



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 05:32 PM EDT

PDB ID : 5SYH / pdb_00005syh
Title : Structure of D141A variant of B. pseudomallei KatG
Authors : Loewen, P.C.
Deposited on : 2016-08-11
Resolution : 1.65 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

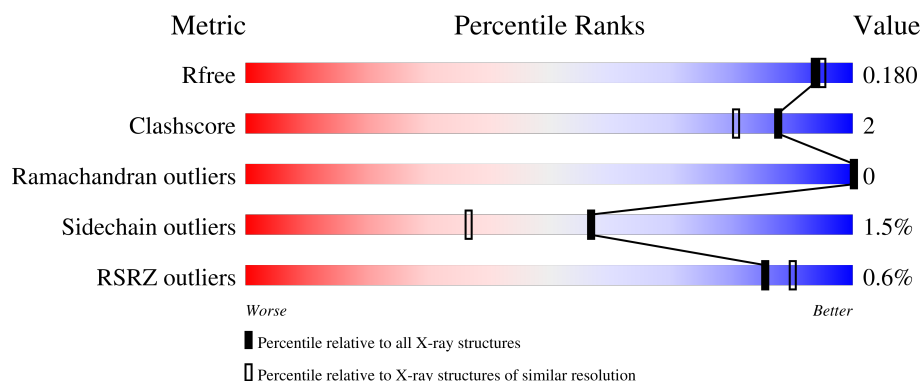
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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	% 85% 13% ..
1	B	728	% 83% 13% ...

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	-	-
7	PO4	B	807	-	X	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12791 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.

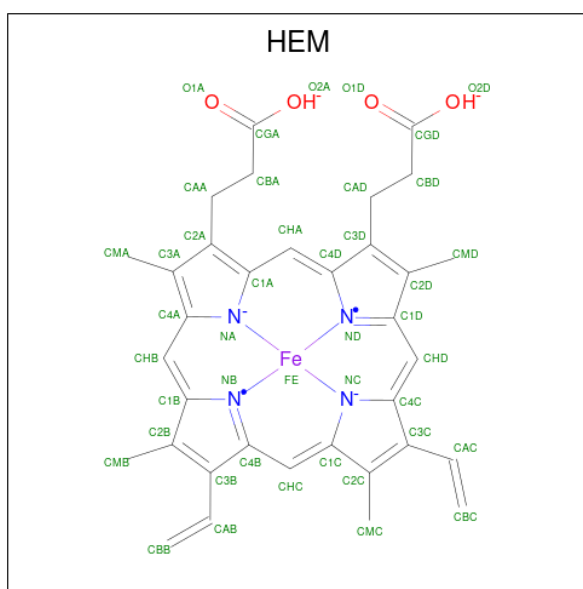
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	7	0
			5543	3500	991	1038	14			
1	B	713	Total	C	N	O	S	0	6	0
			5530	3496	982	1038	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	ALA	ASP	engineered mutation	UNP Q3JNW6
B	141	ALA	ASP	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		

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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

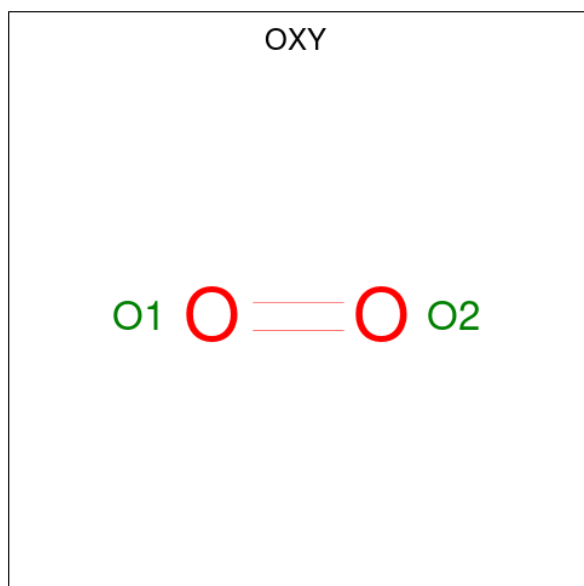
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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).

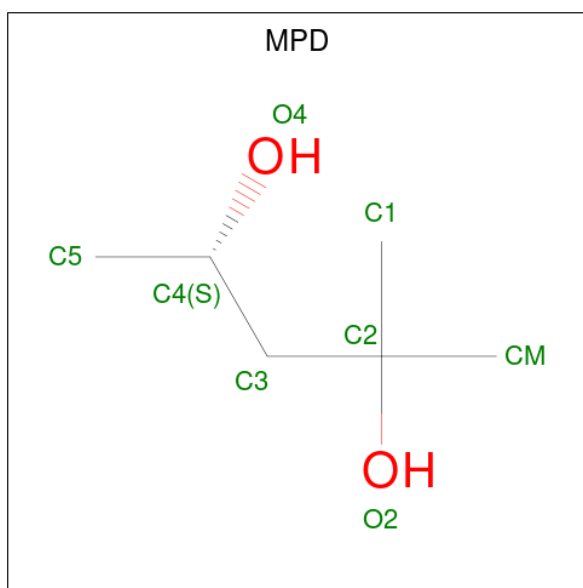
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl		
			1	1	0	0
4	B	1	Total	Cl		
			1	1	0	0

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



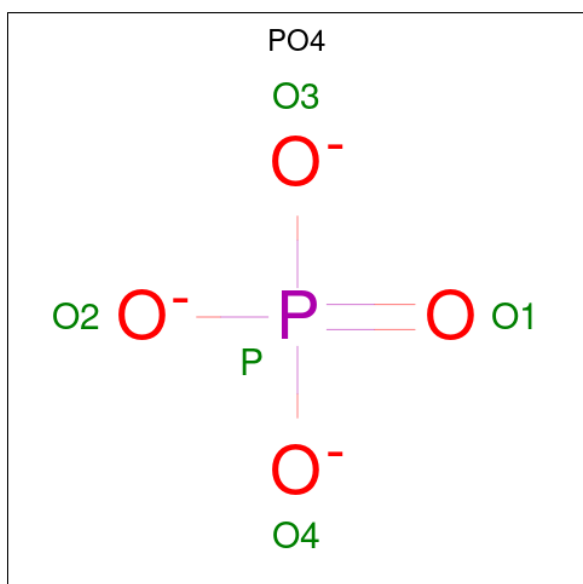
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O		
			2	2	0	0
5	B	1	Total	O		
			2	2	0	0

