



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 06:05 AM EDT

PDB ID : 5SW4 / pdb_00005sw4
Title : Crystal structure of native catalase-peroxidase KatG at pH8.0
Authors : Loewen, P.C.
Deposited on : 2016-08-08
Resolution : 1.90 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

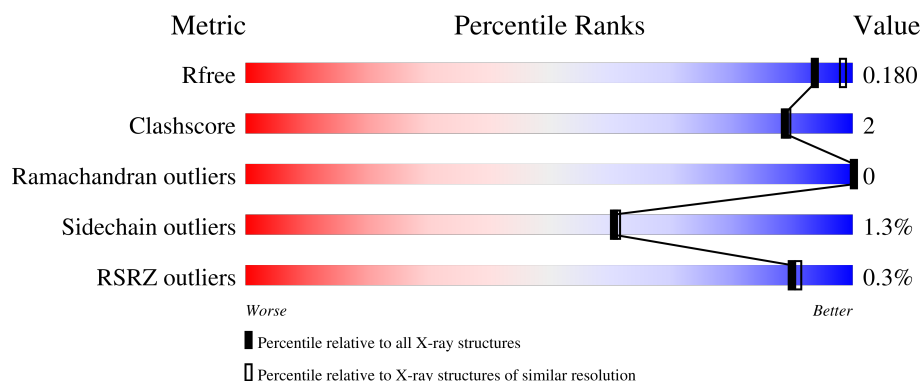
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	
1	B	728	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	TRS	A	807	-	X	-	-

2 Entry composition [i](#)

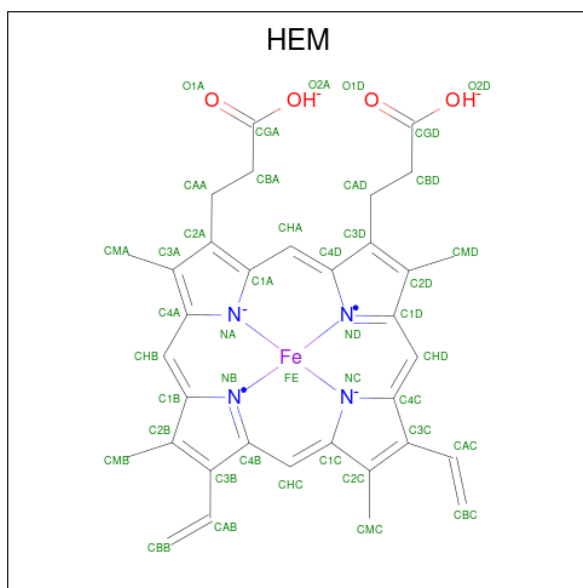
There are 8 unique types of molecules in this entry. The entry contains 12811 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	8	0
			5570	3513	992	1051	14			
1	B	713	Total	C	N	O	S	0	5	0
			5548	3502	989	1043	14			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).

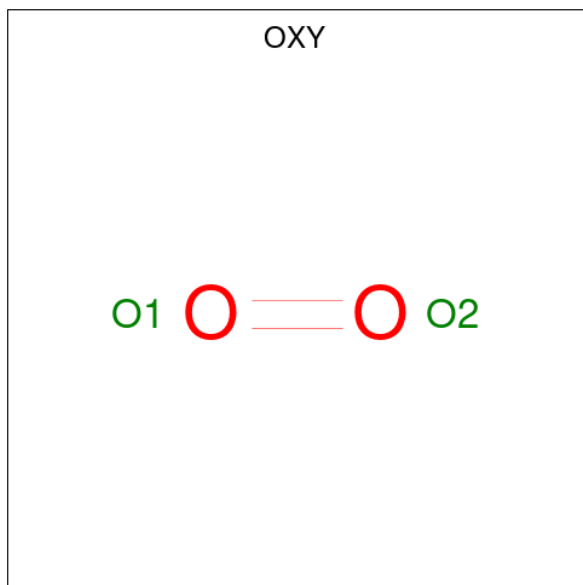


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

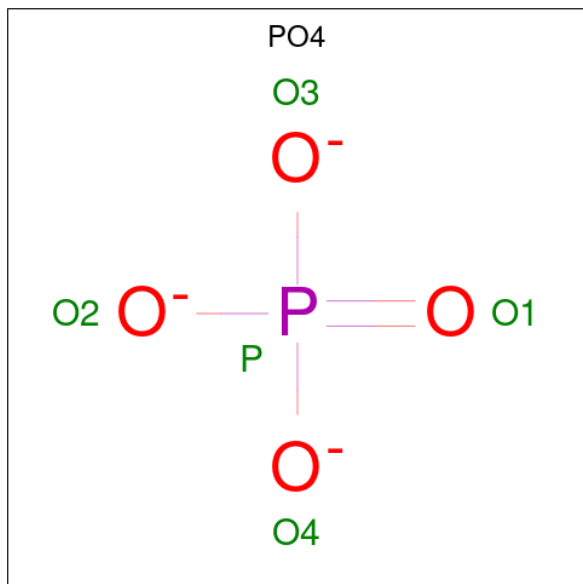
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

- Molecule 4 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



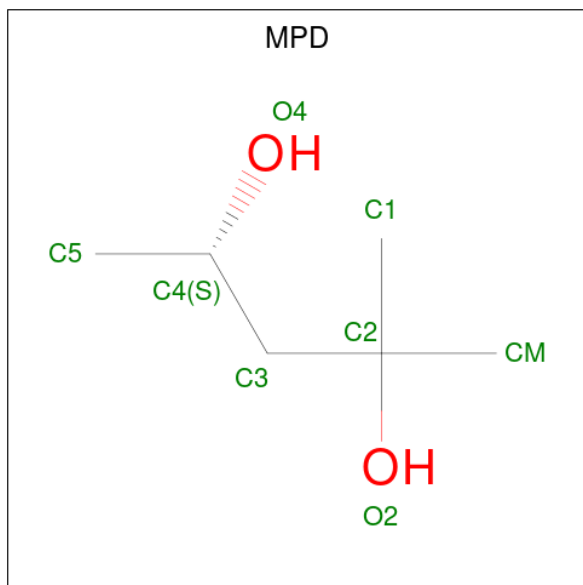
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			2	2		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



