



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 05:21 PM EDT

PDB ID : 5TXQ / pdb_00005txq
Title : Crystal structure of the A143D variant of catalase-peroxidase from *B. pseudo-mallei*
Authors : Loewen, P.C.
Deposited on : 2016-11-17
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

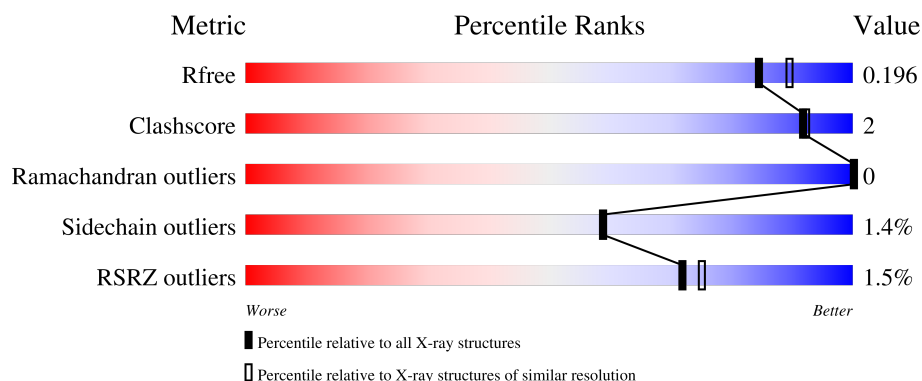
1 Overall quality at a glance

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	% 86% 11% ..
1	B	728	2% 85% 12% ..

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12726 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
			5566	3511	990	1051	14			
1	B	713	Total	C	N	O	S	0	6	0
			5552	3505	989	1044	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	ASP	ALA	engineered mutation	UNP Q3JNW6
B	143	ASP	ALA	engineered mutation	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		

Continued on next page...

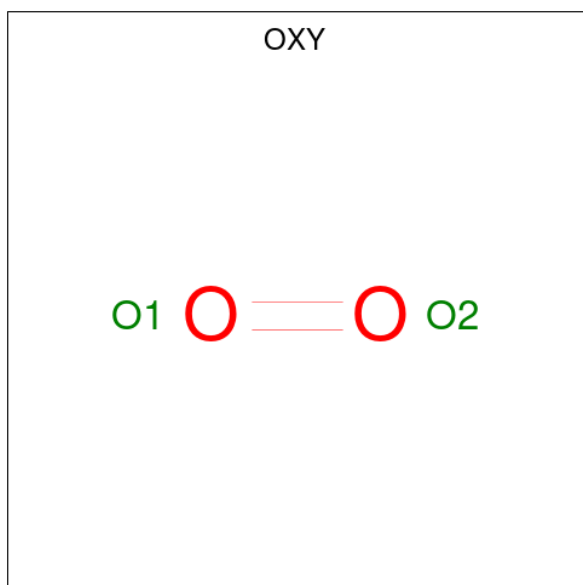
Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	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 OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



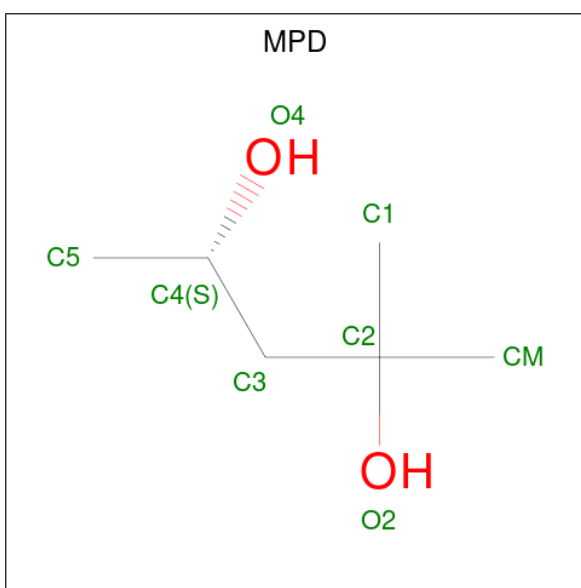
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O		
			2	2	0	0
4	B	1	Total	O		
			2	2	0	0

- 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: $C_6H_{14}O_2$).



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		

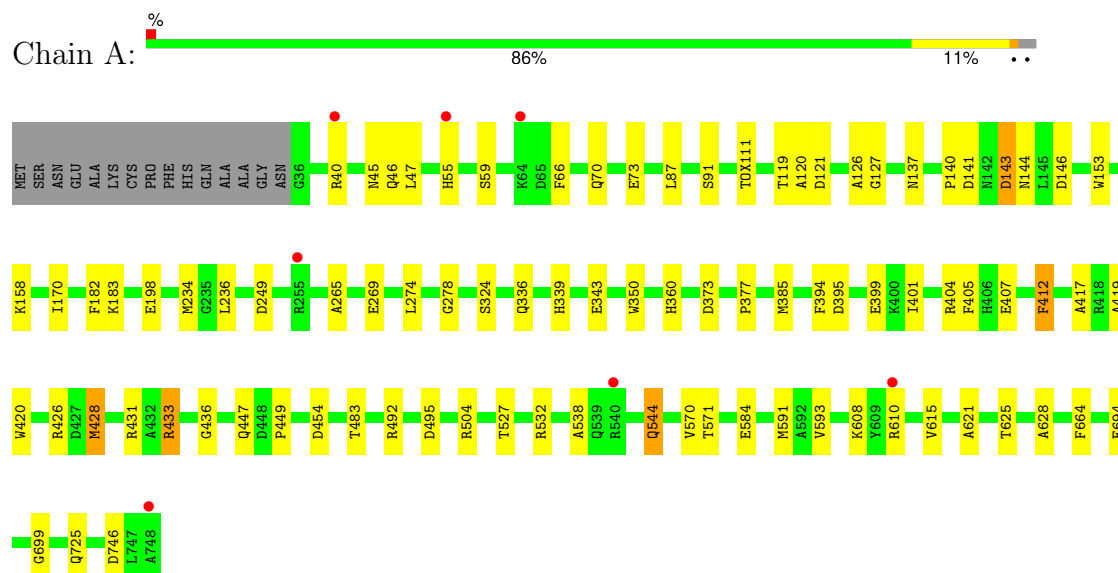
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	756	Total 756	O 756	0	0
7	B	734	Total 734	O 734	0	0

