B	561	GLN
1	B	650	HIS
1	B	725	GLN
1	B	737	ASN
1	B	741	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](#)

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\# Z > 2$
8	NIZ	B	806	-	10,10,10	1.71	2 (20%)	12,12,12	1.86	4 (33%)
5	OXY	B	805	-	1,1,1	0.09	0	-		
9	MPD	B	807	-	7,7,7	0.97	0	9,10,10	1.57	2 (22%)
2	HEM	B	801	11,1	50,50,50	1.78	9 (18%)	67,82,82	1.78	17 (25%)
6	PO4	B	808	-	4,4,4	1.08	0	6,6,6	1.51	1 (16%)
10	AMP	B	809	-	25,25,25	1.94	7 (28%)	37,38,38	2.30	14 (37%)
5	OXY	A	805	-	1,1,1	0.01	0	-		
6	PO4	A	806	-	4,4,4	0.79	0	6,6,6	2.21	1 (16%)
7	MRD	A	807	-	7,7,7	0.59	0	9,10,10	1.48	2 (22%)
2	HEM	A	801	11,1	50,50,50	1.76	15 (30%)	67,82,82	1.50	13 (19%)
5	OXY	A	804	-	1,1,1	0.26	0	-		
5	OXY	B	804	-	1,1,1	0.11	0	-		

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
8	NIZ	B	806	-	-	1/6/6/6	0/1/1/1
9	MPD	B	807	-	-	3/5/5/5	-
2	HEM	B	801	11,1	-	2/14/54/54	-
10	AMP	B	809	-	-	0/10/26/26	0/3/3/3
7	MRD	A	807	-	-	5/5/5/5	-