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

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

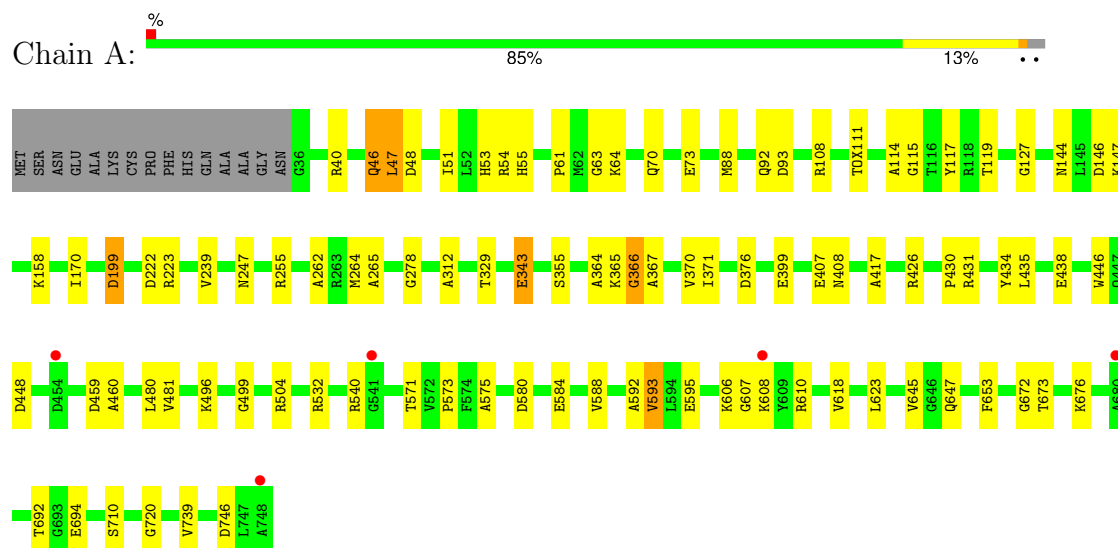
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	784	Total	O	0	0
			784	784		
8	B	798	Total	O	0	0
			798	798		

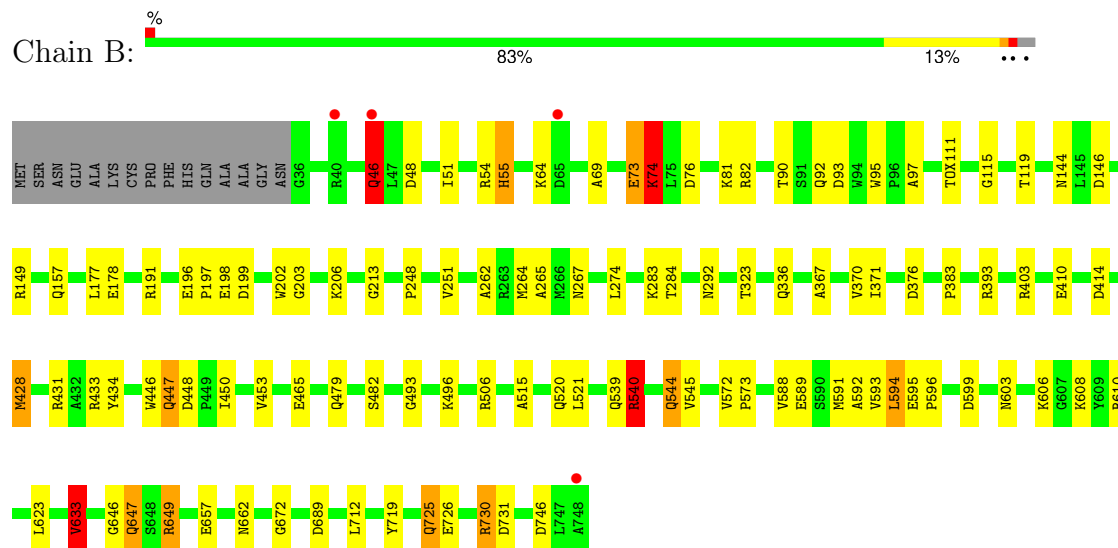
3 Residue-property plots [i](#)

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	100.77Å 113.45Å 174.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.65 20.00 – 1.65	Depositor EDS
% Data completeness (in resolution range)	95.2 (20.00-1.65) 95.1 (20.00-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.140 , 0.171 0.154 , 0.180	Depositor DCC
R_{free} test set	11385 reflections (4.75%)	wwPDB-VP
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12791	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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, PO4, MPD, CL, TOX, HEM, 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	1.81	71/5691 (1.2%)	1.42	23/7732 (0.3%)
1	B	1.84	79/5673 (1.4%)	1.43	20/7711 (0.3%)
All	All	1.82	150/11364 (1.3%)	1.43	43/15443 (0.3%)

