



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:53 AM UTC

PDB ID : 5KSK / pdb_00005ksk
Title : Crystal structure of the catalase-peroxidase from *B. pseudomallei* treated with acetate
Authors : Loewen, P.C.
Deposited on : 2016-07-08
Resolution : 1.69 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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

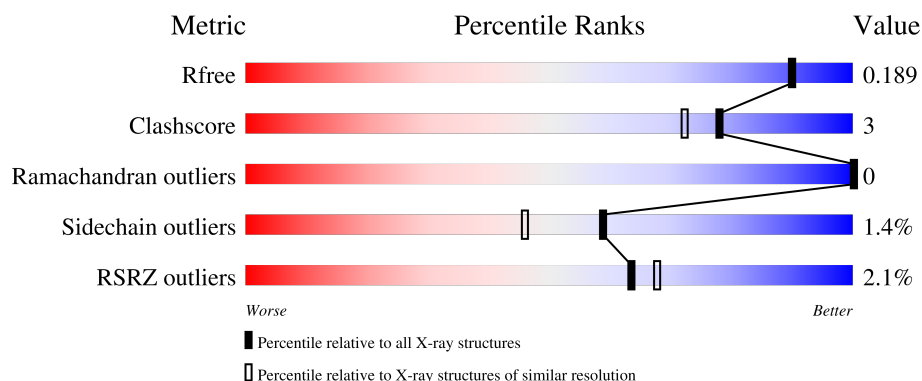
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.69 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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% 84% 13% ..
1	B	728	3% 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	-
6	MPD	B	806	-	X	-	-

2 Entry composition [i](#)

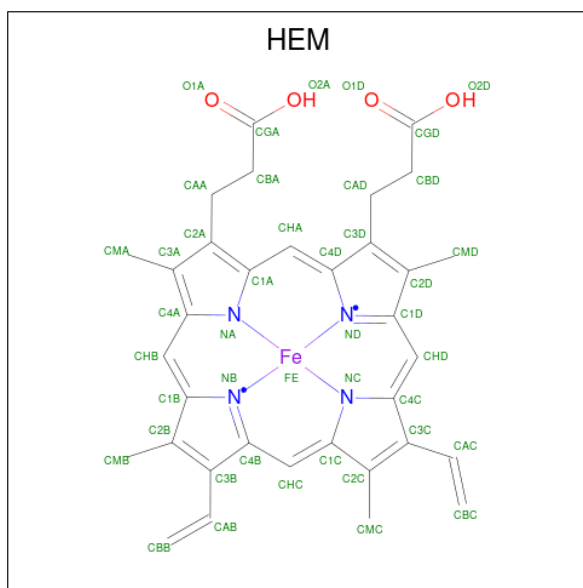
There are 7 unique types of molecules in this entry. The entry contains 12836 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	6	0
			5546	3503	989	1040	14			
1	B	713	Total	C	N	O	S	0	9	0
			5548	3506	987	1041	14			

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



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

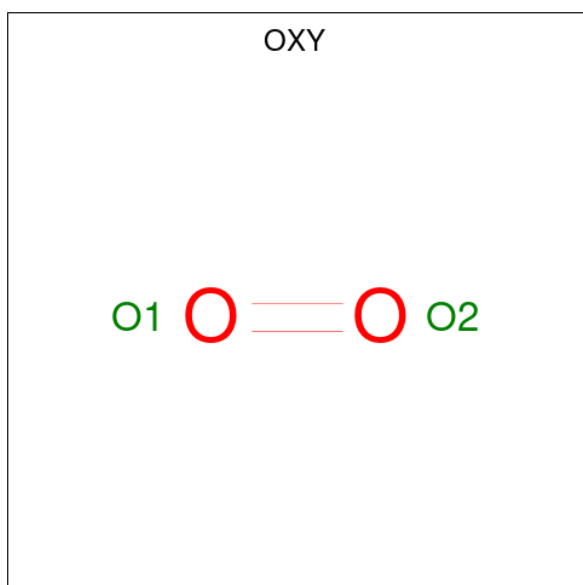
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

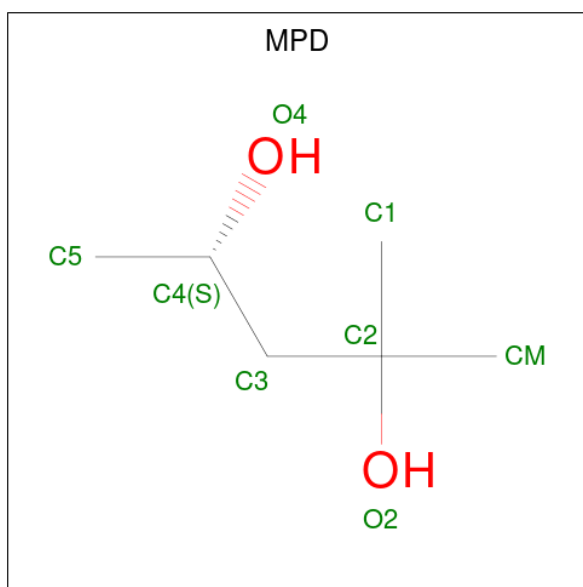
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		

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



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

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



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

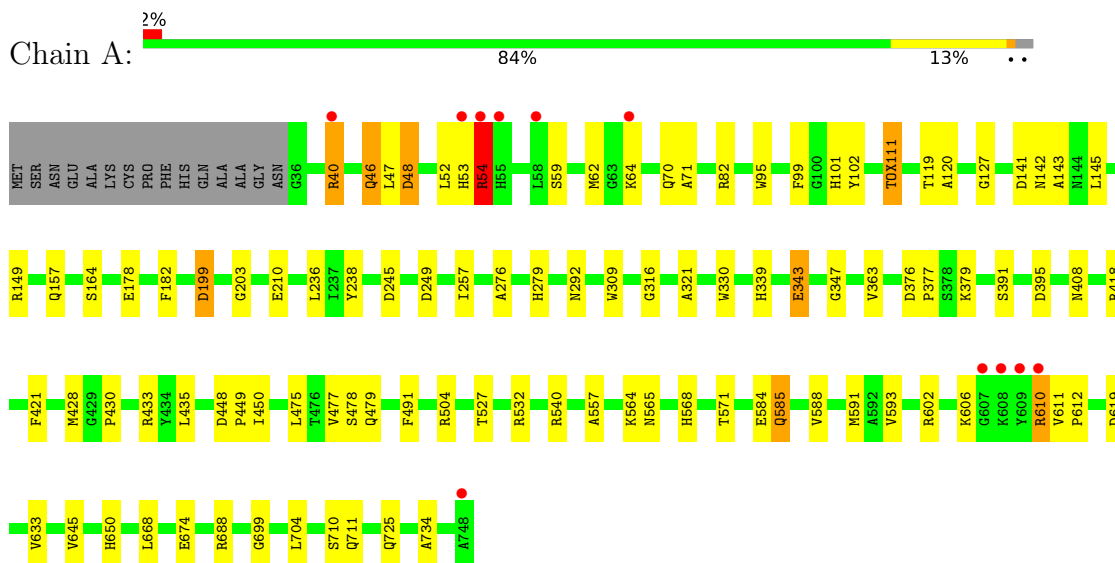
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	821	Total O 821 821	0	0
7	B	787	Total O 787 787	0	0

