



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 09:04 AM UTC

PDB ID : 5SYI / pdb_00005syi
Title : Structure of D141A variant of B. pseudomallei KatG complexed with INH
Authors : Loewen, P.C.
Deposited on : 2016-08-11
Resolution : 1.70 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

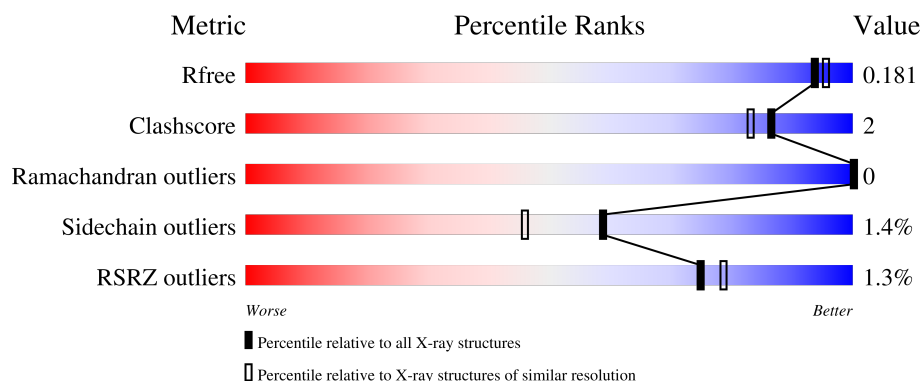
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	% 84% 13% ..
1	B	728	2% 84% 12% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NIZ	B	805	-	X	-	-
8	PO4	B	809	-	X	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12740 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.

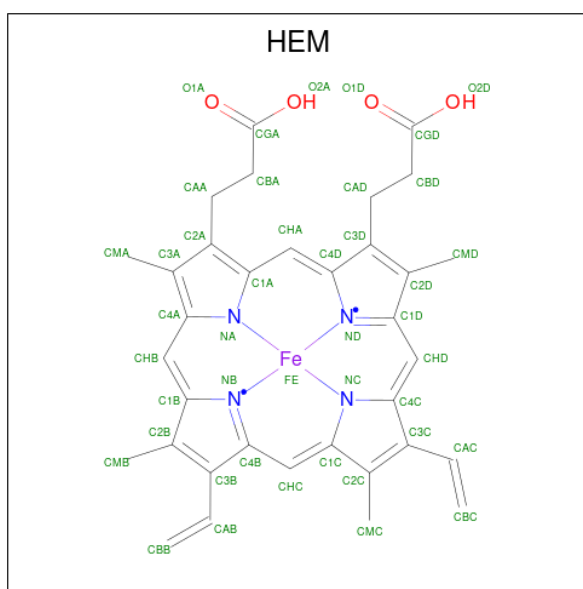
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	4	0
			5523	3490	984	1035	14			
1	B	713	Total	C	N	O	S	0	5	0
			5526	3494	984	1034	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

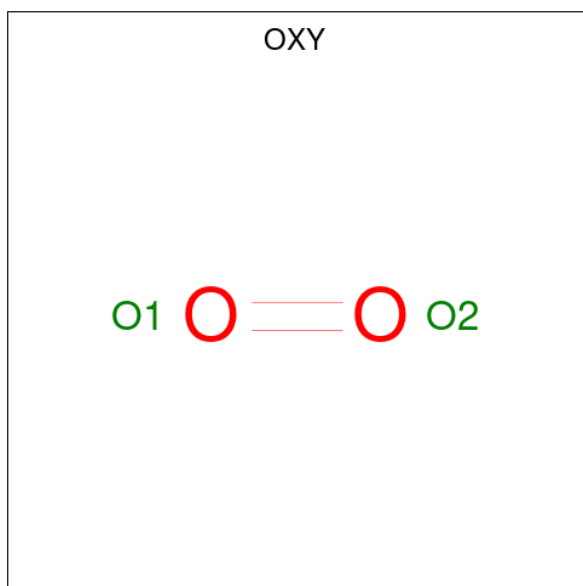
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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).

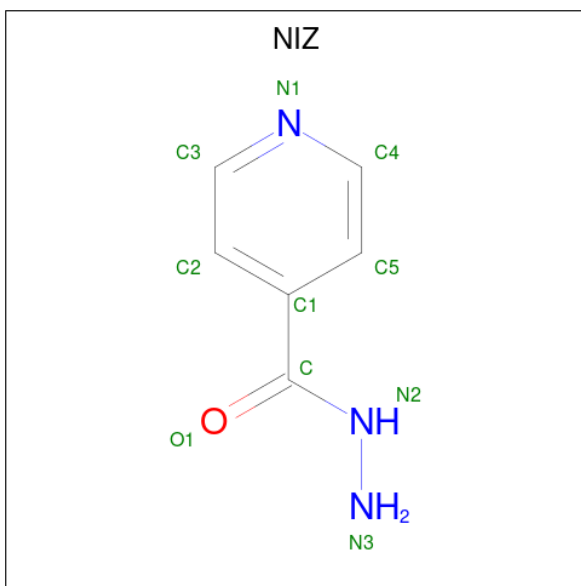
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl		
			1	1	0	0
4	B	1	Total	Cl		
			1	1	0	0

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



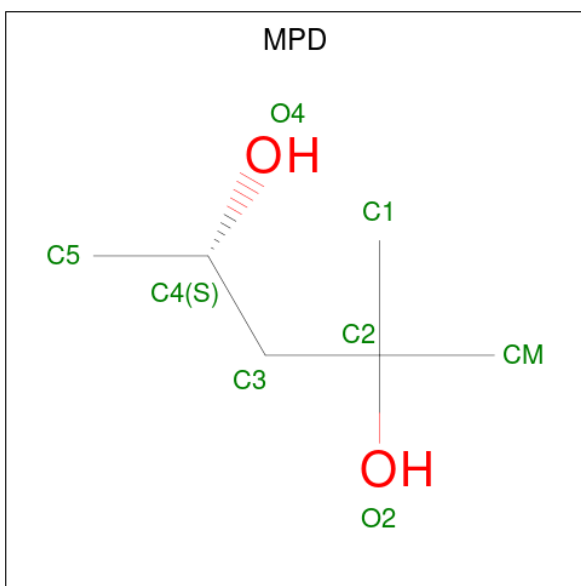
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O		
			2	2	0	0
5	B	1	Total	O		
			2	2	0	0

- Molecule 6 is pyridine-4-carbohydrazide (CCD ID: NIZ) (formula: $C_6H_7N_3O$).