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	A	0	1

All (150) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	532	ARG	NE-CZ	-13.05	1.18	1.33
1	A	448	ASP	C-O	11.29	1.29	1.23
1	A	199	ASP	C-O	10.62	1.36	1.23
1	B	544	GLN	CD-OE1	10.23	1.43	1.23
1	B	453	VAL	C-O	-9.53	1.13	1.24
1	B	54	ARG	CA-C	-9.33	1.40	1.53
1	A	343	GLU	CD-OE1	9.07	1.42	1.25
1	A	365	LYS	N-CA	8.45	1.56	1.46
1	A	343	GLU	N-CA	8.33	1.56	1.46
1	A	376	ASP	N-CA	8.16	1.56	1.46
1	B	448	ASP	N-CA	7.86	1.52	1.46
1	B	730	ARG	CZ-NH2	7.68	1.43	1.33
1	B	199	ASP	C-O	7.59	1.33	1.24
1	B	403	ARG	CD-NE	7.29	1.56	1.46
1	B	248	PRO	CA-C	-7.16	1.46	1.53
1	B	594	LEU	CA-C	7.12	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	GLU	CD-OE2	7.01	1.38	1.25
1	B	336	GLN	CG-CD	7.00	1.69	1.52
1	B	588	VAL	N-CA	-6.91	1.38	1.46
1	B	447	GLN	CA-C	6.90	1.62	1.52
1	B	731	ASP	N-CA	-6.89	1.37	1.46
1	A	88	MET	C-O	-6.85	1.15	1.24
1	A	312	ALA	C-O	6.84	1.33	1.24
1	A	239	VAL	C-O	6.75	1.31	1.23
1	A	364	ALA	CA-C	6.74	1.61	1.52
1	A	571	THR	CA-C	6.68	1.60	1.52
1	A	417	ALA	C-O	6.65	1.31	1.24
1	A	606	LYS	N-CA	6.60	1.54	1.46
1	B	657	GLU	CA-C	6.57	1.61	1.52
1	B	446	TRP	N-CA	-6.52	1.37	1.46
1	B	90	THR	CA-C	-6.51	1.45	1.53
1	A	55	HIS	C-O	-6.48	1.14	1.23
1	B	403	ARG	NE-CZ	6.32	1.40	1.33
1	A	408	ASN	CA-CB	-6.30	1.45	1.53
1	B	540	ARG	C-O	6.29	1.31	1.23
1	A	108	ARG	C-N	-6.26	1.25	1.33
1	A	571	THR	N-CA	-6.26	1.38	1.46
1	A	370	VAL	CA-CB	-6.23	1.48	1.54
1	A	262	ALA	C-N	-6.19	1.25	1.33
1	B	376	ASP	N-CA	6.17	1.54	1.46
1	A	607	GLY	C-O	-6.15	1.19	1.24
1	B	74	LYS	CA-C	6.15	1.60	1.52
1	A	692	THR	CA-C	-6.14	1.44	1.52
1	B	202	TRP	C-N	6.10	1.38	1.33
1	B	482	SER	CA-CB	6.05	1.62	1.53
1	B	251	VAL	CA-C	-6.05	1.45	1.52
1	B	197	PRO	N-CA	-6.04	1.39	1.47
1	A	676	LYS	CA-C	-6.02	1.46	1.52
1	B	95	TRP	C-O	-6.01	1.16	1.24
1	A	739	VAL	C-O	6.00	1.31	1.24
1	A	399	GLU	C-O	-5.98	1.16	1.24
1	B	573	PRO	CA-C	5.96	1.60	1.52
1	B	545	VAL	CA-CB	-5.95	1.47	1.54
1	A	329	THR	C-O	5.94	1.30	1.24
1	B	493	GLY	C-N	-5.89	1.26	1.33
1	B	746	ASP	C-O	-5.88	1.16	1.24
1	B	633[A]	VAL	CA-CB	5.87	1.61	1.54
1	B	633[B]	VAL	CA-CB	5.87	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	448	ASP	N-CA	5.86	1.51	1.46
1	A	329	THR	CA-C	-5.81	1.45	1.52
1	B	81	LYS	CA-C	5.80	1.60	1.52
1	A	720	GLY	N-CA	5.76	1.52	1.45
1	A	573	PRO	N-CA	-5.74	1.40	1.47
1	B	596	PRO	CA-CB	-5.73	1.48	1.54
1	B	434	TYR	N-CA	5.71	1.53	1.46
1	A	147	LYS	N-CA	5.71	1.53	1.46
1	A	117	TYR	N-CA	5.70	1.53	1.46
1	B	251	VAL	CA-CB	5.69	1.61	1.54
1	A	92	GLN	CA-CB	-5.66	1.45	1.53
1	B	672	GLY	C-O	5.65	1.30	1.24
1	B	414	ASP	CG-OD1	-5.64	1.14	1.25
1	A	672	GLY	C-O	5.63	1.30	1.24
1	A	499	GLY	C-O	5.60	1.28	1.23
1	B	726	GLU	CG-CD	5.60	1.66	1.52
1	B	262	ALA	C-O	5.59	1.30	1.24
1	A	63	GLY	N-CA	5.58	1.52	1.45
1	B	730	ARG	CZ-NH1	5.58	1.40	1.32
1	A	61	PRO	N-CA	-5.56	1.39	1.47
1	A	343	GLU	CG-CD	5.56	1.66	1.52
1	B	689	ASP	CA-C	-5.55	1.45	1.52
1	B	92	GLN	CD-NE2	-5.54	1.21	1.33
1	A	371	ILE	N-CA	5.54	1.53	1.46
1	A	540	ARG	C-O	5.53	1.30	1.23
1	B	323	THR	N-CA	-5.53	1.41	1.46
1	B	93	ASP	CA-C	-5.53	1.45	1.52
1	B	515	ALA	N-CA	5.51	1.53	1.46
1	A	223	ARG	CZ-NH1	5.50	1.40	1.32
1	B	606	LYS	N-CA	5.49	1.53	1.46
1	B	177	LEU	N-CA	-5.47	1.39	1.46
1	B	448	ASP	C-O	5.47	1.26	1.23
1	B	213	GLY	C-O	5.46	1.31	1.24
1	A	73	GLU	C-O	5.46	1.30	1.24
1	B	725	GLN	CD-OE1	5.45	1.33	1.23
1	A	746	ASP	C-O	-5.43	1.17	1.24
1	B	191	ARG	NE-CZ	-5.41	1.27	1.33
1	A	446	TRP	N-CA	-5.41	1.39	1.46
1	B	82	ARG	CZ-NH2	-5.39	1.26	1.33
1	B	393	ARG	N-CA	5.39	1.53	1.46
1	A	426	ARG	CZ-NH2	5.38	1.40	1.33
1	B	177	LEU	C-O	5.38	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	69	ALA	N-CA	5.37	1.52	1.46
1	B	196	GLU	C-O	-5.37	1.18	1.24
1	A	673	THR	N-CA	-5.36	1.39	1.46
1	A	434	TYR	CB-CG	-5.36	1.39	1.51
1	A	430	PRO	CA-CB	-5.34	1.46	1.53
1	B	383	PRO	CA-CB	-5.34	1.46	1.53
1	A	580	ASP	CG-OD2	5.32	1.35	1.25
1	A	588	VAL	N-CA	-5.32	1.40	1.46
1	B	371	ILE	N-CA	5.31	1.52	1.46
1	A	93	ASP	C-O	-5.30	1.17	1.24
1	A	247	ASN	CG-ND2	-5.29	1.22	1.33
1	B	649	ARG	CZ-NH1	5.27	1.40	1.32
1	B	592	ALA	C-N	5.27	1.39	1.34
1	A	355	SER	N-CA	-5.25	1.38	1.46
1	A	435	LEU	N-CA	-5.24	1.39	1.45
1	B	506	ARG	CA-C	5.24	1.59	1.52
1	A	366	GLY	N-CA	5.24	1.52	1.45
1	B	496	LYS	N-CA	-5.23	1.38	1.46
1	B	599	ASP	CA-C	-5.23	1.47	1.53
1	B	712	LEU	N-CA	5.22	1.52	1.46
1	A	593	VAL	CA-CB	5.21	1.61	1.54
1	A	127	GLY	CA-C	-5.20	1.43	1.51
1	A	114	ALA	C-O	5.20	1.30	1.24
1	B	267	ASN	C-O	5.20	1.29	1.23
1	A	460	ALA	N-CA	-5.20	1.40	1.46
1	A	278	GLY	CA-C	5.20	1.57	1.52
1	B	572	VAL	C-N	-5.20	1.26	1.33
1	B	283	LYS	N-CA	-5.18	1.40	1.46
1	A	645	VAL	CA-CB	-5.18	1.49	1.54
1	B	292	ASN	N-CA	-5.17	1.39	1.46
1	A	653	PHE	N-CA	-5.16	1.40	1.46
1	A	480	LEU	CA-C	5.15	1.59	1.52
1	A	584	GLU	CG-CD	5.15	1.65	1.52
1	B	149	ARG	CD-NE	5.12	1.53	1.46
1	A	459	ASP	CA-C	-5.11	1.45	1.53
1	A	481	VAL	CA-CB	-5.10	1.47	1.54
1	A	710	SER	C-O	5.10	1.30	1.24
1	A	53	HIS	N-CA	5.09	1.52	1.46
1	A	222	ASP	CA-C	5.09	1.59	1.53
1	A	407	GLU	CG-CD	5.08	1.64	1.52
1	B	367	ALA	N-CA	-5.07	1.39	1.45
1	B	97	ALA	C-O	5.05	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	603	ASN	C-O	5.04	1.30	1.23
1	B	274	LEU	CA-C	-5.04	1.46	1.52
1	B	73	GLU	C-O	5.04	1.30	1.24
1	B	465	GLU	N-CA	-5.04	1.40	1.46
1	B	544	GLN	CA-C	5.03	1.58	1.52
1	A	47	LEU	C-O	5.01	1.29	1.23
1	B	157	GLN	N-CA	-5.00	1.40	1.46
1	B	521	LEU	N-CA	-5.00	1.40	1.46