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

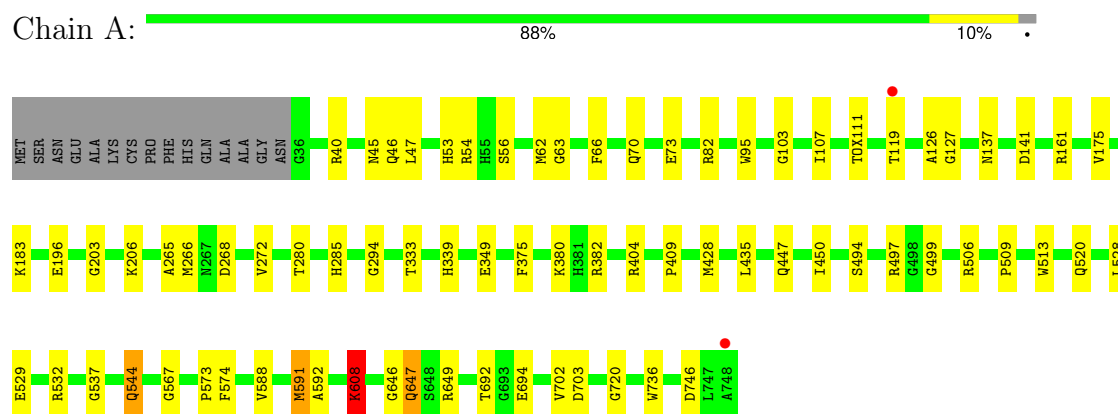
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	762	Total	O	0	0
			762	762		
8	B	791	Total	O	0	0
			791	791		

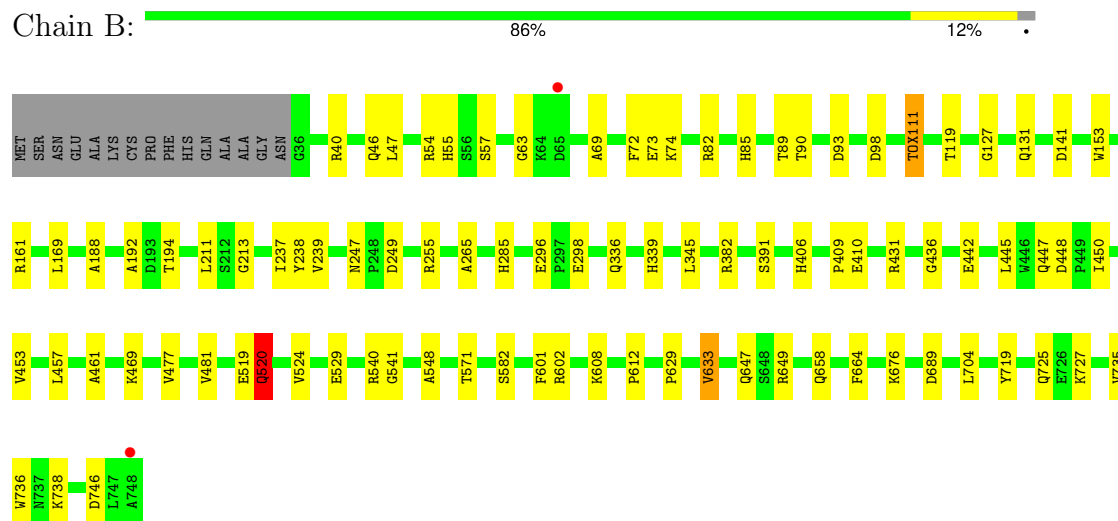
3 Residue-property plots

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	100.78Å 115.98Å 174.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.90 20.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (20.00-1.90) 99.8 (20.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.139 , 0.171 0.153 , 0.180	Depositor DCC
R_{free} test set	15966 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å ²)	20.1	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12811	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.99% 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: MPD, OXY, HEM, NA, PO4, TRS, TOX

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	1.76	57/5693 (1.0%)	1.28	13/7737 (0.2%)
1	B	1.76	59/5675 (1.0%)	1.30	18/7713 (0.2%)
All	All	1.76	116/11368 (1.0%)	1.29	31/15450 (0.2%)

