



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 06:47 AM EDT

PDB ID : 5KQH / pdb_00005kqh
Title : Crystal structure of the V293D variant of catalase-peroxidase from *B. pseudo-mallei*
Authors : Loewen, P.C.
Deposited on : 2016-07-06
Resolution : 1.82 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

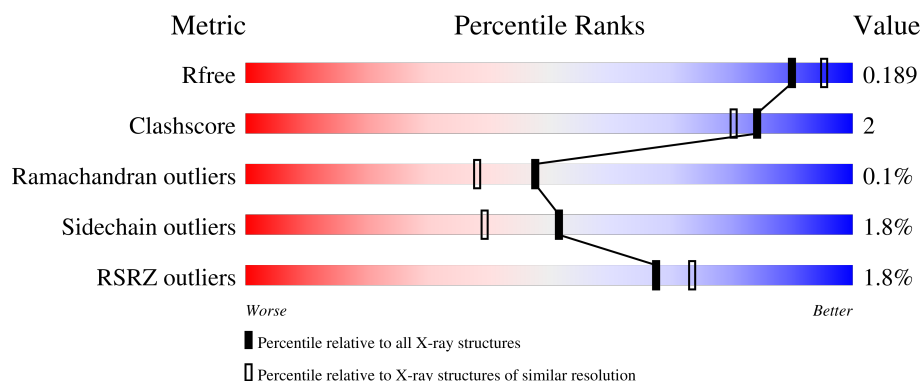
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.82 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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)

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

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12795 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.

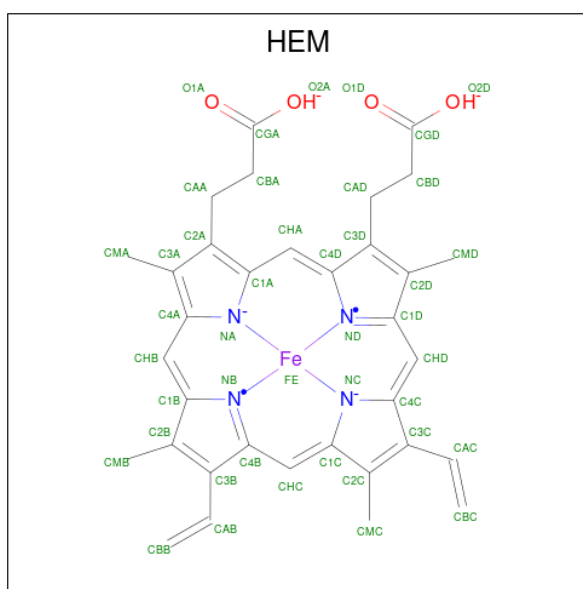
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	8	0
			5566	3510	991	1051	14			
1	B	713	Total	C	N	O	S	0	6	0
			5544	3498	986	1046	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	293	ASP	VAL	conflict	UNP Q3JNW6
B	293	ASP	VAL	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		

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

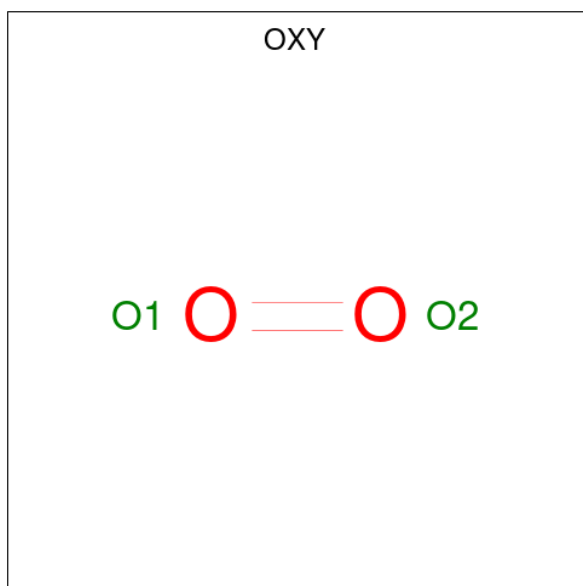
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

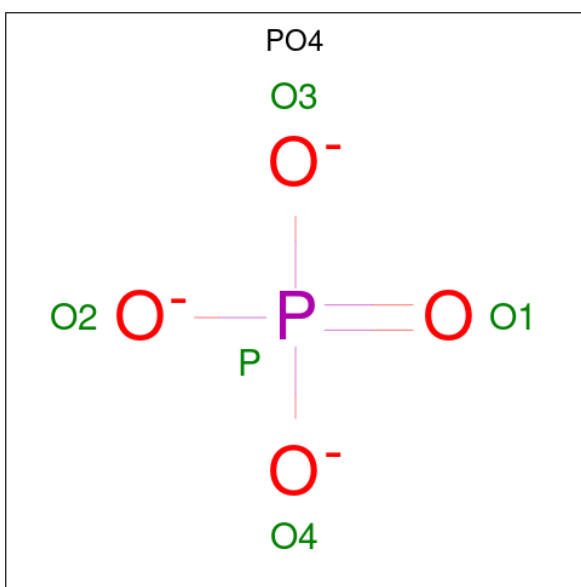
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl		
			1	1	0	0

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



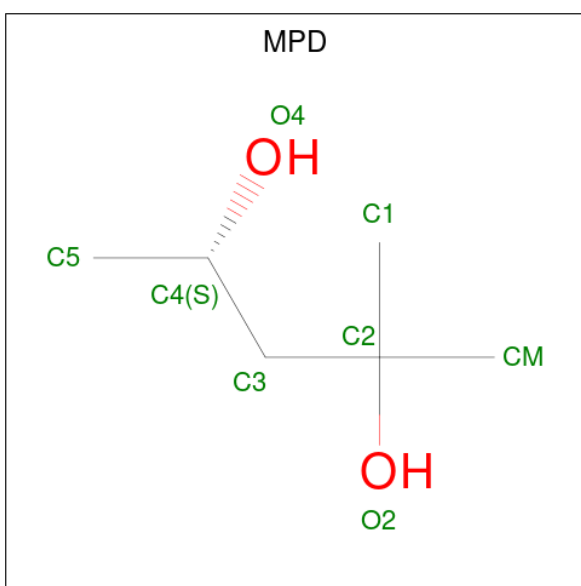
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O		
			2	2	0	0
5	B	1	Total	O		
			2	2	0	0