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	GLU	CG-CD-OE1	8.39	137.69	118.40
1	B	149	ARG	NE-CZ-NH1	7.49	128.99	121.50
1	A	48	ASP	N-CA-C	7.18	120.47	108.20
1	B	46	GLN	CB-CG-CD	7.15	124.76	112.60
1	B	633[A]	VAL	CG1-CB-CG2	-6.67	96.13	110.80
1	B	633[B]	VAL	CG1-CB-CG2	-6.67	96.13	110.80
1	A	694	GLU	CA-CB-CG	6.36	126.82	114.10
1	A	170	ILE	N-CA-C	6.27	116.42	110.53
1	A	595	GLU	O-C-N	6.25	126.75	121.31
1	A	367	ALA	N-CA-C	-6.18	102.20	110.55
1	B	48	ASP	N-CA-C	6.05	118.55	108.20
1	A	407	GLU	CG-CD-OE1	5.99	132.19	118.40
1	A	431	ARG	NE-CZ-NH2	5.87	124.48	119.20
1	B	595	GLU	O-C-N	5.87	126.52	121.30
1	A	127	GLY	N-CA-C	5.71	120.95	114.67
1	B	370	VAL	CA-C-N	-5.69	117.80	123.04
1	B	370	VAL	C-N-CA	-5.69	117.80	123.04
1	A	70	GLN	CA-CB-CG	5.59	125.28	114.10
1	B	54	ARG	CG-CD-NE	-5.49	99.93	112.00
1	B	450	ILE	N-CA-C	-5.45	101.94	107.89
1	B	539	GLN	O-C-N	5.45	129.11	122.96
1	B	544	GLN	CG-CD-NE2	-5.44	108.24	116.40
1	A	532	ARG	NE-CZ-NH2	-5.44	114.30	119.20
1	A	496	LYS	CD-CE-NZ	-5.37	94.72	111.90
1	A	431	ARG	NE-CZ-NH1	-5.35	116.15	121.50
1	B	203	GLY	O-C-N	5.35	127.98	123.43
1	B	54	ARG	N-CA-C	-5.34	103.33	110.55
1	A	343	GLU	CG-CD-OE2	-5.34	106.12	118.40
1	A	592	ALA	N-CA-C	5.31	117.75	111.33
1	A	623	LEU	CA-C-O	5.29	126.06	119.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	GLN	CA-CB-CG	5.15	124.41	114.10
1	A	575	ALA	CA-C-N	-5.13	115.44	120.52
1	A	575	ALA	C-N-CA	-5.13	115.44	120.52
1	B	74	LYS	CB-CA-C	-5.13	100.72	109.65
1	B	206	LYS	CG-CD-CE	5.13	123.09	111.30
1	B	623	LEU	CD1-CG-CD2	5.12	122.06	110.80
1	B	573	PRO	CB-CA-C	-5.11	104.28	110.98
1	A	343	GLU	CB-CG-CD	5.10	121.28	112.60
1	B	428	MET	CA-CB-CG	-5.10	103.90	114.10
1	A	46	GLN	N-CA-CB	5.09	117.53	110.04
1	A	376	ASP	CB-CA-C	5.08	115.81	110.17
1	B	55	HIS	CB-CA-C	5.01	119.15	111.39
1	A	647	GLN	N-CA-CB	-5.00	104.52	112.08

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	366	GLY	Peptide

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	5543	0	5372	13	0
1	B	5530	0	5361	27	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
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	5	0
6	B	16	0	28	0	0
7	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	5	0	0	0	0
8	A	784	0	0	7	0
8	B	798	0	0	8	0
All	All	12791	0	10849	44	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 (44) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119[B]:THR:HG21	8:A:1028:HOH:O	1.68	0.94
1:A:438:GLU:OE2	8:A:901:HOH:O	1.97	0.80
1:B:119[B]:THR:HG23	8:B:1175:HOH:O	1.84	0.77
1:B:410:GLU:OE1	8:B:901:HOH:O	2.02	0.76
1:B:73:GLU:OE2	8:B:902:HOH:O	2.07	0.71
1:B:55:HIS:HD2	8:B:1328:HOH:O	1.72	0.71
1:B:540:ARG:CZ	1:B:540:ARG:HA	2.21	0.70
1:A:343:GLU:HG3	8:A:1494:HOH:O	1.91	0.70
1:B:662:ASN:H	1:B:725:GLN:HE22	1.41	0.68
6:A:806:MPD:O4	6:A:806:MPD:HM1	1.95	0.67
1:B:119[B]:THR:HG22	1:B:593:VAL:HG21	1.84	0.60
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.85	0.59
1:B:46:GLN:NE2	8:B:910:HOH:O	2.38	0.57
1:A:593:VAL:HG13	8:A:1030:HOH:O	2.05	0.57
6:A:806:MPD:O4	6:A:806:MPD:CM	2.52	0.56
1:B:633[A]:VAL:HG22	1:B:719:TYR:CZ	2.42	0.55
1:B:76:ASP:OD2	8:B:903:HOH:O	2.18	0.54
1:B:540:ARG:HA	1:B:540:ARG:NH1	2.25	0.52
1:B:591:MET:SD	1:B:594:LEU:HD12	2.50	0.51
1:B:178:GLU:OE1	8:B:904:HOH:O	2.19	0.51
1:B:633[A]:VAL:HG22	1:B:719:TYR:CE1	2.46	0.51
1:B:479:GLN:HE21	1:B:520[B]:GLN:NE2	2.11	0.48
1:A:144:ASN:HA	1:A:146:ASP:OD1	2.14	0.47
1:B:115:GLY:O	1:B:264:MET:HE1	2.15	0.46
1:A:51:ILE:HD11	1:A:618:VAL:HG12	1.98	0.46
1:A:504:ARG:HD2	8:A:918:HOH:O	2.14	0.46
1:B:646:GLY:C	1:B:647:GLN:HG2	2.40	0.46
6:A:805:MPD:H53	6:A:805:MPD:H11	1.98	0.46
1:A:47:LEU:N	8:A:902:HOH:O	2.25	0.45
1:A:119[A]:THR:CG2	1:A:265:ALA:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:LYS:N	1:B:74:LYS:HD3	2.32	0.45
1:B:119[A]:THR:CG2	1:B:265:ALA:HB2	2.47	0.45
1:B:479:GLN:HE21	1:B:520[B]:GLN:HE22	1.66	0.44
1:A:115:GLY:O	1:A:264:MET:HE1	2.18	0.43
1:B:730:ARG:HD2	8:B:1480:HOH:O	2.17	0.43
1:B:428:MET:O	1:B:433:ARG:HD3	2.19	0.43
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.19	0.43
1:A:158:LYS:HD2	6:A:805:MPD:H13	2.01	0.42
1:B:51:ILE:HD13	1:B:51:ILE:HG21	1.88	0.41
1:A:255[A]:ARG:HG2	8:A:1270:HOH:O	2.21	0.41
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.21	0.41
1:B:284:THR:HG22	2:B:801:HEM:HAA1	2.03	0.41
6:A:805:MPD:H11	6:A:805:MPD:C5	2.50	0.40
1:A:54:ARG:NE	1:A:199:ASP:OD2	2.51	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%)	706 (98%)	11 (2%)	0	100	100
1	B	716/728 (98%)	704 (98%)	12 (2%)	0	100	100
All	All	1433/1456 (98%)	1410 (98%)	23 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	555/559 (99%)	550 (99%)	5 (1%)	70	56
1	B	554/559 (99%)	542 (98%)	12 (2%)	45	23
All	All	1109/1118 (99%)	1092 (98%)	17 (2%)	57	37