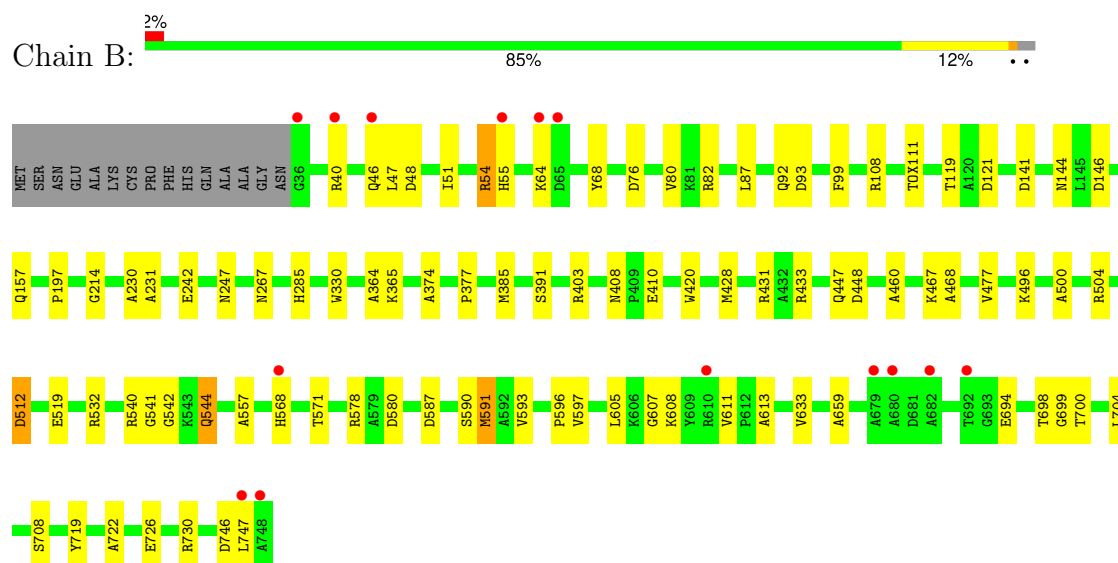
3 Residue-property plots [i](#)

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	100.67Å 115.12Å 174.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.13 – 1.90 96.13 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (96.13-1.90) 99.7 (96.13-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 1.90Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.157 , 0.191 0.168 , 0.196	Depositor DCC
R_{free} test set	7899 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	21.7	Xtriage
Anisotropy	0.667	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.4	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	12726	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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: NA, HEM, TOX, MPD, PO4, OXY