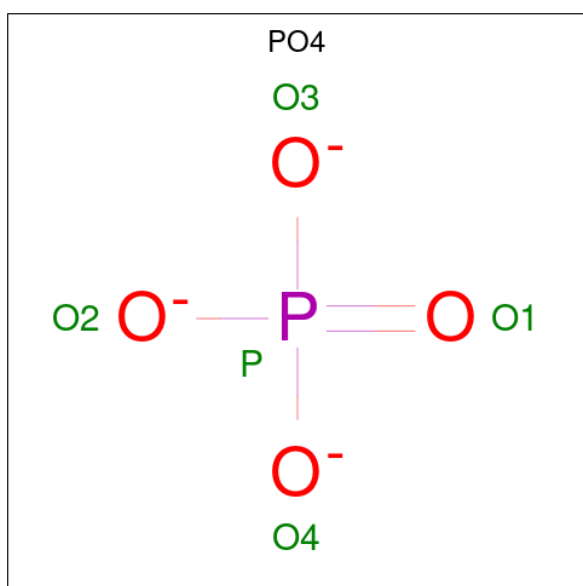
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			10	6	3	1		
6	B	1	Total	C	N	O	0	0
			10	6	3	1		
6	B	1	Total	C	N	O	0	0
			10	6	3	1		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



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

- Molecule 8 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

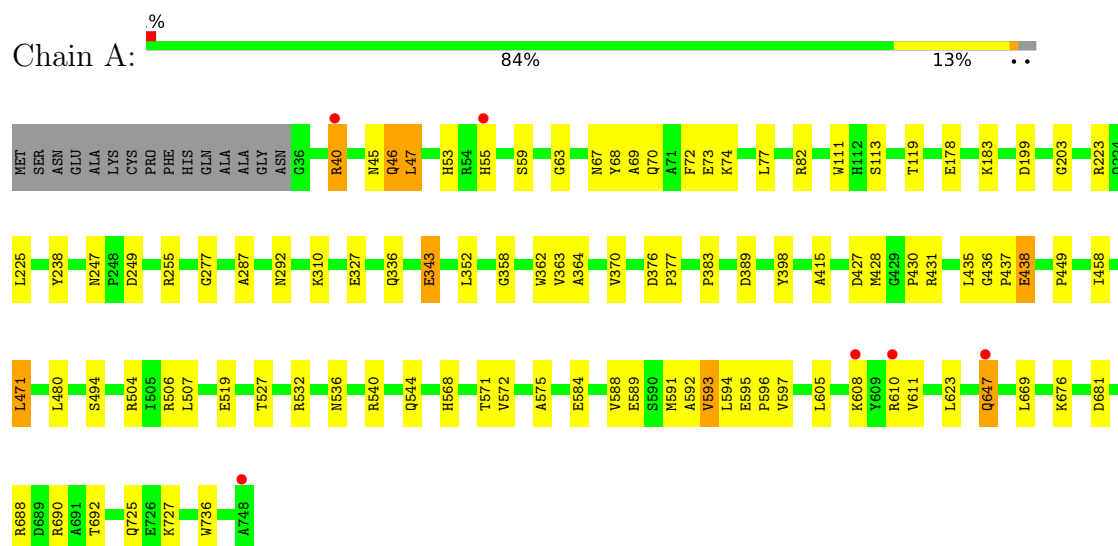
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	783	Total	O	0	0
			783	783		
9	B	742	Total	O	0	0
			742	742		

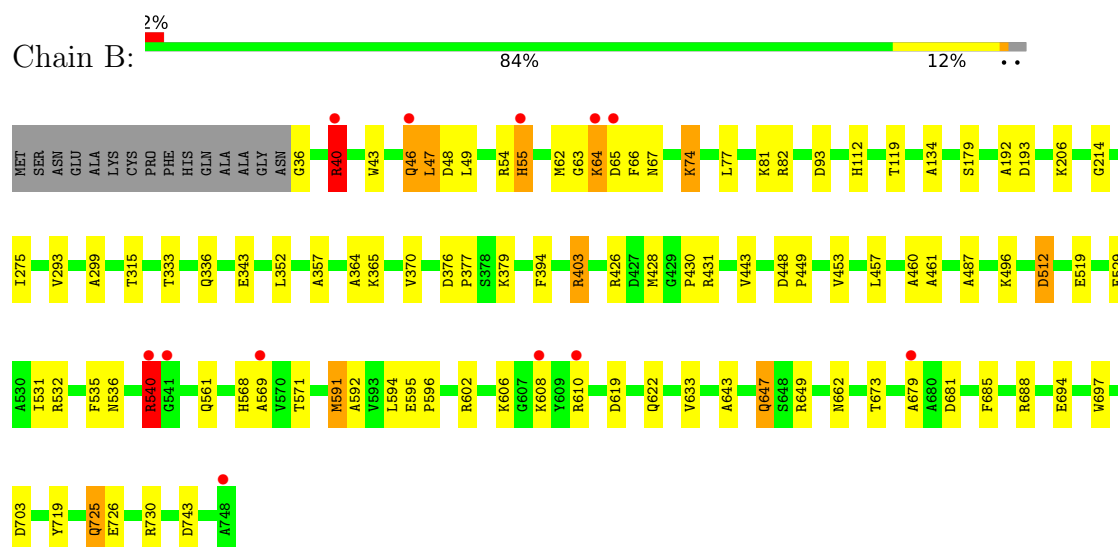
3 Residue-property plots [i](#)

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 115.59Å 174.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.70 20.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (20.00-1.70) 99.3 (20.00-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.145 , 0.170 0.159 , 0.181	Depositor DCC
R_{free} test set	11143 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12740	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 3.22% 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, NIZ, MPD, CL, NA, PO4

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	1.85	87/5677 (1.5%)	1.48	26/7718 (0.3%)
1	B	1.84	76/5685 (1.3%)	1.45	35/7729 (0.5%)
All	All	1.85	163/11362 (1.4%)	1.46	61/15447 (0.4%)