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



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

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



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

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

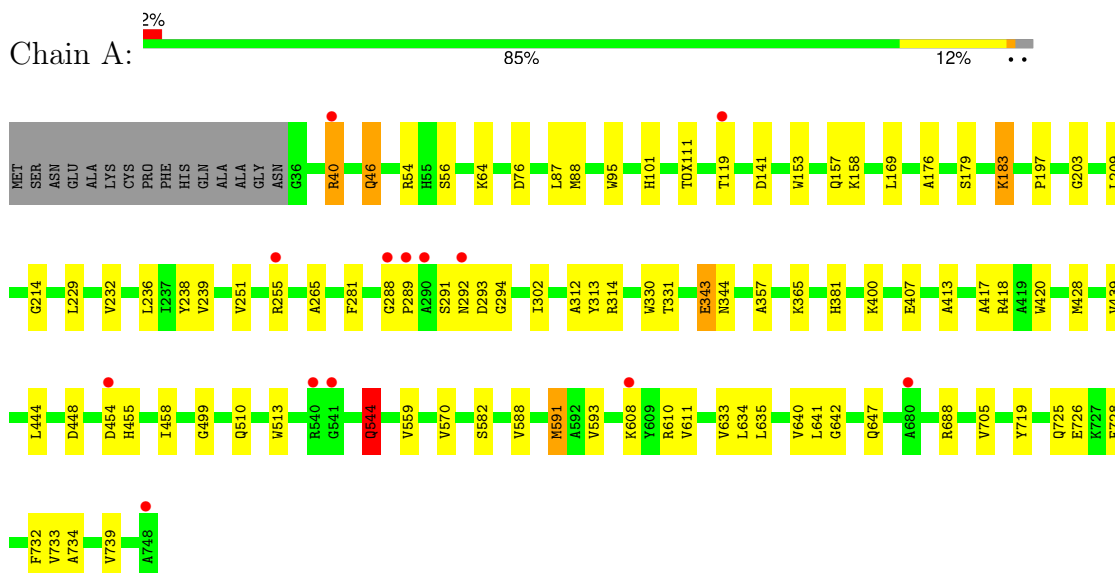
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	786	Total	O	0	0
			786	786		
8	B	764	Total	O	0	0
			764	764		

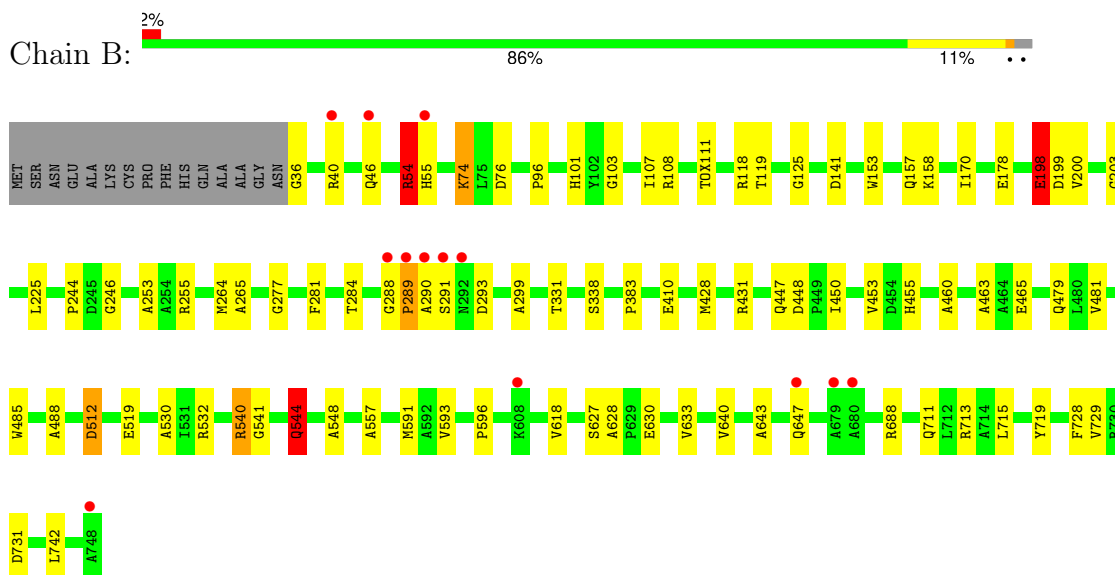
3 Residue-property plots [i](#)

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	100.79Å 113.43Å 174.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.56 – 1.82 47.56 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.56-1.82) 99.8 (47.56-1.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.154 , 0.184 0.165 , 0.189	Depositor DCC
R_{free} test set	8889 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.222	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12795	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 2.76% 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: OXY, PO4, TOX, MPD, NA, HEM, CL

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	1.72	56/5694 (1.0%)	1.30	19/7737 (0.2%)
1	B	1.72	60/5672 (1.1%)	1.30	17/7709 (0.2%)
All	All	1.72	116/11366 (1.0%)	1.30	36/15446 (0.2%)