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	1.67	57/5698 (1.0%)	1.26	16/7742 (0.2%)
1	B	1.68	54/5687 (0.9%)	1.28	14/7728 (0.2%)
All	All	1.68	111/11385 (1.0%)	1.27	30/15470 (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 (111) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	512	ASP	CG-OD2	8.91	1.42	1.25
1	B	540	ARG	C-O	8.91	1.34	1.23
1	A	544	GLN	CD-OE1	8.19	1.39	1.23
1	B	448	ASP	N-CA	7.77	1.51	1.46
1	B	694	GLU	CA-C	7.39	1.62	1.52
1	A	66	PHE	C-O	-7.14	1.15	1.23
1	B	708	SER	C-O	-7.12	1.15	1.24
1	A	417	ALA	N-CA	7.10	1.54	1.46
1	A	584	GLU	C-O	-6.98	1.15	1.24
1	A	725	GLN	CG-CD	6.91	1.69	1.52
1	A	433	ARG	N-CA	-6.89	1.37	1.46
1	B	121	ASP	CA-C	-6.86	1.43	1.52
1	A	628	ALA	N-CA	-6.70	1.39	1.46
1	A	412	PHE	CA-C	6.66	1.61	1.52
1	B	544	GLN	CD-NE2	6.66	1.47	1.33
1	A	385	MET	C-O	6.61	1.31	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	527	THR	N-CA	-6.56	1.38	1.46
1	B	385	MET	C-O	6.56	1.31	1.23
1	B	698	THR	C-O	-6.52	1.15	1.23
1	B	231	ALA	N-CA	-6.50	1.37	1.45
1	B	542	GLY	C-O	-6.48	1.16	1.23
1	B	746	ASP	C-O	-6.38	1.15	1.24
1	B	597	VAL	C-O	-6.32	1.17	1.24
1	B	87	LEU	N-CA	-6.29	1.38	1.46
1	A	236	LEU	CA-C	6.26	1.60	1.52
1	B	596	PRO	C-O	6.26	1.28	1.24
1	B	568	HIS	CA-C	6.26	1.60	1.52
1	A	87	LEU	N-CA	-6.25	1.38	1.46
1	B	285	HIS	C-O	6.24	1.31	1.24
1	B	477	VAL	CA-CB	-6.23	1.47	1.54
1	B	699	GLY	CA-C	-6.22	1.45	1.51
1	B	580	ASP	C-O	-6.22	1.16	1.24
1	A	625	THR	N-CA	6.18	1.54	1.46
1	A	399	GLU	C-O	-6.09	1.17	1.24
1	A	699	GLY	CA-C	-6.08	1.45	1.51
1	A	45	ASN	C-O	-6.00	1.15	1.24
1	B	596	PRO	CA-CB	-5.95	1.47	1.54
1	B	722	ALA	C-O	-5.92	1.16	1.24
1	A	449	PRO	C-O	-5.86	1.16	1.23
1	B	532	ARG	CD-NE	-5.81	1.38	1.46
1	B	391	SER	CA-C	-5.80	1.45	1.52
1	B	460	ALA	CA-C	-5.78	1.45	1.52
1	A	47	LEU	CB-CG	-5.75	1.42	1.53
1	A	746	ASP	C-O	-5.75	1.16	1.24
1	A	127	GLY	C-O	5.65	1.30	1.23
1	B	512	ASP	C-O	-5.61	1.16	1.24
1	B	704	LEU	CA-C	-5.59	1.44	1.52
1	A	143	ASP	C-O	-5.58	1.17	1.23
1	B	590	SER	C-O	-5.54	1.17	1.24
1	B	726	GLU	CD-OE2	5.53	1.35	1.25
1	A	492	ARG	C-O	5.51	1.30	1.23
1	B	700	THR	N-CA	-5.51	1.38	1.45
1	A	91	SER	C-O	-5.49	1.17	1.23
1	A	121	ASP	CA-C	-5.48	1.45	1.52
1	B	587	ASP	CA-C	-5.46	1.45	1.52
1	B	68	TYR	N-CA	5.46	1.52	1.46
1	A	377	PRO	C-O	-5.41	1.16	1.24
1	A	401	ILE	N-CA	5.40	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	247	ASN	CG-OD1	5.39	1.33	1.23
1	A	170	ILE	N-CA	-5.38	1.39	1.46
1	B	607	GLY	C-O	-5.37	1.19	1.24
1	A	407	GLU	CG-CD	5.34	1.65	1.52
1	A	182	PHE	N-CA	-5.33	1.39	1.46
1	B	92	GLN	C-O	5.33	1.30	1.23
1	B	477	VAL	N-CA	5.32	1.52	1.46
1	B	214	GLY	N-CA	-5.32	1.37	1.43
1	A	198	GLU	CG-CD	5.31	1.65	1.52
1	A	126	ALA	C-O	5.30	1.30	1.24
1	A	495	ASP	N-CA	5.30	1.52	1.46
1	A	483	THR	CA-CB	5.29	1.61	1.53
1	A	373	ASP	C-O	-5.29	1.17	1.23
1	A	454	ASP	CB-CG	5.29	1.65	1.52
1	A	725	GLN	N-CA	5.27	1.52	1.46
1	A	694	GLU	CA-C	5.26	1.59	1.52
1	A	59	SER	C-O	-5.25	1.17	1.24
1	A	621	ALA	CA-C	5.24	1.59	1.52
1	B	365	LYS	N-CA	5.24	1.52	1.46
1	A	120	ALA	N-CA	5.22	1.52	1.46
1	A	428	MET	CG-SD	-5.22	1.67	1.80
1	A	571	THR	N-CA	-5.21	1.39	1.46
1	A	70	GLN	CG-CD	5.21	1.65	1.52
1	A	278	GLY	C-O	5.20	1.29	1.23
1	B	157	GLN	N-CA	-5.19	1.40	1.46
1	B	578	ARG	CA-C	-5.19	1.46	1.52
1	A	158	LYS	CA-C	5.18	1.59	1.52
1	A	570	VAL	C-O	-5.17	1.18	1.23
1	B	230	ALA	N-CA	-5.17	1.41	1.46
1	B	420	TRP	CA-C	5.15	1.59	1.52
1	A	419	ALA	C-N	-5.14	1.27	1.33
1	B	267	ASN	CA-CB	5.14	1.60	1.53
1	A	664	PHE	N-CA	-5.14	1.40	1.46
1	A	407	GLU	CD-OE1	5.14	1.35	1.25
1	B	242	GLU	N-CA	5.13	1.52	1.46
1	A	55	HIS	C-O	-5.13	1.16	1.23
1	B	377	PRO	C-O	-5.12	1.17	1.24
1	A	234	MET	C-O	-5.12	1.17	1.24
1	B	694	GLU	N-CA	-5.11	1.39	1.46
1	B	659	ALA	N-CA	-5.11	1.40	1.46
1	A	394	PHE	C-O	-5.11	1.17	1.24
1	A	126	ALA	N-CA	-5.10	1.39	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	SER	CA-C	5.10	1.59	1.52
1	A	420	TRP	N-CA	5.10	1.52	1.46
1	B	51	ILE	C-O	-5.10	1.17	1.24
1	A	538	ALA	C-O	-5.07	1.17	1.24
1	B	364	ALA	C-O	5.07	1.30	1.24
1	B	708	SER	CA-CB	5.05	1.61	1.53
1	B	410	GLU	CG-CD	5.04	1.64	1.52
1	B	500	ALA	N-CA	5.04	1.52	1.46
1	A	436	GLY	C-N	-5.03	1.29	1.33
1	B	80	VAL	N-CA	-5.00	1.40	1.46
1	B	108	ARG	N-CA	-5.00	1.40	1.46