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	2

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	532	ARG	CD-NE	-12.47	1.28	1.46
1	B	540	ARG	C-O	10.06	1.36	1.23
1	B	63	GLY	N-CA	10.02	1.58	1.45
1	A	255	ARG	CD-NE	9.74	1.59	1.46
1	B	179	SER	C-O	9.44	1.35	1.24
1	B	453	VAL	C-O	-8.93	1.13	1.24
1	A	540	ARG	C-O	8.90	1.35	1.23
1	B	512	ASP	CG-OD2	8.89	1.42	1.25
1	B	448	ASP	N-CA	8.27	1.52	1.46
1	A	47	LEU	CB-CG	-8.13	1.37	1.53
1	B	82	ARG	CZ-NH2	-8.08	1.23	1.33
1	A	532	ARG	NE-CZ	-8.04	1.24	1.33
1	A	532	ARG	CZ-NH2	-7.75	1.23	1.33
1	B	535	PHE	CA-C	-7.75	1.43	1.52
1	A	203	GLY	C-O	7.64	1.29	1.23
1	B	606	LYS	N-CA	7.63	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	426	ARG	CZ-NH2	7.61	1.43	1.33
1	B	703	ASP	N-CA	-7.52	1.37	1.46
1	B	726	GLU	CD-OE1	7.16	1.39	1.25
1	B	457	LEU	C-O	7.13	1.32	1.23
1	A	77	LEU	N-CA	-7.13	1.37	1.46
1	B	532	ARG	NE-CZ	-7.12	1.25	1.33
1	A	376	ASP	N-CA	7.10	1.55	1.46
1	A	597	VAL	N-CA	-7.02	1.37	1.46
1	A	363	VAL	C-O	6.98	1.31	1.23
1	A	383	PRO	CA-C	-6.97	1.43	1.52
1	B	568	HIS	CA-C	6.94	1.60	1.52
1	A	536	ASN	CA-C	6.86	1.61	1.52
1	A	45	ASN	C-O	-6.80	1.14	1.24
1	B	293	VAL	N-CA	6.80	1.54	1.46
1	B	688	ARG	N-CA	6.80	1.54	1.45
1	B	47	LEU	CB-CG	-6.67	1.40	1.53
1	B	449	PRO	CA-C	6.61	1.61	1.52
1	B	694	GLU	CA-C	6.60	1.61	1.52
1	B	36	GLY	N-CA	6.60	1.56	1.45
1	A	572	VAL	N-CA	-6.59	1.38	1.46
1	A	247	ASN	CG-ND2	-6.55	1.19	1.33
1	B	681	ASP	CA-C	6.54	1.59	1.52
1	A	676	LYS	CA-C	-6.47	1.45	1.52
1	B	602	ARG	CZ-NH2	-6.44	1.25	1.33
1	A	199	ASP	C-O	6.43	1.31	1.24
1	A	647	GLN	CG-CD	6.42	1.68	1.52
1	A	458	ILE	CA-CB	-6.39	1.47	1.54
1	B	365	LYS	N-CA	6.39	1.53	1.46
1	B	77	LEU	CA-CB	-6.37	1.43	1.53
1	B	343	GLU	C-O	6.36	1.31	1.24
1	A	692	THR	CA-C	-6.35	1.44	1.52
1	A	277	GLY	CA-C	-6.34	1.45	1.52
1	A	647	GLN	CA-C	6.31	1.61	1.53
1	B	647	GLN	CA-C	6.27	1.61	1.53
1	B	592	ALA	CA-C	-6.24	1.44	1.52
1	A	507	LEU	CA-C	-6.24	1.45	1.52
1	B	192	ALA	N-CA	6.21	1.53	1.46
1	A	292	ASN	CA-C	6.17	1.61	1.52
1	A	377	PRO	C-O	-6.12	1.15	1.24
1	B	619	ASP	CG-OD1	-6.12	1.13	1.25
1	A	53	HIS	N-CA	6.12	1.52	1.46
1	A	575	ALA	C-O	-6.08	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	588	VAL	N-CA	-6.07	1.39	1.46
1	A	688	ARG	CA-C	-6.06	1.45	1.52
1	A	255	ARG	NE-CZ	6.02	1.39	1.33
1	B	377	PRO	C-O	-6.00	1.15	1.24
1	A	59	SER	C-O	-5.99	1.16	1.24
1	A	362	TRP	CA-C	-5.98	1.45	1.52
1	A	178	GLU	C-O	5.96	1.31	1.24
1	A	370	VAL	CA-C	5.92	1.59	1.52
1	A	519	GLU	N-CA	5.89	1.53	1.46
1	B	496	LYS	CE-NZ	-5.82	1.31	1.49
1	A	183	LYS	C-O	5.82	1.31	1.24
1	A	593	VAL	CA-CB	5.80	1.62	1.54
1	B	119	THR	CB-CG2	-5.78	1.33	1.52
1	B	376	ASP	N-CA	5.76	1.53	1.46
1	A	63	GLY	N-CA	5.76	1.52	1.45
1	A	471	LEU	CA-C	5.75	1.60	1.52
1	B	370	VAL	N-CA	-5.75	1.40	1.46
1	B	443	VAL	CA-C	-5.74	1.45	1.52
1	A	595	GLU	C-N	-5.73	1.28	1.33
1	B	561	GLN	CA-C	5.71	1.60	1.52
1	B	67	ASN	CA-C	5.69	1.59	1.52
1	B	536	ASN	CA-C	5.68	1.60	1.52
1	A	506	ARG	C-O	5.66	1.31	1.24
1	B	571	THR	C-O	5.63	1.30	1.24
1	A	571	THR	CA-C	5.63	1.59	1.52
1	A	427	ASP	CA-C	-5.60	1.44	1.52
1	A	681	ASP	CA-C	5.59	1.58	1.52
1	A	113	SER	C-O	5.58	1.30	1.24
1	A	532	ARG	CA-C	5.58	1.59	1.52
1	B	55	HIS	C-O	-5.57	1.15	1.23
1	B	315	THR	CA-C	5.55	1.60	1.52
1	A	287	ALA	CA-C	5.55	1.60	1.52
1	B	596	PRO	C-O	5.55	1.28	1.24
1	A	725	GLN	CG-CD	5.54	1.66	1.52
1	B	430	PRO	CA-CB	-5.54	1.46	1.53
1	B	643	ALA	N-CA	-5.54	1.38	1.46
1	B	685	PHE	N-CA	-5.54	1.39	1.46
1	A	449	PRO	C-N	-5.52	1.29	1.33
1	B	679	ALA	N-CA	5.52	1.52	1.46
1	B	529	GLU	N-CA	5.52	1.53	1.46
1	B	743	ASP	N-CA	-5.51	1.39	1.46
1	A	438	GLU	CD-OE1	-5.50	1.14	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	596	PRO	CA-CB	-5.50	1.48	1.54
1	B	46	GLN	N-CA	5.48	1.52	1.45
1	B	394	PHE	N-CA	5.48	1.53	1.46
1	A	74	LYS	CA-C	5.48	1.60	1.52
1	A	336	GLN	CD-NE2	5.46	1.44	1.33
1	B	299	ALA	CA-C	-5.46	1.45	1.52
1	B	647	GLN	CD-OE1	5.44	1.33	1.23
1	A	692	THR	N-CA	5.43	1.53	1.46
1	A	568	HIS	CA-CB	-5.40	1.45	1.53
1	B	571	THR	CA-CB	5.39	1.63	1.53
1	B	461	ALA	CA-C	5.39	1.59	1.52
1	B	697	TRP	CA-C	-5.38	1.46	1.52
1	B	275	ILE	C-O	-5.37	1.18	1.24
1	B	214	GLY	CA-C	-5.37	1.43	1.51
1	A	352	LEU	CA-C	-5.36	1.45	1.52
1	A	428	MET	CG-SD	-5.36	1.67	1.80
1	A	688	ARG	CZ-NH2	-5.36	1.26	1.33
1	A	225	LEU	CA-CB	5.36	1.61	1.53
1	B	49	LEU	CB-CG	-5.36	1.42	1.53
1	A	82	ARG	CZ-NH2	-5.36	1.26	1.33
1	B	591	MET	SD-CE	-5.35	1.66	1.79
1	A	68	TYR	N-CA	5.34	1.52	1.46
1	A	480	LEU	CA-C	5.33	1.59	1.52
1	A	437	PRO	CA-C	-5.32	1.45	1.52
1	A	527	THR	N-CA	-5.31	1.40	1.46
1	B	531	ILE	N-CA	5.31	1.52	1.46
1	B	193	ASP	C-O	5.30	1.30	1.23
1	A	40	ARG	N-CA	5.29	1.52	1.46
1	A	40	ARG	CA-CB	5.28	1.61	1.53
1	A	46	GLN	CG-CD	5.27	1.65	1.52
1	A	669	LEU	N-CA	-5.27	1.39	1.46
1	A	431	ARG	CD-NE	5.26	1.53	1.46
1	B	487	ALA	N-CA	-5.26	1.39	1.46
1	B	448	ASP	CA-CB	-5.24	1.49	1.52
1	A	584	GLU	CG-CD	5.24	1.65	1.52
1	B	571	THR	N-CA	5.23	1.52	1.46
1	A	72	PHE	N-CA	-5.23	1.40	1.46
1	B	596	PRO	N-CA	5.23	1.52	1.47
1	A	358	GLY	C-O	-5.23	1.17	1.24
1	A	310	LYS	CA-C	5.22	1.59	1.52
1	B	364	ALA	CA-CB	-5.21	1.46	1.53
1	B	725	GLN	CD-OE1	5.21	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	327	GLU	CD-OE1	5.21	1.35	1.25
1	A	596	PRO	CA-C	5.20	1.57	1.52
1	B	336	GLN	CA-C	-5.20	1.46	1.52
1	A	67	ASN	CA-C	5.20	1.58	1.52
1	B	65	ASP	CG-OD1	5.18	1.35	1.25
1	A	415	ALA	CA-C	-5.17	1.46	1.52
1	A	370	VAL	C-O	-5.17	1.18	1.24
1	A	494	SER	CA-C	5.15	1.59	1.52
1	B	74	LYS	CA-C	5.14	1.59	1.52
1	A	430	PRO	CA-CB	-5.11	1.46	1.53
1	A	398	TYR	CA-CB	-5.10	1.45	1.53
1	B	673	THR	CA-C	-5.09	1.46	1.52
1	A	736	TRP	N-CA	5.08	1.52	1.46
1	B	352	LEU	CA-C	-5.08	1.46	1.52
1	A	364	ALA	CA-CB	-5.06	1.46	1.53
1	A	436	GLY	C-N	-5.05	1.29	1.34
1	A	611	VAL	CA-C	5.05	1.57	1.53
1	B	40	ARG	N-CA	5.02	1.52	1.46
1	B	357	ALA	C-O	-5.02	1.17	1.24
1	A	435	LEU	N-CA	-5.02	1.39	1.45
1	A	255	ARG	CG-CD	5.02	1.67	1.52