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	ARG	CZ-NH1	9.37	1.45	1.32
1	B	436	GLY	C-O	-9.09	1.11	1.24
1	B	382	ARG	CZ-NH1	8.16	1.44	1.32
1	B	298	GLU	CA-C	8.13	1.64	1.52
1	A	107	ILE	N-CA	8.11	1.56	1.46
1	A	126	ALA	C-O	7.96	1.34	1.24
1	A	66	PHE	C-O	-7.93	1.14	1.23
1	A	544	GLN	CD-OE1	7.74	1.38	1.23
1	B	529	GLU	CA-C	7.70	1.63	1.52
1	B	63	GLY	N-CA	7.56	1.55	1.45
1	A	137	ASN	N-CA	-7.45	1.36	1.46
1	A	285	HIS	N-CA	7.41	1.55	1.46
1	B	746	ASP	C-O	-7.31	1.14	1.24
1	B	345	LEU	CA-C	7.19	1.62	1.52
1	B	285	HIS	C-O	7.19	1.32	1.24
1	A	63	GLY	N-CA	7.06	1.54	1.45
1	B	448	ASP	CA-CB	7.02	1.57	1.52
1	B	477	VAL	N-CA	7.01	1.54	1.46
1	A	703	ASP	CG-OD2	6.93	1.38	1.25
1	B	447	GLN	CA-C	6.76	1.62	1.52
1	B	194	THR	CA-C	6.68	1.61	1.52
1	A	529	GLU	CA-C	6.55	1.61	1.52
1	B	98	ASP	C-O	6.52	1.31	1.23
1	B	445	LEU	CA-C	-6.51	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	457	LEU	C-O	6.45	1.32	1.23
1	A	646	GLY	C-O	-6.40	1.15	1.24
1	A	266	MET	CA-C	6.37	1.60	1.52
1	A	285	HIS	C-O	6.37	1.31	1.23
1	A	746	ASP	C-O	-6.36	1.15	1.24
1	B	169	LEU	CA-C	6.30	1.60	1.52
1	A	499	GLY	C-O	6.29	1.30	1.23
1	A	447	GLN	CA-C	6.24	1.61	1.52
1	A	203	GLY	C-O	6.21	1.28	1.23
1	B	524	VAL	CA-CB	6.19	1.61	1.54
1	B	725	GLN	CD-NE2	6.18	1.46	1.33
1	A	47	LEU	CB-CG	-6.14	1.41	1.53
1	A	736	TRP	N-CA	6.09	1.53	1.46
1	B	582	SER	N-CA	6.06	1.53	1.45
1	B	442	GLU	CA-C	6.04	1.60	1.52
1	B	131	GLN	CA-C	6.01	1.61	1.52
1	A	375	PHE	C-O	-5.99	1.16	1.24
1	B	481	VAL	N-CA	5.98	1.53	1.46
1	A	532	ARG	CD-NE	-5.95	1.38	1.46
1	B	612	PRO	CA-C	5.95	1.59	1.52
1	A	494	SER	CA-C	5.94	1.60	1.52
1	B	736	TRP	N-CA	5.85	1.53	1.46
1	A	333	THR	N-CA	5.79	1.53	1.46
1	A	573	PRO	C-O	5.78	1.30	1.23
1	B	54	ARG	CA-C	-5.75	1.45	1.53
1	B	453	VAL	C-O	-5.75	1.17	1.24
1	A	70	GLN	N-CA	5.74	1.53	1.46
1	A	435	LEU	C-O	5.74	1.30	1.23
1	B	436	GLY	N-CA	5.72	1.52	1.44
1	B	285	HIS	N-CA	5.69	1.53	1.46
1	B	239	VAL	C-O	5.68	1.30	1.23
1	A	54	ARG	CA-C	-5.67	1.45	1.53
1	B	55	HIS	CA-CB	5.66	1.62	1.53
1	B	448	ASP	N-CA	5.63	1.50	1.46
1	B	89	THR	C-O	-5.62	1.16	1.24
1	A	692	THR	C-O	-5.58	1.17	1.24
1	B	85	HIS	CA-C	5.57	1.60	1.52
1	B	192	ALA	N-CA	5.56	1.52	1.46
1	A	694	GLU	CA-C	5.56	1.60	1.52
1	A	45	ASN	C-O	-5.51	1.16	1.24
1	B	247	ASN	C-O	5.50	1.31	1.24
1	A	537	GLY	C-O	-5.47	1.16	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	428	MET	CG-SD	-5.47	1.67	1.80
1	A	82	ARG	CA-C	5.46	1.59	1.52
1	B	548	ALA	N-CA	5.46	1.52	1.46
1	B	47	LEU	CB-CG	-5.42	1.42	1.53
1	A	588	VAL	CA-CB	5.41	1.61	1.54
1	A	574	PHE	N-CA	5.41	1.52	1.46
1	A	95	TRP	N-CA	5.40	1.53	1.46
1	A	175	VAL	N-CA	-5.40	1.39	1.46
1	B	735	VAL	CA-C	5.38	1.59	1.52
1	A	53	HIS	N-CA	5.37	1.52	1.46
1	B	461	ALA	CA-C	5.37	1.59	1.52
1	B	72	PHE	C-O	5.37	1.30	1.24
1	B	153	TRP	CA-C	5.34	1.59	1.52
1	B	602	ARG	CZ-NH2	-5.33	1.26	1.33
1	A	56	SER	N-CA	5.32	1.53	1.45
1	A	567	GLY	C-O	-5.29	1.16	1.24
1	B	704	LEU	CA-C	-5.28	1.45	1.52
1	B	676	LYS	CA-C	-5.28	1.46	1.52
1	B	90	THR	C-O	5.27	1.30	1.23
1	A	702	VAL	C-O	5.26	1.30	1.24
1	A	647	GLN	CA-C	5.26	1.60	1.53
1	B	249	ASP	C-O	5.26	1.30	1.24
1	A	720	GLY	N-CA	5.25	1.51	1.45
1	B	391	SER	CA-CB	5.25	1.62	1.53
1	A	268	ASP	CA-C	5.24	1.59	1.52
1	A	349	GLU	CD-OE2	-5.23	1.15	1.25
1	B	188	ALA	C-O	5.23	1.30	1.24
1	A	528	LEU	CA-CB	5.23	1.61	1.53
1	A	497	ARG	CA-CB	5.22	1.61	1.53
1	A	294	GLY	C-O	5.21	1.28	1.23
1	A	206	LYS	N-CA	5.20	1.52	1.46
1	B	519	GLU	CA-CB	5.19	1.61	1.53
1	B	213	GLY	CA-C	5.18	1.58	1.51
1	B	336	GLN	CD-NE2	5.16	1.44	1.33
1	B	237	ILE	CA-C	5.13	1.58	1.52
1	A	520	GLN	CA-C	5.13	1.59	1.52
1	B	658	GLN	CD-NE2	-5.11	1.22	1.33
1	A	513	TRP	CA-C	-5.10	1.46	1.52
1	A	506	ARG	CA-C	5.09	1.59	1.52
1	B	541	GLY	C-N	-5.09	1.26	1.33
1	B	689	ASP	CG-OD2	-5.09	1.15	1.25
1	A	272	VAL	CA-CB	-5.09	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	103	GLY	N-CA	5.08	1.52	1.45
1	A	404	ARG	CA-C	5.08	1.59	1.52
1	B	410	GLU	CG-CD	5.07	1.64	1.52
1	B	727	LYS	C-O	5.06	1.30	1.24
1	B	601	PHE	CD2-CE2	5.06	1.53	1.38
1	B	296	GLU	N-CA	5.05	1.53	1.45
1	A	196	GLU	CB-CG	-5.04	1.37	1.52
1	A	280	THR	CA-C	5.03	1.59	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	591	MET	CG-SD-CE	7.61	117.63	100.90
1	B	519	GLU	CB-CG-CD	-6.95	100.78	112.60
1	A	608	LYS	CB-CG-CD	6.56	126.38	111.30
1	B	520	GLN	CB-CG-CD	6.41	123.49	112.60
1	B	541	GLY	N-CA-C	-6.38	98.38	112.17
1	A	54	ARG	CG-CD-NE	-6.24	98.27	112.00
1	B	127	GLY	N-CA-C	6.15	121.86	113.99
1	A	70	GLN	CA-CB-CG	6.12	126.34	114.10
1	B	450	ILE	CA-CB-CG1	-6.12	100.00	110.40
1	A	47	LEU	N-CA-CB	-6.09	101.02	109.97
1	B	436	GLY	CA-C-N	6.07	128.23	120.89
1	B	436	GLY	C-N-CA	6.07	128.23	120.89
1	B	704	LEU	CB-CG-CD2	5.73	127.89	110.70
1	B	633[A]	VAL	CB-CA-C	-5.70	104.35	112.22
1	B	633[B]	VAL	CB-CA-C	-5.70	104.35	112.22
1	A	46	GLN	N-CA-C	-5.57	102.65	110.50
1	B	445	LEU	N-CA-C	5.52	117.29	111.28
1	A	520	GLN	CB-CG-CD	5.50	121.95	112.60
1	A	127	GLY	N-CA-C	5.47	120.78	114.16
1	A	73	GLU	CB-CG-CD	5.39	121.77	112.60
1	B	704	LEU	N-CA-C	5.33	119.05	112.54
1	B	93	ASP	N-CA-C	5.29	117.80	111.71
1	B	46	GLN	N-CA-C	-5.27	103.07	110.50
1	A	380	LYS	CA-C-O	-5.16	115.56	121.40
1	A	62	MET	CA-C-N	-5.15	114.83	120.44
1	A	62	MET	C-N-CA	-5.15	114.83	120.44
1	B	82	ARG	NE-CZ-NH2	-5.14	114.58	119.20
1	B	161	ARG	CG-CD-NE	-5.12	100.73	112.00
1	A	592	ALA	N-CA-C	5.12	117.52	111.33
1	B	57	SER	N-CA-C	-5.07	106.92	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	664	PHE	N-CA-C	-5.01	105.82	111.28