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	288	GLY	C-O	13.47	1.42	1.24
1	B	288	GLY	C-O	12.49	1.40	1.24
1	B	485	TRP	N-CA	11.65	1.60	1.46
1	A	544	GLN	CD-OE1	9.75	1.42	1.23
1	B	512	ASP	CG-OD2	9.32	1.43	1.25
1	A	365	LYS	N-CA	8.79	1.57	1.46
1	A	203	GLY	C-O	8.67	1.30	1.23
1	A	499	GLY	C-O	8.50	1.32	1.23
1	A	294	GLY	N-CA	-8.35	1.36	1.45
1	B	244	PRO	CA-C	8.18	1.61	1.52
1	B	448	ASP	C-O	7.75	1.27	1.23
1	B	596	PRO	C-O	7.61	1.29	1.24
1	B	36	GLY	N-CA	7.36	1.57	1.45
1	A	183	LYS	C-O	7.31	1.33	1.24
1	A	153	TRP	C-O	-7.15	1.17	1.24
1	B	448	ASP	CA-CB	7.09	1.57	1.52
1	B	557	ALA	N-CA	-7.05	1.37	1.46
1	B	107	ILE	N-CA	6.90	1.54	1.46
1	B	199	ASP	C-O	6.87	1.32	1.23
1	A	239	VAL	C-O	6.75	1.32	1.23
1	B	203	GLY	C-O	6.69	1.28	1.23
1	A	458	ILE	CA-CB	-6.48	1.48	1.54
1	B	101	HIS	N-CA	6.48	1.54	1.46
1	A	688	ARG	CA-C	-6.43	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	647	GLN	CA-C	6.42	1.61	1.53
1	A	232	VAL	N-CA	6.42	1.54	1.46
1	B	544	GLN	CD-NE2	6.36	1.46	1.33
1	A	739	VAL	N-CA	6.35	1.54	1.46
1	A	56	SER	N-CA	6.26	1.54	1.45
1	B	532	ARG	C-O	-6.25	1.16	1.24
1	A	236	LEU	CA-C	6.22	1.60	1.52
1	B	548	ALA	N-CA	6.19	1.53	1.46
1	A	444	LEU	CA-C	-6.18	1.45	1.52
1	B	630	GLU	N-CA	6.17	1.53	1.46
1	A	294	GLY	C-O	6.13	1.29	1.23
1	B	225	LEU	C-O	6.13	1.31	1.23
1	B	512	ASP	CB-CG	6.13	1.67	1.52
1	A	559	VAL	N-CA	6.04	1.53	1.46
1	B	729	VAL	N-CA	6.04	1.53	1.46
1	A	728	PHE	N-CA	6.04	1.53	1.46
1	A	734	ALA	N-CA	-6.02	1.39	1.46
1	B	628	ALA	CA-C	-5.95	1.45	1.52
1	A	229	LEU	C-O	5.92	1.31	1.23
1	B	281	PHE	N-CA	5.92	1.53	1.45
1	A	732	PHE	N-CA	5.91	1.53	1.46
1	A	169	LEU	N-CA	5.89	1.53	1.46
1	A	312	ALA	N-CA	5.82	1.53	1.46
1	A	330	TRP	N-CA	5.79	1.53	1.46
1	B	153	TRP	C-O	-5.78	1.19	1.24
1	B	118	ARG	C-O	5.77	1.30	1.24
1	A	418	ARG	CA-C	-5.75	1.45	1.52
1	A	197	PRO	CA-C	-5.72	1.45	1.52
1	A	705	VAL	N-CA	-5.68	1.39	1.46
1	A	157	GLN	C-O	5.67	1.30	1.24
1	A	725	GLN	CG-CD	5.66	1.66	1.52
1	A	357	ALA	CA-C	-5.65	1.44	1.52
1	B	291	SER	C-O	5.64	1.31	1.24
1	B	742	LEU	C-O	-5.63	1.17	1.24
1	A	582	SER	CA-C	-5.63	1.45	1.53
1	A	642	GLY	N-CA	5.62	1.52	1.45
1	A	448	ASP	CA-CB	5.61	1.57	1.52
1	B	479	GLN	CA-CB	5.60	1.62	1.53
1	B	291	SER	CA-C	5.58	1.60	1.52
1	A	640	VAL	CA-CB	5.57	1.61	1.54
1	B	277	GLY	C-O	-5.57	1.17	1.23
1	A	288	GLY	C-N	5.54	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	253	ALA	C-O	-5.50	1.17	1.24
1	B	627	SER	C-O	5.50	1.30	1.23
1	B	731	ASP	N-CA	-5.48	1.39	1.46
1	B	158	LYS	C-O	5.47	1.30	1.24
1	A	291	SER	CA-C	5.47	1.60	1.52
1	B	410	GLU	CG-CD	5.46	1.65	1.52
1	B	54	ARG	CA-C	-5.46	1.45	1.53
1	B	170	ILE	N-CA	5.45	1.52	1.46
1	B	453	VAL	C-O	-5.44	1.17	1.24
1	A	87	LEU	N-CA	-5.44	1.39	1.46
1	B	463	ALA	N-CA	-5.44	1.39	1.46
1	B	465	GLU	CA-C	5.42	1.59	1.52
1	A	733	VAL	CA-CB	5.41	1.61	1.54
1	A	344	ASN	CA-C	-5.39	1.46	1.52
1	B	530	ALA	N-CA	5.38	1.52	1.46
1	B	338	SER	C-O	5.36	1.29	1.23
1	A	417	ALA	N-CA	5.35	1.52	1.46
1	A	95	TRP	N-CA	5.33	1.53	1.46
1	B	299	ALA	C-O	5.33	1.31	1.24
1	B	465	GLU	C-O	-5.32	1.18	1.24
1	B	688	ARG	CA-C	-5.32	1.46	1.52
1	B	200	VAL	C-O	5.28	1.29	1.24
1	A	588	VAL	N-CA	-5.27	1.40	1.46
1	A	634	LEU	N-CA	-5.27	1.40	1.46
1	B	170	ILE	CA-CB	-5.27	1.48	1.54
1	B	711	GLN	CD-NE2	-5.27	1.22	1.33
1	B	96	PRO	C-O	5.25	1.29	1.23
1	B	715	LEU	C-O	5.24	1.30	1.24
1	B	488	ALA	N-CA	5.23	1.52	1.46
1	B	103	GLY	C-O	5.22	1.29	1.23
1	B	125	GLY	C-O	5.22	1.30	1.23
1	A	641	LEU	CA-CB	-5.21	1.44	1.53
1	B	157	GLN	N-CA	-5.20	1.40	1.46
1	A	454	ASP	CB-CG	5.18	1.65	1.52
1	B	532	ARG	CD-NE	-5.15	1.39	1.46
1	A	209	LEU	N-CA	-5.14	1.39	1.46
1	A	413	ALA	N-CA	5.10	1.52	1.46
1	B	618	VAL	N-CA	-5.10	1.39	1.46
1	B	643	ALA	CA-CB	-5.10	1.44	1.53
1	A	281	PHE	N-CA	5.09	1.52	1.45
1	B	108	ARG	CD-NE	-5.09	1.39	1.46
1	A	251	VAL	CA-CB	5.08	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	GLY	C-O	-5.07	1.17	1.24
1	B	481	VAL	C-O	5.07	1.30	1.24
1	B	383	PRO	CA-CB	5.07	1.60	1.53
1	A	641	LEU	CA-C	5.05	1.59	1.52
1	B	640	VAL	C-O	-5.05	1.18	1.24
1	A	570	VAL	C-O	5.03	1.28	1.24
1	A	176	ALA	C-O	5.02	1.29	1.24
1	A	420	TRP	N-CA	5.01	1.52	1.46

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	293	ASP	N-CA-CB	8.97	123.60	110.06
1	A	293	ASP	N-CA-CB	8.42	122.77	110.06
1	B	591	MET	CG-SD-CE	-7.55	84.28	100.90
1	B	541	GLY	N-CA-C	-7.40	98.78	112.62
1	B	46	GLN	CB-CG-CD	7.13	124.72	112.60
1	A	54	ARG	CG-CD-NE	-6.83	96.97	112.00
1	A	46	GLN	N-CA-C	-6.83	101.52	110.53
1	B	288	GLY	CA-C-N	6.56	126.58	119.89
1	B	288	GLY	C-N-CA	6.56	126.58	119.89
1	A	343	GLU	CA-CB-CG	6.52	127.14	114.10
1	A	293	ASP	CA-C-N	6.16	128.37	122.27
1	A	293	ASP	C-N-CA	6.16	128.37	122.27
1	B	460	ALA	N-CA-C	6.13	117.96	111.28
1	A	365	LYS	N-CA-C	6.00	118.59	111.33
1	A	591	MET	CG-SD-CE	-5.84	88.05	100.90
1	B	46	GLN	N-CA-C	-5.77	102.91	110.53
1	A	302	ILE	CB-CA-C	5.75	121.08	112.16
1	B	46	GLN	CA-CB-CG	5.67	125.45	114.10
1	A	179	SER	CA-CB-OG	5.63	122.36	111.10
1	B	246	GLY	N-CA-C	5.60	123.05	115.32
1	A	331	THR	N-CA-C	5.57	118.33	109.81
1	B	512	ASP	CA-CB-CG	5.54	118.14	112.60
1	B	198	GLU	CA-CB-CG	5.49	125.09	114.10
1	A	46	GLN	CB-CG-CD	5.46	121.88	112.60
1	A	407	GLU	CG-CD-OE1	5.34	130.69	118.40
1	A	544	GLN	CG-CD-NE2	-5.34	108.39	116.40
1	B	331	THR	N-CA-C	5.30	118.22	109.85
1	A	46	GLN	CA-CB-CG	5.25	124.59	114.10
1	A	439	VAL	N-CA-C	5.24	114.67	108.96
1	B	450	ILE	CB-CA-C	-5.22	104.85	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	713	ARG	N-CA-C	-5.17	105.65	111.28
1	A	635	LEU	N-CA-C	-5.11	105.79	111.36
1	B	290	ALA	CA-C-N	5.08	127.59	120.28
1	B	290	ALA	C-N-CA	5.08	127.59	120.28
1	A	288	GLY	CA-C-N	5.06	125.06	119.90
1	A	288	GLY	C-N-CA	5.06	125.06	119.90

