



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 04:34 PM EDT

PDB ID : 5SYJ / pdb_00005syj
Title : Crystal structure of the D141A variant of B. pseudomallei KatGin complex with isoniazid
Authors : Loewen, P.C.
Deposited on : 2016-08-11
Resolution : 1.88 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

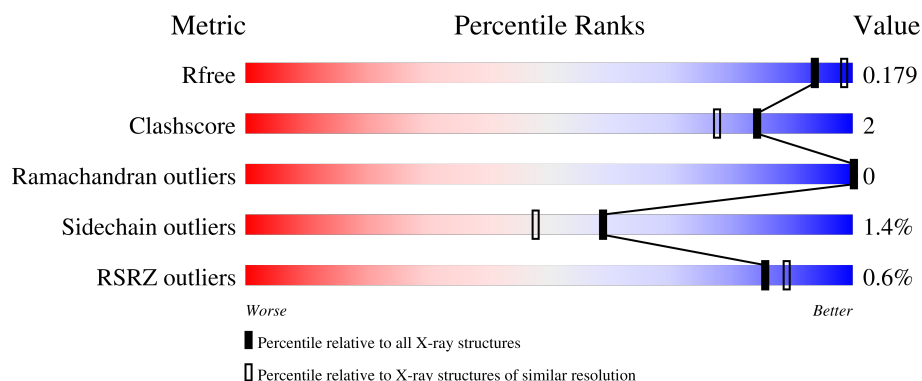
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	
1	B	728	

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
5	MPD	B	804	-	X	-	-
7	NIZ	A	809	-	X	-	-
7	NIZ	A	810	-	X	-	-
7	NIZ	B	810	-	X	X	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12427 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.

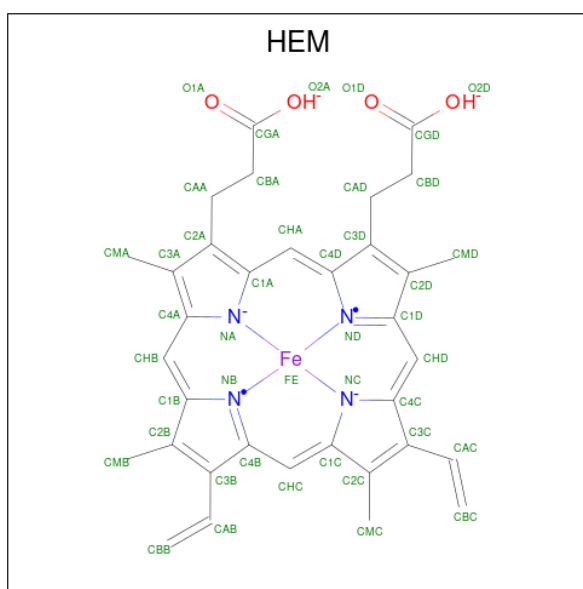
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	7	0
			5539	3500	990	1035	14			
1	B	713	Total	C	N	O	S	0	5	0
			5525	3492	984	1035	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		

Continued on next page...

Continued from previous page...

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

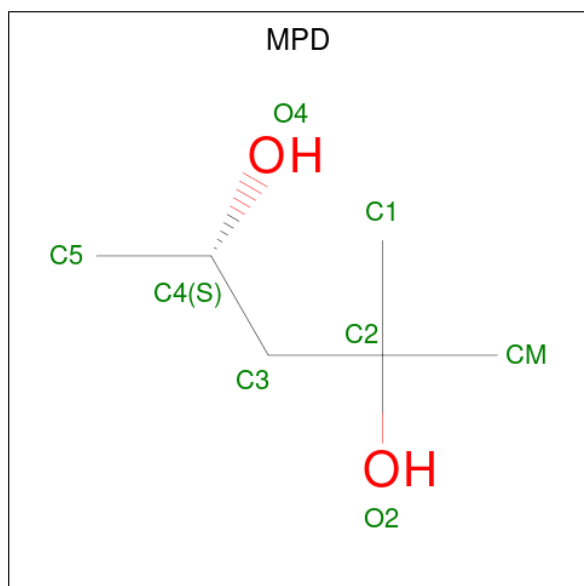
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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



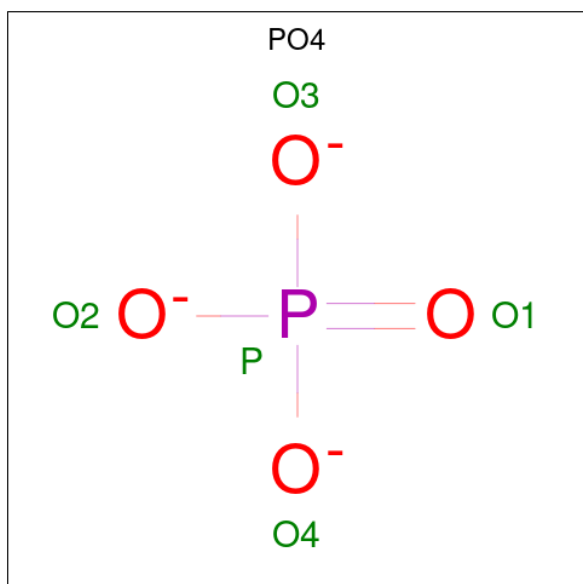
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		

Continued on next page...