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	5570	0	5356	10	0
1	B	5548	0	5354	23	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	2	0	0	1	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	16	0	28	5	0
6	B	8	0	14	2	0
7	A	8	0	12	0	0
7	B	8	0	11	0	0
8	A	762	0	0	7	0
8	B	791	0	0	11	0
All	All	12811	0	10835	41	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (41) 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:B:339[B]:HIS:HE1	1:B:406:HIS:HA	1.38	0.89
1:B:520:GLN:HG3	8:B:1383:HOH:O	1.73	0.87
1:B:647:GLN:HG2	8:B:1050:HOH:O	1.75	0.86
1:B:571:THR:HG23	8:B:1239:HOH:O	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339[B]:HIS:CE1	8:A:925:HOH:O	2.33	0.80
1:B:431:ARG:CD	8:B:1510:HOH:O	2.33	0.76
1:B:69:ALA:O	1:B:73:GLU:HG2	1.86	0.74
1:B:339[B]:HIS:CE1	1:B:406:HIS:HA	2.23	0.72
1:A:339[B]:HIS:CD2	1:A:409:PRO:HB3	2.26	0.71
1:B:431:ARG:HD2	8:B:1510:HOH:O	1.90	0.71
1:B:255[A]:ARG:HD3	8:B:1370:HOH:O	1.91	0.70
6:A:805:MPD:H51	8:A:1524:HOH:O	1.98	0.64
1:B:255[B]:ARG:HG2	8:B:1633:HOH:O	1.99	0.62
6:A:805:MPD:CM	6:A:805:MPD:O4	2.47	0.62
1:B:540:ARG:NE	1:B:540:ARG:HA	2.17	0.59
6:B:804:MPD:O4	6:B:804:MPD:H12	2.03	0.59
1:B:119[A]:THR:CG2	1:B:265:ALA:HB2	2.32	0.59
1:B:119[A]:THR:HG22	1:B:265:ALA:HB2	1.86	0.57
1:A:119[A]:THR:CG2	1:A:265:ALA:HB2	2.35	0.56
1:A:119[A]:THR:HG22	1:A:265:ALA:HB2	1.90	0.54
1:B:633[B]:VAL:CG1	1:B:719:TYR:CZ	2.91	0.54
1:B:339[A]:HIS:CD2	1:B:409:PRO:HB3	2.47	0.50
6:A:805:MPD:O4	6:A:805:MPD:HM1	2.12	0.50
1:A:339[B]:HIS:HE1	8:A:925:HOH:O	1.82	0.49
1:B:111:TOX:H9	1:B:238:TYR:OH	2.13	0.49
4:A:803:OXY:O2	8:A:901:HOH:O	2.20	0.47
1:B:629:PRO:O	1:B:633[A]:VAL:HG23	2.14	0.47
1:A:647:GLN:CD	1:A:647:GLN:N	2.74	0.45
6:A:806:MPD:HM2	8:A:1476:HOH:O	2.16	0.45
1:A:608:LYS:HA	1:A:608:LYS:HE2	1.98	0.45
6:B:804:MPD:O4	6:B:804:MPD:C1	2.60	0.44
1:B:255[B]:ARG:CG	8:B:1633:HOH:O	2.64	0.43
1:A:509:PRO:HD2	1:A:591:MET:HG2	2.00	0.43
6:A:806:MPD:CM	8:A:1476:HOH:O	2.67	0.43
1:B:211:LEU:HB2	8:B:1469:HOH:O	2.18	0.43
1:B:469:LYS:HD3	8:B:1385:HOH:O	2.19	0.41
1:A:339[A]:HIS:HB2	8:A:1442:HOH:O	2.20	0.41
1:A:339[B]:HIS:CG	1:A:409:PRO:HB3	2.54	0.41
1:B:339[B]:HIS:HE1	1:B:406:HIS:CA	2.21	0.41
1:B:738:LYS:NZ	8:B:914:HOH:O	2.47	0.41
1:B:633[A]:VAL:HG22	1:B:719:TYR:CZ	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	717/728 (98%)	709 (99%)	8 (1%)	0	100	100
1	B	715/728 (98%)	704 (98%)	11 (2%)	0	100	100
All	All	1432/1456 (98%)	1413 (99%)	19 (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	556/560 (99%)	548 (99%)	8 (1%)	59	59
1	B	554/560 (99%)	548 (99%)	6 (1%)	65	67
All	All	1110/1120 (99%)	1096 (99%)	14 (1%)	61	61

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	141	ASP
1	A	161	ARG
1	A	183	LYS
1	A	450	ILE
1	A	544	GLN
1	A	608	LYS
1	A	649	ARG

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Mol	Chain	Res	Type
1	B	40	ARG
1	B	74	LYS
1	B	141	ASP
1	B	520	GLN
1	B	608	LYS
1	B	649	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	737	ASN
1	B	737	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues 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
1	TOX	A	111[A]	2	14,17,18	1.81	6 (42%)	12,23,25	2.36	4 (33%)
1	TOX	B	111	1,2	14,17,18	2.49	6 (42%)	12,23,25	2.29	5 (41%)
1	TOX	A	111[B]	-	14,17,18	1.81	6 (42%)	12,23,25	2.36	4 (33%)