All (17) 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	608	LYS
1	A	610	ARG
1	B	46	GLN
1	B	64	LYS
1	B	74	LYS
1	B	540	ARG
1	B	544	GLN
1	B	589	GLU
1	B	608	LYS
1	B	610	ARG
1	B	633[A]	VAL
1	B	633[B]	VAL
1	B	647	GLN
1	B	649	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	247	ASN
1	A	339	HIS
1	A	647	GLN
1	A	737	ASN
1	B	46	GLN
1	B	55	HIS
1	B	647	GLN
1	B	650	HIS
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	B	111	1	14,17,18	1.51	3 (21%)	12,23,25	1.86	3 (25%)
1	TOX	A	111	1	14,17,18	2.08	6 (42%)	12,23,25	1.92	3 (25%)

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	B	111	1	-	3/5/8/10	0/2/2/2
1	TOX	A	111	1	-	2/5/8/10	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	TOX	O1-NE1	3.89	1.44	1.39
1	A	111	TOX	CE3-CD2	-3.58	1.34	1.39
1	A	111	TOX	CD1-CG	3.57	1.44	1.36
1	A	111	TOX	CD2-CG	3.25	1.49	1.44
1	A	111	TOX	O-C	3.20	1.32	1.20
1	B	111	TOX	O-C	2.90	1.31	1.20
1	B	111	TOX	CA-N	-2.16	1.42	1.48
1	A	111	TOX	CA-N	-2.11	1.42	1.48
1	A	111	TOX	CD2-CE2	-2.03	1.38	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	TOX	CE3-CD2-CE2	3.78	123.60	119.24
1	B	111	TOX	CH2-CZ3-CE3	3.71	124.82	120.24
1	B	111	TOX	CZ2-CE2-CD2	2.90	125.19	121.95
1	A	111	TOX	CE3-CD2-CG	-2.68	129.86	133.85
1	A	111	TOX	CB-CG-CD1	-2.52	123.17	126.67
1	B	111	TOX	CB-CG-CD1	-2.05	123.82	126.67

There are no chirality outliers.

All (5) 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
1	B	111	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 14 ligands modelled in this entry, 4 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	$\# Z > 2$
5	OXY	B	804	-	1,1,1	0.41	0	-		
5	OXY	A	804	-	1,1,1	0.28	0	-		
6	MPD	A	806	-	7,7,7	0.78	0	9,10,10	2.10	4 (44%)

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	1.47	10 (20%)	67,82,82	1.61	13 (19%)
2	HEM	B	801	1	50,50,50	1.68	10 (20%)	67,82,82	1.74	19 (28%)
6	MPD	A	805	-	7,7,7	1.09	0	9,10,10	1.81	1 (11%)
6	MPD	B	805	-	7,7,7	1.26	1 (14%)	9,10,10	2.05	4 (44%)
7	PO4	B	807	-	4,4,4	1.83	2 (50%)	6,6,6	2.56	2 (33%)
6	MPD	B	806	-	7,7,7	1.65	1 (14%)	9,10,10	1.85	4 (44%)
7	PO4	A	807	-	4,4,4	1.42	1 (25%)	6,6,6	1.04	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
6	MPD	A	806	-	-	2/5/5/5	-
2	HEM	A	801	1	-	2/14/54/54	-
2	HEM	B	801	1	-	2/14/54/54	-
6	MPD	A	805	-	-	3/5/5/5	-
6	MPD	B	805	-	-	4/5/5/5	-
6	MPD	B	806	-	-	3/5/5/5	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C1B-NB	-4.85	1.31	1.40
2	B	801	HEM	FE-NB	4.12	2.07	1.94
2	A	801	HEM	C4D-C3D	-3.94	1.38	1.45
2	B	801	HEM	C4C-NC	-3.43	1.33	1.39
2	B	801	HEM	FE-NC	3.18	2.05	1.95
2	A	801	HEM	FE-NC	3.10	2.05	1.95
2	A	801	HEM	FE-NB	2.94	2.04	1.94
2	B	801	HEM	CHA-C4D	-2.89	1.32	1.38
7	A	807	PO4	P-O1	2.81	1.57	1.50
2	B	801	HEM	C4A-NA	2.80	1.44	1.39
7	B	807	PO4	P-O3	-2.67	1.46	1.54
2	B	801	HEM	CMB-C2B	2.64	1.56	1.50
2	A	801	HEM	O1A-CGA	2.63	1.30	1.22
2	A	801	HEM	C4C-NC	-2.57	1.34	1.39
2	A	801	HEM	C4D-ND	-2.56	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	CMD-C2D	-2.54	1.45	1.50
2	A	801	HEM	C1B-C2B	-2.37	1.39	1.44
2	A	801	HEM	O2A-CGA	-2.34	1.23	1.30
2	B	801	HEM	CBD-CGD	2.28	1.55	1.50
2	A	801	HEM	FE-NA	2.24	2.02	1.95
6	B	805	MPD	O2-C2	-2.20	1.39	1.44
2	B	801	HEM	C4D-C3D	-2.11	1.41	1.45
6	B	806	MPD	C5-C4	2.06	1.60	1.51
2	A	801	HEM	C4B-NB	-2.05	1.34	1.38
7	B	807	PO4	P-O1	2.04	1.55	1.50