2	HEM	A	801	11,1	-	2/14/54/54	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C1B-NB	-6.25	1.29	1.40
10	B	809	AMP	C5-C4	5.37	1.48	1.39
2	A	801	HEM	FE-NC	4.11	2.08	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	FE-NA	4.09	2.08	1.95
10	B	809	AMP	C8-N7	3.81	1.39	1.31
2	B	801	HEM	C1D-ND	-3.70	1.31	1.38
2	B	801	HEM	C4D-ND	-3.56	1.34	1.40
2	A	801	HEM	C4B-NB	-3.56	1.31	1.38
2	B	801	HEM	FE-NB	3.54	2.05	1.94
2	B	801	HEM	C4B-NB	-3.31	1.32	1.38
8	B	806	NIZ	C5-C1	3.24	1.44	1.39
8	B	806	NIZ	C-N2	3.15	1.37	1.33
2	A	801	HEM	C1B-NB	-3.14	1.34	1.40
10	B	809	AMP	C5-C6	3.10	1.49	1.41
2	A	801	HEM	C1A-NA	-3.07	1.33	1.39
10	B	809	AMP	C2-N3	3.03	1.39	1.33
10	B	809	AMP	C4-N3	3.02	1.40	1.34
2	A	801	HEM	C4A-NA	-3.00	1.34	1.39
2	A	801	HEM	FE-NB	2.98	2.04	1.94
2	B	801	HEM	C2A-C3A	-2.87	1.31	1.38
2	B	801	HEM	FE-NC	2.82	2.04	1.95
2	A	801	HEM	C1C-NC	-2.59	1.34	1.39
2	A	801	HEM	CHD-C1D	-2.57	1.33	1.39
2	A	801	HEM	O1A-CGA	2.50	1.30	1.22
2	B	801	HEM	O1D-CGD	2.45	1.30	1.22