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	5566	0	5359	19	0
1	B	5544	0	5343	22	0
2	A	43	0	30	0	0
2	B	43	0	30	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	1	0
6	A	5	0	0	1	0
6	B	5	0	0	0	0
7	A	24	0	42	7	0
7	B	8	0	14	2	0
8	A	786	0	0	9	0
8	B	764	0	0	11	0
All	All	12795	0	10818	50	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 (50) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:808:MPD:H11	8:A:1330:HOH:O	1.71	0.90
1:B:647:GLN:HG2	8:B:1417:HOH:O	1.75	0.85
1:B:289:PRO:HD2	8:B:1562:HOH:O	1.77	0.85
1:B:512:ASP:OD1	8:B:901:HOH:O	1.94	0.85
1:B:76:ASP:OD2	8:B:902:HOH:O	1.96	0.82
1:B:519:GLU:OE1	8:B:903:HOH:O	1.97	0.82
1:A:119[B]:THR:HG21	8:A:1074:HOH:O	1.80	0.81
1:B:198:GLU:OE1	8:B:904:HOH:O	2.08	0.71
7:B:805:MPD:HM2	7:B:805:MPD:H52	1.81	0.63
5:B:803:OXY:O2	8:B:905:HOH:O	2.16	0.63
1:B:54:ARG:HB3	1:B:55:HIS:CD2	2.35	0.61
7:A:806:MPD:O4	7:A:806:MPD:H12	2.00	0.61
1:A:610:ARG:HG3	1:A:611:VAL:HG23	1.82	0.60
1:A:633[A]:VAL:CG2	1:A:719:TYR:CZ	2.86	0.58
1:B:540:ARG:NE	1:B:540:ARG:HA	2.18	0.58
1:A:255[B]:ARG:HG2	8:A:905:HOH:O	2.04	0.57
7:A:806:MPD:O4	7:A:806:MPD:C1	2.52	0.56
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.90	0.55
1:A:593:VAL:HG13	8:A:1042:HOH:O	2.07	0.55
1:B:178:GLU:OE1	8:B:906:HOH:O	2.18	0.54
7:A:808:MPD:C1	8:A:1330:HOH:O	2.45	0.51
1:B:540:ARG:HA	1:B:540:ARG:CZ	2.40	0.51
1:A:455:HIS:CE1	1:A:544:GLN:HG3	2.46	0.51
1:A:400:LYS:NZ	8:A:916:HOH:O	2.44	0.50
1:A:119[A]:THR:CG2	1:A:265:ALA:HB2	2.42	0.50
1:B:284:THR:HG22	2:B:801:HEM:HAA1	1.94	0.50
1:B:255:ARG:HB2	8:B:1604:HOH:O	2.11	0.50
1:B:119[B]:THR:HG23	1:B:593:VAL:HG11	1.95	0.47
1:A:343:GLU:HG3	8:A:1508:HOH:O	2.14	0.47
1:B:119[A]:THR:CG2	1:B:265:ALA:HB2	2.45	0.46
1:A:76:ASP:OD2	8:A:903:HOH:O	2.20	0.46
1:A:158:LYS:HD2	7:A:808:MPD:H13	1.97	0.46
7:B:805:MPD:H52	7:B:805:MPD:CM	2.44	0.46
1:A:119[A]:THR:HG22	1:A:265:ALA:HB2	1.99	0.45
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.17	0.44
1:A:40:ARG:NH1	8:A:930:HOH:O	2.51	0.44
7:A:807:MPD:HM1	7:A:807:MPD:O4	2.18	0.44
7:A:808:MPD:H11	7:A:808:MPD:H52	2.00	0.44
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.99	0.44
1:B:512:ASP:CB	8:B:901:HOH:O	2.66	0.43
1:A:313:TYR:CZ	1:A:314:ARG:HD3	2.54	0.43
1:B:74:LYS:HD3	8:B:1443:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:MET:O	1:B:265:ALA:HB3	2.20	0.42
1:A:381:HIS:ND1	6:A:805:PO4:O4	2.42	0.41
1:A:510:GLN:HG2	1:A:513:TRP:CH2	2.56	0.41
1:A:88:MET:HB3	1:A:101:HIS:CE1	2.55	0.41
1:B:633[A]:VAL:HG22	1:B:719:TYR:CZ	2.55	0.41
1:B:633[B]:VAL:HG12	1:B:728:PHE:CD1	2.56	0.40
1:B:455:HIS:CE1	1:B:544:GLN:HG3	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	717/728 (98%)	708 (99%)	8 (1%)	1 (0%)	48	38
1	B	715/728 (98%)	707 (99%)	8 (1%)	0	100	100
All	All	1432/1456 (98%)	1415 (99%)	16 (1%)	1 (0%)	48	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	292	ASN

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	556/560 (99%)	544 (98%)	12 (2%)	45	30
1	B	554/560 (99%)	545 (98%)	9 (2%)	55	44
All	All	1110/1120 (99%)	1089 (98%)	21 (2%)	51	37

All (21) 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	141	ASP
1	A	183	LYS
1	A	289	PRO
1	A	428	MET
1	A	544	GLN
1	A	591	MET
1	A	608	LYS
1	A	726[A]	GLU
1	A	726[B]	GLU
1	B	40	ARG
1	B	54	ARG
1	B	74	LYS
1	B	141	ASP
1	B	198	GLU
1	B	289	PRO
1	B	428	MET
1	B	540	ARG
1	B	544	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	B	406	HIS
1	B	520	GLN
1	B	647	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 ⓘ

4 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[B]	-	14,17,18	1.76	4 (28%)	12,23,25	1.56	3 (25%)
1	TOX	A	111[A]	2	14,17,18	1.76	4 (28%)	12,23,25	1.56	3 (25%)
1	TOX	B	111[A]	2	14,17,18	1.96	3 (21%)	12,23,25	2.71	5 (41%)
1	TOX	B	111[B]	-	14,17,18	1.96	3 (21%)	12,23,25	2.71	5 (41%)

