



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 2, 2026 – 10:13 PM EDT

PDB ID : 5KQK / pdb_00005kqk
Title : Crystal structure of the Q233E/N240D variant of the catalase-peroxidase from *B. pseudomallei*
Authors : Loewen, P.C.
Deposited on : 2016-07-06
Resolution : 1.75 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

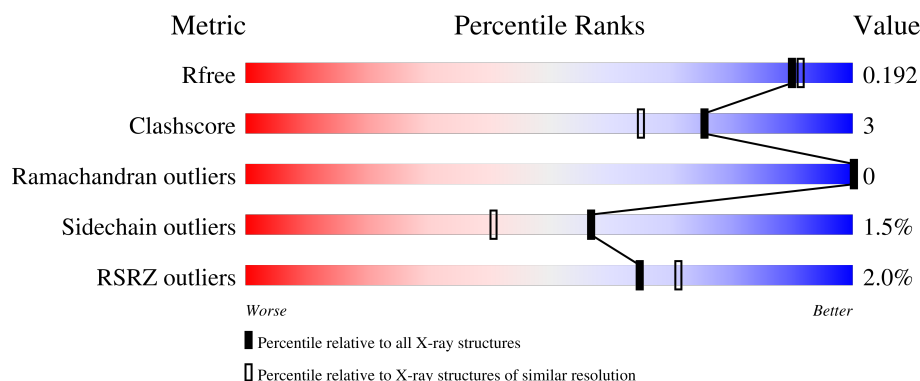
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	2% 87% 10% ..
1	B	728	2% 85% 12% ..

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
6	MPD	B	805	-	-	X	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12860 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.

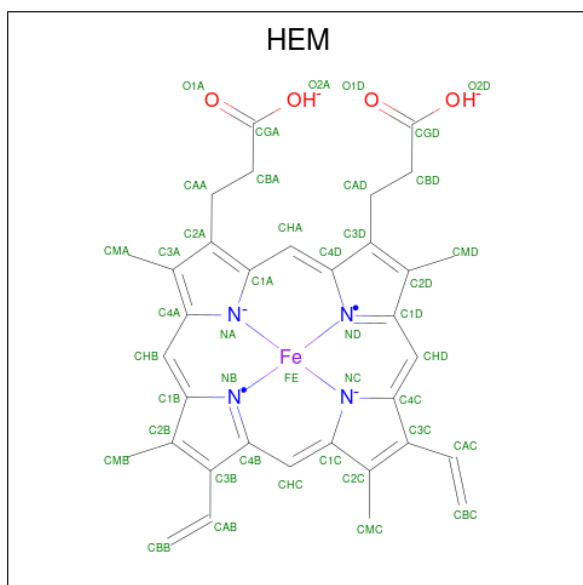
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	7	0
			5548	3506	985	1043	14			
1	B	713	Total	C	N	O	S	0	10	0
			5557	3514	986	1043	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	233	GLU	GLN	conflict	UNP Q3JNW6
A	240	ASP	ASN	conflict	UNP Q3JNW6
B	233	GLU	GLN	conflict	UNP Q3JNW6
B	240	ASP	ASN	conflict	UNP Q3JNW6

- 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		

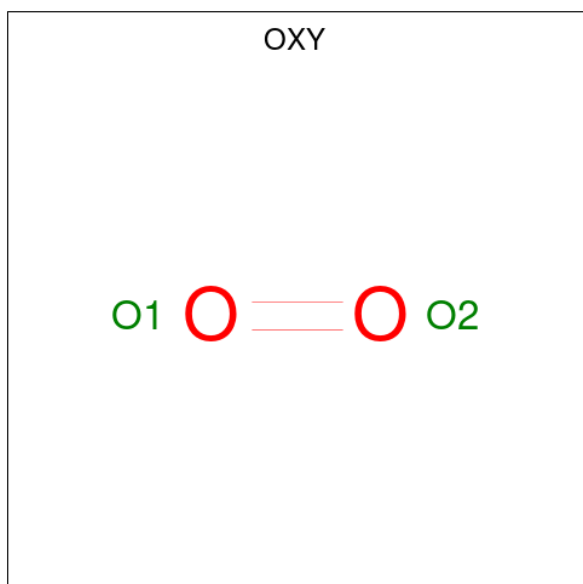
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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 CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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



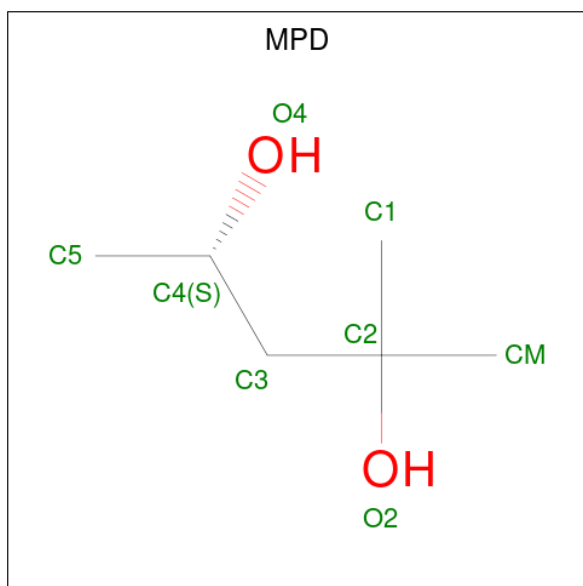
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			2	2		

Continued on next page...

Continued from previous page...

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

- 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 8 6 2	0	0
6	A	1	Total C O 8 6 2	0	0
6	B	1	Total C O 8 6 2	0	0
6	B	1	Total C O 8 6 2	0	0

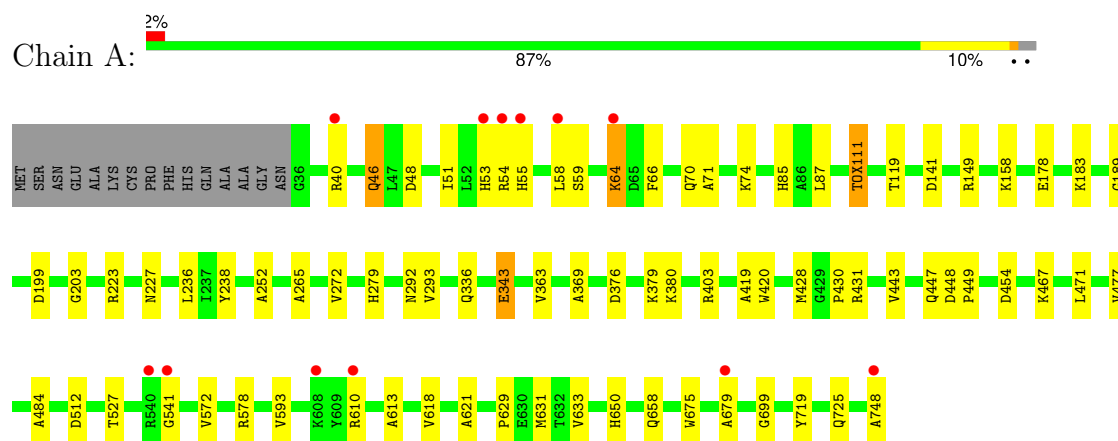
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	817	Total O 817 817	0	0
7	B	812	Total O 812 812	0	0