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	ARG	NE-CZ-NH2	-23.23	98.30	119.20
1	A	532	ARG	NE-CZ-NH1	15.84	137.34	121.50
1	A	532	ARG	CD-NE-CZ	10.51	139.12	124.40
1	B	46	GLN	N-CA-C	-9.04	98.34	110.55
1	B	47	LEU	N-CA-CB	-8.94	97.30	110.17
1	B	46	GLN	CA-CB-CG	8.71	131.51	114.10
1	A	46	GLN	N-CA-C	-8.69	99.07	110.53
1	A	47	LEU	N-CA-CB	-8.63	97.75	110.17
1	B	571	THR	CA-C-O	8.06	129.06	120.36
1	B	571	THR	CB-CA-C	7.69	123.78	109.71
1	A	46	GLN	CA-CB-CG	7.65	129.39	114.10
1	B	431	ARG	NE-CZ-NH2	7.14	125.62	119.20
1	A	532	ARG	CB-CG-CD	-6.65	96.00	111.30
1	B	55	HIS	CB-CA-C	6.20	120.99	111.39
1	B	428	MET	CA-CB-CG	-6.13	101.83	114.10
1	B	66	PHE	CA-C-N	-6.10	114.20	122.86
1	B	66	PHE	C-N-CA	-6.10	114.20	122.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	403	ARG	CG-CD-NE	-6.08	98.62	112.00
1	B	54	ARG	CG-CD-NE	-6.03	98.73	112.00
1	B	571	THR	CA-C-N	-5.96	117.56	123.04
1	B	571	THR	C-N-CA	-5.96	117.56	123.04
1	B	93	ASP	N-CA-C	5.93	118.53	111.71
1	B	206	LYS	CG-CD-CE	5.74	124.49	111.30
1	A	431	ARG	NE-CZ-NH2	5.70	124.33	119.20
1	A	47	LEU	CA-C-O	-5.69	115.36	121.56
1	B	40	ARG	CA-CB-CG	5.69	125.47	114.10
1	A	592	ALA	N-CA-C	5.66	118.17	111.33
1	A	40	ARG	CA-CB-CG	5.65	125.41	114.10
1	B	48	ASP	N-CA-C	5.65	118.75	107.62
1	B	529	GLU	CB-CG-CD	5.60	122.13	112.60
1	B	460	ALA	N-CA-C	5.60	118.31	111.82
1	B	571	THR	O-C-N	-5.58	116.66	123.30
1	B	529	GLU	N-CA-C	-5.57	105.36	111.82
1	A	70	GLN	CA-CB-CG	5.57	125.23	114.10
1	B	81	LYS	CA-C-O	-5.53	114.69	120.55
1	A	727	LYS	N-CA-C	5.51	117.28	111.28
1	B	569	ALA	CA-C-O	-5.44	114.76	120.58
1	A	249	ASP	O-C-N	5.43	127.31	121.12
1	B	595	GLU	O-C-N	5.42	126.13	121.30
1	A	343	GLU	CB-CG-CD	5.40	121.78	112.60
1	A	605	LEU	CB-CA-C	-5.33	101.93	110.14
1	B	62	MET	CA-C-N	-5.31	114.53	120.53
1	B	62	MET	C-N-CA	-5.31	114.53	120.53
1	A	584	GLU	CB-CG-CD	5.28	121.58	112.60
1	A	389	ASP	CA-C-O	5.27	126.01	120.42
1	A	623	LEU	CA-C-O	5.27	126.14	120.55
1	A	46	GLN	CB-CG-CD	5.24	121.51	112.60
1	A	55	HIS	CB-CA-C	5.19	119.44	111.39
1	A	223	ARG	CA-CB-CG	-5.17	103.75	114.10
1	B	54	ARG	CA-C-N	-5.17	115.30	122.74
1	B	54	ARG	C-N-CA	-5.17	115.30	122.74
1	B	134	ALA	CA-C-O	-5.17	115.07	120.70
1	A	690	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	B	43	TRP	CA-C-N	-5.12	114.51	120.04
1	B	43	TRP	C-N-CA	-5.12	114.51	120.04
1	A	588	VAL	N-CA-C	5.10	115.82	110.62
1	B	333	THR	CA-C-N	-5.09	114.58	119.87
1	B	333	THR	C-N-CA	-5.09	114.58	119.87
1	A	519	GLU	CA-CB-CG	-5.07	103.96	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	ARG	CD-NE-CZ	5.04	131.46	124.40
1	B	592	ALA	N-CA-C	5.00	117.47	111.71