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	807	PO4	O2-P-O1	-4.77	94.09	110.95
2	A	801	HEM	O1A-CGA-CBA	-4.20	109.77	123.09
6	A	806	MPD	O4-C4-C3	-4.08	95.13	111.35
6	B	805	MPD	CM-C2-C1	3.91	119.37	110.63
2	B	801	HEM	C1D-C2D-C3D	-3.86	102.92	106.98
2	A	801	HEM	C1D-C2D-C3D	-3.84	102.94	106.98
7	B	807	PO4	O3-P-O2	3.78	119.66	107.91
2	A	801	HEM	C4C-C3C-C2C	3.66	109.98	106.81
2	B	801	HEM	CMA-C3A-C2A	3.65	133.37	125.62
2	B	801	HEM	O1A-CGA-CBA	-3.51	111.97	123.09
2	B	801	HEM	CHD-C1D-ND	-3.44	120.72	124.42
2	A	801	HEM	CHC-C1C-NC	3.32	128.07	124.45
2	B	801	HEM	CHA-C4D-ND	-3.28	120.31	124.37
6	A	806	MPD	O4-C4-C5	3.23	123.36	109.45
2	B	801	HEM	C1B-NB-C4B	3.18	108.98	105.21
6	A	805	MPD	CM-C2-C1	-3.10	103.69	110.63
2	A	801	HEM	O2A-CGA-CBA	3.05	123.65	114.00
2	B	801	HEM	C3B-C4B-NB	-3.00	107.31	109.47
6	B	806	MPD	O4-C4-C5	2.98	122.28	109.45
2	A	801	HEM	C3C-C2C-C1C	-2.93	104.27	107.05
6	B	806	MPD	O2-C2-CM	2.81	116.76	107.99
2	B	801	HEM	CAA-C2A-C1A	2.79	130.39	124.94
2	B	801	HEM	C4D-ND-C1D	-2.78	101.91	105.21
2	B	801	HEM	CAA-C2A-C3A	-2.77	120.85	127.07
2	A	801	HEM	CAA-C2A-C1A	2.76	130.33	124.94
2	B	801	HEM	CMA-C3A-C4A	-2.66	121.37	125.42
2	B	801	HEM	C2D-C1D-ND	2.55	112.86	109.90
2	B	801	HEM	CHC-C4B-NB	2.52	127.14	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	806	MPD	CM-C2-C3	-2.51	99.38	110.20
2	B	801	HEM	C4D-C3D-C2D	2.48	110.50	106.89
6	B	805	MPD	O2-C2-C1	-2.42	100.44	107.99
2	A	801	HEM	CAD-CBD-CGD	2.41	120.05	113.67
2	A	801	HEM	CMD-C2D-C1D	2.34	128.69	125.03
2	A	801	HEM	CBD-CAD-C3D	2.30	118.91	112.53
6	A	806	MPD	O2-C2-C1	2.22	114.89	107.99
2	B	801	HEM	CBB-CAB-C3B	-2.18	116.64	127.53
2	B	801	HEM	O2D-CGD-O1D	2.16	128.89	123.33
6	B	806	MPD	CM-C2-C1	2.12	115.37	110.63
6	A	806	MPD	C1-C2-C3	-2.11	101.11	110.20
6	B	805	MPD	O2-C2-CM	-2.10	101.43	107.99
2	A	801	HEM	CAA-CBA-CGA	-2.10	108.11	113.67
2	B	801	HEM	CHB-C4A-NA	-2.09	120.07	123.86
2	B	801	HEM	CHB-C1B-NB	2.09	126.95	124.37
6	B	805	MPD	O2-C2-C3	2.06	116.96	109.27
2	B	801	HEM	CHA-C4D-C3D	2.05	129.00	125.23
2	A	801	HEM	CHD-C4C-C3C	2.01	128.60	125.21
2	A	801	HEM	CBB-CAB-C3B	-2.01	117.49	127.53

There are no chirality outliers.

All (16) torsion outliers are listed below:

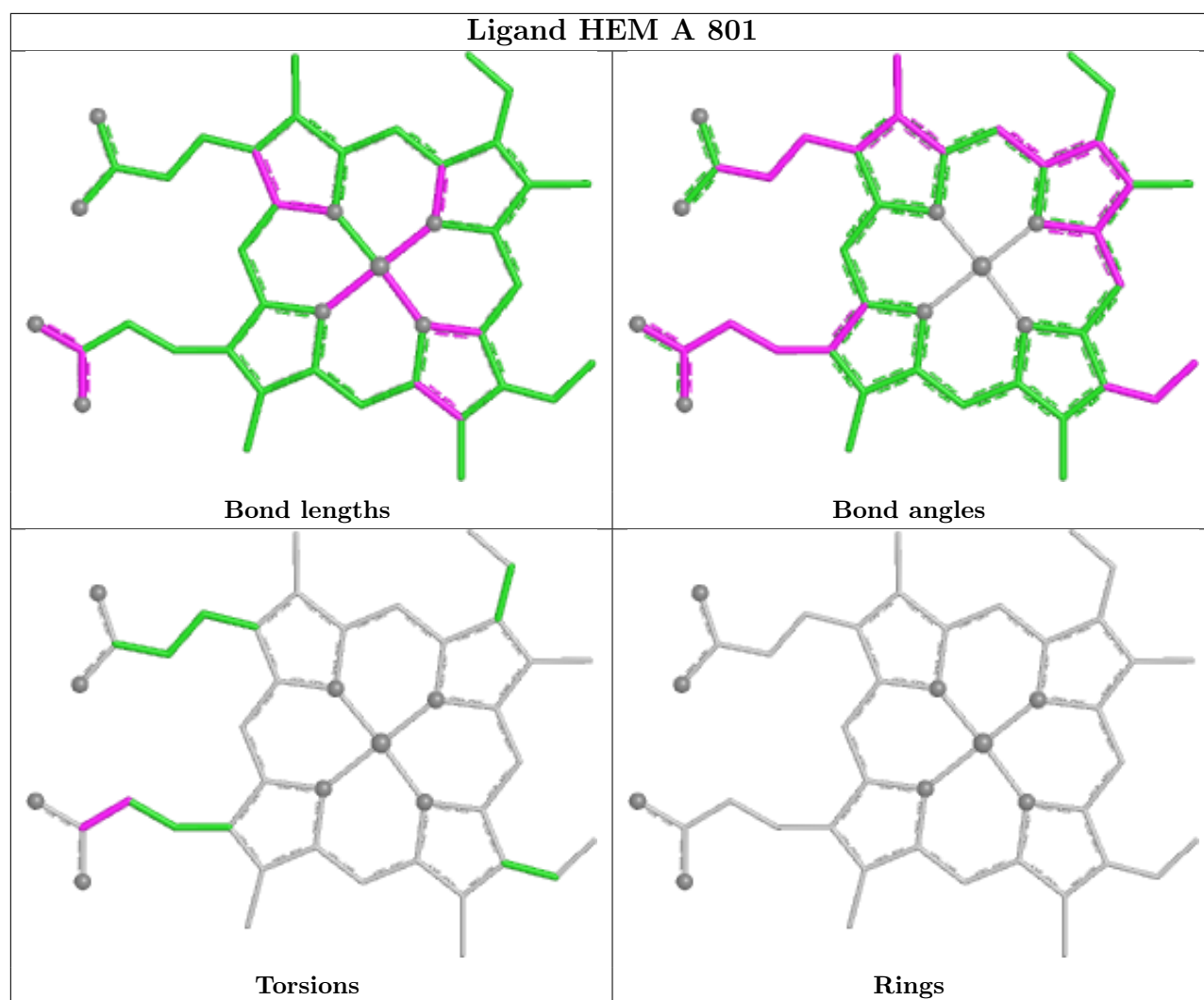
Mol	Chain	Res	Type	Atoms
6	A	805	MPD	C2-C3-C4-C5
6	A	805	MPD	O2-C2-C3-C4
6	B	806	MPD	O2-C2-C3-C4
6	A	806	MPD	C1-C2-C3-C4
6	B	805	MPD	C1-C2-C3-C4
6	B	805	MPD	CM-C2-C3-C4
6	B	806	MPD	C1-C2-C3-C4
6	B	806	MPD	CM-C2-C3-C4
2	A	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O1A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