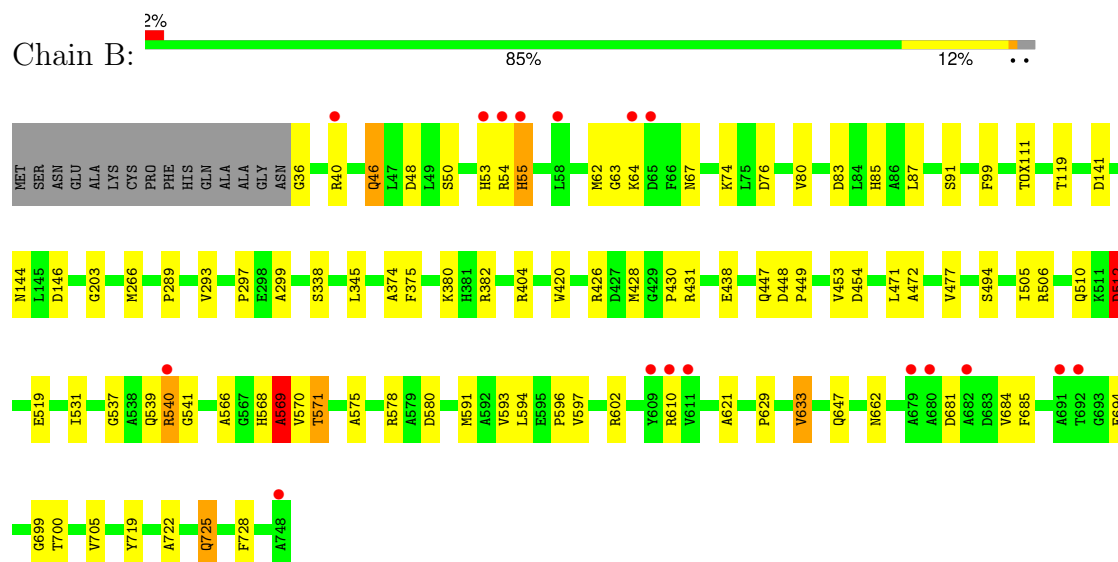
3 Residue-property plots [i](#)