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[B]	-	-	3/5/8/10	0/2/2/2
1	TOX	A	111[A]	2	-	3/5/8/10	0/2/2/2
1	TOX	B	111[A]	2	-	3/5/8/10	0/2/2/2
1	TOX	B	111[B]	-	-	3/5/8/10	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[A]	TOX	CH2-CZ2	4.32	1.46	1.38
1	B	111[B]	TOX	CH2-CZ2	4.32	1.46	1.38
1	B	111[A]	TOX	O-C	3.76	1.34	1.20
1	B	111[B]	TOX	O-C	3.76	1.34	1.20
1	A	111[A]	TOX	CD2-CE2	3.56	1.45	1.41
1	A	111[B]	TOX	CD2-CE2	3.56	1.45	1.41
1	A	111[A]	TOX	CE2-NE1	-3.36	1.33	1.39
1	A	111[B]	TOX	CE2-NE1	-3.36	1.33	1.39
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111[A]	TOX	CE2-NE1	-2.72	1.34	1.39
1	B	111[B]	TOX	CE2-NE1	-2.72	1.34	1.39
1	A	111[A]	TOX	CH2-CZ3	2.38	1.43	1.38
1	A	111[B]	TOX	CH2-CZ3	2.38	1.43	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111[A]	TOX	CB-CG-CD1	-4.38	120.57	126.67
1	B	111[B]	TOX	CB-CG-CD1	-4.38	120.57	126.67
1	B	111[A]	TOX	CH2-CZ3-CE3	4.18	125.40	120.24
1	B	111[B]	TOX	CH2-CZ3-CE3	4.18	125.40	120.24
1	B	111[A]	TOX	CZ3-CH2-CZ2	-3.97	115.34	120.24
1	B	111[B]	TOX	CZ3-CH2-CZ2	-3.97	115.34	120.24
1	B	111[A]	TOX	CZ2-CE2-NE1	3.74	135.32	129.37
1	B	111[B]	TOX	CZ2-CE2-NE1	3.74	135.32	129.37
1	B	111[A]	TOX	CB-CG-CD2	3.58	133.57	126.70
1	B	111[B]	TOX	CB-CG-CD2	3.58	133.57	126.70
1	A	111[A]	TOX	CZ3-CE3-CD2	-2.40	115.45	119.80
1	A	111[B]	TOX	CZ3-CE3-CD2	-2.40	115.45	119.80
1	A	111[A]	TOX	CE3-CD2-CE2	2.14	121.70	119.24
1	A	111[B]	TOX	CE3-CD2-CE2	2.14	121.70	119.24
1	A	111[A]	TOX	CH2-CZ3-CE3	2.01	122.71	120.24
1	A	111[B]	TOX	CH2-CZ3-CE3	2.01	122.71	120.24

There are no chirality outliers.

All (12) 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[A]	TOX	N-CA-CB-CG
1	B	111[A]	TOX	C-CA-CB-CG
1	B	111[B]	TOX	N-CA-CB-CG
1	B	111[B]	TOX	C-CA-CB-CG
1	B	111[A]	TOX	CA-CB-CG-CD2
1	B	111[B]	TOX	CA-CB-CG-CD2
1	A	111[A]	TOX	CA-CB-CG-CD2
1	A	111[B]	TOX	CA-CB-CG-CD2

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 13 ligands modelled in this entry, 3 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
2	HEM	B	801	1	50,50,50	1.71	11 (22%)	67,82,82	1.82	20 (29%)
6	PO4	B	804	-	4,4,4	0.73	0	6,6,6	2.27	2 (33%)
7	MPD	A	807	-	7,7,7	0.70	0	9,10,10	1.24	0
5	OXY	A	804	-	1,1,1	0.06	0	-		
5	OXY	B	803	-	1,1,1	0.33	0	-		
2	HEM	A	801	1	50,50,50	1.89	14 (28%)	67,82,82	1.63	13 (19%)
7	MPD	A	806	-	7,7,7	1.02	1 (14%)	9,10,10	0.85	0
6	PO4	A	805	-	4,4,4	0.78	0	6,6,6	1.31	1 (16%)
7	MPD	B	805	-	7,7,7	1.04	1 (14%)	9,10,10	2.13	3 (33%)
7	MPD	A	808	-	7,7,7	0.94	0	9,10,10	1.71	2 (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
2	HEM	B	801	1	-	3/14/54/54	-
7	MPD	A	807	-	-	1/5/5/5	-
2	HEM	A	801	1	-	2/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MPD	A	806	-	-	3/5/5/5	-
7	MPD	B	805	-	-	1/5/5/5	-
7	MPD	A	808	-	-	4/5/5/5	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C4D-ND	-4.84	1.31	1.40
2	B	801	HEM	FE-NB	4.19	2.07	1.94
2	B	801	HEM	C1B-NB	-4.15	1.33	1.40
2	A	801	HEM	FE-NC	3.90	2.08	1.95
2	A	801	HEM	FE-NB	3.59	2.06	1.94
2	A	801	HEM	FE-NA	3.55	2.06	1.95
2	B	801	HEM	CMA-C3A	3.53	1.58	1.50
2	A	801	HEM	CHD-C4C	-3.44	1.31	1.38
2	A	801	HEM	C1C-NC	-3.37	1.33	1.39
2	A	801	HEM	C1B-NB	-3.36	1.34	1.40
2	B	801	HEM	CHC-C4B	-3.26	1.31	1.39
2	A	801	HEM	CHD-C1D	3.11	1.46	1.39
2	B	801	HEM	C4B-NB	-2.99	1.33	1.38
2	A	801	HEM	C1D-ND	-2.99	1.33	1.38
2	B	801	HEM	C1C-C2C	2.93	1.51	1.45
2	B	801	HEM	CMD-C2D	-2.84	1.44	1.50
2	A	801	HEM	O1D-CGD	2.73	1.31	1.22
2	B	801	HEM	C4D-ND	-2.62	1.35	1.40
2	A	801	HEM	O1A-CGA	2.51	1.30	1.22
2	B	801	HEM	O2D-CGD	-2.44	1.22	1.30
2	B	801	HEM	CMB-C2B	2.44	1.55	1.50
2	A	801	HEM	FE-ND	2.43	2.02	1.94
2	A	801	HEM	CBA-CGA	2.40	1.56	1.50
2	A	801	HEM	C4B-NB	-2.29	1.34	1.38
2	B	801	HEM	O2A-CGA	-2.09	1.23	1.30
7	B	805	MPD	O2-C2	-2.06	1.39	1.44
7	A	806	MPD	O2-C2	2.01	1.49	1.44