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	438	GLU	Sidechain
1	A	47	LEU	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	5523	0	5351	12	0
1	B	5526	0	5360	17	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	1	0
5	B	2	0	0	1	0
6	A	10	0	7	2	0
6	B	20	0	14	4	0
7	A	16	0	28	10	0
7	B	16	0	28	4	0
8	A	5	0	0	0	0
8	B	5	0	0	0	0
9	A	783	0	0	11	1
9	B	742	0	0	8	1
All	All	12740	0	10848	46	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (46) 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:806:MPD:H11	7:A:806:MPD:O4	1.44	1.14
5:B:804:OXY:O1	6:B:806:NIZ:N2	1.85	1.08
1:A:119[B]:THR:HG21	9:A:1012:HOH:O	1.73	0.88
7:A:806:MPD:H53	9:A:1185:HOH:O	1.75	0.85
5:A:804:OXY:O1	6:A:805:NIZ:N2	2.11	0.84
7:A:806:MPD:H11	7:A:806:MPD:HO4	1.46	0.80
7:A:806:MPD:O4	7:A:806:MPD:C1	2.25	0.80
1:B:47:LEU:O	9:B:901:HOH:O	2.00	0.79
7:A:806:MPD:H51	9:A:1600:HOH:O	1.83	0.77
7:A:807:MPD:H12	7:A:807:MPD:C5	2.14	0.77
1:B:622:GLN:OE1	6:B:805:NIZ:O1	2.08	0.72
1:A:343:GLU:OE1	9:A:901:HOH:O	2.12	0.67
7:B:807:MPD:HM1	9:B:1374:HOH:O	1.93	0.67
1:B:55:HIS:HD2	9:B:1287:HOH:O	1.81	0.62
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.81	0.62
1:A:593:VAL:HG13	9:A:926:HOH:O	2.00	0.62
7:A:807:MPD:H12	7:A:807:MPD:H52	1.83	0.59
1:B:519:GLU:OE1	9:B:902:HOH:O	2.16	0.59
1:B:40:ARG:NH1	9:B:908:HOH:O	2.35	0.58
1:B:730[A]:ARG:HD2	9:B:1519:HOH:O	2.04	0.58
7:B:808:MPD:C5	7:B:808:MPD:HM2	2.34	0.58
7:B:808:MPD:HM2	7:B:808:MPD:H52	1.84	0.58
1:B:403:ARG:NH1	9:B:910:HOH:O	2.38	0.57
1:B:591:MET:SD	1:B:594:LEU:HD12	2.46	0.56
1:A:69:ALA:O	1:A:73:GLU:HG3	2.06	0.56
1:A:647:GLN:HG2	9:A:1127:HOH:O	2.04	0.56
1:B:512:ASP:OD1	9:B:903:HOH:O	2.18	0.55
1:A:343:GLU:HG3	9:A:901:HOH:O	2.07	0.53
1:A:591:MET:SD	1:A:594:LEU:HD12	2.48	0.53
7:A:807:MPD:H12	7:A:807:MPD:H53	1.88	0.53
7:B:807:MPD:O4	7:B:807:MPD:O2	2.27	0.50
1:B:662:ASN:H	1:B:725:GLN:HE22	1.60	0.48
1:B:64:LYS:O	1:B:64:LYS:HD3	2.15	0.46
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.99	0.46
1:B:622:GLN:HE22	6:B:805:NIZ:C1	2.30	0.44
1:A:504:ARG:HD2	9:A:932:HOH:O	2.18	0.43
1:B:540:ARG:CZ	1:B:540:ARG:HA	2.48	0.43
1:A:544:GLN:OE1	9:A:902:HOH:O	2.21	0.43
7:A:807:MPD:C5	7:A:807:MPD:C1	2.88	0.43
7:A:807:MPD:HM3	9:A:1039:HOH:O	2.17	0.43
1:A:111:TRP:HZ3	1:A:238:TYR:HH	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:540:ARG:HA	1:B:540:ARG:NH1	2.34	0.42
6:A:805:NIZ:H4	9:A:1191:HOH:O	2.20	0.42
1:B:633[A]:VAL:HG22	1:B:719:TYR:CZ	2.55	0.41
1:A:471:LEU:HD23	1:A:471:LEU:HA	1.94	0.41
1:B:112:HIS:NE2	6:B:806:NIZ:N2	2.69	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1132:HOH:O	9:B:1056:HOH:O[2_444]	2.16	0.04

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	715/728 (98%)	706 (99%)	9 (1%)	0	100	100
1	B	716/728 (98%)	709 (99%)	7 (1%)	0	100	100
All	All	1431/1456 (98%)	1415 (99%)	16 (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	553/560 (99%)	548 (99%)	5 (1%)	70	62
1	B	554/560 (99%)	544 (98%)	10 (2%)	51	36
All	All	1107/1120 (99%)	1092 (99%)	15 (1%)	59	46

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	46	GLN
1	A	589	GLU
1	A	608	LYS
1	A	610	ARG
1	B	40	ARG
1	B	46	GLN
1	B	64	LYS
1	B	74	LYS
1	B	379	LYS
1	B	540	ARG
1	B	608	LYS
1	B	610	ARG
1	B	647	GLN
1	B	649	ARG

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

Mol	Chain	Res	Type
1	A	227	ASN
1	A	247	ASN
1	A	568	HIS
1	A	737	ASN
1	B	55	HIS
1	B	622	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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 17 ligands modelled in this entry, 4 are monoatomic - leaving 13 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
7	MPD	A	807	-	7,7,7	0.79	0	9,10,10	2.53	4 (44%)
6	NIZ	B	805	-	10,10,10	4.84	7 (70%)	12,12,12	4.14	8 (66%)
5	OXY	B	804	-	1,1,1	0.08	0	-		
5	OXY	A	804	-	1,1,1	0.18	0	-		
7	MPD	B	808	-	7,7,7	1.18	0	9,10,10	1.24	2 (22%)
2	HEM	A	801	1,6	50,50,50	1.55	10 (20%)	67,82,82	1.54	13 (19%)
8	PO4	A	808	-	4,4,4	1.21	1 (25%)	6,6,6	2.76	2 (33%)
2	HEM	B	801	1,6	50,50,50	2.00	16 (32%)	67,82,82	1.63	15 (22%)
7	MPD	A	806	-	7,7,7	1.51	2 (28%)	9,10,10	1.45	3 (33%)
6	NIZ	B	806	2	10,10,10	3.77	4 (40%)	12,12,12	3.05	7 (58%)
8	PO4	B	809	-	4,4,4	2.02	1 (25%)	6,6,6	4.11	3 (50%)
7	MPD	B	807	-	7,7,7	0.70	0	9,10,10	1.34	2 (22%)
6	NIZ	A	805	2	10,10,10	3.63	6 (60%)	12,12,12	1.74	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
7	MPD	A	807	-	-	2/5/5/5	-
6	NIZ	B	805	-	-	1/6/6/6	0/1/1/1
7	MPD	B	808	-	-	3/5/5/5	-
2	HEM	A	801	1,6	-	2/14/54/54	-
2	HEM	B	801	1,6	-	2/14/54/54	-
7	MPD	A	806	-	-	3/5/5/5	-
6	NIZ	B	806	2	-	0/6/6/6	0/1/1/1
7	MPD	B	807	-	-	3/5/5/5	-
6	NIZ	A	805	2	-	0/6/6/6	0/1/1/1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	805	NIZ	C4-N1	9.71	1.60	1.33
6	B	806	NIZ	C-N2	7.74	1.41	1.33
6	B	805	NIZ	C5-C1	7.28	1.50	1.39
6	A	805	NIZ	C-N2	6.88	1.40	1.33
6	B	805	NIZ	C2-C1	6.43	1.49	1.39
6	A	805	NIZ	C2-C1	6.11	1.48	1.39
2	B	801	HEM	C1A-NA	-5.83	1.28	1.39
6	B	806	NIZ	C2-C1	5.33	1.47	1.39
6	B	806	NIZ	C4-N1	4.95	1.47	1.33
2	B	801	HEM	C4A-NA	4.66	1.48	1.39
6	B	805	NIZ	N3-N2	-4.58	1.35	1.41
2	A	801	HEM	O1A-CGA	4.20	1.35	1.22
6	A	805	NIZ	C3-N1	4.11	1.45	1.33
6	B	806	NIZ	C3-N1	3.94	1.44	1.33
8	B	809	PO4	P-O3	-3.49	1.44	1.54
2	B	801	HEM	C4C-NC	-3.44	1.33	1.39
6	A	805	NIZ	C5-C1	3.39	1.44	1.39
6	A	805	NIZ	C4-N1	3.25	1.42	1.33
6	B	805	NIZ	C-N2	3.16	1.37	1.33
2	B	801	HEM	C1B-NB	-3.15	1.34	1.40
2	A	801	HEM	FE-NB	3.08	2.04	1.94
2	A	801	HEM	FE-NC	3.06	2.05	1.95
2	A	801	HEM	CMA-C3A	3.05	1.57	1.50
2	B	801	HEM	C1C-C2C	-3.05	1.39	1.45
2	B	801	HEM	CAC-C3C	-2.89	1.39	1.47
6	B	805	NIZ	C2-C3	2.86	1.44	1.38
2	B	801	HEM	C1D-ND	-2.81	1.33	1.38
2	B	801	HEM	CMB-C2B	2.80	1.56	1.50
2	B	801	HEM	C3B-C2B	-2.78	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C3B-C2B	2.67	1.42	1.37
2	A	801	HEM	FE-NA	2.63	2.03	1.95
2	A	801	HEM	C1B-NB	-2.62	1.35	1.40
2	B	801	HEM	FE-NC	2.60	2.03	1.95
2	A	801	HEM	CMD-C2D	-2.59	1.45	1.50
2	B	801	HEM	FE-ND	2.52	2.02	1.94
2	B	801	HEM	CHC-C1C	2.41	1.43	1.38
2	B	801	HEM	CHB-C4A	-2.32	1.34	1.39
2	B	801	HEM	C1D-C2D	2.31	1.49	1.44
2	A	801	HEM	O2A-CGA	-2.22	1.23	1.30
6	B	805	NIZ	C1-C	-2.17	1.45	1.50
6	A	805	NIZ	O1-C	-2.17	1.18	1.23
2	B	801	HEM	CBA-CGA	2.16	1.55	1.50
2	A	801	HEM	CAD-C3D	-2.09	1.46	1.51
7	A	806	MPD	O4-C4	2.08	1.51	1.43
7	A	806	MPD	C3-C2	-2.08	1.48	1.54
8	A	808	PO4	P-O4	-2.02	1.48	1.54
2	B	801	HEM	O2D-CGD	-2.00	1.24	1.30