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	100.72Å 115.05Å 174.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.06 – 1.75 96.06 – 1.75	Depositor EDS
% Data completeness (in resolution range)	98.0 (96.06-1.75) 98.0 (96.06-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 1.75Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.152 , 0.182 0.165 , 0.192	Depositor DCC
R_{free} test set	10034 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	16.2	Xtriage
Anisotropy	0.643	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.7	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	12860	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MPD, OXY, CL, HEM, NA, 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	1.71	45/5692 (0.8%)	1.27	11/7736 (0.1%)
1	B	1.69	54/5710 (0.9%)	1.30	15/7764 (0.2%)
All	All	1.70	99/11402 (0.9%)	1.28	26/15500 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	512	ASP	CG-OD2	10.07	1.44	1.25
1	A	363	VAL	C-O	9.42	1.33	1.24
1	A	471	LEU	CA-C	8.81	1.64	1.52
1	B	448	ASP	N-CA	8.77	1.52	1.46
1	A	420	TRP	N-CA	8.51	1.56	1.46
1	B	725	GLN	CD-OE1	8.33	1.39	1.23
1	B	426	ARG	CZ-NH2	7.65	1.43	1.33
1	A	477	VAL	N-CA	7.25	1.54	1.46
1	A	203	GLY	N-CA	7.18	1.52	1.45
1	A	236	LEU	CA-C	7.03	1.61	1.52
1	B	375	PHE	CA-CB	-6.94	1.41	1.53
1	A	527	THR	N-CA	-6.75	1.38	1.46
1	B	728	PHE	CA-C	6.71	1.61	1.52
1	B	63	GLY	N-CA	6.69	1.53	1.45
1	B	722	ALA	C-O	-6.61	1.15	1.24
1	A	572	VAL	N-CA	-6.59	1.40	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	602	ARG	N-CA	-6.53	1.38	1.46
1	B	430	PRO	C-O	6.50	1.31	1.23
1	A	430	PRO	C-O	6.37	1.31	1.23
1	B	621	ALA	N-CA	-6.36	1.38	1.46
1	A	621	ALA	CA-C	6.30	1.60	1.52
1	B	203	GLY	C-O	6.29	1.28	1.23
1	A	149	ARG	CA-CB	6.23	1.63	1.53
1	B	297	PRO	CA-CB	6.22	1.63	1.53
1	B	293	VAL	C-O	-6.19	1.17	1.24
1	B	684	VAL	N-CA	-6.17	1.39	1.46
1	A	292	ASN	N-CA	-6.17	1.38	1.46
1	B	420	TRP	N-CA	6.16	1.53	1.46
1	B	699	GLY	CA-C	-6.13	1.45	1.51
1	A	87	LEU	N-CA	-6.12	1.38	1.46
1	B	91	SER	C-O	-6.12	1.16	1.23
1	A	448	ASP	N-CA	6.09	1.51	1.46
1	B	67	ASN	CA-C	6.09	1.59	1.52
1	A	59	SER	C-O	-6.08	1.16	1.24
1	B	540	ARG	C-O	5.98	1.32	1.23
1	B	694	GLU	CA-C	5.97	1.60	1.52
1	A	158	LYS	CA-C	5.92	1.60	1.52
1	A	71	ALA	C-O	5.89	1.30	1.24
1	A	448	ASP	CA-CB	5.87	1.57	1.52
1	A	443	VAL	C-O	-5.84	1.17	1.24
1	B	404	ARG	CA-C	5.79	1.60	1.52
1	A	484	ALA	CA-C	5.75	1.60	1.52
1	B	531	ILE	N-CA	5.69	1.53	1.46
1	A	272	VAL	CA-CB	5.67	1.61	1.54
1	A	578	ARG	CZ-NH1	5.66	1.40	1.32
1	A	675	TRP	N-CA	-5.66	1.39	1.46
1	B	471	LEU	CA-C	5.65	1.60	1.52
1	A	178	GLU	C-O	5.63	1.30	1.24
1	B	477	VAL	N-CA	5.61	1.53	1.46
1	B	338	SER	C-O	5.61	1.30	1.23
1	A	679	ALA	N-CA	5.60	1.53	1.46
1	A	227	ASN	CA-C	-5.58	1.47	1.53
1	A	279	HIS	CE1-NE2	5.58	1.38	1.32
1	A	512	ASP	N-CA	5.58	1.52	1.46
1	B	299	ALA	CA-C	-5.58	1.45	1.52
1	B	700	THR	N-CA	-5.55	1.39	1.45
1	A	70	GLN	CG-CD	5.53	1.65	1.52
1	B	602	ARG	CZ-NH2	-5.52	1.26	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	647	GLN	CA-C	5.51	1.61	1.52
1	B	578	ARG	CA-C	-5.48	1.45	1.52
1	A	725	GLN	CG-CD	5.47	1.65	1.52
1	B	87	LEU	N-CA	-5.45	1.39	1.46
1	A	428	MET	CG-SD	-5.44	1.67	1.80
1	B	80	VAL	N-CA	-5.39	1.40	1.46
1	B	449	PRO	CA-C	5.39	1.59	1.52
1	A	419	ALA	C-N	-5.38	1.26	1.33
1	A	236	LEU	C-O	-5.37	1.17	1.23
1	A	223	ARG	CZ-NH2	5.36	1.40	1.33
1	B	597	VAL	C-O	-5.36	1.18	1.24
1	A	46	GLN	CG-CD	5.35	1.65	1.52
1	B	694	GLU	N-CA	-5.32	1.39	1.46
1	B	453	VAL	C-O	-5.30	1.17	1.24
1	A	178	GLU	CA-C	-5.30	1.45	1.52
1	B	266	MET	CA-CB	-5.29	1.45	1.53
1	B	472	ALA	N-CA	5.26	1.53	1.46
1	B	685	PHE	CA-C	-5.25	1.46	1.52
1	B	438	GLU	CA-C	-5.25	1.46	1.52
1	B	289	PRO	C-O	5.23	1.29	1.23
1	B	681	ASP	CA-C	5.22	1.58	1.52
1	B	85	HIS	CA-C	5.21	1.59	1.52
1	B	596	PRO	C-O	5.16	1.28	1.23
1	A	621	ALA	N-CA	-5.16	1.40	1.46
1	A	293	VAL	C-O	-5.14	1.18	1.24
1	B	705	VAL	N-CA	-5.14	1.40	1.46
1	A	449	PRO	N-CA	-5.13	1.40	1.47
1	B	83	ASP	C-O	5.12	1.30	1.24
1	B	575	ALA	CA-CB	-5.12	1.46	1.53
1	A	343	GLU	CD-OE2	5.12	1.35	1.25
1	A	189	GLY	N-CA	-5.11	1.39	1.45
1	A	658	GLN	CD-NE2	-5.09	1.22	1.33
1	B	36	GLY	N-CA	5.08	1.53	1.45
1	B	580	ASP	C-O	-5.08	1.17	1.24
1	A	252	ALA	CA-C	5.06	1.59	1.52
1	B	537	GLY	N-CA	5.05	1.52	1.45
1	A	66	PHE	C-O	-5.04	1.17	1.23
1	B	505	ILE	CA-C	5.04	1.60	1.52
1	B	512	ASP	CB-CG	5.02	1.64	1.52
1	A	699	GLY	CA-C	-5.01	1.46	1.51
1	B	510	GLN	CA-C	-5.00	1.46	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	GLN	N-CA-C	-8.45	99.38	110.53
1	A	403	ARG	CG-CD-NE	7.84	129.25	112.00
1	B	46	GLN	N-CA-C	-7.78	100.26	110.53
1	A	541	GLY	N-CA-C	-7.67	98.28	112.62
1	B	541	GLY	N-CA-C	-6.93	97.90	112.45
1	B	55	HIS	CB-CA-C	6.71	121.79	111.39
1	B	540	ARG	CB-CA-C	6.39	124.12	111.22
1	A	48	ASP	N-CA-C	6.34	119.04	108.20
1	B	48	ASP	N-CA-C	6.12	118.66	108.20
1	A	55	HIS	CB-CA-C	5.76	120.32	111.39
1	B	428	MET	CA-CB-CG	-5.72	102.67	114.10
1	A	46	GLN	CB-CG-CD	5.70	122.29	112.60
1	B	62	MET	CA-C-N	-5.63	114.17	120.53
1	B	62	MET	C-N-CA	-5.63	114.17	120.53
1	B	382	ARG	CG-CD-NE	-5.51	99.87	112.00
1	B	46	GLN	CB-CG-CD	5.47	121.90	112.60
1	A	613	ALA	N-CA-C	5.40	118.66	111.75
1	B	494	SER	N-CA-C	5.32	116.76	111.07
1	B	345	LEU	O-C-N	5.28	127.59	122.09
1	B	539	GLN	CA-C-N	-5.20	113.55	123.32
1	B	539	GLN	C-N-CA	-5.20	113.55	123.32
1	A	467	LYS	N-CA-C	-5.17	105.65	111.28
1	B	569	ALA	N-CA-C	-5.11	102.13	110.20
1	A	149	ARG	NE-CZ-NH1	5.07	126.56	121.50
1	A	64	LYS	CB-CG-CD	5.06	122.95	111.30
1	A	631	MET	N-CA-C	-5.00	105.72	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	569	ALA	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5548	0	5374	26	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5557	0	5389	33	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	2	0	0	0	0
5	B	2	0	0	0	0
6	A	16	0	28	3	0
6	B	16	0	28	10	0
7	A	817	0	0	11	1
7	B	812	0	0	12	1
All	All	12860	0	10879	67	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 3.