2	A	801	HEM	C1D-C2D	2.41	1.49	1.44
2	A	801	HEM	C2A-C3A	-2.38	1.32	1.38
2	A	801	HEM	C4C-NC	-2.28	1.35	1.39
10	B	809	AMP	C6-N6	2.20	1.39	1.34
2	A	801	HEM	CHB-C1B	2.14	1.42	1.38
2	B	801	HEM	C3B-C4B	2.12	1.49	1.44
10	B	809	AMP	C8-N9	2.04	1.41	1.37
2	A	801	HEM	C3C-C2C	2.03	1.41	1.37

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CHC-C4B-NB	6.32	131.22	124.42
10	B	809	AMP	N3-C2-N1	-5.05	120.94	128.58
6	A	806	PO4	O4-P-O3	4.78	122.78	107.91
10	B	809	AMP	C2-N1-C6	4.61	126.31	118.73
2	A	801	HEM	C3D-C4D-ND	4.55	115.16	110.17
8	B	806	NIZ	C1-C-N2	4.44	121.26	116.33
2	B	801	HEM	CHD-C1D-ND	4.23	128.98	124.42
10	B	809	AMP	N3-C4-N9	4.09	134.12	127.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	809	AMP	C4-N9-C8	3.84	109.77	105.74
10	B	809	AMP	N6-C6-N1	3.78	126.80	118.38
10	B	809	AMP	O2P-P-O5'	-3.75	96.90	106.67
2	B	801	HEM	CHA-C4D-ND	3.54	128.75	124.37
10	B	809	AMP	O2P-P-O1P	3.49	124.45	110.83
2	B	801	HEM	CHA-C4D-C3D	-3.37	119.02	125.23