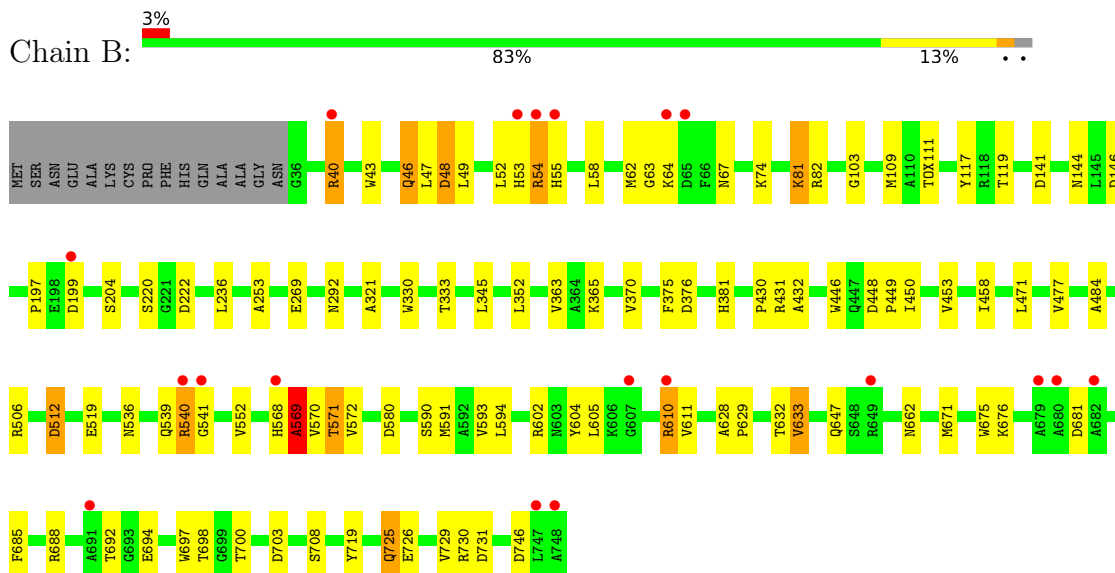
3 Residue-property plots [i](#)

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	100.70Å 115.48Å 174.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.39 – 1.69 48.39 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.39-1.69) 99.2 (48.39-1.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.152 , 0.180 0.164 , 0.189	Depositor DCC
R_{free} test set	11167 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 36.6	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	12836	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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: HEM, OXY, NA, TOX, MPD, 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	1.83	71/5688 (1.2%)	1.40	15/7729 (0.2%)
1	B	1.82	74/5696 (1.3%)	1.40	23/7741 (0.3%)
All	All	1.82	145/11384 (1.3%)	1.40	38/15470 (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	A	0	1
1	B	0	3
All	All	0	4