All (67) 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:569:ALA:O	1:B:570[A]:VAL:HG23	1.58	1.02
1:B:568:HIS:ND1	7:B:901:HOH:O	1.94	1.01
1:B:55:HIS:HD2	7:B:1347:HOH:O	1.48	0.96
1:B:506:ARG:HE	6:B:805:MPD:H12	1.38	0.88
1:A:119[B]:THR:HG21	7:A:1138:HOH:O	1.80	0.81
1:B:119[B]:THR:HG23	7:B:1081:HOH:O	1.82	0.79
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.67	0.77
1:B:512:ASP:OD1	7:B:902:HOH:O	2.02	0.77
6:B:806:MPD:O4	6:B:806:MPD:H12	1.85	0.77
6:B:805:MPD:H51	7:B:1269:HOH:O	1.84	0.76
1:B:119[B]:THR:HG22	1:B:593:VAL:HG21	1.66	0.76
1:B:569:ALA:O	1:B:570[A]:VAL:CG2	2.35	0.75
6:A:805:MPD:H52	6:A:805:MPD:H11	1.69	0.73
6:A:805:MPD:H11	6:A:805:MPD:C5	2.20	0.71
6:B:805:MPD:H13	7:B:1555:HOH:O	1.91	0.70
1:B:519:GLU:OE1	7:B:903:HOH:O	2.09	0.69
6:B:806:MPD:O2	6:B:806:MPD:H53	1.97	0.65
1:A:85:HIS:HD2	7:A:1502:HOH:O	1.82	0.61
1:A:593:VAL:HG13	7:A:926:HOH:O	2.02	0.60
1:A:376:ASP:OD2	1:A:379:LYS:HE3	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:MET:SD	1:B:594:LEU:HD12	2.45	0.57
1:A:343:GLU:OE1	7:A:903:HOH:O	2.17	0.56
1:A:58:LEU:HB3	1:B:53[A]:HIS:HD2	1.71	0.55
1:B:380:LYS:NZ	7:B:909:HOH:O	2.36	0.54
1:B:629:PRO:O	1:B:633[A]:VAL:HG23	2.08	0.54
6:B:805:MPD:H52	6:B:805:MPD:C1	2.38	0.54
1:A:748:ALA:C	7:A:1564:HOH:O	2.53	0.52
1:B:568:HIS:CE1	7:B:901:HOH:O	2.51	0.52
1:B:506:ARG:NE	6:B:805:MPD:H12	2.17	0.52
1:B:662:ASN:H	1:B:725:GLN:HE22	1.57	0.51
1:A:119[B]:THR:CG2	1:A:593:VAL:HG11	2.40	0.51
1:A:58:LEU:HB3	1:B:53[A]:HIS:CD2	2.46	0.51
1:A:629:PRO:O	1:A:633[B]:VAL:HG23	2.11	0.51
1:B:74:LYS:HB2	7:B:1037:HOH:O	2.11	0.50
1:B:566:ALA:O	1:B:568:HIS:HD2	1.95	0.49
1:A:650:HIS:HE1	7:A:1562:HOH:O	1.96	0.48
1:B:506:ARG:HE	6:B:805:MPD:C1	2.18	0.48
1:A:633[B]:VAL:HG22	1:A:719:TYR:CE2	2.48	0.48
1:B:76:ASP:OD2	7:B:904:HOH:O	2.20	0.47
1:A:51:ILE:HD11	1:A:618:VAL:HG12	1.96	0.47
6:A:805:MPD:HM2	7:A:1460:HOH:O	2.13	0.47
1:A:53:HIS:CD2	7:A:958:HOH:O	2.68	0.47
6:B:805:MPD:H52	6:B:805:MPD:H11	1.97	0.46
1:B:54:ARG:HB3	1:B:55:HIS:ND1	2.30	0.46
1:A:119[A]:THR:CG2	1:A:265:ALA:HB2	2.46	0.46
1:A:336:GLN:HG2	7:A:1648:HOH:O	2.15	0.46
1:A:650:HIS:HD2	7:A:1346:HOH:O	1.98	0.46
1:A:633[B]:VAL:HG22	1:A:719:TYR:CZ	2.52	0.45
1:B:571[A]:THR:OG1	7:B:905:HOH:O	2.20	0.45
1:A:54:ARG:NE	1:A:199:ASP:OD2	2.50	0.44
1:A:633[B]:VAL:CG2	1:A:719:TYR:CZ	3.01	0.44
1:B:50[B]:SER:OG	1:B:53[B]:HIS:CE1	2.71	0.44
1:B:454:ASP:OD1	1:B:454:ASP:N	2.51	0.43
1:A:454:ASP:OD1	1:A:454:ASP:N	2.50	0.43
1:B:566:ALA:O	1:B:568:HIS:CD2	2.71	0.43
1:B:633[A]:VAL:HG22	1:B:719:TYR:CZ	2.55	0.42
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.19	0.42
1:B:633[A]:VAL:HG22	1:B:719:TYR:CE2	2.54	0.42
1:A:111:TOX:H9	1:A:238:TYR:OH	2.19	0.42
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.20	0.41
1:A:431:ARG:HD2	1:A:447:GLN:OE1	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:PHE:CD1	1:B:374:ALA:HA	2.56	0.41
6:B:806:MPD:O2	6:B:806:MPD:C5	2.63	0.41
1:A:369:ALA:O	1:A:380:LYS:HD2	2.21	0.41
1:B:50[B]:SER:HA	1:B:53[B]:HIS:CE1	2.56	0.40
1:A:431:ARG:HD3	7:A:1447:HOH:O	2.22	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)
7:A:1372:HOH:O	7:B:1232:HOH:O[2_444]	2.02	0.18

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%)	706 (98%)	11 (2%)	0	100	100
1	B	720/728 (99%)	709 (98%)	11 (2%)	0	100	100
All	All	1437/1456 (99%)	1415 (98%)	22 (2%)	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%)	549 (99%)	7 (1%)	61	46
1	B	559/560 (100%)	548 (98%)	11 (2%)	48	29
All	All	1115/1120 (100%)	1097 (98%)	18 (2%)	57	38

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	46	GLN
1	A	64	LYS
1	A	74	LYS
1	A	141	ASP
1	A	183	LYS
1	A	610	ARG
1	B	40	ARG
1	B	46	GLN
1	B	64	LYS
1	B	141	ASP
1	B	512	ASP
1	B	540	ARG
1	B	571[A]	THR
1	B	571[B]	THR
1	B	610	ARG
1	B	633[A]	VAL
1	B	633[B]	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	650	HIS
1	B	55	HIS
1	B	568	HIS
1	B	650	HIS
1	B	711	GLN
1	B	725	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	1	14,17,18	1.85	4 (28%)	12,23,25	1.82	3 (25%)
1	TOX	B	111	1,2	14,17,18	1.90	3 (21%)	12,23,25	2.62	7 (58%)