10	B	809	AMP	C5-C4-N3	-3.31	122.15	126.72
2	A	801	HEM	CAA-CBA-CGA	-3.28	104.95	113.67
2	A	801	HEM	CBD-CAD-C3D	3.14	121.21	112.53
2	A	801	HEM	C4B-C3B-C2B	-3.11	104.42	107.28
2	B	801	HEM	C4D-C3D-C2D	-3.10	102.38	106.89
2	A	801	HEM	C2A-C1A-NA	-3.03	106.79	110.15
2	B	801	HEM	CAA-CBA-CGA	-3.00	105.71	113.67
2	A	801	HEM	C4C-NC-C1C	2.98	110.67	105.82
2	B	801	HEM	C1B-NB-C4B	2.97	108.73	105.21
6	B	808	PO4	O4-P-O1	-2.94	100.55	110.95
2	B	801	HEM	C4B-C3B-C2B	-2.85	104.66	107.28
7	A	807	MRD	C1-C2-C3	2.82	122.35	110.20
9	B	807	MPD	O2-C2-C3	-2.72	99.09	109.27
10	B	809	AMP	C2-N3-C4	2.69	118.41	111.83
10	B	809	AMP	C4-N9-C1'	-2.62	120.50	126.63
10	B	809	AMP	C5-C6-N6	-2.62	116.79	123.29
10	B	809	AMP	N9-C8-N7	-2.57	110.29	113.94
2	A	801	HEM	C4D-C3D-C2D	-2.57	103.15	106.89
2	B	801	HEM	CHC-C4B-C3B	-2.50	120.09	125.07
2	B	801	HEM	CHD-C1D-C2D	-2.47	121.13	125.03
2	A	801	HEM	CHA-C4D-C3D	-2.44	120.73	125.23
8	B	806	NIZ	C4-N1-C3	2.40	122.34	116.86