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	541	GLY	N-CA-C	-7.80	98.03	112.62
1	B	46	GLN	N-CA-C	-6.58	101.85	110.53
1	A	55	HIS	CB-CA-C	6.32	121.18	111.39
1	A	198	GLU	CG-CD-OE1	6.22	132.71	118.40
1	B	330	TRP	N-CA-C	6.18	119.30	111.69
1	B	93	ASP	N-CA-C	6.18	118.01	111.28
1	A	46	GLN	N-CA-C	-6.11	102.47	110.53
1	B	591	MET	CG-SD-CE	-6.08	87.54	100.90
1	A	591	MET	CG-SD-CE	-6.04	87.62	100.90
1	B	611	VAL	N-CA-C	5.87	113.68	108.63
1	A	395	ASP	N-CA-C	-5.85	102.41	109.72
1	A	70	GLN	CA-CB-CG	5.76	125.61	114.10
1	B	468	ALA	N-CA-C	-5.70	105.15	111.36
1	A	153	TRP	CA-C-N	-5.70	113.02	119.28
1	A	153	TRP	C-N-CA	-5.70	113.02	119.28
1	A	532	ARG	NE-CZ-NH2	-5.69	114.08	119.20
1	A	249	ASP	CA-C-N	5.45	125.27	119.28
1	A	249	ASP	C-N-CA	5.45	125.27	119.28
1	B	47	LEU	N-CA-CB	-5.41	102.02	109.97
1	A	137	ASN	N-CA-C	5.35	118.90	112.38
1	B	408	ASN	CA-C-N	-5.33	114.13	119.56
1	B	408	ASN	C-N-CA	-5.33	114.13	119.56
1	B	403	ARG	CG-CD-NE	-5.31	100.33	112.00
1	A	615	VAL	N-CA-C	-5.22	105.45	110.72
1	B	197	PRO	N-CA-C	5.14	119.16	111.14
1	A	198	GLU	CB-CG-CD	5.12	121.31	112.60
1	B	46	GLN	CB-CG-CD	5.11	121.28	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	LEU	N-CA-CB	-5.11	102.47	109.97
1	A	532	ARG	NE-CZ-NH1	5.07	126.56	121.50
1	B	48	ASP	N-CA-C	5.05	117.57	107.62

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	747	LEU	Peptide

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	5566	0	5368	16	1
1	B	5552	0	5369	15	1
2	A	43	0	30	1	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
4	B	2	0	0	1	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	16	0	28	3	0
7	A	756	0	0	6	0
7	B	734	0	0	6	0
All	All	12726	0	10825	35	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 (35) 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:512:ASP:OD1	7:B:901:HOH:O	2.04	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:803:OXY:O2	7:B:902:HOH:O	2.08	0.72
1:B:519:GLU:OE1	7:B:903:HOH:O	2.10	0.69
1:B:730[A]:ARG:HD2	7:B:1501:HOH:O	1.94	0.68
1:A:119[B]:THR:CG2	1:A:265:ALA:HB2	2.27	0.65
1:A:119[B]:THR:HG21	1:A:265:ALA:HB2	1.82	0.62
4:A:803:OXY:O2	7:A:904:HOH:O	2.16	0.61
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.84	0.60
1:B:76:ASP:OD2	7:B:904:HOH:O	2.16	0.57
1:A:360:HIS:ND1	7:A:908:HOH:O	2.33	0.55
1:B:54:ARG:HB3	1:B:55:HIS:CD2	2.43	0.54
1:A:339:HIS:O	1:A:343[B]:GLU:HG3	2.09	0.53
1:B:730[B]:ARG:HD2	7:B:1122:HOH:O	2.10	0.52
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.12	0.48
1:A:336:GLN:NE2	7:A:903:HOH:O	2.15	0.48
1:A:350:TRP:O	6:A:805:MPD:H51	2.14	0.48
1:A:504:ARG:HD2	7:A:1170:HOH:O	2.14	0.47
6:A:806:MPD:HM2	7:A:1144:HOH:O	2.13	0.47
1:A:431:ARG:HD2	1:A:447:GLN:OE1	2.15	0.47
6:A:805:MPD:H4	7:A:1436:HOH:O	2.16	0.46
1:B:99:PHE:CD2	1:B:374:ALA:HA	2.52	0.45
1:A:405:PHE:HB3	1:A:412:PHE:HB2	2.00	0.43
1:A:144:ASN:HA	1:A:146:ASP:OD1	2.18	0.43
1:B:504:ARG:HD3	1:B:591:MET:HE3	2.01	0.43
1:B:119:THR:HG23	1:B:593:VAL:HG11	2.01	0.42
1:A:269:GLU:OE1	1:A:404:ARG:NH2	2.47	0.42
1:A:428:MET:O	1:A:433:ARG:HD3	2.20	0.42
1:A:119[A]:THR:HG23	1:A:593:VAL:HG11	2.02	0.42
1:A:274:LEU:O	2:A:801:HEM:HBC2	2.21	0.41
1:B:467:LYS:HG2	1:B:557:ALA:HB2	2.02	0.41
1:B:428:MET:O	1:B:433:ARG:HD3	2.20	0.41
1:A:426[B]:ARG:HA	1:A:426[B]:ARG:HD2	1.87	0.41
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.21	0.41
1:B:605:LEU:HD11	1:B:613:ALA:HB2	2.03	0.41
1:A:140:PRO:O	1:A:143:ASP:HB2	2.21	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)
1:A:343[A]:GLU:OE2	1:B:82:ARG:NE[2_444]	2.18	0.02

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	716/728 (98%)	703 (98%)	13 (2%)	0	100	100
All	All	1433/1456 (98%)	1409 (98%)	24 (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	557/561 (99%)	550 (99%)	7 (1%)	61	61
1	B	556/561 (99%)	547 (98%)	9 (2%)	55	54
All	All	1113/1122 (99%)	1097 (99%)	16 (1%)	59	59

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	73	GLU
1	A	141	ASP
1	A	183	LYS
1	A	544	GLN
1	A	608	LYS
1	A	610	ARG
1	B	40	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	54	ARG
1	B	64	LYS
1	B	141	ASP
1	B	496	LYS
1	B	544	GLN
1	B	571[A]	THR
1	B	571[B]	THR
1	B	608	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	ASN
1	A	520	GLN
1	A	647	GLN
1	B	406	HIS
1	B	544	GLN
1	B	568	HIS
1	B	711	GLN
1	B	725	GLN
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 ⓘ