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	TOX	A	111[A]	2	-	2/5/8/10	0/2/2/2
1	TOX	B	111	1,2	-	2/5/8/10	0/2/2/2
1	TOX	A	111[B]	-	-	2/5/8/10	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	TOX	O-C	4.30	1.36	1.20
1	B	111	TOX	CZ2-CE2	-4.25	1.33	1.39
1	B	111	TOX	CD2-CE2	4.15	1.46	1.41
1	B	111	TOX	CD1-CG	3.14	1.43	1.36
1	A	111[A]	TOX	O-C	3.05	1.31	1.20
1	A	111[B]	TOX	O-C	3.05	1.31	1.20
1	A	111[A]	TOX	CD2-CG	2.98	1.48	1.44
1	A	111[B]	TOX	CD2-CG	2.98	1.48	1.44
1	A	111[A]	TOX	CD2-CE2	2.62	1.44	1.41
1	A	111[B]	TOX	CD2-CE2	2.62	1.44	1.41
1	B	111	TOX	O1-NE1	2.44	1.42	1.39
1	B	111	TOX	CD2-CG	2.31	1.47	1.44
1	A	111[A]	TOX	CE2-NE1	-2.30	1.35	1.39
1	A	111[B]	TOX	CE2-NE1	-2.30	1.35	1.39
1	A	111[A]	TOX	CZ3-CE3	2.26	1.42	1.38
1	A	111[B]	TOX	CZ3-CE3	2.26	1.42	1.38
1	A	111[A]	TOX	CH2-CZ3	2.04	1.42	1.38
1	A	111[B]	TOX	CH2-CZ3	2.04	1.42	1.38

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111[A]	TOX	CZ2-CE2-NE1	4.77	136.97	129.37
1	A	111[B]	TOX	CZ2-CE2-NE1	4.77	136.97	129.37
1	B	111	TOX	CZ2-CE2-NE1	4.49	136.52	129.37
1	A	111[A]	TOX	CZ2-CE2-CD2	-3.94	117.55	121.95
1	A	111[B]	TOX	CZ2-CE2-CD2	-3.94	117.55	121.95
1	B	111	TOX	CZ2-CE2-CD2	-3.87	117.63	121.95
1	A	111[A]	TOX	CE2-CD2-CG	-3.79	103.91	107.39
1	A	111[B]	TOX	CE2-CD2-CG	-3.79	103.91	107.39
1	B	111	TOX	CB-CG-CD1	-3.56	121.72	126.67
1	A	111[A]	TOX	CE3-CD2-CE2	2.65	122.30	119.24
1	A	111[B]	TOX	CE3-CD2-CE2	2.65	122.30	119.24
1	B	111	TOX	CB-CG-CD2	2.49	131.48	126.70
1	B	111	TOX	CH2-CZ2-CE2	2.37	123.07	118.28

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	111[A]	TOX	N-CA-CB-CG
1	A	111[A]	TOX	C-CA-CB-CG
1	A	111[B]	TOX	N-CA-CB-CG
1	A	111[B]	TOX	C-CA-CB-CG
1	B	111	TOX	N-CA-CB-CG
1	B	111	TOX	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	111	TOX	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 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	$\# Z > 2$
6	MPD	A	805	-	7,7,7	0.98	1 (14%)	9,10,10	1.94	3 (33%)
7	TRS	A	807	-	7,7,7	1.42	2 (28%)	9,9,9	2.80	4 (44%)
7	TRS	B	805	-	7,7,7	1.33	1 (14%)	9,9,9	1.64	1 (11%)
4	OXY	A	803	-	1,1,1	0.02	0	-		
6	MPD	B	804	-	7,7,7	0.81	0	9,10,10	1.55	3 (33%)
6	MPD	A	806	-	7,7,7	0.86	0	9,10,10	1.73	3 (33%)
2	HEM	A	801	1	50,50,50	1.77	10 (20%)	67,82,82	1.36	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	PO4	A	804	-	4,4,4	2.33	1 (25%)	6,6,6	2.05	2 (33%)
5	PO4	B	803	-	4,4,4	1.42	1 (25%)	6,6,6	2.12	2 (33%)
2	HEM	B	801	1	50,50,50	1.63	13 (26%)	67,82,82	1.72	15 (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
6	MPD	A	805	-	-	0/5/5/5	-
7	TRS	A	807	-	-	5/9/9/9	-
7	TRS	B	805	-	-	3/9/9/9	-
6	MPD	B	804	-	-	3/5/5/5	-
6	MPD	A	806	-	-	5/5/5/5	-
2	HEM	A	801	1	-	3/14/54/54	-
2	HEM	B	801	1	-	2/14/54/54	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	FE-NB	5.00	2.10	1.94
5	A	804	PO4	P-O1	4.64	1.61	1.50
2	A	801	HEM	C4D-C3D	4.39	1.52	1.45
2	A	801	HEM	C1B-NB	-4.31	1.32	1.40
2	A	801	HEM	C4D-ND	-4.03	1.33	1.40
2	B	801	HEM	FE-NB	3.61	2.06	1.94
2	B	801	HEM	C4B-NB	-3.55	1.31	1.38
2	B	801	HEM	C1B-NB	-3.11	1.34	1.40
2	B	801	HEM	FE-NA	2.96	2.04	1.95
2	B	801	HEM	CMA-C3A	2.76	1.56	1.50
2	B	801	HEM	C2A-C3A	-2.59	1.32	1.38
2	B	801	HEM	C4A-NA	-2.58	1.34	1.39
2	B	801	HEM	CHB-C1B	2.55	1.43	1.38
2	B	801	HEM	O1A-CGA	2.54	1.30	1.22
2	B	801	HEM	O1D-CGD	2.51	1.30	1.22
2	B	801	HEM	FE-NC	2.49	2.03	1.95
2	A	801	HEM	CBA-CGA	2.48	1.56	1.50
2	A	801	HEM	CHB-C1B	2.47	1.43	1.38
2	A	801	HEM	FE-NC	2.45	2.03	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	CBA-CGA	2.44	1.56	1.50
7	B	805	TRS	O3-C3	-2.31	1.34	1.42
7	A	807	TRS	C1-C	2.30	1.59	1.53
2	A	801	HEM	FE-NA	2.29	2.02	1.95
2	B	801	HEM	CBD-CAD	-2.26	1.44	1.51
6	A	805	MPD	C5-C4	2.16	1.60	1.51
2	A	801	HEM	FE-ND	2.14	2.01	1.94
7	A	807	TRS	O1-C1	2.14	1.49	1.42
5	B	803	PO4	P-O1	2.07	1.55	1.50
2	A	801	HEM	C1C-NC	-2.04	1.35	1.39