2	B	801	HEM	CMC-C2C-C3C	-2.39	122.64	128.43
2	A	801	HEM	C3C-C2C-C1C	-2.34	104.83	107.05
10	B	809	AMP	O5'-P-O1P	-2.31	100.21	106.44
2	A	801	HEM	O2A-CGA-CBA	2.29	121.24	114.00
10	B	809	AMP	O3'-C3'-C4'	2.23	117.50	111.08
2	B	801	HEM	CMD-C2D-C1D	2.22	128.51	125.03
2	A	801	HEM	C1B-NB-C4B	2.19	107.80	105.21
8	B	806	NIZ	O1-C-C1	-2.17	116.60	120.90
7	A	807	MRD	CM-C2-C1	-2.16	105.79	110.63
8	B	806	NIZ	C2-C3-N1	-2.13	119.97	123.60
2	B	801	HEM	CAD-CBD-CGD	2.12	119.30	113.67
2	B	801	HEM	CBD-CAD-C3D	2.08	118.28	112.53
2	A	801	HEM	CAD-C3D-C4D	2.06	128.29	124.70
2	B	801	HEM	CHC-C1C-NC	-2.05	122.22	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	807	MPD	C1-C2-C3	2.04	118.99	110.20
2	B	801	HEM	CAB-C3B-C2B	2.04	135.05	128.43
2	A	801	HEM	C4D-ND-C1D	-2.03	102.80	105.21
2	B	801	HEM	CMC-C2C-C1C	2.03	128.30	124.73

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	807	MRD	C1-C2-C3-C4
7	A	807	MRD	O2-C2-C3-C4
7	A	807	MRD	C2-C3-C4-C5
8	B	806	NIZ	C1-C-N2-N3