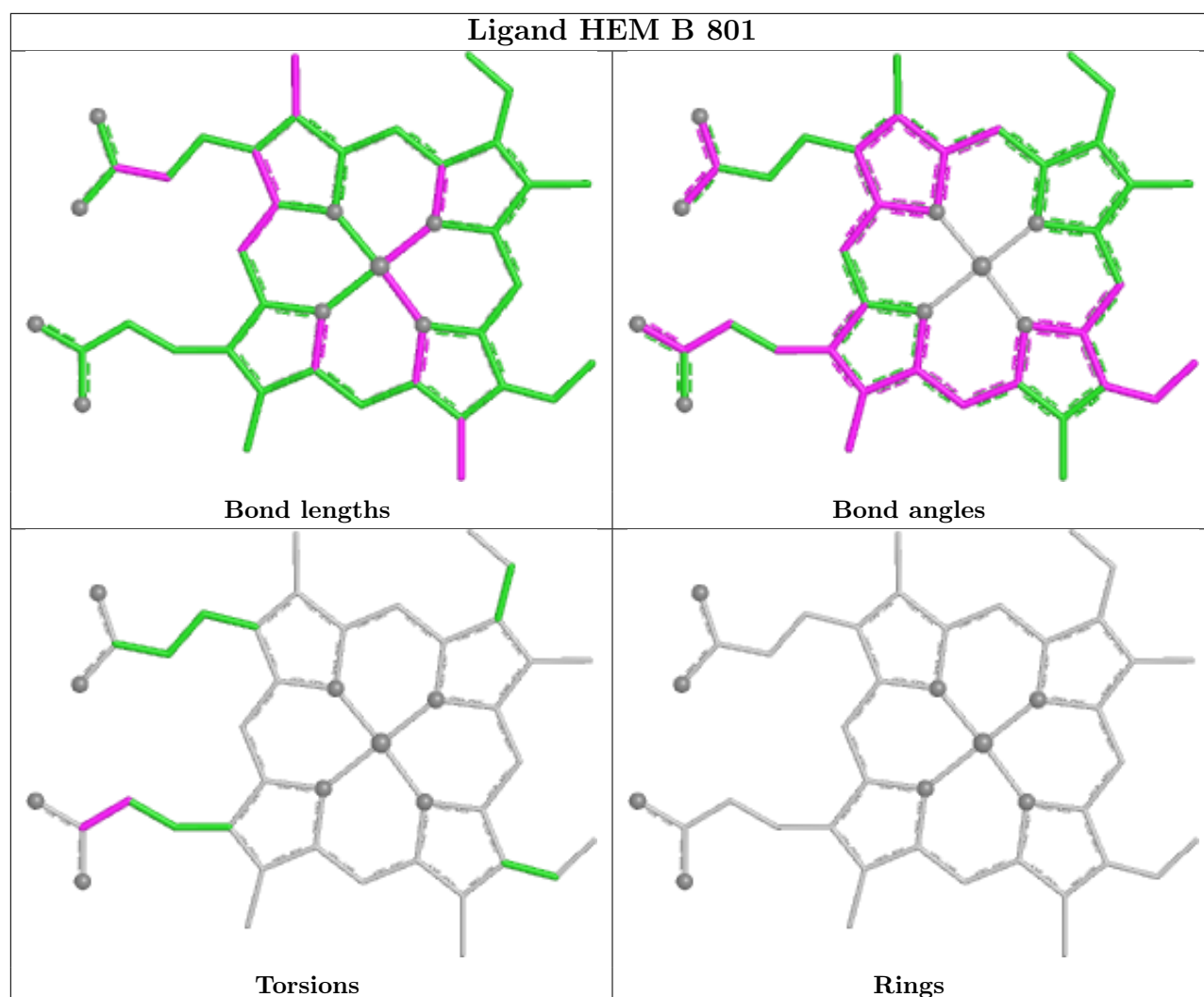
There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	806	MPD	2	0
2	B	801	HEM	1	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 [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%)	-0.45	5 (0%)	84 89	10, 19, 37, 77	7 (0%)
1	B	712/728 (97%)	-0.50	4 (0%)	85 90	10, 18, 36, 79	6 (0%)
All	All	1424/1456 (97%)	-0.48	9 (0%)	85 90	10, 18, 37, 79	13 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	3.6
1	A	608	LYS	2.7
1	B	65	ASP	2.5
1	A	541	GLY	2.5
1	A	454	ASP	2.5
1	B	748	ALA	2.2
1	B	40	ARG	2.1
1	A	680	ALA	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	A	111	16/17	0.98	0.04	11,14,21,22	2
1	TOX	B	111	16/17	0.98	0.04	12,13,18,21	2