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	805	NIZ	C1-C-N2	8.56	125.83	116.33
8	B	809	PO4	O3-P-O2	8.39	134.02	107.91
6	B	806	NIZ	C1-C-N2	7.55	124.70	116.33
6	B	805	NIZ	C5-C4-N1	-6.10	113.20	123.60
2	B	801	HEM	C1D-C2D-C3D	-5.52	101.17	106.98
6	B	805	NIZ	C5-C1-C2	5.20	125.18	118.57
8	A	808	PO4	O3-P-O1	-4.87	93.72	110.95
8	B	809	PO4	O2-P-O1	-4.75	94.15	110.95
6	B	805	NIZ	C3-C2-C1	-4.43	114.21	119.05
6	B	805	NIZ	O1-C-C1	-4.38	112.22	120.90
2	A	801	HEM	CAA-CBA-CGA	-4.37	102.08	113.67
2	A	801	HEM	CHC-C1C-NC	4.30	129.14	124.45
6	B	806	NIZ	C5-C1-C2	4.06	123.74	118.57
8	A	808	PO4	O4-P-O3	3.83	119.82	107.91
2	A	801	HEM	O2A-CGA-CBA	3.75	125.85	114.00
7	A	807	MPD	CM-C2-C1	-3.70	102.34	110.63
7	A	807	MPD	C5-C4-C3	3.62	128.48	111.67
2	B	801	HEM	C2D-C1D-ND	3.62	114.08	109.90
7	A	807	MPD	O4-C4-C3	-3.60	97.02	111.35
6	B	805	NIZ	C4-N1-C3	3.52	124.92	116.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	C4B-C3B-C2B	-3.37	104.18	107.28
6	A	805	NIZ	C1-C-N2	3.24	119.93	116.33
2	A	801	HEM	O1A-CGA-CBA	-3.03	113.48	123.09
6	B	806	NIZ	C5-C1-C	-2.88	111.28	120.60
6	B	806	NIZ	O1-C-N2	-2.86	119.03	122.46
8	B	809	PO4	O3-P-O1	-2.82	100.98	110.95
2	B	801	HEM	O1A-CGA-CBA	-2.80	114.22	123.09
2	A	801	HEM	C4C-NC-C1C	2.74	110.28	105.82
7	A	806	MPD	CM-C2-C1	2.72	116.73	110.63
2	A	801	HEM	CHC-C4B-NB	2.71	127.34	124.42
6	B	806	NIZ	C3-C2-C1	-2.60	116.20	119.05
2	A	801	HEM	C2D-C1D-ND	2.57	112.87	109.90
2	B	801	HEM	CMD-C2D-C3D	2.48	132.86	126.15
6	B	805	NIZ	O1-C-N2	-2.42	119.55	122.46
7	A	807	MPD	O2-C2-CM	2.42	115.52	107.99
2	B	801	HEM	C3A-C4A-NA	-2.42	106.27	110.14
2	A	801	HEM	CHA-C4D-ND	-2.38	121.42	124.37
6	B	806	NIZ	O1-C-C1	-2.38	116.19	120.90
2	B	801	HEM	C2A-C1A-NA	2.37	112.78	110.15
7	B	807	MPD	O2-C2-C1	-2.36	100.63	107.99
2	A	801	HEM	C4C-C3C-C2C	2.36	108.86	106.81
6	A	805	NIZ	C5-C4-N1	-2.36	119.58	123.60
2	A	801	HEM	C4D-ND-C1D	-2.34	102.43	105.21
2	B	801	HEM	CBD-CAD-C3D	2.34	118.99	112.53
7	B	808	MPD	CM-C2-C1	2.33	115.85	110.63
2	B	801	HEM	C2B-C1B-NB	2.27	112.45	109.84
7	A	806	MPD	O4-C4-C5	2.27	119.21	109.45
6	B	805	NIZ	C-N2-N3	-2.26	117.97	121.50
2	B	801	HEM	CMB-C2B-C1B	-2.24	121.54	125.03
2	B	801	HEM	CMC-C2C-C1C	2.23	128.66	124.73
6	B	806	NIZ	C4-C5-C1	-2.18	116.66	119.05
2	B	801	HEM	CAA-CBA-CGA	-2.18	107.88	113.67
6	A	805	NIZ	O1-C-C1	-2.18	116.58	120.90
2	B	801	HEM	O2A-CGA-O1A	2.14	128.83	123.33
2	B	801	HEM	O1D-CGD-CBD	-2.13	116.34	123.09
2	B	801	HEM	CAD-CBD-CGD	2.11	119.26	113.67
7	B	807	MPD	CM-C2-C1	2.06	115.25	110.63
7	A	806	MPD	CM-C2-C3	-2.06	101.30	110.20
2	B	801	HEM	O2D-CGD-CBD	2.06	120.51	114.00
2	A	801	HEM	C1D-C2D-C3D	-2.04	104.83	106.98
2	A	801	HEM	CBD-CAD-C3D	2.02	118.11	112.53
7	B	808	MPD	C5-C4-C3	2.02	121.04	111.67

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	805	NIZ	C1-C-N2-N3
7	A	806	MPD	C2-C3-C4-O4
7	A	807	MPD	C2-C3-C4-C5
7	A	807	MPD	C2-C3-C4-O4
7	B	808	MPD	C2-C3-C4-O4
7	B	807	MPD	C1-C2-C3-C4
7	B	807	MPD	CM-C2-C3-C4
7	B	808	MPD	C2-C3-C4-C5
2	A	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O1A
7	A	806	MPD	O2-C2-C3-C4
7	B	807	MPD	O2-C2-C3-C4
7	B	808	MPD	O2-C2-C3-C4
7	A	806	MPD	CM-C2-C3-C4