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	C4B-C3B-C2B	-4.94	102.74	107.28
2	B	801	HEM	CMD-C2D-C1D	4.84	132.60	125.03
6	B	804	PO4	O3-P-O2	4.79	122.81	107.91
2	A	801	HEM	CMB-C2B-C1B	-4.50	118.00	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	C4C-C3C-C2C	-4.39	103.01	106.81
2	A	801	HEM	CAA-CBA-CGA	-4.06	102.89	113.67
7	B	805	MPD	CM-C2-C1	3.97	119.51	110.63
7	A	808	MPD	O4-C4-C3	-3.70	96.64	111.35
2	B	801	HEM	CBD-CAD-C3D	3.58	122.43	112.53
7	B	805	MPD	O2-C2-C3	-3.45	96.37	109.27
2	B	801	HEM	CAD-C3D-C2D	-3.33	121.64	127.87
2	B	801	HEM	CAD-C3D-C4D	3.12	130.13	124.70
2	B	801	HEM	C1B-NB-C4B	3.10	108.88	105.21
7	B	805	MPD	O2-C2-CM	-3.10	98.33	107.99
2	B	801	HEM	C4C-CHD-C1D	-3.08	119.48	126.02
2	A	801	HEM	C3B-C2B-C1B	3.07	108.72	106.41
2	A	801	HEM	O2A-CGA-CBA	2.93	123.26	114.00
2	A	801	HEM	CBD-CAD-C3D	2.92	120.60	112.53
2	B	801	HEM	C2A-C1A-NA	-2.85	107.00	110.15
2	B	801	HEM	C3B-C4B-NB	-2.81	107.45	109.47
2	B	801	HEM	CHD-C1D-ND	2.73	127.36	124.42
2	B	801	HEM	CMA-C3A-C4A	-2.69	121.32	125.42
2	B	801	HEM	CHD-C4C-C3C	-2.66	120.73	125.21
2	B	801	HEM	CAA-CBA-CGA	-2.64	106.68	113.67
2	B	801	HEM	C1D-C2D-C3D	-2.61	104.23	106.98
2	A	801	HEM	C4C-C3C-C2C	2.52	109.00	106.81
2	B	801	HEM	CHD-C1D-C2D	-2.51	121.07	125.03
2	B	801	HEM	CMA-C3A-C2A	2.40	130.71	125.62
6	A	805	PO4	O3-P-O2	2.28	115.02	107.91
7	A	808	MPD	O2-C2-CM	-2.28	100.88	107.99
2	A	801	HEM	CHB-C1B-NB	2.19	127.07	124.37
2	B	801	HEM	CAA-C2A-C3A	-2.17	122.20	127.07
2	B	801	HEM	CAA-C2A-C1A	2.15	129.15	124.94
2	A	801	HEM	C3D-C4D-ND	2.14	112.52	110.17
2	A	801	HEM	C3C-C2C-C1C	-2.14	105.02	107.05
2	B	801	HEM	O2A-CGA-CBA	2.12	120.69	114.00
2	A	801	HEM	O2D-CGD-CBD	2.11	120.66	114.00
2	A	801	HEM	CHD-C1D-ND	2.09	126.67	124.42
2	A	801	HEM	CMD-C2D-C1D	2.03	128.21	125.03
6	B	804	PO4	O3-P-O1	-2.03	103.78	110.95
2	B	801	HEM	CHC-C4B-NB	2.01	126.59	124.42

There are no chirality outliers.

All (14) torsion outliers are listed below:

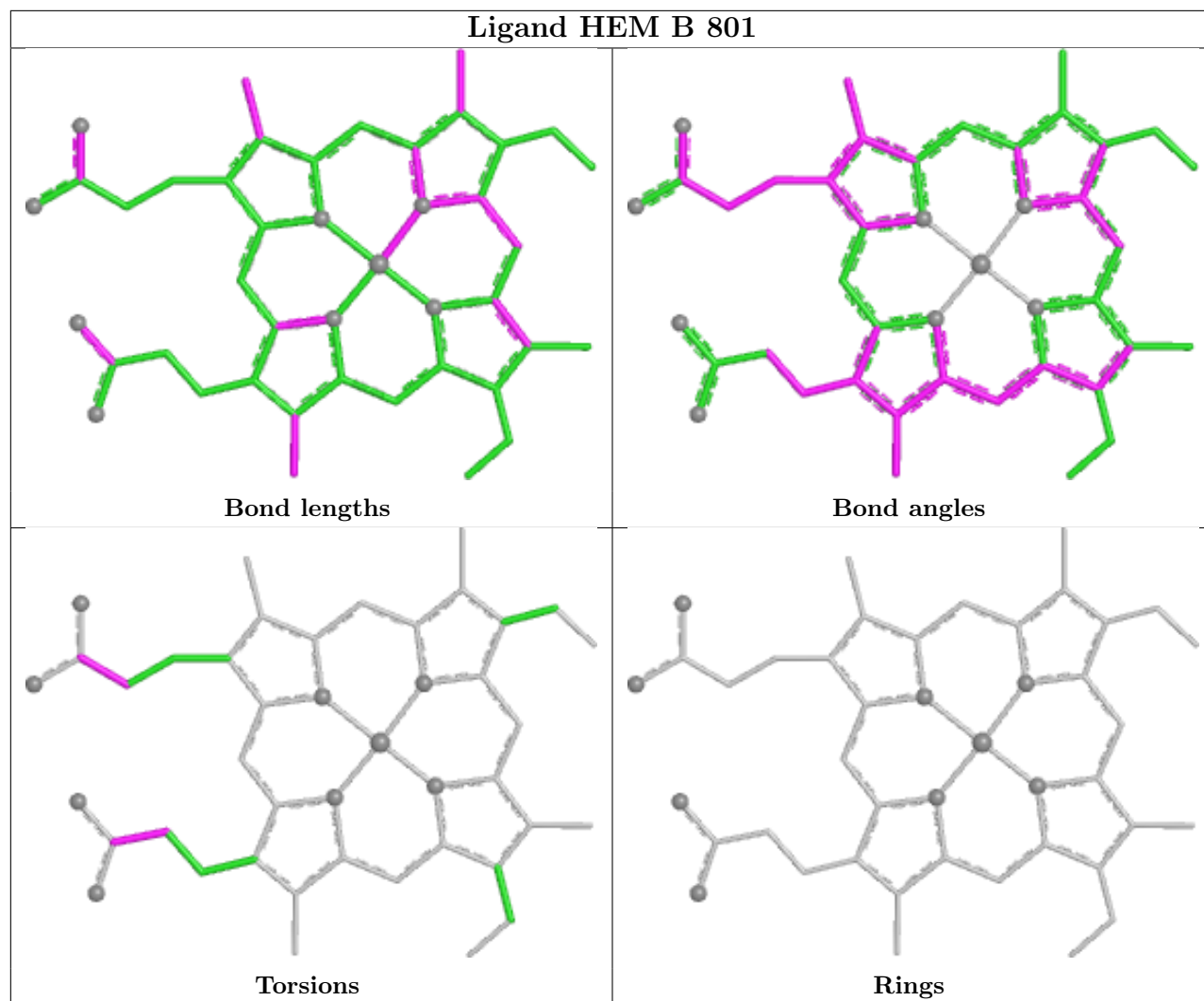
Mol	Chain	Res	Type	Atoms
7	A	806	MPD	C1-C2-C3-C4
7	A	806	MPD	O2-C2-C3-C4
7	A	808	MPD	C2-C3-C4-O4
7	A	808	MPD	C2-C3-C4-C5
7	A	808	MPD	O2-C2-C3-C4
7	A	806	MPD	CM-C2-C3-C4
7	A	808	MPD	C1-C2-C3-C4
2	A	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O1A
2	A	801	HEM	CAA-CBA-CGA-O1A
7	A	807	MPD	O2-C2-C3-C4
7	B	805	MPD	O2-C2-C3-C4
2	B	801	HEM	CAD-CBD-CGD-O1D