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

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	TOX	O-C	4.29	1.36	1.20
1	A	111	TOX	CH2-CZ3	4.05	1.47	1.38
1	A	111	TOX	CD2-CE2	3.49	1.45	1.41
1	B	111	TOX	CE2-NE1	-3.20	1.34	1.39
1	A	111	TOX	O-C	2.78	1.30	1.20
1	B	111	TOX	CE3-CD2	-2.34	1.36	1.39
1	A	111	TOX	CD2-CG	2.02	1.47	1.44

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	TOX	CZ2-CE2-CD2	-4.24	117.22	121.95
1	B	111	TOX	CZ3-CH2-CZ2	-4.08	115.20	120.24
1	A	111	TOX	CZ2-CE2-NE1	3.70	135.27	129.37
1	B	111	TOX	CE2-CD2-CG	-3.53	104.15	107.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	TOX	CH2-CZ2-CE2	3.37	125.09	118.28
1	B	111	TOX	CZ2-CE2-NE1	2.88	133.96	129.37
1	B	111	TOX	CD2-CG-CD1	2.59	108.69	106.34
1	A	111	TOX	CZ3-CH2-CZ2	-2.29	117.41	120.24
1	B	111	TOX	CE3-CD2-CG	2.19	137.12	133.85
1	A	111	TOX	CH2-CZ2-CE2	2.00	122.32	118.28

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	111	TOX	N-CA-CB-CG
1	A	111	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	A	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, 4 are monoatomic - leaving 8 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	$\# Z > 2$
2	HEM	B	801	1	50,50,50	2.08	13 (26%)	67,82,82	1.36	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	801	1	50,50,50	2.20	18 (36%)	67,82,82	1.86	18 (26%)
6	MPD	B	806	-	7,7,7	0.74	0	9,10,10	1.42	1 (11%)
5	OXY	A	804	-	1,1,1	0.03	0	-		
6	MPD	B	805	-	7,7,7	1.04	0	9,10,10	1.36	1 (11%)
6	MPD	A	805	-	7,7,7	0.77	0	9,10,10	1.11	1 (11%)
6	MPD	A	806	-	7,7,7	0.75	0	9,10,10	1.34	1 (11%)
5	OXY	B	804	-	1,1,1	0.07	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
2	HEM	B	801	1	-	2/14/54/54	-
2	HEM	A	801	1	-	2/14/54/54	-
6	MPD	B	806	-	-	1/5/5/5	-
6	MPD	A	806	-	-	3/5/5/5	-
6	MPD	A	805	-	-	4/5/5/5	-
6	MPD	B	805	-	-	4/5/5/5	-

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C1C-NC	-7.56	1.25	1.39
2	A	801	HEM	C1B-NB	-6.34	1.29	1.40
2	A	801	HEM	FE-NB	5.13	2.10	1.94
2	B	801	HEM	C1B-NB	-4.69	1.32	1.40
2	A	801	HEM	C1C-NC	-4.63	1.30	1.39
2	A	801	HEM	C4C-NC	3.64	1.46	1.39
2	A	801	HEM	FE-NC	3.58	2.07	1.95
2	B	801	HEM	C4C-NC	3.58	1.46	1.39
2	B	801	HEM	C3C-C4C	-3.54	1.39	1.46
2	A	801	HEM	C4A-NA	-3.53	1.33	1.39
2	B	801	HEM	CMD-C2D	-3.52	1.43	1.50
2	B	801	HEM	FE-NB	3.48	2.05	1.94
2	B	801	HEM	C4A-NA	-3.40	1.33	1.39
2	B	801	HEM	C1C-C2C	3.38	1.52	1.45
2	A	801	HEM	FE-NA	3.34	2.06	1.95
2	B	801	HEM	C2A-C3A	-3.04	1.31	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	CHD-C4C	-3.03	1.32	1.38
2	A	801	HEM	CHC-C1C	-2.91	1.32	1.38
2	A	801	HEM	C3C-C4C	2.81	1.50	1.46
2	A	801	HEM	CMA-C3A	2.79	1.56	1.50
2	A	801	HEM	C1B-C2B	-2.64	1.39	1.44
2	B	801	HEM	FE-NC	2.63	2.03	1.95
2	A	801	HEM	O1D-CGD	2.46	1.30	1.22
2	B	801	HEM	CMC-C2C	-2.30	1.46	1.50
2	A	801	HEM	O1A-CGA	2.29	1.29	1.22
2	B	801	HEM	C3D-C2D	2.25	1.41	1.36
2	A	801	HEM	C3B-C2B	2.17	1.41	1.37
2	A	801	HEM	CMB-C2B	2.16	1.55	1.50
2	B	801	HEM	FE-ND	2.16	2.01	1.94
2	A	801	HEM	CAB-C3B	-2.13	1.41	1.47
2	A	801	HEM	CHC-C4B	-2.09	1.34	1.39

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	CHD-C4C-NC	4.65	129.51	124.45
2	A	801	HEM	C2A-C1A-NA	-4.32	105.36	110.15
2	A	801	HEM	O2A-CGA-CBA	4.20	127.28	114.00
2	B	801	HEM	CMD-C2D-C1D	3.88	131.10	125.03
2	A	801	HEM	C4C-NC-C1C	3.79	112.01	105.82
2	A	801	HEM	C4B-C3B-C2B	-3.76	103.82	107.28
2	A	801	HEM	C1C-CHC-C4B	3.47	133.39	126.02
2	A	801	HEM	C4A-NA-C1A	3.42	111.40	105.82
2	A	801	HEM	CHC-C1C-NC	-3.36	120.80	124.45
2	A	801	HEM	O1A-CGA-CBA	-3.15	113.09	123.09
2	A	801	HEM	CHB-C4A-NA	3.12	129.52	123.86
2	A	801	HEM	CHB-C1B-NB	-3.07	120.58	124.37
6	A	806	MPD	O2-C2-CM	2.83	116.82	107.99
2	B	801	HEM	C2A-C1A-NA	-2.83	107.01	110.15
6	B	806	MPD	O2-C2-CM	-2.66	99.70	107.99
2	B	801	HEM	CAA-CBA-CGA	-2.65	106.63	113.67
2	B	801	HEM	CBA-CAA-C2A	2.63	119.79	112.53
2	A	801	HEM	CBD-CAD-C3D	2.62	119.78	112.53
2	A	801	HEM	O2D-CGD-CBD	2.59	122.19	114.00
2	A	801	HEM	O1D-CGD-CBD	-2.54	115.05	123.09
2	A	801	HEM	C2B-C1B-NB	2.53	112.75	109.84
2	A	801	HEM	C3A-C4A-NA	-2.40	106.29	110.14
2	B	801	HEM	C4A-C3A-C2A	2.40	109.56	106.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	C4B-C3B-C2B	-2.37	105.10	107.28
2	A	801	HEM	CHC-C1C-C2C	2.33	130.33	125.49
6	A	805	MPD	O2-C2-CM	-2.33	100.73	107.99
2	B	801	HEM	O2A-CGA-CBA	2.31	121.31	114.00
2	A	801	HEM	CAA-CBA-CGA	-2.23	107.74	113.67
6	B	805	MPD	CM-C2-C1	-2.20	105.70	110.63
2	B	801	HEM	C2B-C1B-NB	2.04	112.19	109.84
2	B	801	HEM	C4D-ND-C1D	2.04	107.62	105.21