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	807	TRS	O1-C1-C	6.27	128.34	110.88
2	B	801	HEM	CHC-C1C-NC	-4.74	119.29	124.45
7	B	805	TRS	O1-C1-C	4.47	123.32	110.88
2	B	801	HEM	CHC-C4B-NB	4.41	129.17	124.42
5	A	804	PO4	O4-P-O2	-4.37	94.33	107.91
2	B	801	HEM	C1B-NB-C4B	3.81	109.71	105.21
2	A	801	HEM	CAA-CBA-CGA	-3.75	103.73	113.67
6	A	806	MPD	C5-C4-C3	3.47	127.78	111.67
2	B	801	HEM	CAA-CBA-CGA	-3.38	104.70	113.67
5	B	803	PO4	O3-P-O1	-3.29	99.32	110.95
2	A	801	HEM	C1B-NB-C4B	3.29	109.10	105.21
2	A	801	HEM	C4B-C3B-C2B	-3.26	104.28	107.28
6	A	805	MPD	O4-C4-C3	-3.21	98.60	111.35
2	B	801	HEM	C2D-C1D-ND	3.19	113.59	109.90
7	A	807	TRS	C3-C-C2	-3.18	102.20	110.66
7	A	807	TRS	C3-C-C1	3.13	119.00	110.66
5	B	803	PO4	O4-P-O3	3.11	117.58	107.91
2	B	801	HEM	C3C-C2C-C1C	-3.05	104.16	107.05
2	A	801	HEM	C1D-C2D-C3D	-3.03	103.79	106.98
2	B	801	HEM	CMA-C3A-C2A	2.98	131.94	125.62
2	B	801	HEM	C3B-C4B-NB	-2.88	107.40	109.47
2	B	801	HEM	C1D-C2D-C3D	-2.88	103.95	106.98
6	A	806	MPD	CM-C2-C1	-2.81	104.33	110.63
2	A	801	HEM	C3B-C2B-C1B	2.80	108.52	106.41
6	A	805	MPD	O4-C4-C5	2.77	121.38	109.45
2	B	801	HEM	CAD-CBD-CGD	2.71	120.86	113.67
6	B	804	MPD	C1-C2-C3	2.54	121.16	110.20
2	A	801	HEM	C2D-C1D-ND	2.49	112.79	109.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	805	MPD	C1-C2-C3	-2.48	99.52	110.20
6	B	804	MPD	CM-C2-C3	-2.40	99.84	110.20
2	B	801	HEM	CBB-CAB-C3B	-2.35	115.81	127.53
2	B	801	HEM	O2A-CGA-CBA	2.31	121.31	114.00
2	B	801	HEM	CAA-C2A-C1A	2.30	129.43	124.94
6	B	804	MPD	O4-C4-C5	2.26	119.20	109.45
7	A	807	TRS	O3-C3-C	2.26	117.18	110.88
2	A	801	HEM	CMD-C2D-C1D	2.20	128.47	125.03
2	A	801	HEM	O1D-CGD-CBD	-2.13	116.35	123.09
2	B	801	HEM	CBD-CAD-C3D	2.12	118.39	112.53
5	A	804	PO4	O2-P-O1	2.06	118.23	110.95
6	A	806	MPD	O4-C4-C3	-2.04	103.23	111.35
2	B	801	HEM	CHD-C1D-C2D	-2.02	121.83	125.03

There are no chirality outliers.

All (21) torsion outliers are listed below:

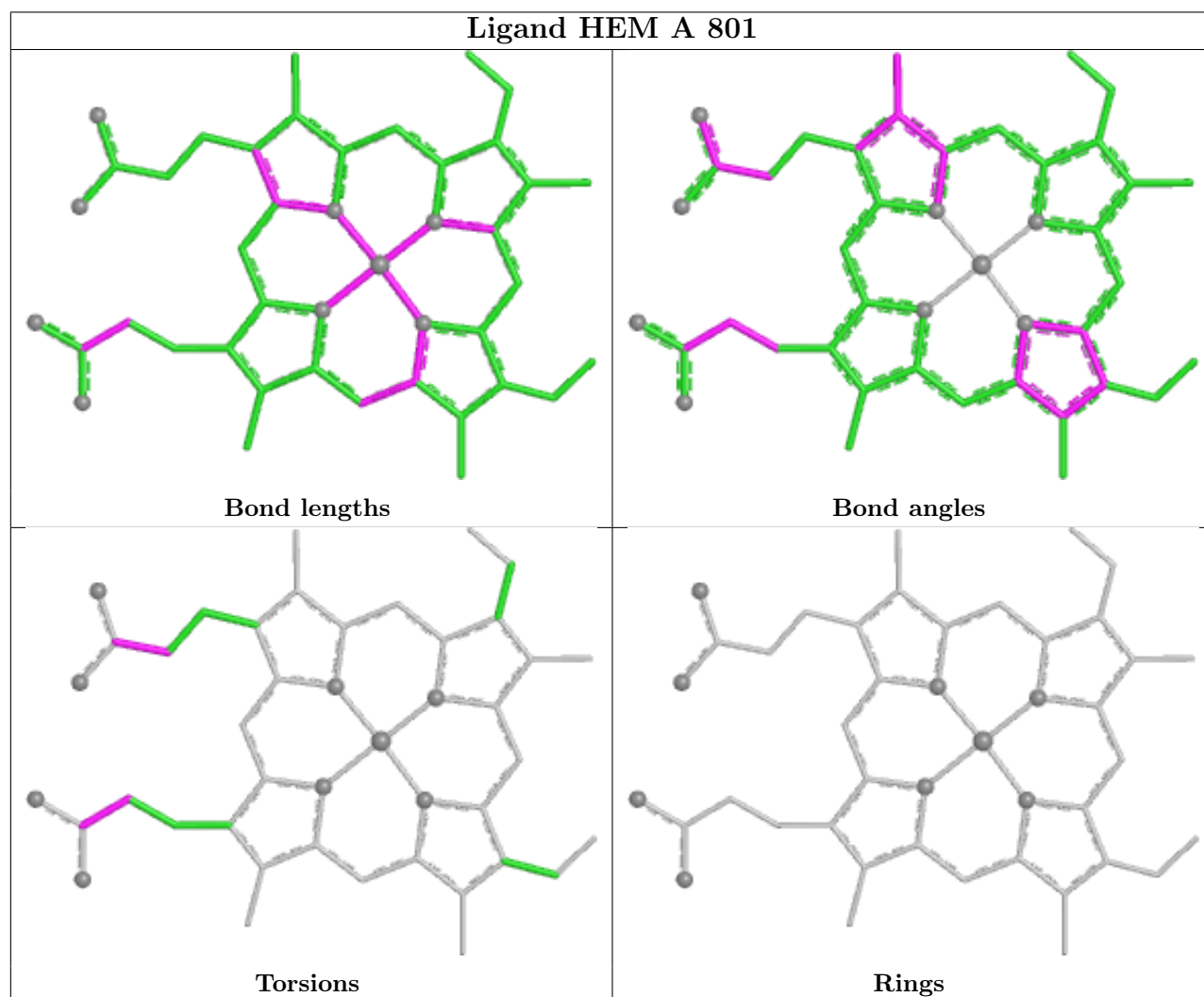
Mol	Chain	Res	Type	Atoms
6	A	806	MPD	C1-C2-C3-C4
6	A	806	MPD	C2-C3-C4-C5
6	B	804	MPD	C1-C2-C3-C4
6	B	804	MPD	O2-C2-C3-C4
7	A	807	TRS	C2-C-C1-O1
7	A	807	TRS	N-C-C1-O1
7	B	805	TRS	C2-C-C3-O3
7	B	805	TRS	N-C-C3-O3
6	A	806	MPD	O2-C2-C3-C4
6	A	806	MPD	CM-C2-C3-C4
7	A	807	TRS	C3-C-C1-O1
7	B	805	TRS	C1-C-C3-O3
2	A	801	HEM	CAA-CBA-CGA-O2A
7	A	807	TRS	C1-C-C3-O3
2	B	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	CAA-CBA-CGA-O1A
6	A	806	MPD	C2-C3-C4-O4
6	B	804	MPD	CM-C2-C3-C4
7	A	807	TRS	N-C-C3-O3
2	A	801	HEM	CAD-CBD-CGD-O2D