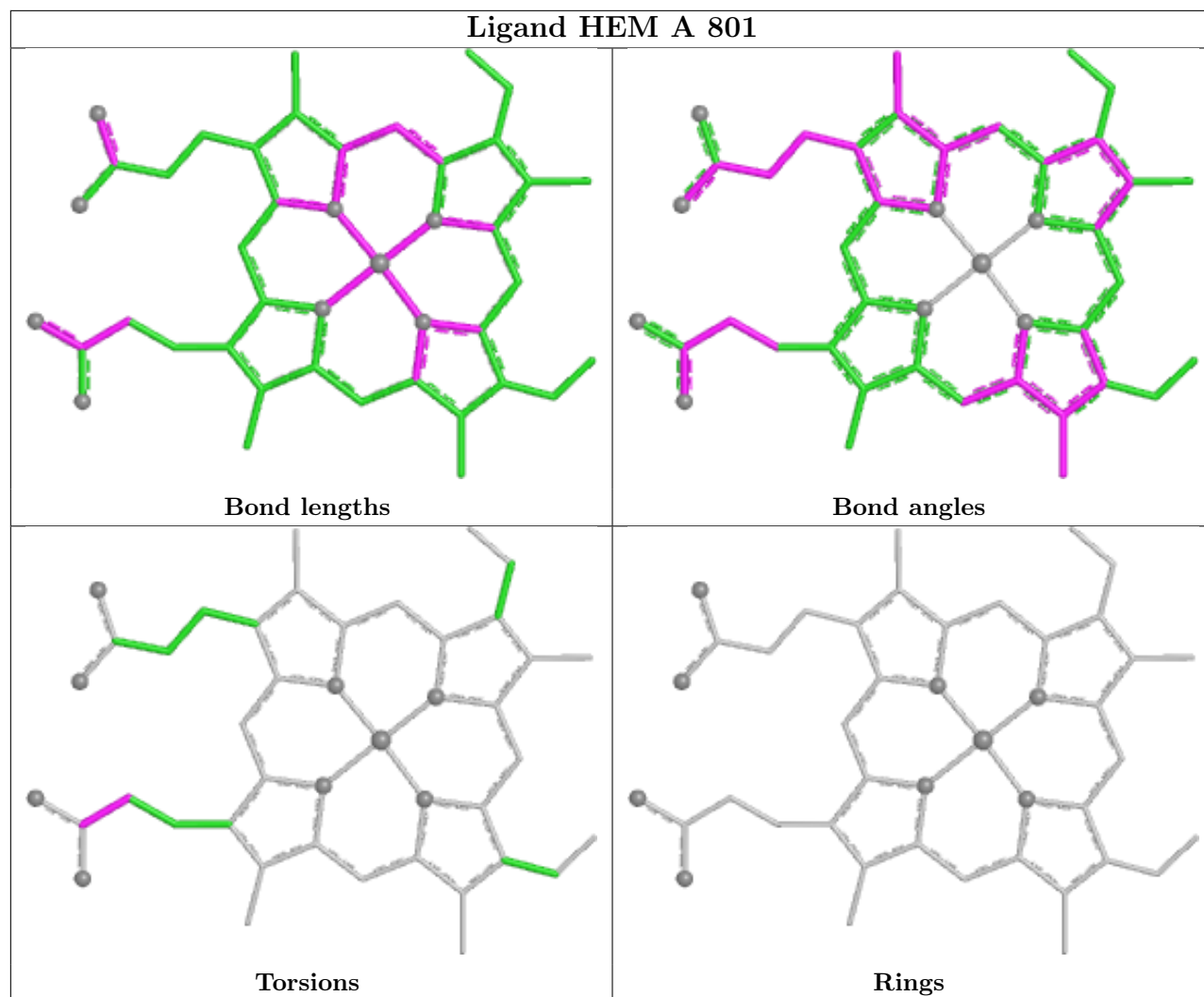
There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	HEM	1	0
7	A	807	MPD	1	0
5	B	803	OXY	1	0
7	A	806	MPD	2	0
6	A	805	PO4	1	0
7	B	805	MPD	2	0
7	A	808	MPD	4	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	-0.39	13 (1%) 67 73	8, 20, 38, 73	7 (0%)
1	B	712/728 (97%)	-0.44	13 (1%) 67 73	8, 19, 36, 72	5 (0%)
All	All	1424/1456 (97%)	-0.42	26 (1%) 67 73	8, 20, 37, 73	12 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	4.7
1	A	292	ASN	4.1
1	B	748	ALA	3.5
1	A	541	GLY	3.5
1	A	289	PRO	3.3
1	B	289	PRO	3.1
1	A	290	ALA	3.0
1	B	55	HIS	2.8
1	B	292	ASN	2.8
1	A	680	ALA	2.7
1	B	679	ALA	2.6
1	A	40	ARG	2.6
1	B	647	GLN	2.4
1	B	680	ALA	2.4
1	A	540	ARG	2.4
1	A	255[A]	ARG	2.4
1	B	40	ARG	2.4
1	A	288	GLY	2.3
1	A	608	LYS	2.2
1	B	290	ALA	2.2
1	A	119[A]	THR	2.2
1	B	288	GLY	2.2
1	B	608	LYS	2.2
1	A	454	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	291	SER	2.1
1	B	46	GLN	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	B	111[A]	16/17	0.97	0.05	12,15,22,22	1
1	TOX	B	111[B]	16/17	0.97	0.05	12,15,18,22	1
1	TOX	A	111[A]	16/17	0.98	0.05	13,15,21,27	1
1	TOX	A	111[B]	16/17	0.98	0.05	13,15,18,21	1