All (145) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	512	ASP	CG-OD2	12.05	1.48	1.25
1	B	448	ASP	N-CA	11.42	1.56	1.46
1	A	448	ASP	N-CA	9.58	1.53	1.46
1	B	540	ARG	C-O	9.46	1.36	1.23
1	B	694	GLU	CA-C	9.05	1.64	1.52
1	A	668	LEU	CA-C	-8.79	1.41	1.52
1	B	571	THR	CA-C	-8.56	1.42	1.52
1	B	370	VAL	N-CA	-8.35	1.37	1.46
1	A	699	GLY	N-CA	7.87	1.53	1.45
1	B	512	ASP	CB-CG	7.68	1.71	1.52
1	A	449	PRO	C-O	-7.29	1.15	1.23
1	B	676	LYS	C-O	-7.21	1.16	1.24
1	A	408	ASN	CA-CB	-7.10	1.45	1.53
1	A	279	HIS	CE1-NE2	7.05	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	532	ARG	NE-CZ	-6.97	1.25	1.33
1	B	103	GLY	CA-C	6.96	1.59	1.52
1	A	203	GLY	N-CA	6.91	1.52	1.45
1	A	478	SER	CA-C	-6.89	1.44	1.52
1	B	333	THR	CA-C	6.77	1.60	1.52
1	A	477	VAL	CA-CB	-6.74	1.47	1.54
1	B	74	LYS	CA-C	6.73	1.61	1.52
1	A	59	SER	C-O	-6.72	1.15	1.24
1	A	725	GLN	CG-CD	6.68	1.68	1.52
1	B	671	MET	CG-SD	-6.67	1.64	1.80
1	B	590	SER	N-CA	6.61	1.54	1.46
1	A	585	GLN	CD-OE1	6.57	1.36	1.23
1	B	746	ASP	CB-CG	6.52	1.68	1.52
1	A	711	GLN	CD-NE2	-6.51	1.19	1.33
1	B	67	ASN	CA-C	6.44	1.60	1.52
1	A	571	THR	CA-C	6.38	1.60	1.52
1	B	52	LEU	N-CA	6.37	1.54	1.46
1	B	700	THR	N-CA	-6.30	1.38	1.45
1	A	347	GLY	N-CA	6.29	1.53	1.45
1	A	236	LEU	CA-C	6.28	1.60	1.52
1	B	222	ASP	CA-CB	6.26	1.60	1.52
1	A	257	ILE	N-CA	6.24	1.53	1.46
1	A	182	PHE	C-O	-6.24	1.16	1.24
1	B	726	GLU	CD-OE1	6.24	1.37	1.25
1	A	674	GLU	C-O	6.23	1.31	1.24
1	A	527	THR	N-CA	-6.22	1.39	1.46
1	B	63	GLY	N-CA	6.20	1.53	1.45
1	A	149	ARG	CA-CB	6.18	1.62	1.53
1	B	103	GLY	C-N	6.18	1.41	1.33
1	B	602	ARG	CZ-NH2	-6.17	1.25	1.33
1	A	178	GLU	C-O	6.10	1.31	1.24
1	B	571	THR	CA-CB	6.05	1.62	1.53
1	A	568	HIS	CA-CB	-6.02	1.44	1.53
1	B	46	GLN	N-CA	5.98	1.53	1.45
1	A	82	ARG	CZ-NH2	-5.94	1.25	1.33
1	B	725	GLN	CD-OE1	5.94	1.34	1.23
1	B	572	VAL	N-CA	-5.94	1.41	1.46
1	B	292	ASN	N-CA	-5.93	1.38	1.46
1	B	453	VAL	C-O	-5.92	1.17	1.24
1	A	70	GLN	CG-CD	5.90	1.66	1.52
1	A	565	ASN	C-O	5.86	1.31	1.24
1	A	377	PRO	C-O	-5.85	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	343	GLU	CD-OE2	5.83	1.36	1.25
1	B	82	ARG	CZ-NH2	-5.82	1.25	1.33
1	A	157	GLN	C-O	5.81	1.30	1.24
1	B	708	SER	N-CA	5.80	1.52	1.46
1	A	421	PHE	N-CA	5.79	1.53	1.46
1	A	363	VAL	C-O	5.79	1.29	1.24
1	B	628	ALA	C-O	-5.79	1.19	1.24
1	A	120	ALA	CA-C	-5.78	1.45	1.52
1	B	81	LYS	CE-NZ	5.78	1.66	1.49
1	B	605	LEU	C-O	-5.78	1.17	1.23
1	B	220	SER	C-O	5.73	1.30	1.23
1	B	568	HIS	CA-C	5.72	1.59	1.52
1	B	604	TYR	C-O	5.72	1.30	1.24
1	A	588	VAL	N-CA	-5.72	1.39	1.46
1	A	330	TRP	N-CA	-5.70	1.39	1.46
1	B	647	GLN	CA-C	5.68	1.60	1.53
1	B	681	ASP	CA-C	5.68	1.58	1.52
1	A	62	MET	C-N	-5.68	1.23	1.33
1	B	698	THR	N-CA	-5.67	1.38	1.45
1	B	446	TRP	C-O	-5.65	1.16	1.24
1	A	688	ARG	CA-C	-5.59	1.46	1.52
1	A	245	ASP	CG-OD1	5.56	1.35	1.25
1	A	540	ARG	C-O	5.52	1.30	1.23
1	B	477	VAL	CA-CB	-5.52	1.48	1.54
1	B	580	ASP	CA-C	5.51	1.59	1.52
1	A	564	LYS	C-O	5.51	1.30	1.24
1	A	527	THR	C-O	5.50	1.30	1.24
1	B	685	PHE	CA-C	-5.50	1.46	1.52
1	A	557	ALA	CA-CB	-5.50	1.44	1.53
1	A	95	TRP	N-CA	5.48	1.53	1.46
1	A	430	PRO	C-O	5.48	1.30	1.23
1	B	448	ASP	C-O	5.47	1.26	1.23
1	B	571	THR	C-O	5.44	1.30	1.24
1	A	584	GLU	N-CA	5.43	1.53	1.46
1	A	619	ASP	N-CA	5.43	1.52	1.46
1	B	352	LEU	CA-C	-5.43	1.45	1.52
1	A	142	ASN	C-O	-5.43	1.16	1.24
1	B	109	MET	C-O	5.42	1.30	1.24
1	B	363	VAL	N-CA	5.42	1.52	1.46
1	B	688	ARG	NE-CZ	5.41	1.39	1.33
1	B	47	LEU	CB-CG	-5.39	1.42	1.53
1	B	552	VAL	CA-CB	-5.38	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	704	LEU	N-CA	-5.37	1.39	1.46
1	A	391	SER	N-CA	-5.34	1.39	1.46
1	B	703	ASP	N-CA	-5.34	1.40	1.46
1	B	236	LEU	C-O	5.32	1.30	1.23
1	A	532	ARG	CD-NE	5.30	1.53	1.46
1	A	316	GLY	N-CA	5.29	1.53	1.45
1	B	471	LEU	CA-C	5.29	1.59	1.52
1	B	484	ALA	CA-C	5.29	1.59	1.52
1	B	458	ILE	CA-CB	-5.27	1.48	1.54
1	A	450	ILE	N-CA	5.27	1.50	1.46
1	A	52	LEU	C-O	5.25	1.30	1.24
1	A	491	PHE	C-O	5.25	1.30	1.23
1	B	675	TRP	N-CA	-5.25	1.39	1.46
1	A	127	GLY	C-O	5.23	1.29	1.24
1	A	145	LEU	CA-C	-5.23	1.45	1.52
1	B	632	THR	CA-C	5.21	1.59	1.52
1	B	365	LYS	N-CA	5.21	1.52	1.46
1	B	49	LEU	CB-CG	-5.21	1.43	1.53
1	B	269	GLU	C-O	-5.21	1.18	1.24
1	B	729	VAL	N-CA	5.21	1.52	1.46
1	A	450	ILE	CA-CB	-5.20	1.49	1.54
1	B	376	ASP	CA-C	-5.19	1.46	1.52
1	B	708	SER	CA-C	-5.19	1.47	1.52
1	B	536	ASN	N-CA	-5.17	1.39	1.46
1	B	204	SER	C-O	-5.17	1.16	1.24
1	B	731	ASP	N-CA	-5.17	1.40	1.46
1	A	612	PRO	CA-C	5.16	1.59	1.52
1	B	449	PRO	C-O	-5.16	1.17	1.23
1	A	210	GLU	N-CA	5.15	1.52	1.46
1	A	292	ASN	N-CA	-5.15	1.39	1.46
1	B	197	PRO	N-CA	-5.15	1.40	1.47
1	A	47	LEU	CB-CG	-5.09	1.43	1.53
1	B	74	LYS	N-CA	-5.09	1.39	1.46
1	A	102	TYR	N-CA	5.09	1.52	1.46
1	A	475	LEU	CA-C	-5.09	1.46	1.52
1	A	418	ARG	NE-CZ	5.09	1.38	1.33
1	B	430	PRO	C-O	5.08	1.29	1.23
1	A	164	SER	N-CA	5.07	1.52	1.45
1	A	70	GLN	CD-OE1	5.07	1.33	1.23
1	A	606	LYS	N-CA	5.07	1.52	1.46
1	A	71	ALA	CA-C	-5.06	1.46	1.52
1	A	734	ALA	CA-CB	-5.06	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	435	LEU	N-CA	-5.06	1.39	1.45
1	A	479	GLN	C-N	-5.05	1.27	1.33
1	B	375	PHE	CA-C	5.05	1.59	1.52
1	B	43	TRP	CA-CB	5.02	1.59	1.53
1	B	381	HIS	N-CA	5.02	1.52	1.45