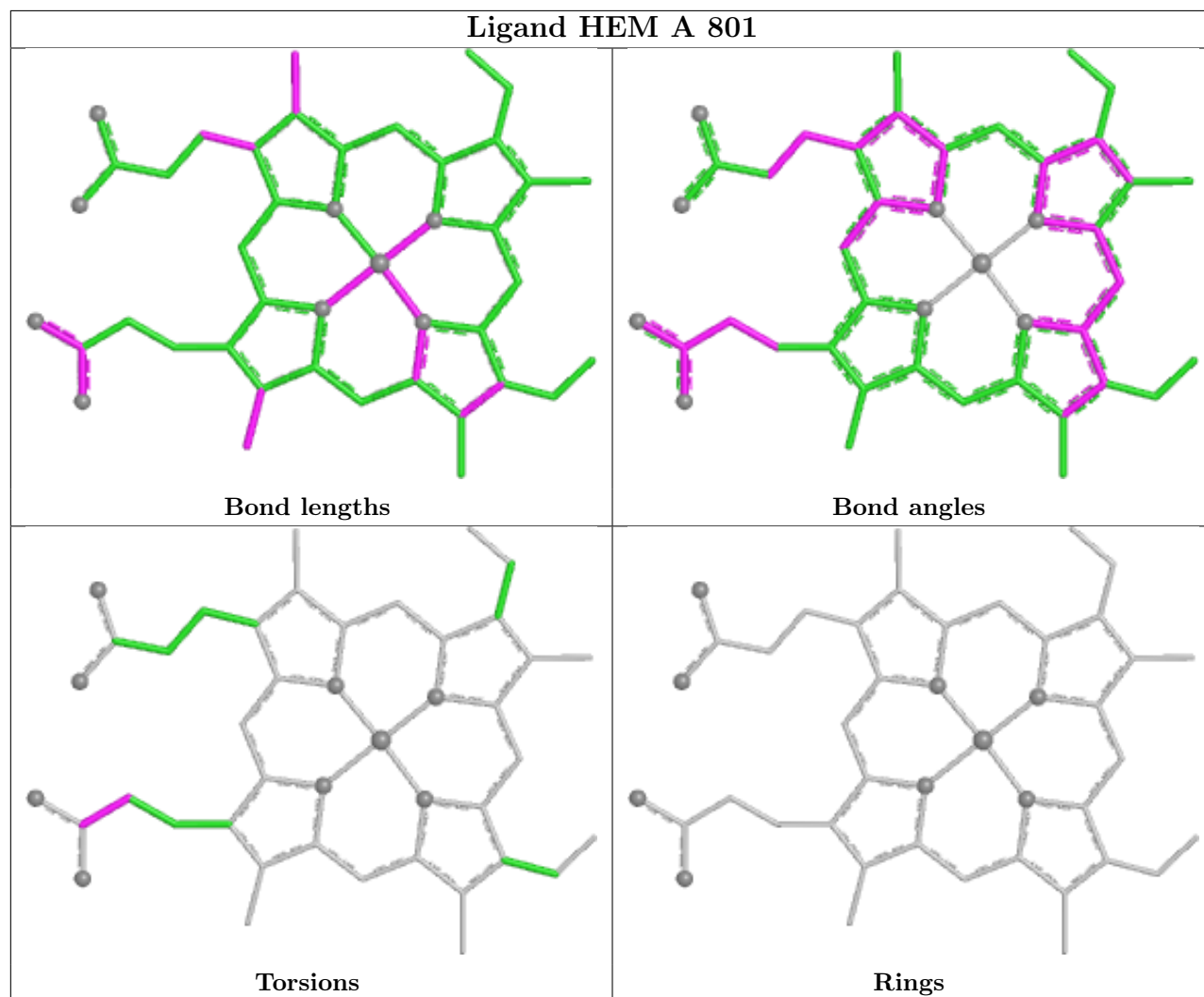
There are no ring outliers.

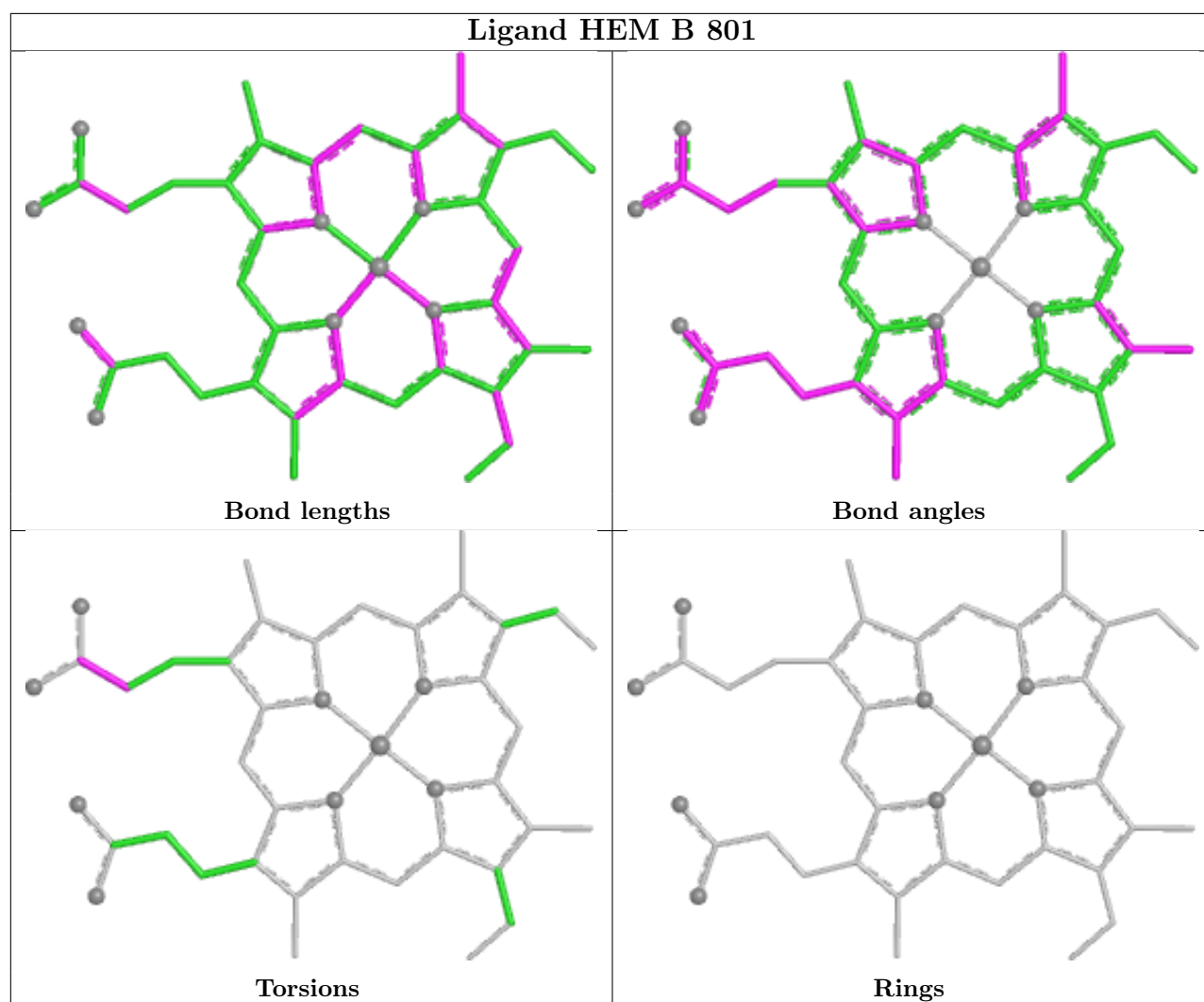
9 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	807	MPD	5	0
6	B	805	NIZ	2	0
5	B	804	OXY	1	0
5	A	804	OXY	1	0
7	B	808	MPD	2	0
7	A	806	MPD	5	0
6	B	806	NIZ	2	0
7	B	807	MPD	2	0
6	A	805	NIZ	2	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	713/728 (97%)	-0.38	6 (0%) 82 85	9, 20, 37, 80	4 (0%)
1	B	713/728 (97%)	-0.41	12 (1%) 69 73	10, 19, 37, 82	5 (0%)
All	All	1426/1456 (97%)	-0.40	18 (1%) 75 79	9, 20, 37, 82	9 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	5.2
1	B	748	ALA	3.5
1	B	569	ALA	3.2
1	B	64	LYS	2.9
1	B	610	ARG	2.7
1	A	608	LYS	2.7
1	B	55	HIS	2.7
1	A	647	GLN	2.7
1	B	608	LYS	2.6
1	B	65	ASP	2.6
1	B	46	GLN	2.5
1	A	40	ARG	2.5
1	A	55	HIS	2.4
1	B	541	GLY	2.4
1	B	40	ARG	2.3
1	B	679	ALA	2.1
1	A	610	ARG	2.0
1	B	540	ARG	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