9	B	807	MPD	C1-C2-C3-C4
9	B	807	MPD	CM-C2-C3-C4
2	A	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O1A
7	A	807	MRD	C2-C3-C4-O4
9	B	807	MPD	C2-C3-C4-O4
7	A	807	MRD	CM-C2-C3-C4

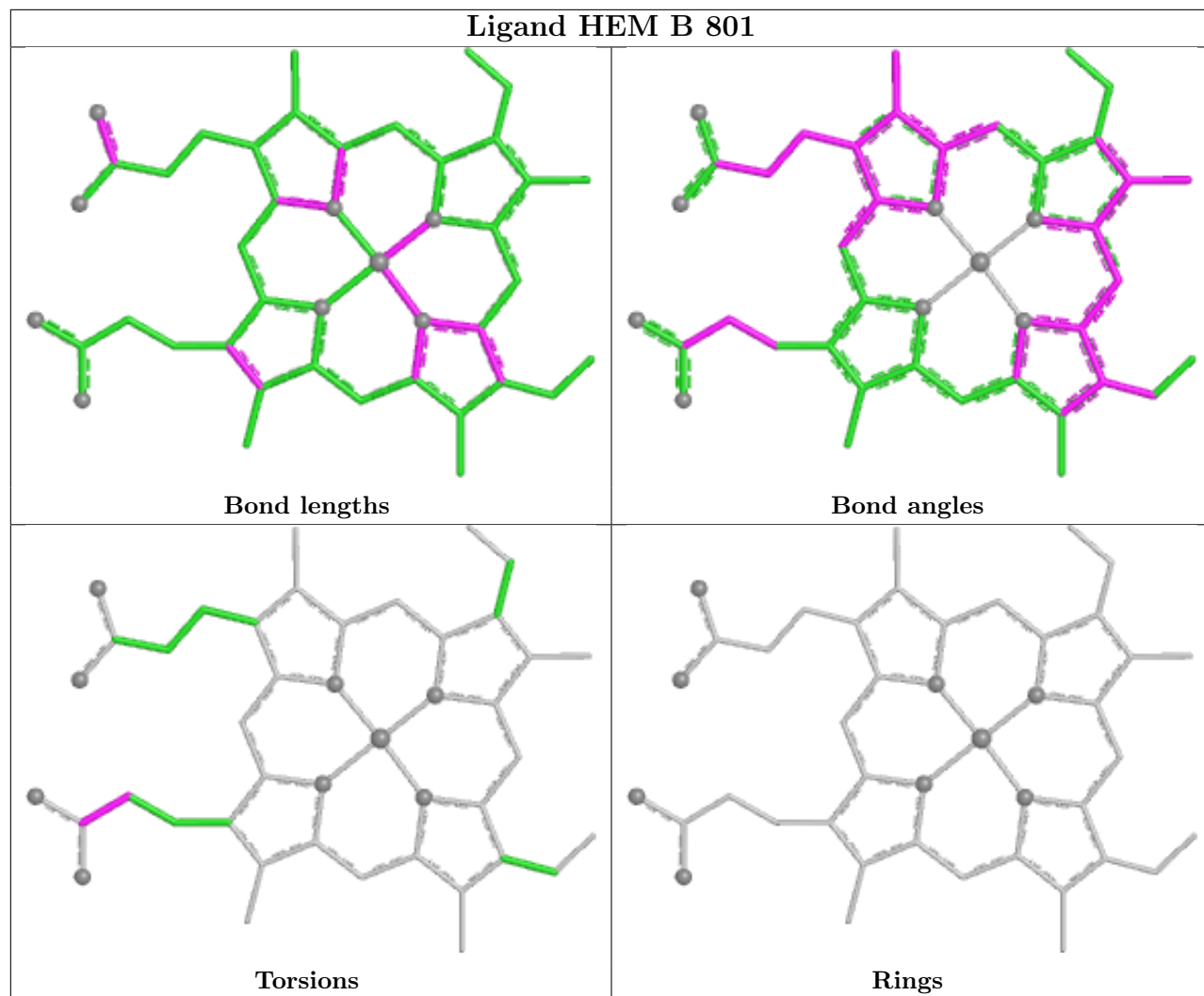
There are no ring outliers.

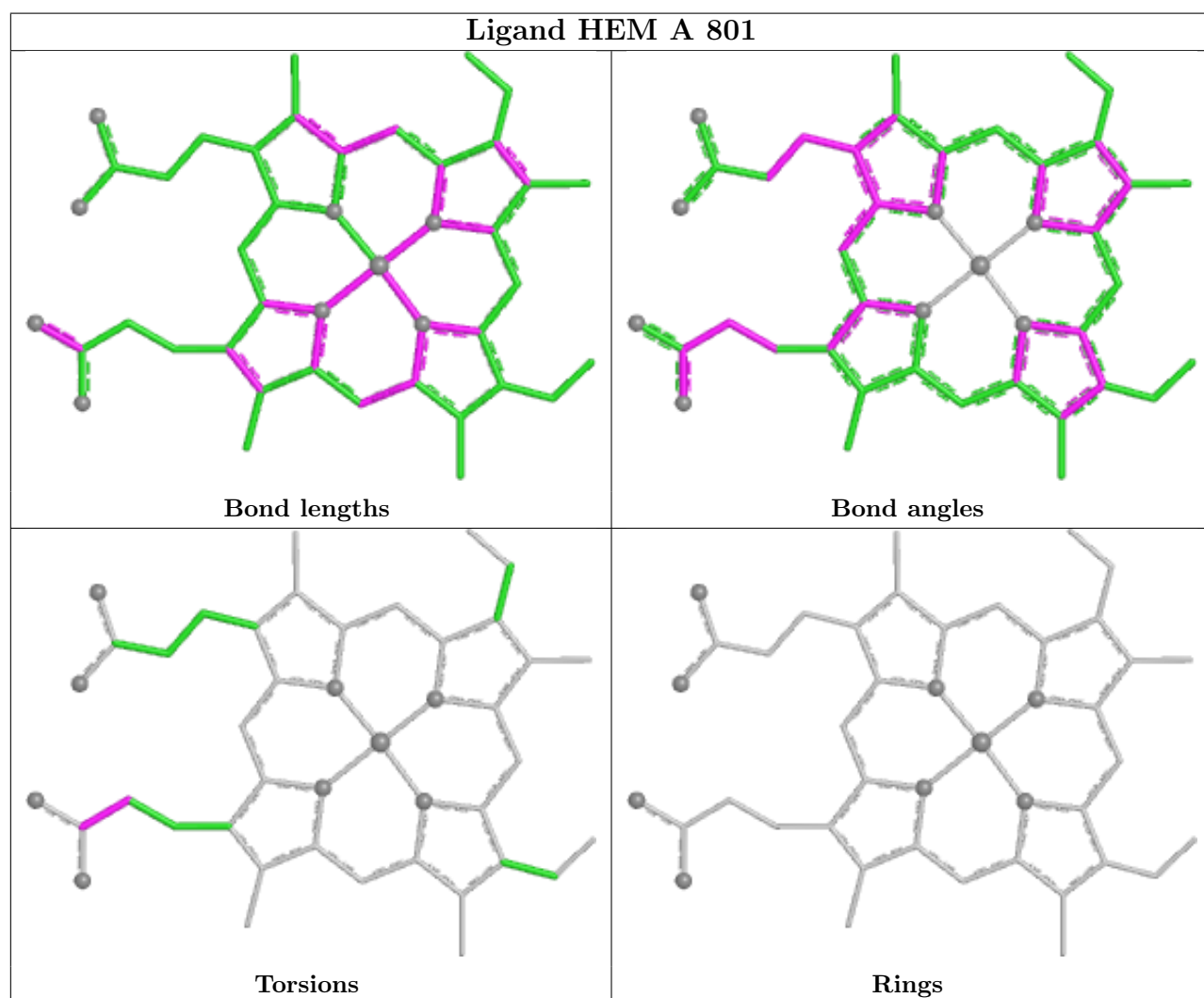
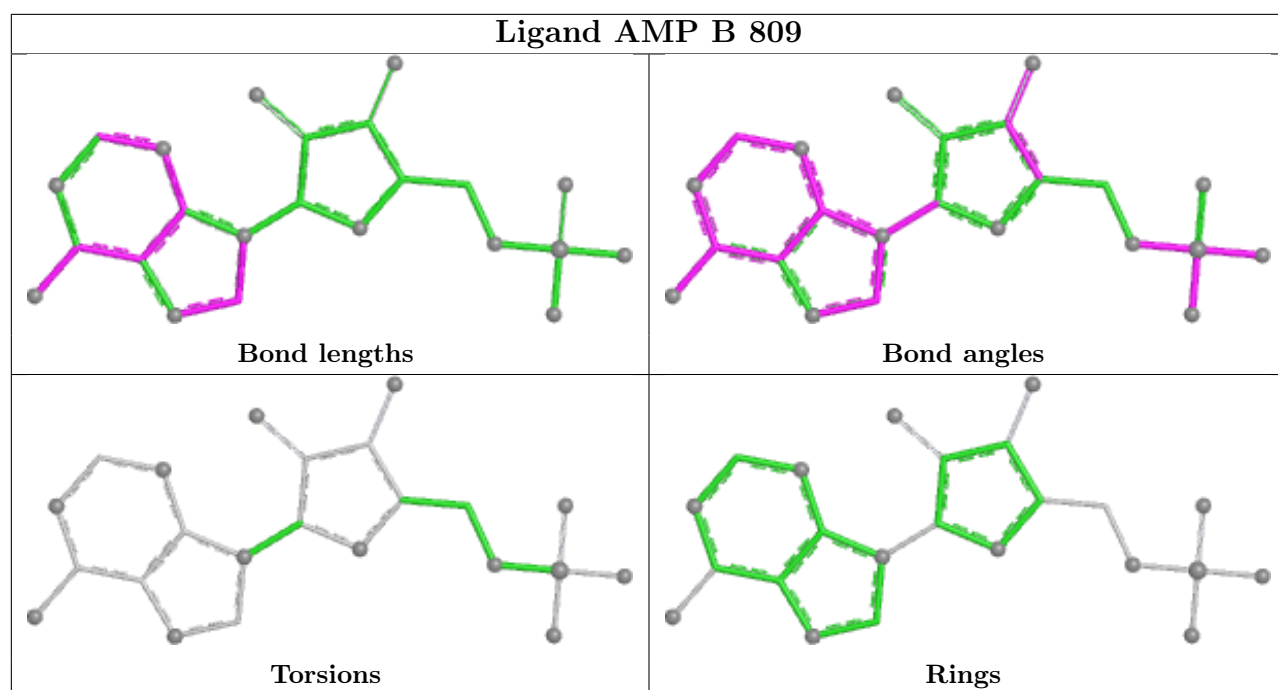
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	806	NIZ	2	0
9	B	807	MPD	2	0
7	A	807	MRD	4	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	713/728 (97%)	-0.47	2 (0%)	90 93	10, 23, 45, 83	7 (0%)
1	B	713/728 (97%)	-0.58	5 (0%)	84 88	11, 21, 40, 73	4 (0%)
All	All	1426/1456 (97%)	-0.53	7 (0%)	87 90	10, 22, 43, 83	11 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	3.0
1	B	748	ALA	2.9
1	B	36	GLY	2.4
1	B	680	ALA	2.4
1	A	541	GLY	2.1
1	B	608	LYS	2.1
1	B	692	THR	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](#)

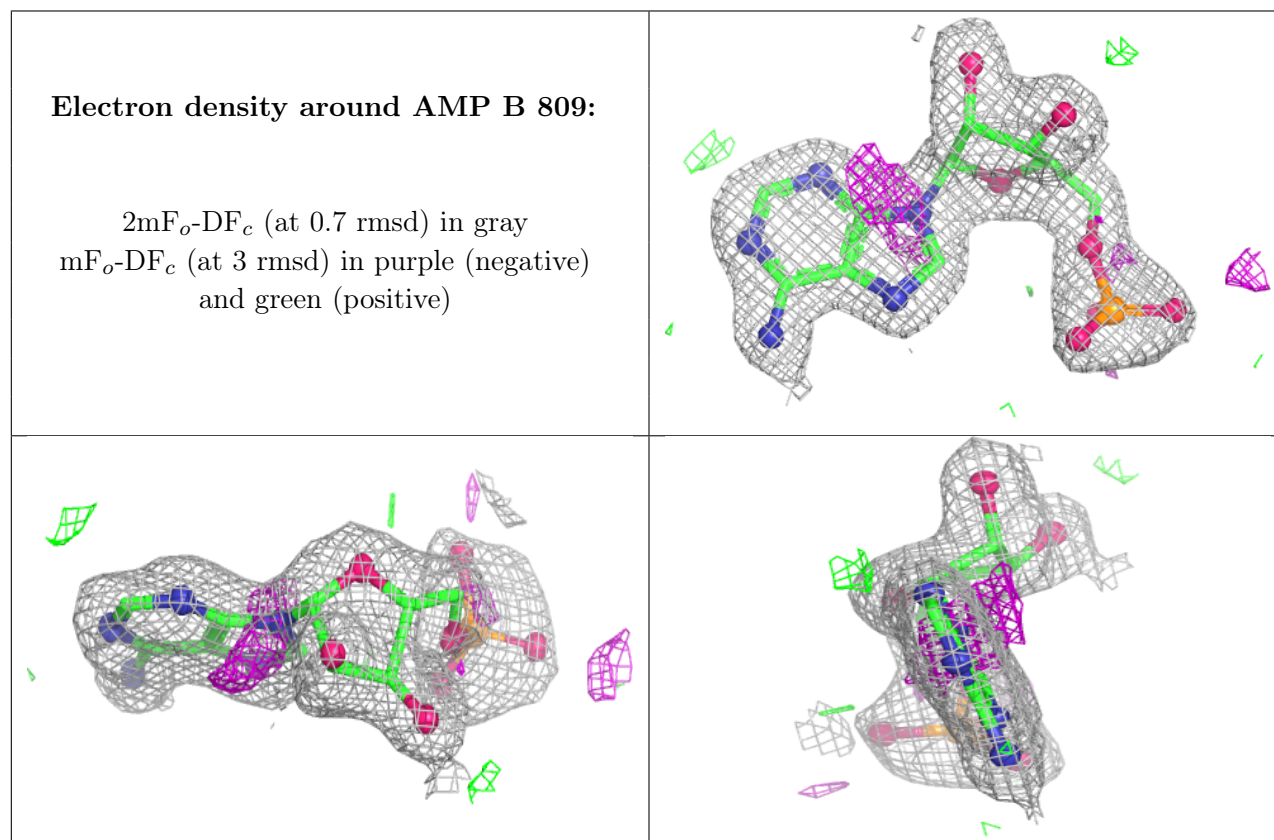
There are no oligosaccharides in this entry.