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	710	SER	N-CA-C	10.23	123.48	111.71
1	A	48	ASP	N-CA-C	7.67	121.31	108.20
1	B	48	ASP	N-CA-C	7.53	121.08	108.20
1	B	46	GLN	N-CA-C	-7.49	99.40	110.48
1	B	46	GLN	CB-CG-CD	7.32	125.04	112.60
1	A	46	GLN	N-CA-C	-7.27	100.24	110.50
1	B	569	ALA	N-CA-C	-7.27	97.74	109.96
1	A	46	GLN	CA-CB-CG	7.02	128.13	114.10
1	A	330	TRP	N-CA-C	6.77	120.01	111.69
1	A	321	ALA	N-CA-C	6.52	119.69	110.23
1	B	62	MET	CA-C-N	-6.47	111.82	121.01
1	B	62	MET	C-N-CA	-6.47	111.82	121.01
1	A	54	ARG	N-CA-C	-6.44	101.86	110.55
1	A	395	ASP	N-CA-C	-6.17	102.01	109.72
1	B	512	ASP	CA-CB-CG	6.13	118.73	112.60
1	A	46	GLN	CB-CG-CD	6.11	122.99	112.60
1	B	54	ARG	N-CA-C	-6.08	102.34	110.55
1	B	512	ASP	CB-CG-OD1	-6.00	104.60	118.40
1	A	279	HIS	CE1-NE2-CD2	-5.90	103.10	109.00
1	B	330	TRP	N-CA-C	5.88	118.93	111.69
1	B	345	LEU	O-C-N	5.78	128.25	122.12
1	A	478	SER	N-CA-C	5.76	117.23	111.07
1	A	448	ASP	CA-C-O	5.66	124.84	120.48
1	B	58	LEU	CA-C-O	-5.59	114.95	120.82
1	A	249	ASP	CB-CA-C	-5.35	104.24	110.17
1	B	540	ARG	N-CA-CB	5.35	119.67	111.22
1	B	697	TRP	O-C-N	-5.27	117.24	123.25
1	B	253	ALA	N-CA-C	-5.19	105.62	111.28
1	B	46	GLN	CA-CB-CG	5.15	124.40	114.10
1	B	541	GLY	N-CA-C	-5.15	108.22	115.32
1	B	321	ALA	N-CA-C	5.14	117.69	110.23
1	B	449	PRO	O-C-N	5.13	129.37	123.01
1	B	450	ILE	CB-CA-C	-5.12	105.17	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	633	VAL	CG1-CB-CG2	-5.10	99.58	110.80
1	B	117	TYR	N-CA-C	5.03	117.63	110.24
1	B	697	TRP	CA-CB-CG	5.03	123.15	113.60
1	A	276	ALA	CA-C-O	5.01	125.73	120.42
1	B	432	ALA	N-CA-C	5.01	118.49	112.38

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	ASP	Mainchain
1	B	199	ASP	Mainchain
1	B	539	GLN	Peptide
1	B	569	ALA	Mainchain

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	5546	0	5370	20	0
1	B	5548	0	5378	33	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	24	0	42	2	0
6	B	16	0	28	10	0
7	A	821	0	0	8	0
7	B	787	0	0	17	0
All	All	12836	0	10878	62	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 3.

All (62) 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:506:ARG:HE	6:B:805:MPD:H12	1.31	0.94
1:A:119[B]:THR:HG21	7:A:1049:HOH:O	1.72	0.87
6:B:805:MPD:H51	7:B:1353:HOH:O	1.81	0.79
6:B:805:MPD:H13	7:B:1543:HOH:O	1.85	0.75
1:B:512:ASP:OD1	7:B:903:HOH:O	2.02	0.75
1:B:55:HIS:HD2	7:B:1386:HOH:O	1.72	0.72
6:B:806:MPD:O4	6:B:806:MPD:C1	2.40	0.70
1:B:431:ARG:HD2	7:B:1468:HOH:O	1.92	0.68
1:B:519:GLU:OE1	7:B:904:HOH:O	2.11	0.68
1:B:54:ARG:O	7:B:906:HOH:O	2.12	0.68
1:B:569:ALA:O	1:B:570:VAL:HG23	1.96	0.66
1:A:53:HIS:NE2	7:A:908:HOH:O	2.30	0.64
1:B:81:LYS:CE	7:B:1097:HOH:O	2.46	0.62
1:B:431:ARG:CD	7:B:1468:HOH:O	2.46	0.61
6:A:805:MPD:H53	6:A:805:MPD:H11	1.81	0.61
1:B:81:LYS:HD3	7:B:1097:HOH:O	2.00	0.61
6:A:806:MPD:O2	6:A:806:MPD:O4	2.14	0.60
1:A:99:PHE:O	1:A:101[B]:HIS:HD2	1.86	0.59
1:B:81:LYS:CD	7:B:1097:HOH:O	2.49	0.59
1:B:506:ARG:HE	6:B:805:MPD:C1	2.10	0.58
1:B:506:ARG:NE	6:B:805:MPD:H12	2.12	0.58
1:B:53:HIS:CD2	7:B:1347:HOH:O	2.57	0.57
1:B:662:ASN:H	1:B:725:GLN:HE22	1.52	0.56
1:B:53:HIS:HD2	7:B:1347:HOH:O	1.87	0.56
1:B:591:MET:SD	1:B:594:LEU:HD12	2.47	0.55
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.87	0.55
6:B:805:MPD:C1	6:B:805:MPD:H52	2.37	0.54
1:B:119[B]:THR:CG2	7:B:1119:HOH:O	2.54	0.54
1:A:343:GLU:OE1	7:A:906:HOH:O	2.19	0.52
1:B:610:ARG:HD2	1:B:611:VAL:HG23	1.91	0.51
1:A:376:ASP:OD2	1:A:379:LYS:HE3	2.11	0.50
1:B:569:ALA:O	1:B:570:VAL:CG2	2.59	0.50
1:A:585:GLN:NE2	7:A:921:HOH:O	2.45	0.50
1:A:593:VAL:HG13	7:A:912:HOH:O	2.12	0.49
1:A:610:ARG:HD2	1:A:611:VAL:HG23	1.95	0.49
1:A:504:ARG:HD2	7:A:951:HOH:O	2.12	0.48
1:B:119[B]:THR:HG22	7:B:1119:HOH:O	2.13	0.48
1:B:633[A]:VAL:HG22	1:B:719:TYR:CZ	2.49	0.48
1:B:629:PRO:O	1:B:633[A]:VAL:HG23	2.13	0.47
1:B:119[B]:THR:HG22	1:B:593:VAL:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:HIS:HE1	7:A:1555:HOH:O	1.96	0.47
1:A:54:ARG:HG3	1:A:199:ASP:OD2	2.16	0.46
1:B:40:ARG:NH2	1:B:48:ASP:HB2	2.30	0.46
1:B:512:ASP:HB2	7:B:1447:HOH:O	2.17	0.44
1:A:40:ARG:NH2	1:A:48:ASP:HB2	2.32	0.44
1:B:633[A]:VAL:HG22	1:B:719:TYR:CE2	2.52	0.44
6:B:806:MPD:O4	6:B:806:MPD:H12	2.16	0.43
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.18	0.43
1:B:119[B]:THR:HG23	7:B:1119:HOH:O	2.19	0.43
6:B:806:MPD:O4	6:B:806:MPD:H11	2.16	0.43
1:A:339:HIS:HB2	7:A:1372:HOH:O	2.19	0.42
1:A:591:MET:HB2	1:A:591:MET:HE2	1.85	0.42
1:A:602:ARG:HB3	1:A:645:VAL:HG23	2.01	0.42
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	3.03	0.42
6:B:805:MPD:H12	6:B:805:MPD:H52	2.00	0.42
1:A:111:TOX:H9	1:A:238:TYR:OH	2.19	0.42
1:A:143:ALA:HA	1:A:309:TRP:CH2	2.55	0.42
1:B:591:MET:HE2	1:B:591:MET:HB2	1.90	0.41
1:A:428:MET:O	1:A:433:ARG:HD3	2.20	0.41
1:A:376:ASP:OD2	1:A:379:LYS:CE	2.68	0.41