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	2.30	7 (50%)	12,23,25	1.69	4 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TOX	B	111	2,1	14,17,18	2.93	7 (50%)	12,23,25	2.48	6 (50%)

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	2,1	-	2/5/8/10	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	TOX	O-C	6.23	1.43	1.20
1	B	111	TOX	CE3-CD2	-4.55	1.33	1.39
1	B	111	TOX	CE2-NE1	-4.08	1.32	1.39
1	A	111	TOX	O-C	4.02	1.35	1.20
1	A	111	TOX	CE2-NE1	-3.71	1.33	1.39
1	B	111	TOX	CD2-CE2	3.61	1.45	1.41
1	A	111	TOX	CD2-CE2	3.59	1.45	1.41
1	A	111	TOX	CZ2-CE2	-3.09	1.34	1.39
1	B	111	TOX	CZ2-CE2	-2.97	1.35	1.39
1	B	111	TOX	CD2-CG	2.69	1.48	1.44
1	B	111	TOX	O1-NE1	2.57	1.42	1.39
1	A	111	TOX	CH2-CZ3	2.51	1.43	1.38
1	A	111	TOX	CA-N	-2.31	1.41	1.48
1	A	111	TOX	CE3-CD2	-2.29	1.36	1.39

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	TOX	CH2-CZ3-CE3	4.72	126.06	120.24
1	B	111	TOX	CZ3-CH2-CZ2	-3.99	115.32	120.24
1	A	111	TOX	CZ3-CH2-CZ2	-3.17	116.33	120.24
1	B	111	TOX	CZ2-CE2-NE1	2.89	133.97	129.37
1	B	111	TOX	CE3-CD2-CE2	-2.81	116.00	119.24
1	B	111	TOX	CD2-CG-CD1	-2.69	103.90	106.34
1	A	111	TOX	CZ2-CE2-NE1	2.57	133.47	129.37
1	B	111	TOX	CB-CG-CD2	2.47	131.45	126.70
1	A	111	TOX	CE2-CD2-CG	-2.34	105.24	107.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	TOX	CH2-CZ3-CE3	2.30	123.07	120.24

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.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 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	$\# Z > 2$
6	MPD	A	805	-	7,7,7	1.20	0	9,10,10	1.12	0
4	OXY	B	803	-	1,1,1	0.04	0	-		
5	PO4	B	804	-	4,4,4	1.05	0	6,6,6	2.05	2 (33%)
4	OXY	A	803	-	1,1,1	0.07	0	-		
6	MPD	A	806	-	7,7,7	0.92	0	9,10,10	1.89	2 (22%)
2	HEM	B	801	1	50,50,50	1.67	13 (26%)	67,82,82	1.85	15 (22%)
2	HEM	A	801	1	50,50,50	1.76	10 (20%)	67,82,82	1.48	9 (13%)
5	PO4	A	804	-	4,4,4	0.97	0	6,6,6	1.66	1 (16%)

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	806	-	-	2/5/5/5	-
6	MPD	A	805	-	-	1/5/5/5	-
2	HEM	B	801	1	-	2/14/54/54	-
2	HEM	A	801	1	-	3/14/54/54	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C1B-NB	-4.84	1.31	1.40
2	A	801	HEM	FE-NC	4.84	2.11	1.95
2	A	801	HEM	FE-NB	4.50	2.08	1.94
2	A	801	HEM	FE-NA	3.83	2.07	1.95
2	A	801	HEM	C1B-NB	-3.72	1.33	1.40
2	B	801	HEM	C1C-NC	-3.38	1.33	1.39
2	A	801	HEM	CAC-C3C	3.28	1.56	1.47
2	B	801	HEM	C3B-C4B	2.84	1.50	1.44
2	B	801	HEM	CHB-C1B	2.79	1.44	1.38
2	B	801	HEM	C3C-C4C	-2.76	1.41	1.46
2	B	801	HEM	FE-NC	2.71	2.04	1.95
2	A	801	HEM	CBA-CGA	2.63	1.56	1.50
2	B	801	HEM	O1D-CGD	2.53	1.30	1.22
2	B	801	HEM	C1C-C2C	-2.48	1.40	1.45
2	B	801	HEM	FE-NB	2.47	2.02	1.94
2	A	801	HEM	O1D-CGD	2.45	1.30	1.22
2	B	801	HEM	C2A-C3A	-2.45	1.32	1.38
2	B	801	HEM	C1A-NA	-2.43	1.35	1.39
2	A	801	HEM	O1A-CGA	2.30	1.29	1.22
2	A	801	HEM	C3B-C2B	2.28	1.41	1.37
2	A	801	HEM	C3D-C2D	-2.11	1.32	1.36
2	B	801	HEM	CBA-CGA	2.05	1.55	1.50
2	B	801	HEM	CHD-C4C	2.04	1.42	1.38