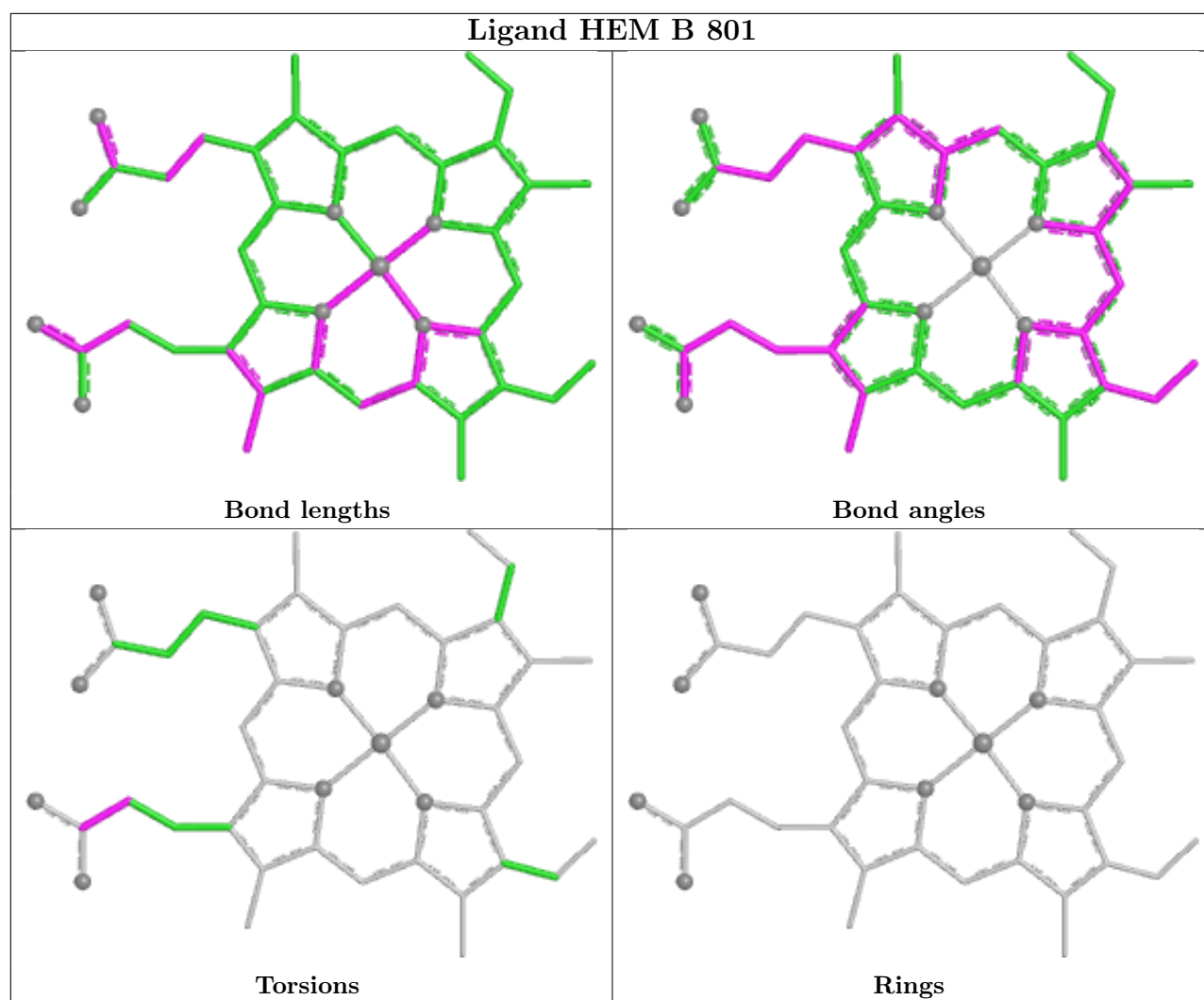
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	805	MPD	3	0
4	A	803	OXY	1	0
6	B	804	MPD	2	0
6	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%)	-0.54	2 (0%) 90 91	8, 21, 37, 74	7 (0%)
1	B	712/728 (97%)	-0.64	2 (0%) 90 91	8, 19, 34, 68	5 (0%)
All	All	1424/1456 (97%)	-0.59	4 (0%) 90 91	8, 20, 36, 74	12 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	3.4
1	B	748	ALA	2.8
1	A	119[A]	THR	2.4
1	B	65	ASP	2.2

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	TOX	A	111[A]	16/17	0.96	0.06	13,17,31,32	0
1	TOX	A	111[B]	16/17	0.96	0.06	13,17,24,32	1
1	TOX	B	111	16/17	0.97	0.05	13,16,26,28	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