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	716/728 (98%)	707 (99%)	9 (1%)	0	100	100
1	B	718/728 (99%)	710 (99%)	8 (1%)	0	100	100
All	All	1434/1456 (98%)	1417 (99%)	17 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	555/560 (99%)	549 (99%)	6 (1%)	65	54
1	B	557/560 (100%)	547 (98%)	10 (2%)	51	36
All	All	1112/1120 (99%)	1096 (99%)	16 (1%)	59	46

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

Mol	Chain	Res	Type
1	A	40	ARG
1	A	46	GLN
1	A	54	ARG
1	A	64	LYS
1	A	141	ASP
1	A	610	ARG
1	B	40	ARG
1	B	46	GLN
1	B	64	LYS
1	B	141	ASP
1	B	540	ARG
1	B	571	THR
1	B	610	ARG
1	B	633[A]	VAL
1	B	633[B]	VAL
1	B	730	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	53	HIS
1	A	85	HIS
1	A	247	ASN
1	A	520	GLN
1	A	544	GLN

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Mol	Chain	Res	Type
1	A	647	GLN
1	B	53	HIS
1	B	55	HIS
1	B	725	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	TOX	B	111[B]	-	14,17,18	2.48	5 (35%)	12,23,25	3.14	7 (58%)
1	TOX	B	111[A]	2	14,17,18	2.48	5 (35%)	12,23,25	3.14	7 (58%)
1	TOX	A	111	1	14,17,18	2.01	5 (35%)	12,23,25	2.61	7 (58%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TOX	B	111[B]	-	-	2/5/8/10	0/2/2/2
1	TOX	B	111[A]	2	-	2/5/8/10	0/2/2/2
1	TOX	A	111	1	-	4/5/8/10	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111[A]	TOX	O-C	4.94	1.38	1.20
1	B	111[B]	TOX	O-C	4.94	1.38	1.20
1	B	111[A]	TOX	CE2-NE1	-4.77	1.31	1.39
1	B	111[B]	TOX	CE2-NE1	-4.77	1.31	1.39
1	A	111	TOX	CD2-CE2	4.02	1.46	1.41
1	B	111[A]	TOX	CB-CA	-2.82	1.47	1.53
1	B	111[B]	TOX	CB-CA	-2.82	1.47	1.53
1	A	111	TOX	CH2-CZ3	2.81	1.44	1.38
1	A	111	TOX	O-C	2.79	1.30	1.20
1	B	111[A]	TOX	CD1-CG	2.68	1.42	1.36
1	B	111[B]	TOX	CD1-CG	2.68	1.42	1.36
1	A	111	TOX	CB-CG	2.60	1.55	1.50
1	B	111[A]	TOX	CZ2-CE2	-2.60	1.35	1.39
1	B	111[B]	TOX	CZ2-CE2	-2.60	1.35	1.39
1	A	111	TOX	O1-NE1	2.42	1.42	1.39

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111[A]	TOX	CZ2-CE2-CD2	-5.59	115.71	121.95
1	B	111[B]	TOX	CZ2-CE2-CD2	-5.59	115.71	121.95
1	B	111[A]	TOX	CZ3-CH2-CZ2	-5.44	113.53	120.24
1	B	111[B]	TOX	CZ3-CH2-CZ2	-5.44	113.53	120.24
1	B	111[A]	TOX	CH2-CZ2-CE2	4.49	127.33	118.28
1	B	111[B]	TOX	CH2-CZ2-CE2	4.49	127.33	118.28
1	A	111	TOX	CD2-CG-CD1	3.92	109.90	106.34
1	A	111	TOX	CZ2-CE2-NE1	3.84	135.48	129.37
1	A	111	TOX	CE2-CD2-CG	-3.73	103.96	107.39
1	A	111	TOX	CB-CG-CD1	-3.56	121.73	126.67
1	B	111[A]	TOX	CE3-CD2-CE2	3.05	122.76	119.24
1	B	111[B]	TOX	CE3-CD2-CE2	3.05	122.76	119.24
1	B	111[A]	TOX	CE2-CD2-CG	-2.98	104.65	107.39
1	B	111[B]	TOX	CE2-CD2-CG	-2.98	104.65	107.39
1	A	111	TOX	CZ2-CE2-CD2	-2.72	118.92	121.95
1	A	111	TOX	CE3-CD2-CG	2.68	137.84	133.85
1	B	111[A]	TOX	CH2-CZ3-CE3	2.19	122.95	120.24
1	B	111[B]	TOX	CH2-CZ3-CE3	2.19	122.95	120.24
1	B	111[A]	TOX	CZ2-CE2-NE1	2.06	132.66	129.37
1	B	111[B]	TOX	CZ2-CE2-NE1	2.06	132.66	129.37
1	A	111	TOX	CH2-CZ2-CE2	2.04	122.41	118.28

There are no chirality outliers.

All (8) 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[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	A	111	TOX	CA-CB-CG-CD2
1	A	111	TOX	CA-CB-CG-CD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 4 are monoatomic - leaving 9 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	807	-	7,7,7	0.76	0	9,10,10	1.37	1 (11%)
5	OXY	B	804	-	1,1,1	0.40	0	-		
5	OXY	A	804	-	1,1,1	0.27	0	-		
6	MPD	B	806	-	7,7,7	0.64	0	9,10,10	2.00	4 (44%)
6	MPD	A	806	-	7,7,7	0.57	0	9,10,10	1.62	2 (22%)
2	HEM	A	801	1	50,50,50	2.09	11 (22%)	67,82,82	2.02	18 (26%)
2	HEM	B	801	1	50,50,50	2.07	14 (28%)	67,82,82	1.51	13 (19%)
6	MPD	A	805	-	7,7,7	0.62	0	9,10,10	1.53	2 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MPD	B	805	-	7,7,7	1.18	1 (14%)	9,10,10	1.05	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	807	-	-	0/5/5/5	-
6	MPD	B	806	-	-	5/5/5/5	-
6	MPD	A	806	-	-	2/5/5/5	-
2	HEM	A	801	1	-	2/14/54/54	-
2	HEM	B	801	1	-	3/14/54/54	-
6	MPD	A	805	-	-	1/5/5/5	-
6	MPD	B	805	-	-	2/5/5/5	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C1B-NB	-7.15	1.27	1.40
2	A	801	HEM	FE-NB	5.79	2.12	1.94
2	B	801	HEM	C1B-NB	-5.50	1.30	1.40
2	B	801	HEM	C4A-NA	-5.18	1.29	1.39
2	B	801	HEM	C1C-NC	-4.96	1.30	1.39
2	A	801	HEM	FE-NC	4.39	2.09	1.95
2	B	801	HEM	C3C-C4C	-4.38	1.38	1.46
2	A	801	HEM	C1D-ND	3.68	1.46	1.38
2	A	801	HEM	FE-NA	3.45	2.06	1.95
2	A	801	HEM	C1D-C2D	3.44	1.51	1.44
2	B	801	HEM	FE-NB	3.33	2.05	1.94
2	B	801	HEM	CHC-C4B	3.07	1.46	1.39
2	B	801	HEM	C4D-ND	-3.06	1.34	1.40
2	A	801	HEM	C3B-C2B	2.86	1.43	1.37
2	A	801	HEM	CMA-C3A	2.78	1.56	1.50
2	B	801	HEM	CMD-C2D	-2.76	1.45	1.50
2	A	801	HEM	CHA-C1A	-2.72	1.33	1.39
2	A	801	HEM	C4C-NC	-2.45	1.35	1.39
2	B	801	HEM	FE-ND	2.44	2.02	1.94
2	B	801	HEM	C2A-C3A	-2.42	1.32	1.38
2	B	801	HEM	CHB-C1B	2.38	1.43	1.38
2	B	801	HEM	C4D-C3D	2.35	1.49	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C4C-NC	2.29	1.43	1.39
2	B	801	HEM	C3D-C2D	2.10	1.41	1.36
2	A	801	HEM	CHD-C4C	-2.04	1.34	1.38
6	B	805	MPD	C3-C2	2.04	1.60	1.54