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	PO4	A	805	5/5	0.69	0.16	53,75,81,85	0
7	MPD	A	807	8/8	0.76	0.31	72,78,82,85	0
7	MPD	B	805	8/8	0.78	0.28	46,57,77,77	0
7	MPD	A	806	8/8	0.88	0.14	27,36,46,50	0
6	PO4	B	804	5/5	0.89	0.10	37,54,55,59	0
7	MPD	A	808	8/8	0.91	0.13	33,36,53,55	0
5	OXY	B	803	2/2	0.91	0.21	30,30,30,32	0
5	OXY	A	804	2/2	0.93	0.20	37,37,37,47	0
4	CL	A	803	1/1	0.98	0.07	32,32,32,32	0
2	HEM	B	801	43/43	0.99	0.05	13,14,16,17	0
2	HEM	A	801	43/43	0.99	0.05	12,15,18,18	0
3	NA	B	802	1/1	1.00	0.04	15,15,15,15	0

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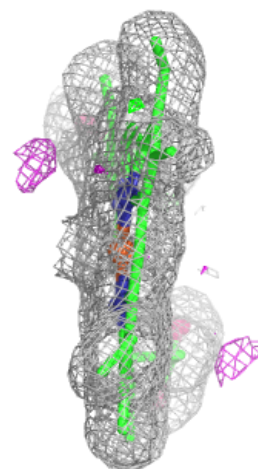
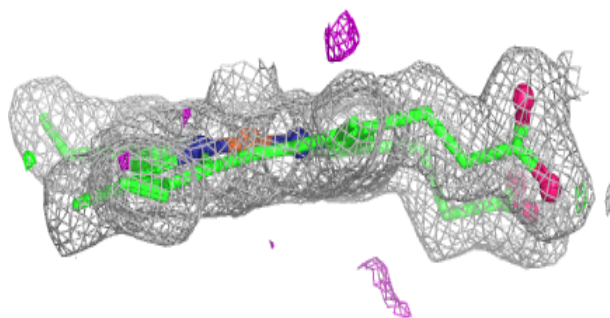
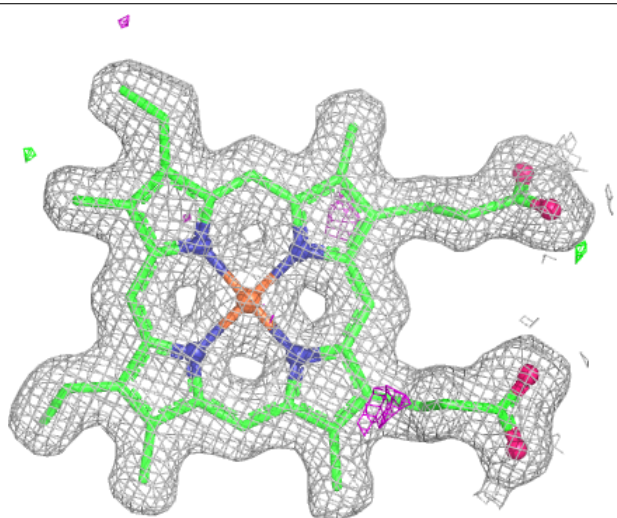
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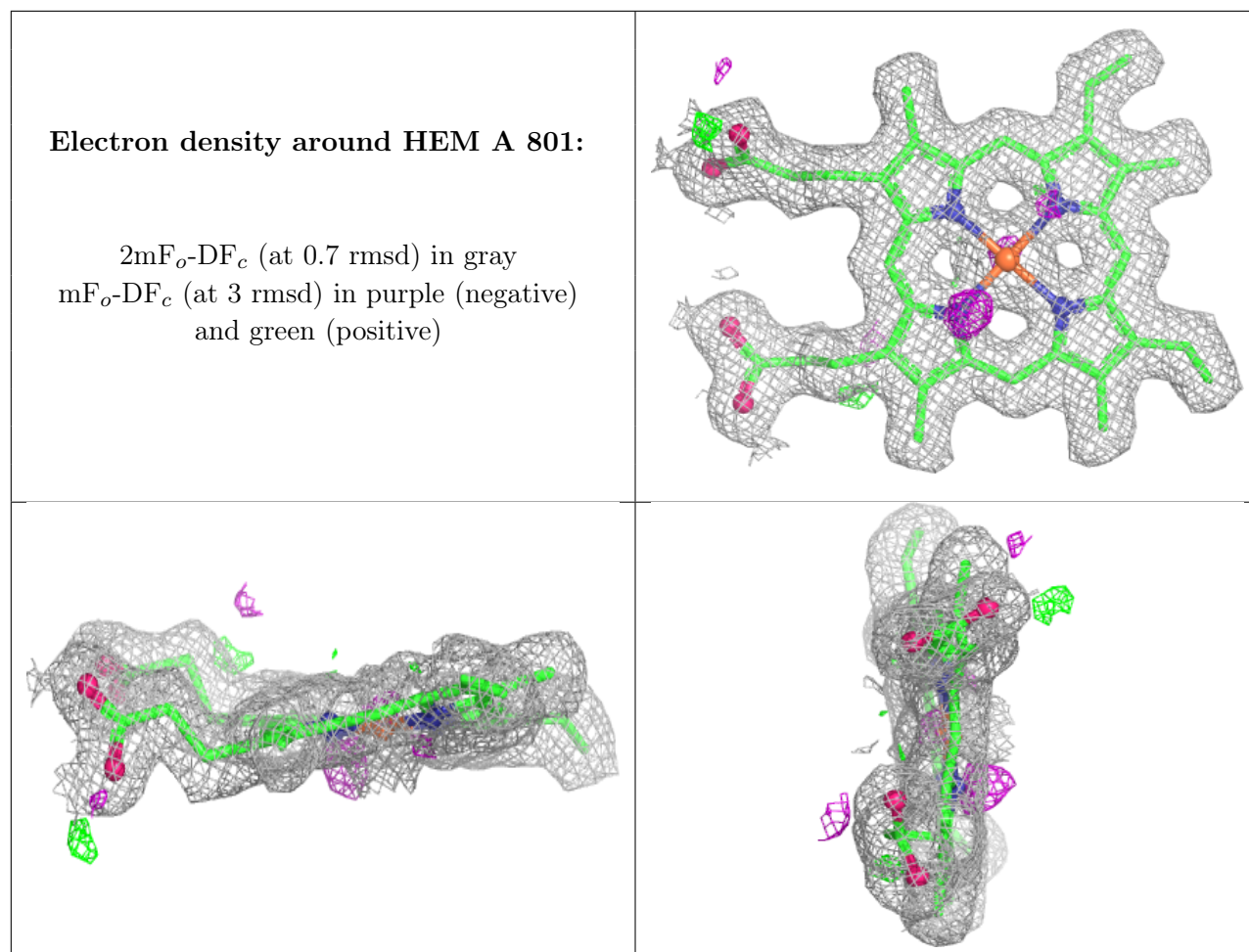
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	A	802	1/1	1.00	0.06	15,15,15,15	0

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 B 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 ⓘ

There are no such residues in this entry.