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	CHC-C4B-NB	7.07	132.03	124.42
2	B	801	HEM	CAA-CBA-CGA	-4.83	100.85	113.67
2	A	801	HEM	C1B-NB-C4B	4.32	110.32	105.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	CAA-CBA-CGA	-3.95	103.18	113.67
6	A	806	MPD	CM-C2-C1	-3.88	101.94	110.63
2	B	801	HEM	C1B-NB-C4B	3.62	109.49	105.21
2	B	801	HEM	C3B-C4B-NB	-3.57	106.90	109.47
5	B	804	PO4	O4-P-O1	-3.46	98.71	110.95
2	A	801	HEM	O2A-CGA-CBA	3.31	124.46	114.00
2	A	801	HEM	C4B-C3B-C2B	-3.30	104.25	107.28
2	B	801	HEM	C4C-C3C-C2C	-3.02	104.19	106.81
5	B	804	PO4	O3-P-O2	3.01	117.28	107.91
2	B	801	HEM	C4C-CHD-C1D	-3.00	119.64	126.02
2	A	801	HEM	O2D-CGD-CBD	2.88	123.09	114.00
2	B	801	HEM	CBD-CAD-C3D	2.74	120.11	112.53
2	B	801	HEM	C3C-C2C-C1C	2.72	109.61	107.05
2	A	801	HEM	O1A-CGA-CBA	-2.63	114.75	123.09
5	A	804	PO4	O4-P-O1	-2.63	101.67	110.95
2	B	801	HEM	CAD-CBD-CGD	2.62	120.61	113.67
2	A	801	HEM	CMA-C3A-C2A	2.47	130.87	125.62
2	B	801	HEM	O2A-CGA-CBA	2.42	121.65	114.00
2	B	801	HEM	CHD-C4C-C3C	-2.36	121.22	125.21
6	A	806	MPD	O4-C4-C3	-2.31	102.17	111.35
2	A	801	HEM	O1D-CGD-CBD	-2.25	115.94	123.09
2	A	801	HEM	C4A-CHB-C1B	2.23	131.50	126.25
2	B	801	HEM	CHD-C4C-NC	2.21	126.86	124.45
2	B	801	HEM	CHC-C1C-NC	-2.19	122.07	124.45
2	B	801	HEM	C4B-C3B-C2B	-2.03	105.41	107.28
2	B	801	HEM	CHC-C4B-C3B	-2.02	121.04	125.07

There are no chirality outliers.

All (8) torsion outliers are listed below:

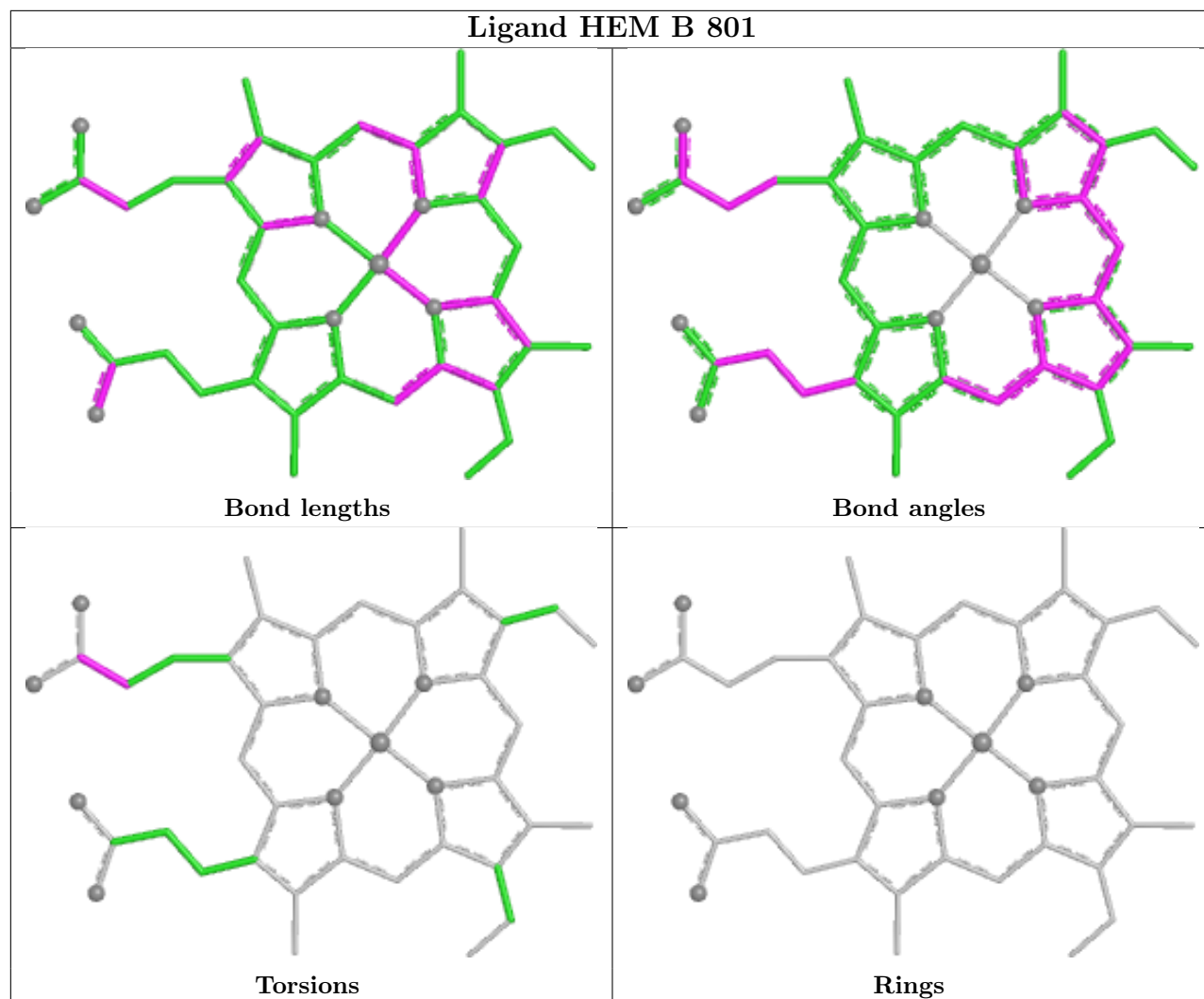
Mol	Chain	Res	Type	Atoms
6	A	805	MPD	C2-C3-C4-C5
6	A	806	MPD	C1-C2-C3-C4
2	B	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O1A
2	A	801	HEM	CAA-CBA-CGA-O1A
6	A	806	MPD	CM-C2-C3-C4
2	A	801	HEM	CAD-CBD-CGD-O2D