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

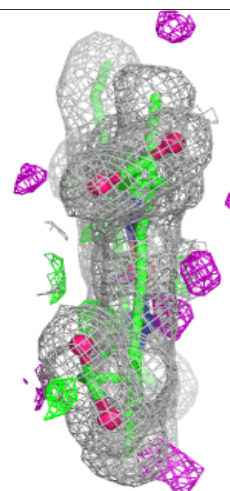
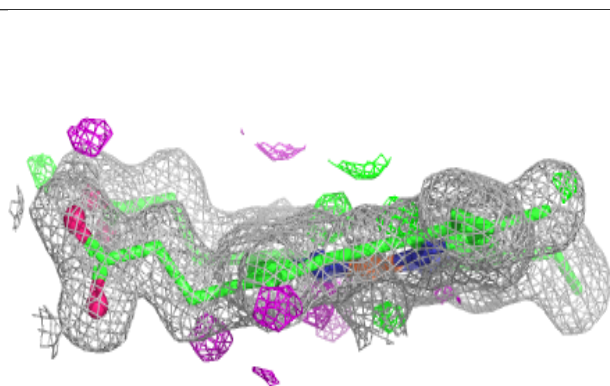
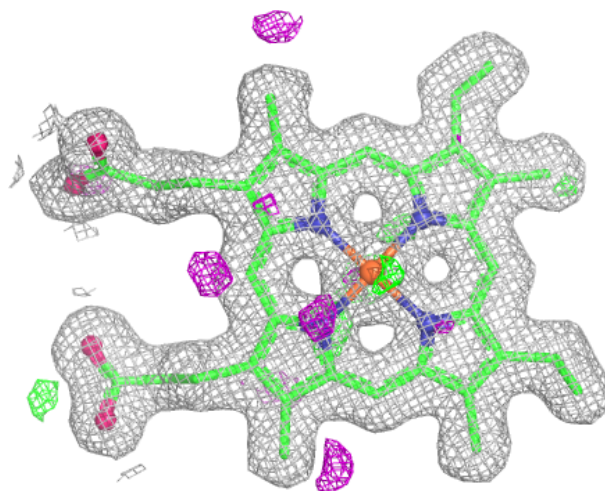
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

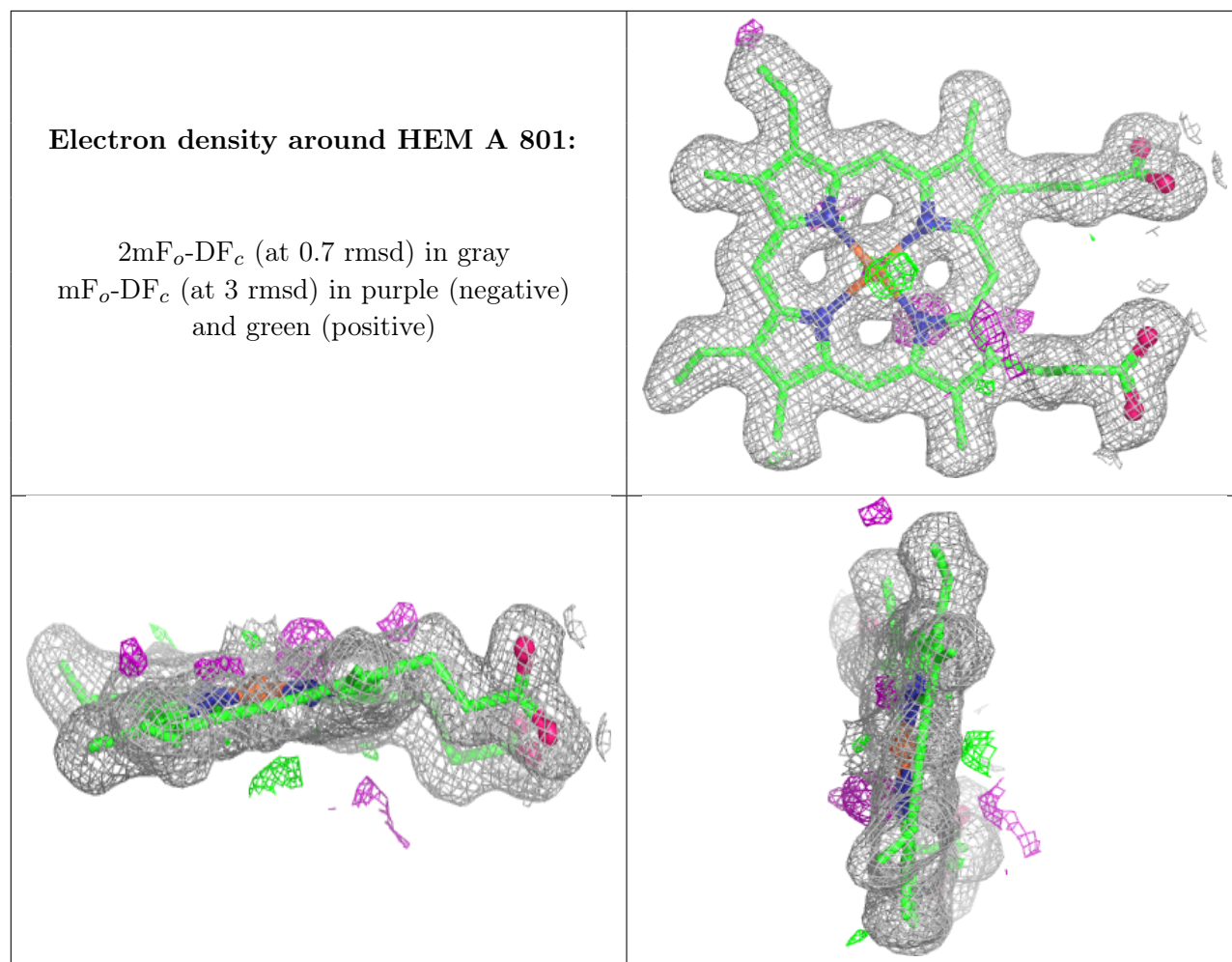
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MPD	B	806	8/8	0.68	0.28	49,67,71,74	0
7	PO4	A	807	5/5	0.79	0.14	42,60,78,79	0
5	OXY	B	804	2/2	0.86	0.19	31,31,31,39	0
6	MPD	A	806	8/8	0.86	0.15	52,64,66,67	0
6	MPD	A	805	8/8	0.89	0.13	37,43,53,53	0
6	MPD	B	805	8/8	0.90	0.11	42,44,53,55	0
7	PO4	B	807	5/5	0.91	0.10	34,48,55,56	0
5	OXY	A	804	2/2	0.92	0.20	33,33,33,39	0
4	CL	B	803	1/1	0.96	0.10	33,33,33,33	0
4	CL	A	803	1/1	0.97	0.09	33,33,33,33	0
2	HEM	B	801	43/43	0.99	0.04	12,13,16,20	0
3	NA	B	802	1/1	0.99	0.03	15,15,15,15	0
2	HEM	A	801	43/43	0.99	0.04	11,13,17,22	0
3	NA	A	802	1/1	1.00	0.03	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.