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	C4B-C3B-C2B	-7.15	100.70	107.28
2	B	801	HEM	CAA-C2A-C1A	4.34	133.41	124.94
2	A	801	HEM	C4C-NC-C1C	4.27	112.79	105.82
2	A	801	HEM	O2A-CGA-CBA	3.91	126.35	114.00
2	A	801	HEM	C4D-ND-C1D	-3.83	100.67	105.21
2	A	801	HEM	CHA-C4D-ND	-3.67	119.83	124.37
2	A	801	HEM	O1A-CGA-CBA	-3.60	111.66	123.09
2	A	801	HEM	CMB-C2B-C1B	-3.52	119.54	125.03
2	A	801	HEM	CHD-C4C-NC	3.49	128.26	124.45
2	A	801	HEM	CAA-CBA-CGA	-3.36	104.75	113.67
2	A	801	HEM	C2A-C1A-NA	-3.24	106.56	110.15
2	A	801	HEM	C3D-C4D-ND	3.23	113.72	110.17
6	B	806	MPD	CM-C2-C1	-3.23	103.39	110.63
2	A	801	HEM	C1B-NB-C4B	3.20	108.99	105.21
2	B	801	HEM	CMA-C3A-C2A	3.17	132.35	125.62
2	B	801	HEM	CMA-C3A-C4A	-3.12	120.67	125.42
6	A	806	MPD	O2-C2-CM	3.08	117.58	107.99
2	B	801	HEM	CAA-C2A-C3A	-2.98	120.39	127.07
6	B	806	MPD	C1-C2-C3	2.85	122.51	110.20
2	B	801	HEM	CAD-CBD-CGD	2.83	121.17	113.67
6	A	807	MPD	O2-C2-CM	-2.83	99.17	107.99
6	B	806	MPD	O2-C2-C3	-2.71	99.14	109.27
2	B	801	HEM	C3C-C2C-C1C	-2.61	104.57	107.05
6	B	806	MPD	O4-C4-C5	-2.52	98.62	109.45
6	A	805	MPD	CM-C2-C1	-2.43	105.18	110.63
2	A	801	HEM	CBD-CAD-C3D	2.42	119.24	112.53
2	B	801	HEM	C2B-C1B-NB	2.42	112.63	109.84
2	B	801	HEM	CHC-C1C-NC	2.41	127.08	124.45
2	B	801	HEM	CHC-C1C-C2C	-2.41	120.47	125.49
2	B	801	HEM	C4D-ND-C1D	2.34	107.98	105.21
2	A	801	HEM	CHB-C1B-NB	-2.32	121.50	124.37
6	A	805	MPD	O4-C4-C3	-2.29	102.24	111.35
2	A	801	HEM	O2D-CGD-O1D	2.25	129.12	123.33
6	A	806	MPD	CM-C2-C1	-2.25	105.59	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	C2C-C1C-NC	-2.24	105.49	109.64
2	A	801	HEM	CAD-CBD-CGD	2.19	119.48	113.67
2	B	801	HEM	C4B-C3B-C2B	-2.17	105.29	107.28
2	B	801	HEM	C4C-C3C-C2C	2.16	108.69	106.81
2	A	801	HEM	O1D-CGD-CBD	-2.12	116.38	123.09
2	B	801	HEM	C4D-C3D-C2D	-2.05	103.90	106.89

There are no chirality outliers.

All (15) torsion outliers are listed below:

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

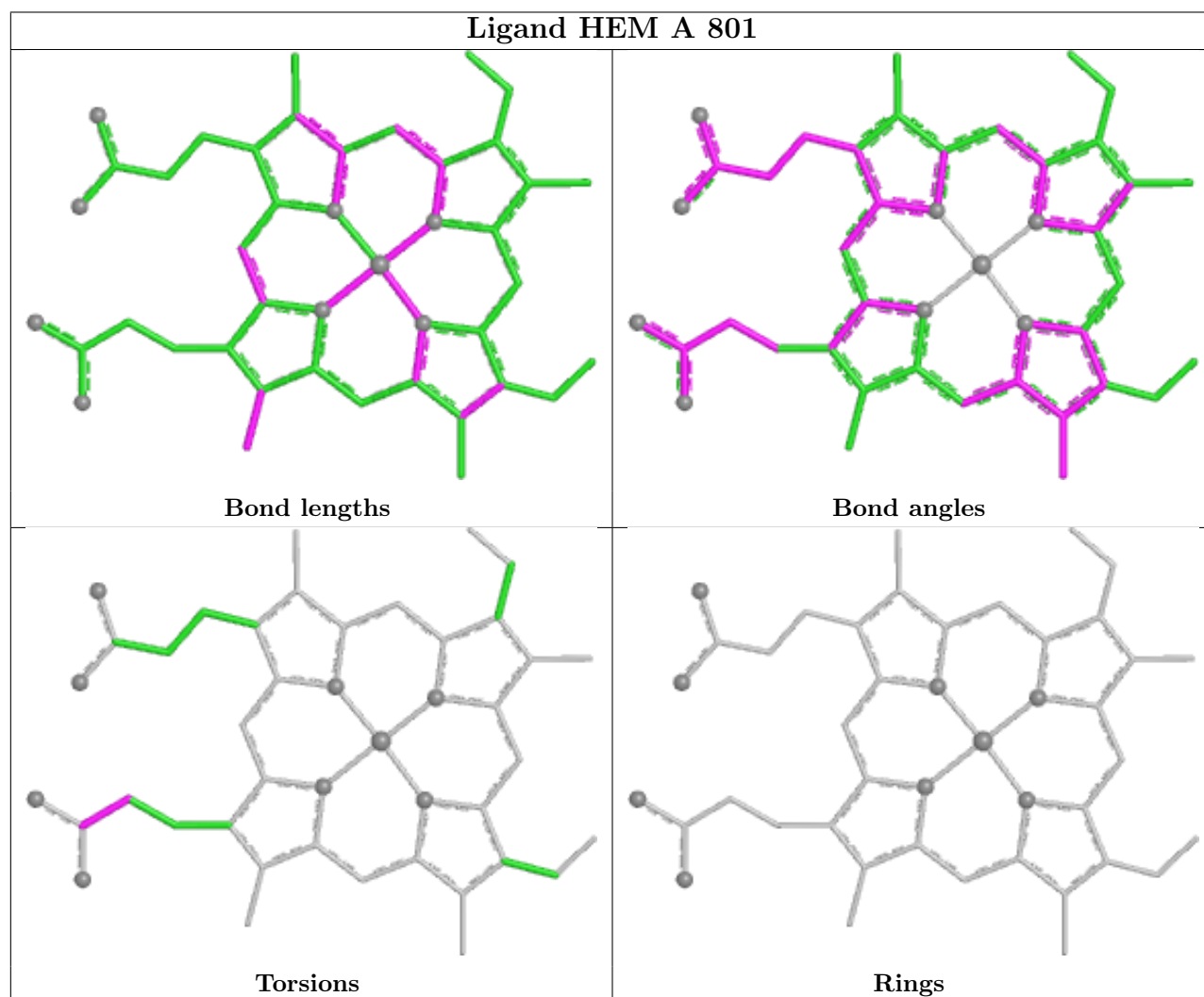
There are no ring outliers.