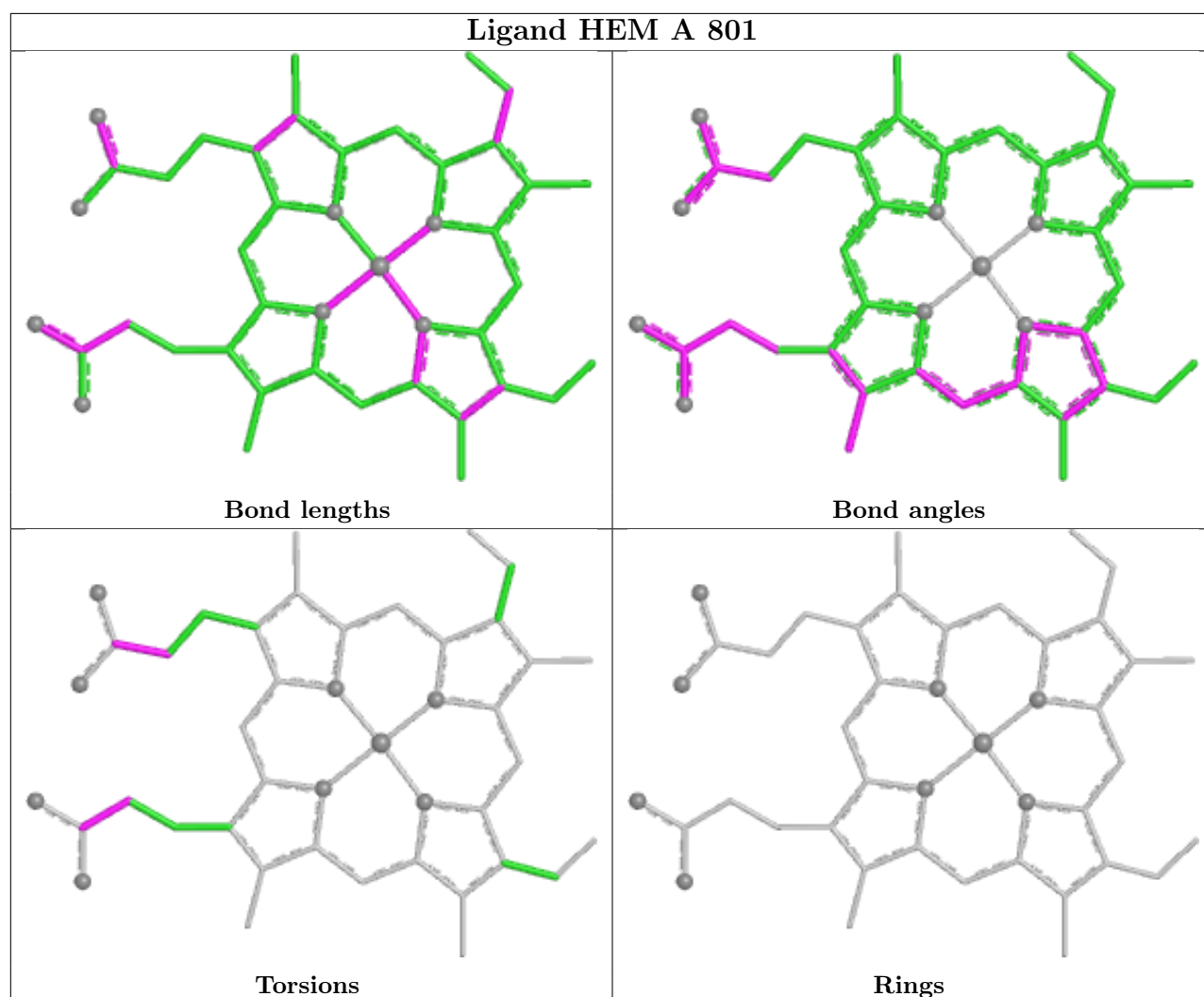
There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	805	MPD	2	0
4	B	803	OXY	1	0
4	A	803	OXY	1	0
6	A	806	MPD	1	0
2	A	801	HEM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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%)	-0.35	7 (0%) 79 82	12, 24, 42, 89	7 (0%)
1	B	712/728 (97%)	-0.39	14 (1%) 65 69	8, 23, 42, 87	6 (0%)
All	All	1424/1456 (97%)	-0.37	21 (1%) 72 75	8, 23, 42, 89	13 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	748	ALA	6.0
1	A	748	ALA	5.3
1	B	55	HIS	4.1
1	B	692	THR	2.9
1	B	680	ALA	2.9
1	B	610	ARG	2.8
1	A	64	LYS	2.8
1	B	679	ALA	2.7
1	A	55	HIS	2.7
1	B	40	ARG	2.6
1	B	747	LEU	2.4
1	A	610	ARG	2.3
1	A	540	ARG	2.2
1	B	64	LYS	2.2
1	B	568	HIS	2.1
1	B	36	GLY	2.1
1	B	46	GLN	2.1
1	B	682	ALA	2.1
1	B	65	ASP	2.1
1	A	255[A]	ARG	2.0
1	A	40	ARG	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	TOX	A	111	16/17	0.97	0.05	16,19,27,30	0
1	TOX	B	111	16/17	0.97	0.05	16,19,26,26	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