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.

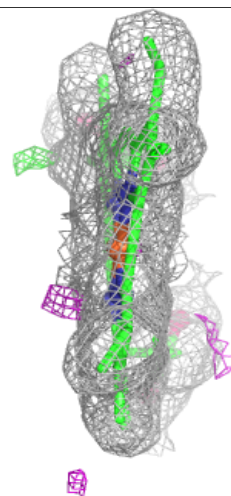
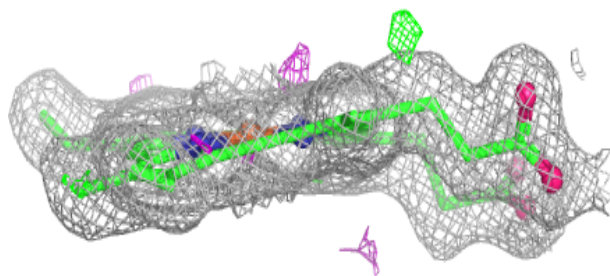
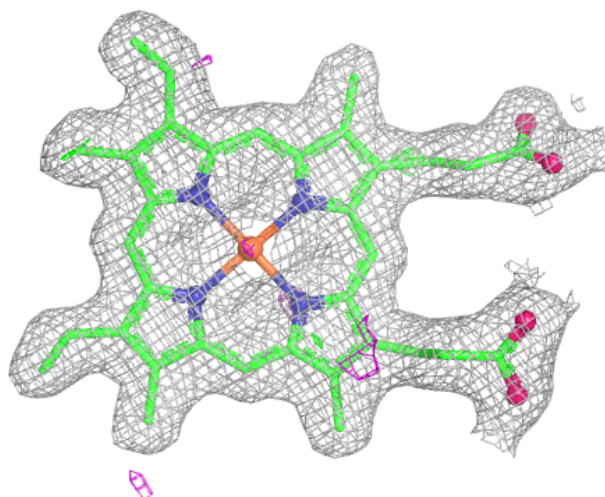
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	OXY	A	805	2/2	0.88	0.13	47,47,47,52	0
6	PO4	A	806	5/5	0.88	0.08	57,59,66,67	0
8	NIZ	B	806	10/10	0.89	0.10	36,42,48,49	0
7	MRD	A	807	8/8	0.91	0.12	48,55,61,62	0
5	OXY	B	805	2/2	0.91	0.16	36,36,36,52	0
9	MPD	B	807	8/8	0.91	0.12	42,46,53,54	0
6	PO4	B	808	5/5	0.94	0.10	45,54,57,61	0