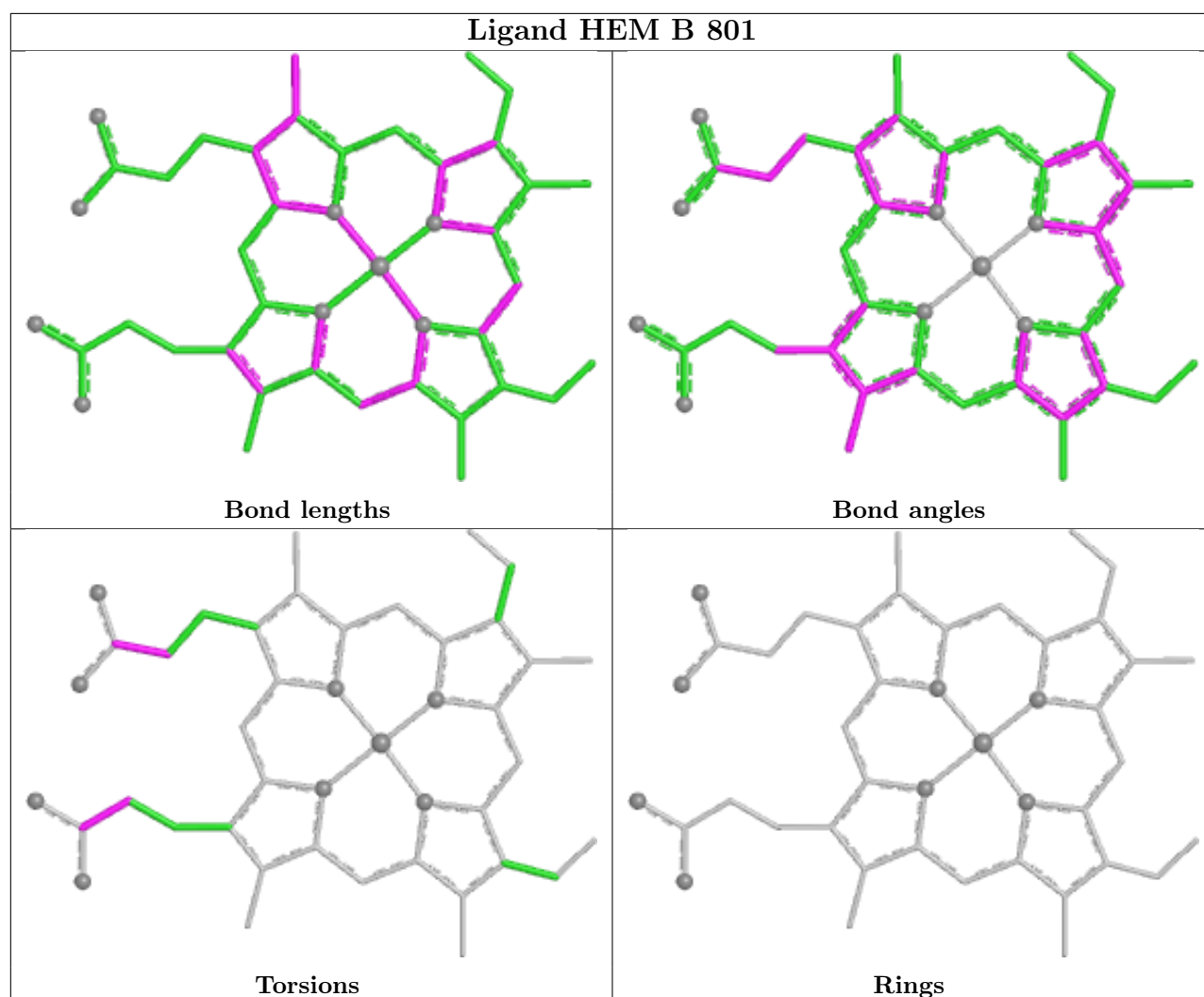
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	806	MPD	3	0
6	A	806	MPD	1	0
6	A	805	MPD	1	0
6	B	805	MPD	7	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%)	-0.22	11 (1%) 72 76	10, 22, 41, 81	6 (0%)
1	B	712/728 (97%)	-0.24	19 (2%) 56 60	11, 22, 41, 91	8 (1%)
All	All	1424/1456 (97%)	-0.23	30 (2%) 63 68	10, 22, 41, 91	14 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	5.5
1	B	748	ALA	4.6
1	B	680	ALA	4.3
1	A	53	HIS	4.0
1	B	64	LYS	3.9
1	B	53	HIS	3.9
1	B	610	ARG	3.8
1	B	679	ALA	3.7
1	B	54	ARG	3.7
1	B	65	ASP	3.7
1	A	610	ARG	3.6
1	B	568	HIS	3.3
1	B	55	HIS	3.3
1	A	55	HIS	3.1
1	A	54	ARG	3.0
1	A	64	LYS	2.8
1	B	541	GLY	2.6
1	B	540	ARG	2.6
1	A	40	ARG	2.6
1	B	682	ALA	2.5
1	B	40	ARG	2.5
1	A	58	LEU	2.4
1	A	609	TYR	2.3
1	B	691	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	607	GLY	2.2
1	B	199	ASP	2.2
1	B	607	GLY	2.2
1	B	649[A]	ARG	2.1
1	A	608	LYS	2.1
1	B	747	LEU	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	14,16,25,26	2
1	TOX	B	111[A]	16/17	0.99	0.03	15,16,21,22	3
1	TOX	B	111[B]	16/17	0.99	0.03	15,16,18,22	3

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.