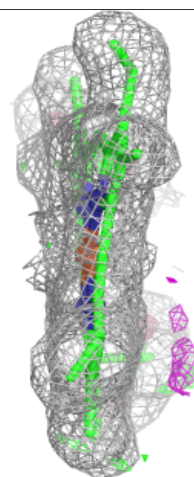
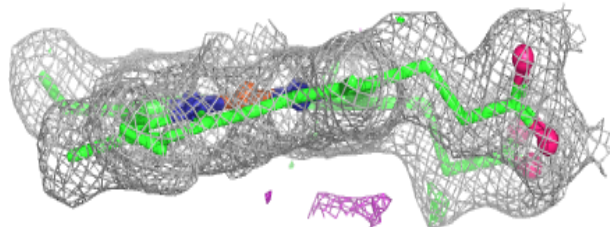
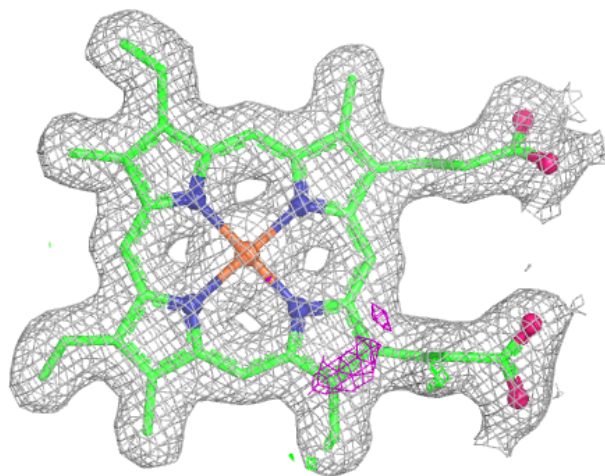
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

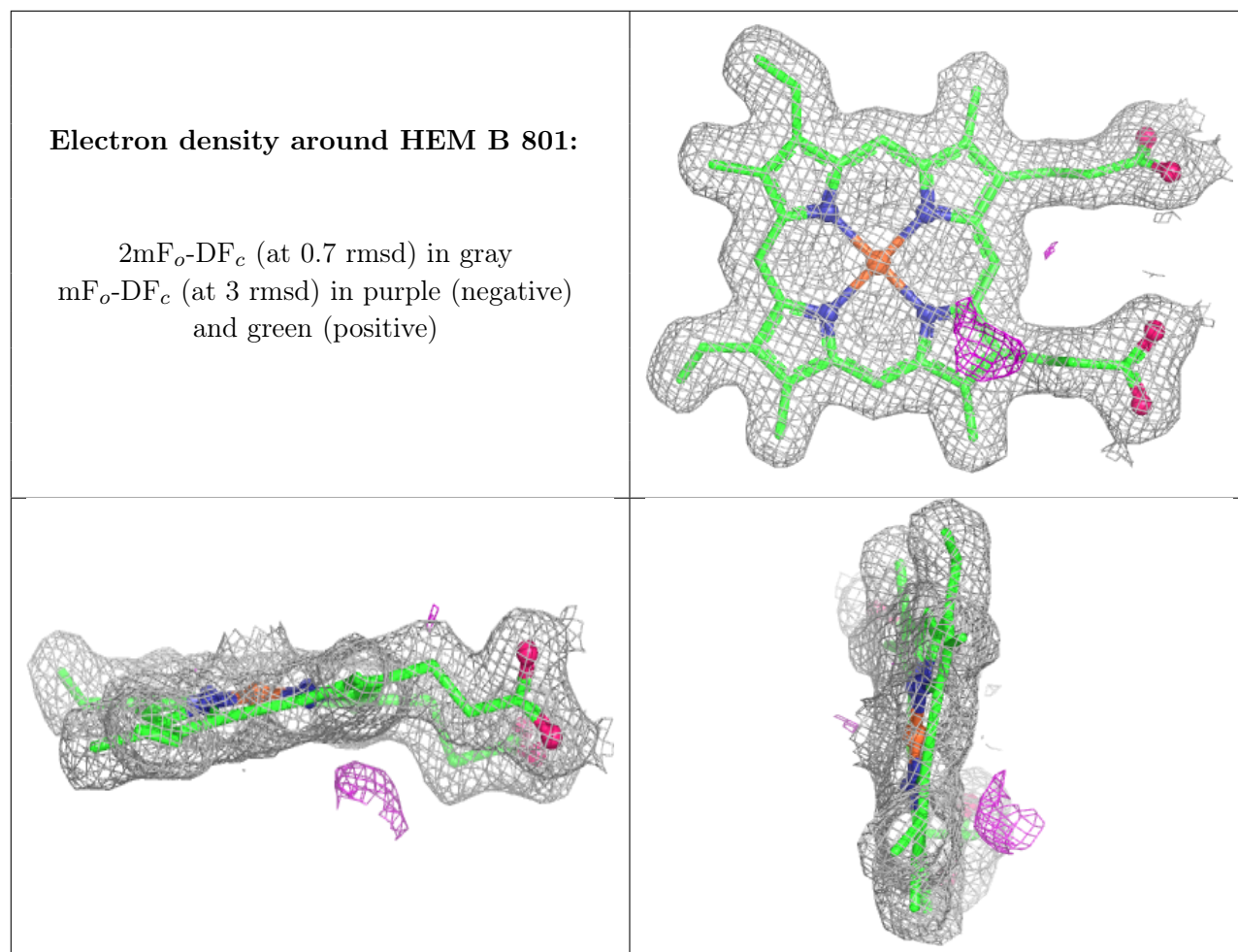
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MPD	A	805	8/8	0.73	0.25	60,64,68,69	0
6	MPD	A	806	8/8	0.85	0.17	44,47,56,59	0
5	PO4	B	804	5/5	0.90	0.09	43,61,70,71	0
4	OXY	A	803	2/2	0.90	0.27	48,48,48,48	0
5	PO4	A	804	5/5	0.90	0.10	58,65,72,75	0
4	OXY	B	803	2/2	0.93	0.26	34,34,34,42	0
2	HEM	A	801	43/43	0.98	0.06	17,21,24,25	0
3	NA	B	802	1/1	0.98	0.05	20,20,20,20	0
3	NA	A	802	1/1	0.99	0.04	19,19,19,19	0
2	HEM	B	801	43/43	0.99	0.05	16,18,20,21	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.