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	805	MPD	C2-C3-C4-C5
6	B	806	MPD	C2-C3-C4-C5
6	A	805	MPD	O2-C2-C3-C4
6	B	805	MPD	O2-C2-C3-C4
6	A	805	MPD	C2-C3-C4-O4
6	A	806	MPD	C1-C2-C3-C4
6	B	805	MPD	C1-C2-C3-C4
6	B	805	MPD	C2-C3-C4-C5
2	B	801	HEM	CAA-CBA-CGA-O1A
2	A	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O2A
6	A	806	MPD	O2-C2-C3-C4
6	A	805	MPD	CM-C2-C3-C4
6	A	806	MPD	CM-C2-C3-C4
6	B	805	MPD	CM-C2-C3-C4

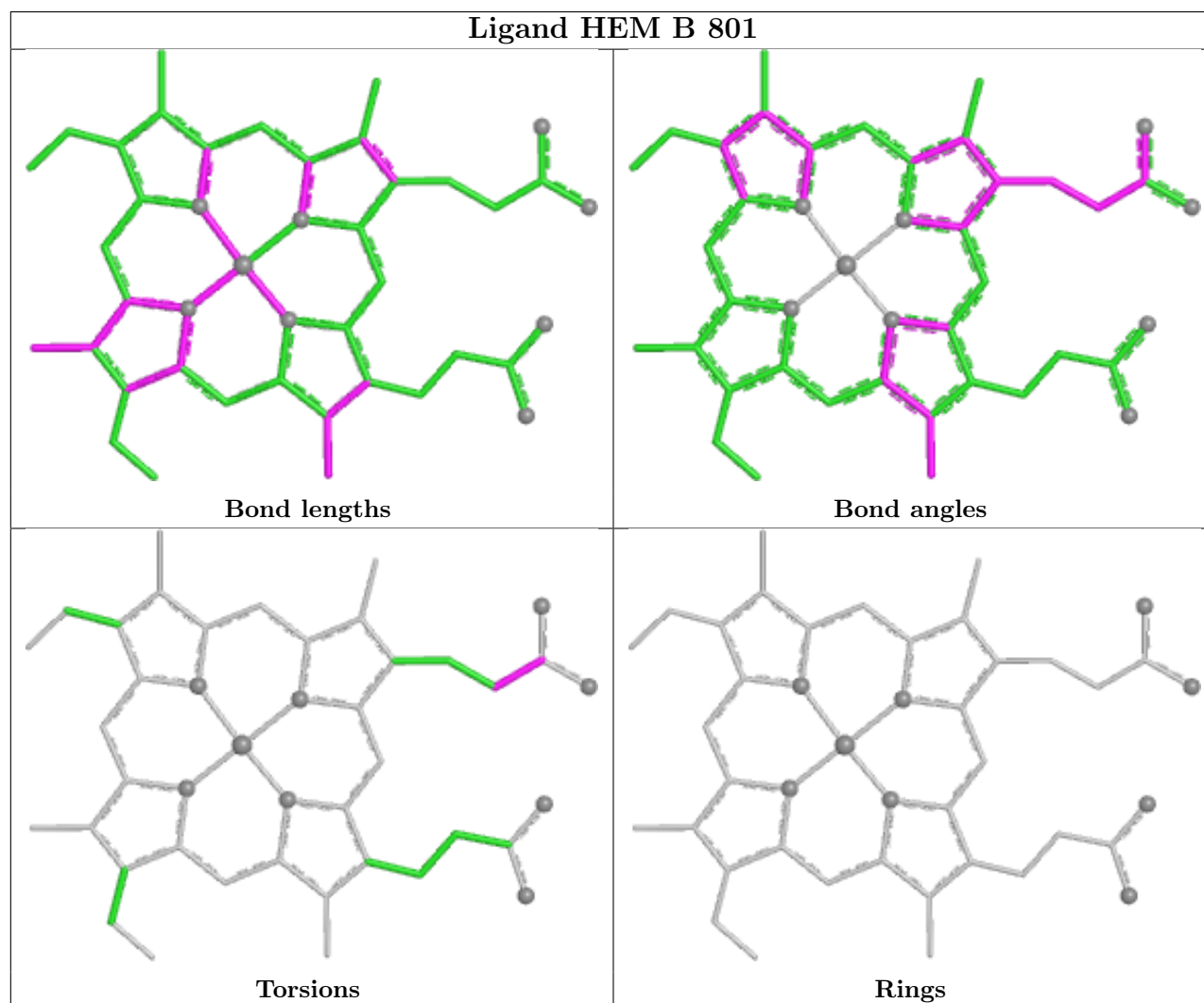
There are no ring outliers.