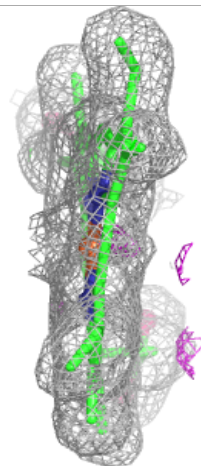
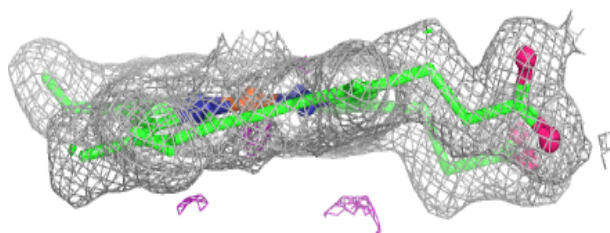
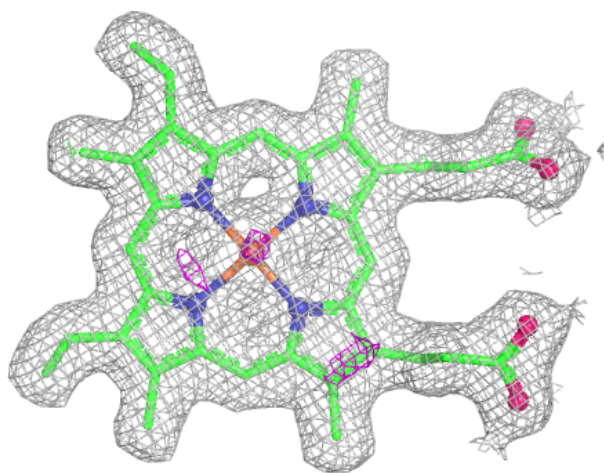
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

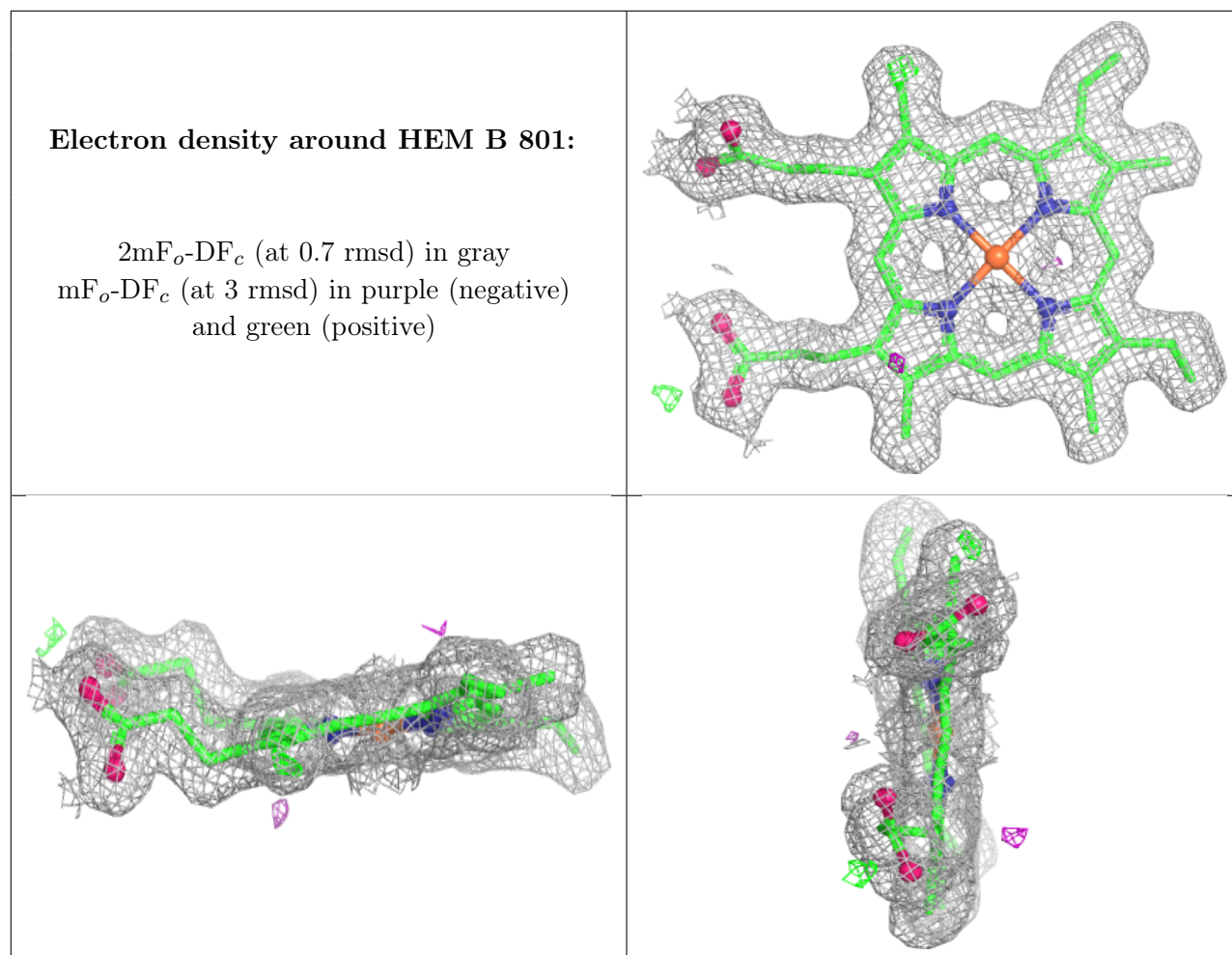
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MPD	A	805	8/8	0.74	0.22	48,55,70,71	0
5	PO4	A	804	5/5	0.80	0.11	59,67,76,89	0
5	PO4	B	803	5/5	0.82	0.11	56,63,68,78	0
6	MPD	A	806	8/8	0.86	0.13	43,45,56,60	0
6	MPD	B	804	8/8	0.90	0.13	46,53,60,61	0
7	TRS	A	807	8/8	0.92	0.11	30,37,43,52	0
4	OXY	A	803	2/2	0.95	0.22	31,31,31,37	0
7	TRS	B	805	8/8	0.95	0.09	24,31,33,34	0
2	HEM	A	801	43/43	0.99	0.04	14,16,18,19	0
2	HEM	B	801	43/43	0.99	0.04	13,15,16,18	0
3	NA	A	802	1/1	0.99	0.06	17,17,17,17	0
3	NA	B	802	1/1	0.99	0.05	16,16,16,16	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.