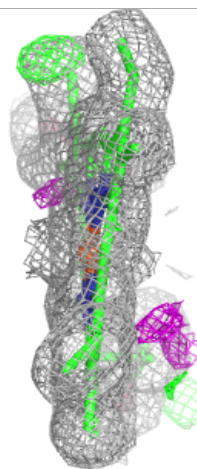
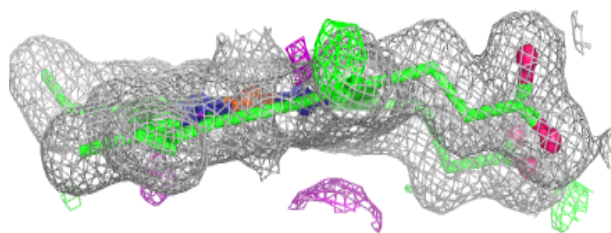
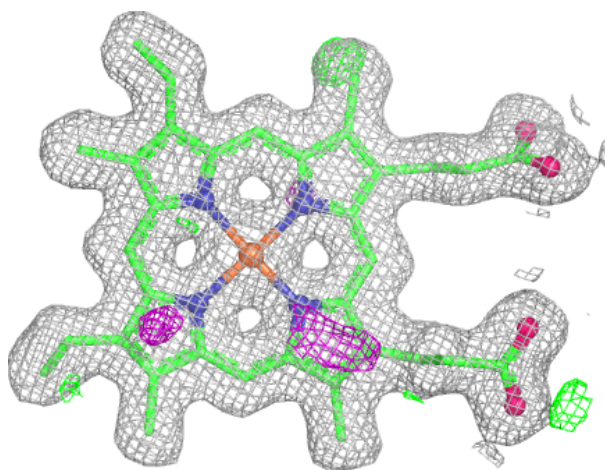
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

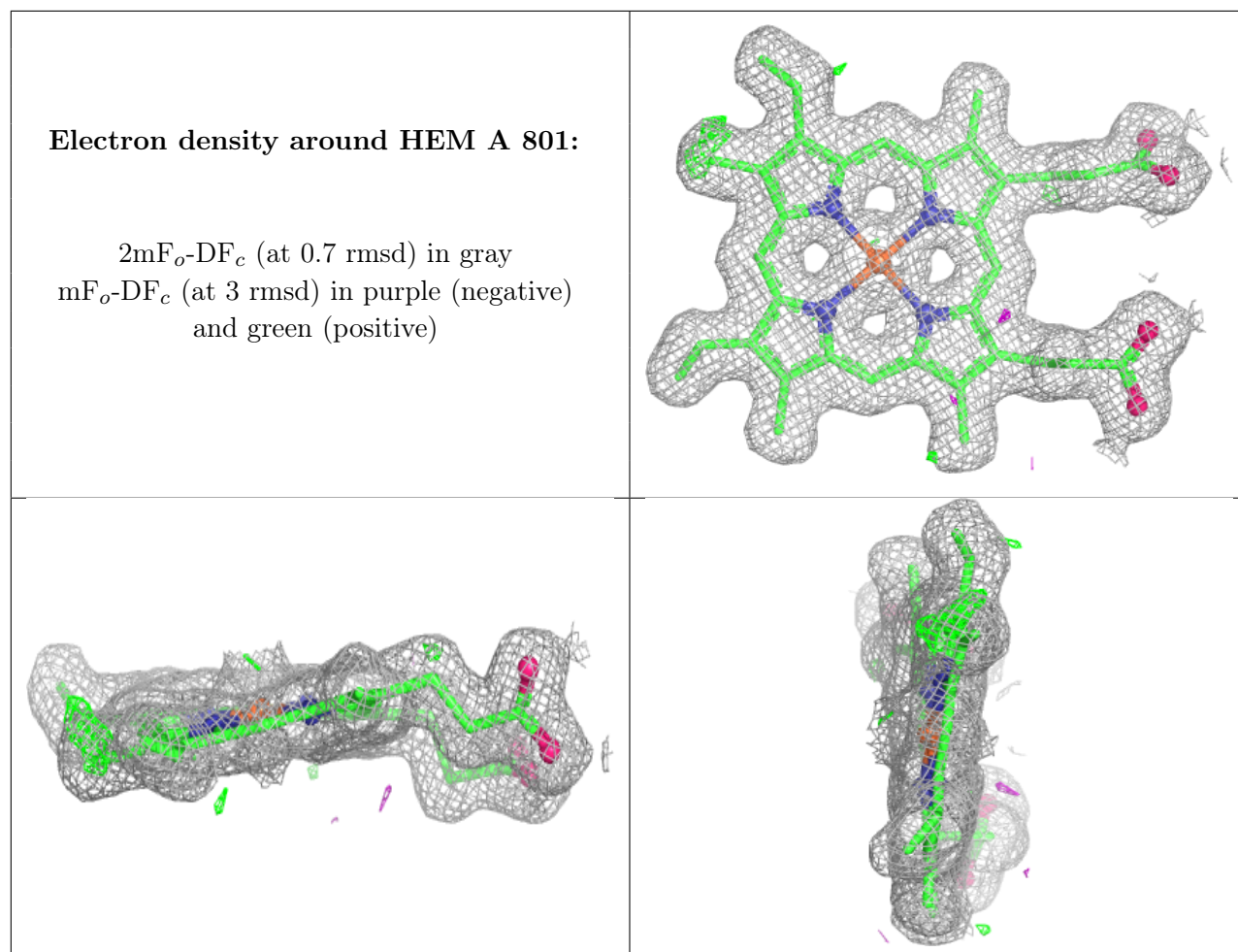
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MPD	B	808	8/8	0.72	0.27	44,63,71,74	0
6	NIZ	B	805	10/10	0.75	0.17	26,39,48,49	0
7	MPD	A	807	8/8	0.82	0.14	42,50,57,68	0
7	MPD	A	806	8/8	0.82	0.15	38,41,55,59	0
6	NIZ	B	806	10/10	0.88	0.10	26,30,34,35	0
6	NIZ	A	805	10/10	0.89	0.10	28,32,35,35	0
7	MPD	B	807	8/8	0.90	0.11	46,54,59,60	0
8	PO4	A	808	5/5	0.93	0.08	44,54,60,61	0
8	PO4	B	809	5/5	0.93	0.09	35,46,50,54	0
5	OXY	B	804	2/2	0.94	0.14	26,26,26,40	0
5	OXY	A	804	2/2	0.96	0.13	23,23,23,38	0
4	CL	B	803	1/1	0.98	0.05	31,31,31,31	0
4	CL	A	803	1/1	0.98	0.08	33,33,33,33	0
2	HEM	B	801	43/43	0.99	0.04	12,14,17,20	0
3	NA	B	802	1/1	0.99	0.05	17,17,17,17	0
2	HEM	A	801	43/43	0.99	0.04	12,15,19,20	0
3	NA	A	802	1/1	1.00	0.06	16,16,16,16	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.