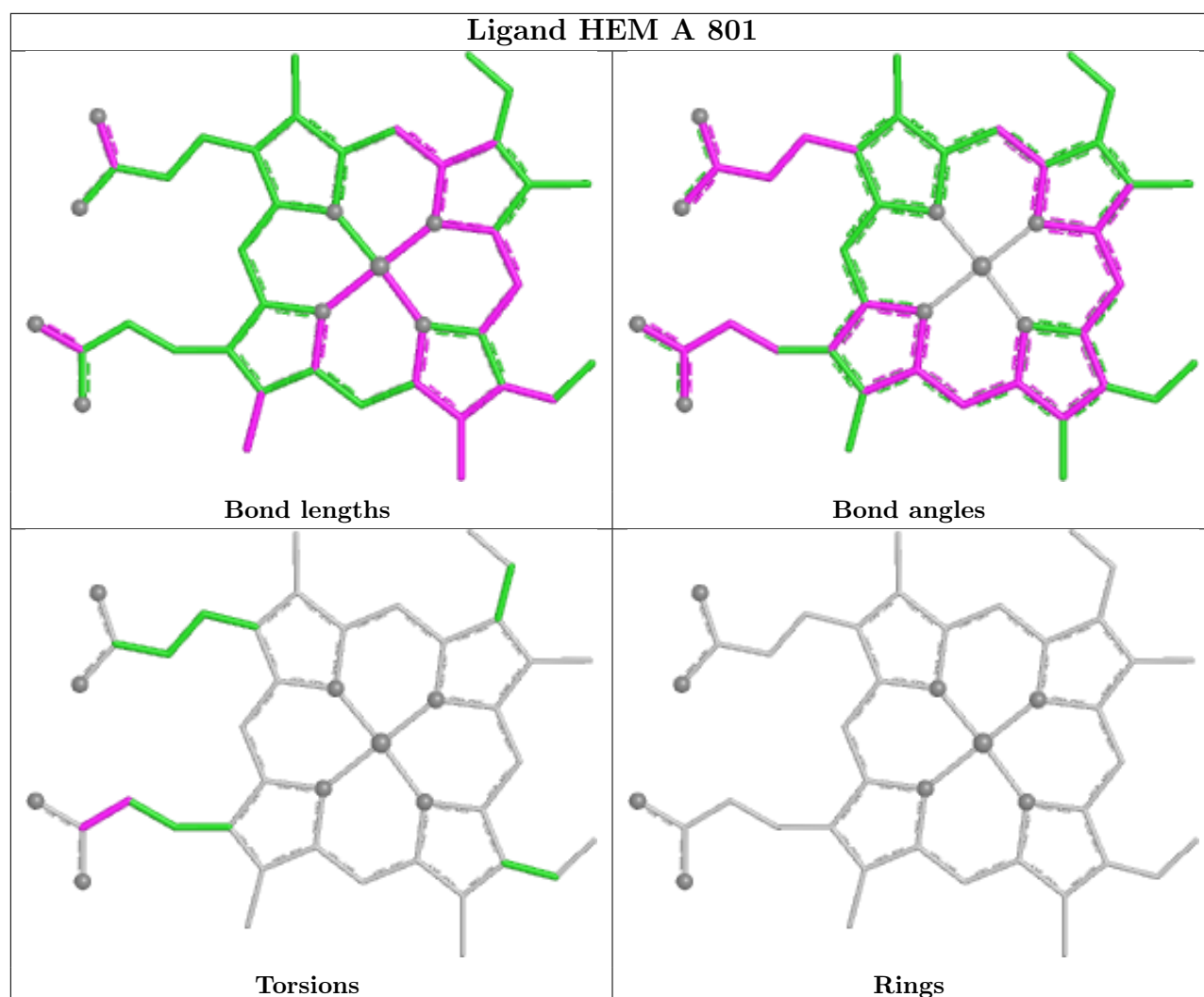
3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	806	MPD	3	0
6	B	805	MPD	7	0
6	A	805	MPD	3	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	712/728 (97%)	-0.26	12 (1%)	69 75	8, 17, 36, 87	7 (0%)
1	B	712/728 (97%)	-0.29	17 (2%)	59 66	9, 16, 36, 88	10 (1%)
All	All	1424/1456 (97%)	-0.28	29 (2%)	65 71	8, 17, 36, 88	17 (1%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	55	HIS	6.2
1	A	53	HIS	5.4
1	B	64	LYS	5.0
1	B	748	ALA	4.9
1	B	53[A]	HIS	4.5
1	A	55	HIS	4.4
1	A	748	ALA	4.2
1	B	692	THR	4.0
1	A	64	LYS	4.0
1	B	680	ALA	3.9
1	B	54	ARG	3.5
1	A	608	LYS	3.4
1	B	679	ALA	3.3
1	B	691	ALA	3.3
1	B	610	ARG	3.2
1	B	40	ARG	3.1
1	B	540	ARG	3.1
1	A	58	LEU	2.9
1	A	541	GLY	2.8
1	B	611	VAL	2.7
1	B	65	ASP	2.7
1	B	58	LEU	2.7
1	A	54	ARG	2.6
1	A	40	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	609	TYR	2.4
1	A	540	ARG	2.3
1	A	610	ARG	2.3
1	B	682	ALA	2.2
1	A	679	ALA	2.1

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	16/17	0.97	0.06	10,12,23,23	0
1	TOX	B	111	16/17	0.98	0.04	10,12,18,18	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.