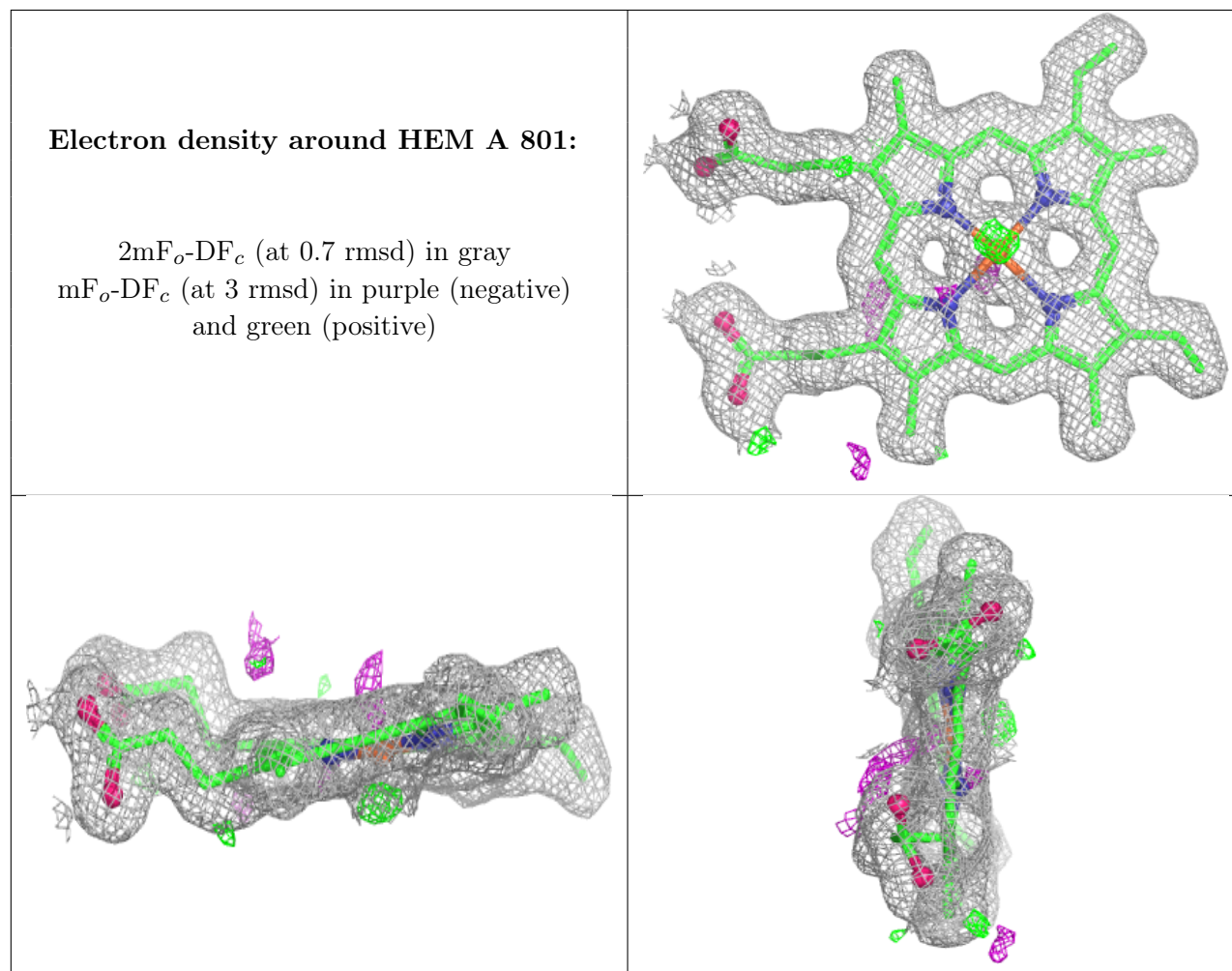
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MPD	A	807	8/8	0.80	0.24	60,68,73,74	0
6	MPD	A	805	8/8	0.85	0.17	44,50,61,63	0
6	MPD	B	806	8/8	0.86	0.22	56,66,71,75	0
6	MPD	A	806	8/8	0.87	0.19	51,59,73,75	0
6	MPD	B	805	8/8	0.88	0.14	32,44,48,48	0
5	OXY	A	804	2/2	0.90	0.19	42,42,42,43	0
5	OXY	B	804	2/2	0.91	0.18	35,35,35,36	0
3	NA	B	802	1/1	0.98	0.06	20,20,20,20	0
4	CL	B	803	1/1	0.98	0.09	32,32,32,32	0

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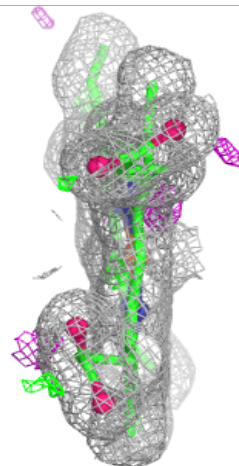
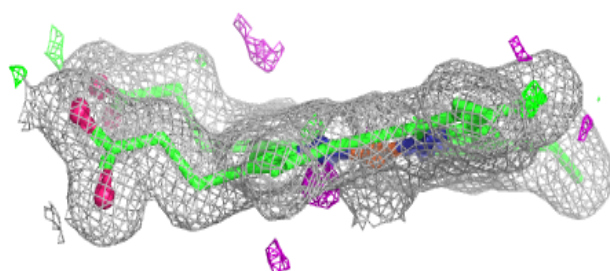
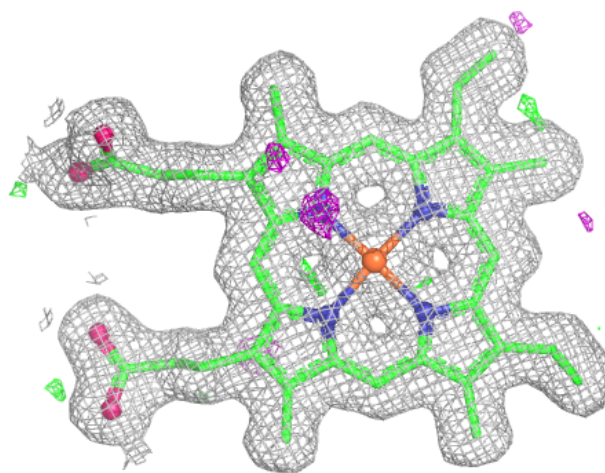
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NA	A	802	1/1	0.98	0.04	19,19,19,19	0
4	CL	A	803	1/1	0.99	0.09	30,30,30,30	0
2	HEM	A	801	43/43	0.99	0.05	16,19,22,23	0
2	HEM	B	801	43/43	0.99	0.05	15,16,19,24	0

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 [i](#)

There are no such residues in this entry.