5	OXY	A	804	2/2	0.95	0.12	34,34,34,35	0
10	AMP	B	809	23/23	0.95	0.07	29,32,51,54	0
5	OXY	B	804	2/2	0.97	0.10	26,26,26,28	0
2	HEM	A	801	43/43	0.98	0.05	18,20,23,24	0
3	NA	A	802	1/1	0.98	0.04	16,16,16,16	0
4	CL	A	803	1/1	0.99	0.04	25,25,25,25	1
4	CL	B	803	1/1	0.99	0.02	20,20,20,20	1
2	HEM	B	801	43/43	0.99	0.04	14,15,17,18	0
3	NA	B	802	1/1	0.99	0.05	18,18,18,18	0

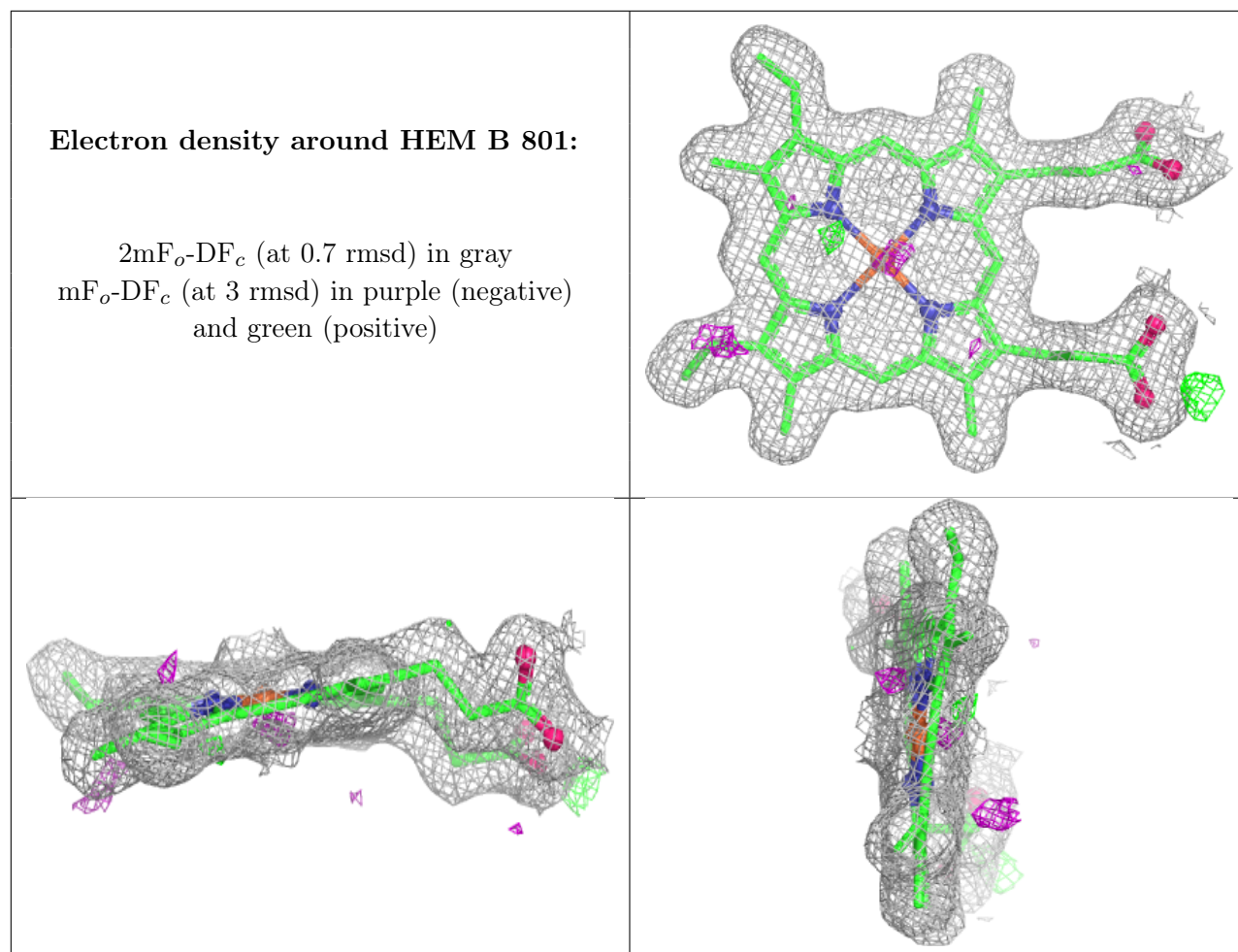
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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