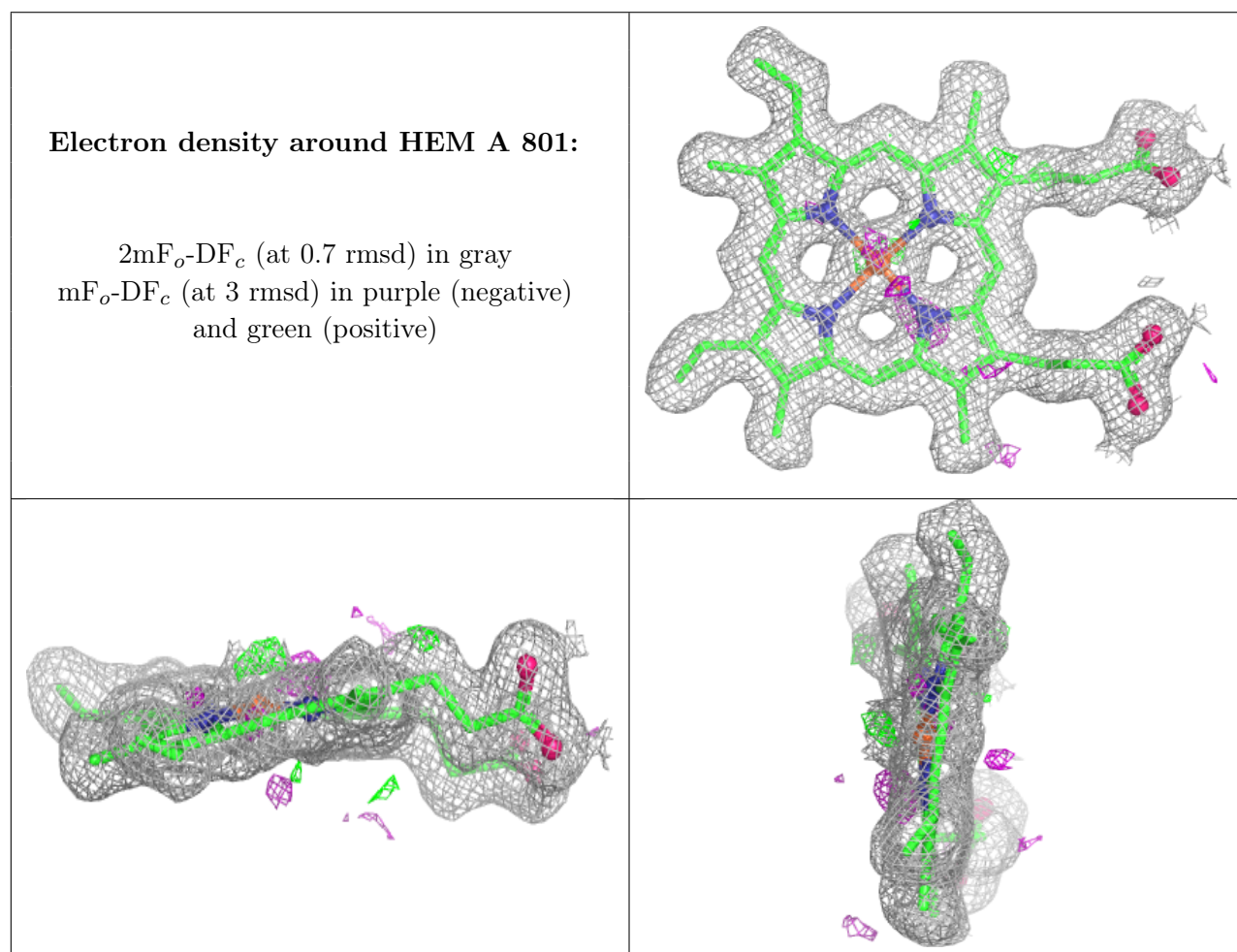
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MPD	B	805	8/8	0.87	0.15	29,35,35,37	0
6	MPD	B	806	8/8	0.88	0.21	50,58,65,65	0
6	MPD	A	805	8/8	0.89	0.14	37,39,46,47	0
6	MPD	A	806	8/8	0.90	0.18	45,51,62,64	0
5	OXY	A	804	2/2	0.93	0.22	36,36,36,37	0
5	OXY	B	804	2/2	0.96	0.14	25,25,25,28	0
2	HEM	A	801	43/43	0.99	0.05	11,14,16,17	0
2	HEM	B	801	43/43	0.99	0.04	10,11,13,16	0
3	NA	A	802	1/1	0.99	0.03	14,14,14,14	0
3	NA	B	802	1/1	0.99	0.03	14,14,14,14	0
4	CL	A	803	1/1	0.99	0.07	26,26,26,26	0

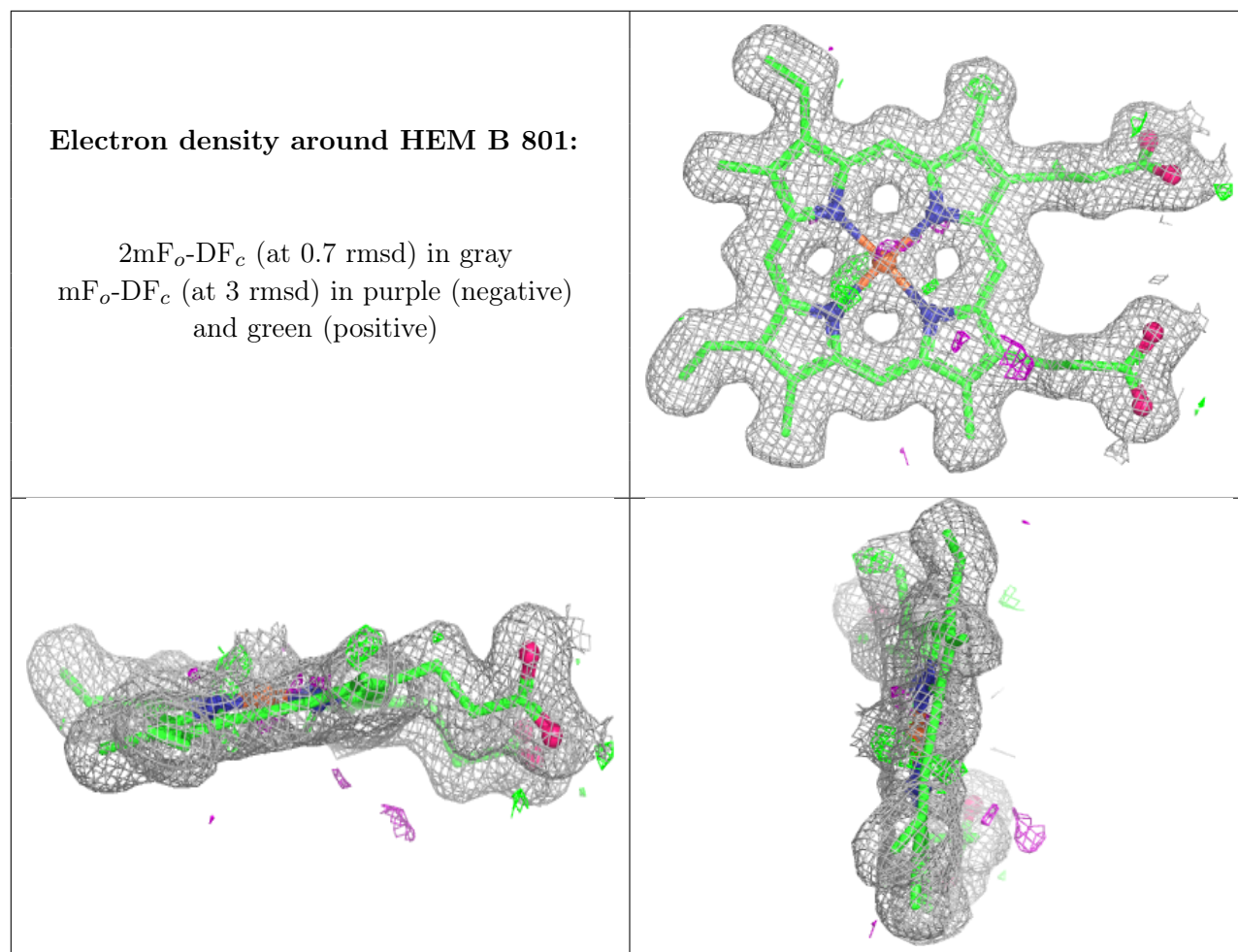
Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CL	B	803	1/1	0.99	0.07	26,26,26,26	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.