Continued from previous page...

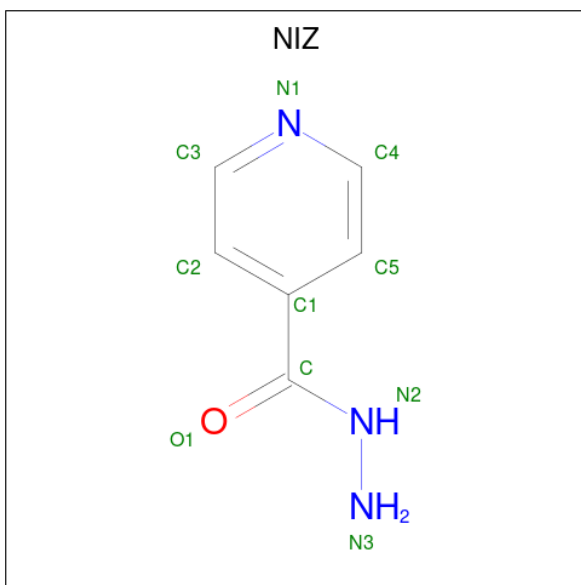
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			8	6	2		
5	A	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		
5	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 7 is pyridine-4-carbohydrazide (CCD ID: NIZ) (formula: $C_6H_7N_3O$).



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

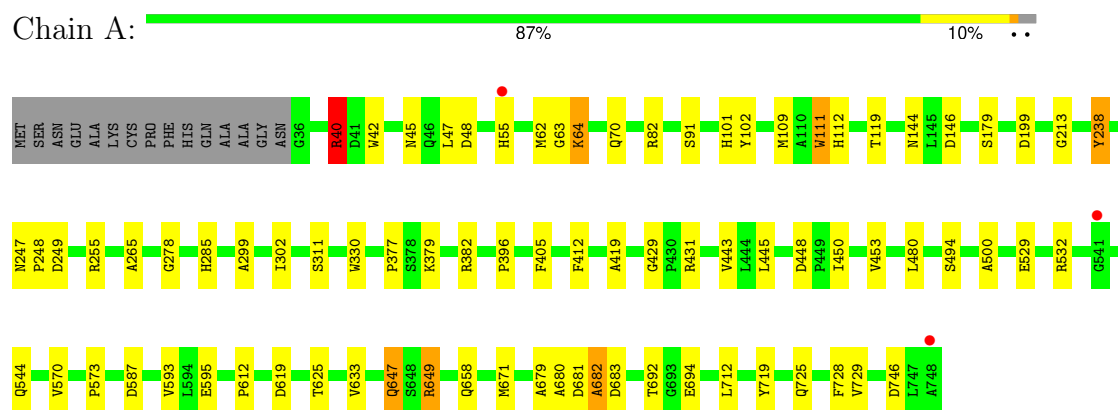
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	576	Total	O	0	0
			576	576		
8	B	583	Total	O	0	0
			583	583		

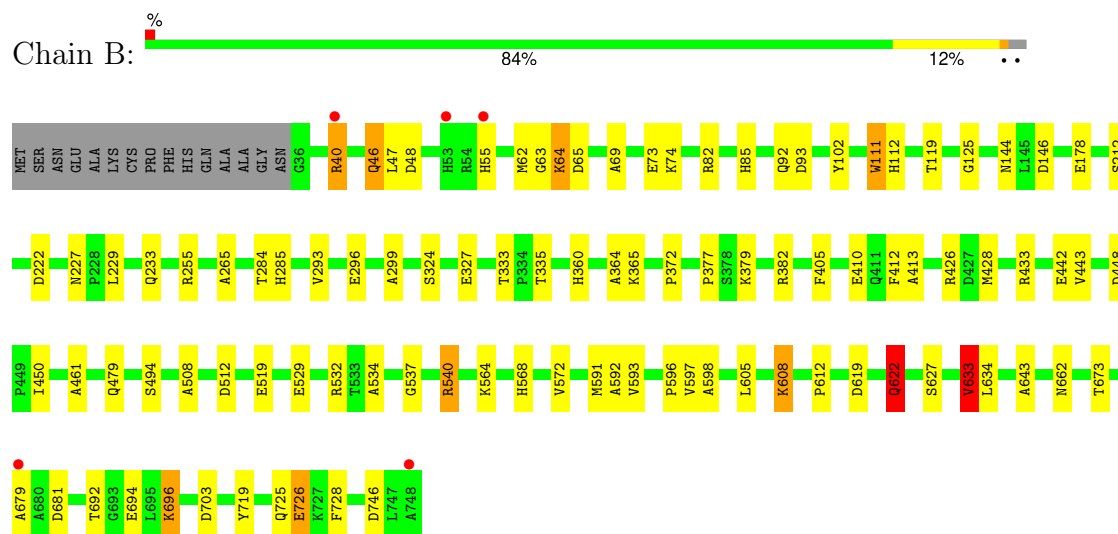
3 Residue-property plots [i](#)

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	100.64Å 114.64Å 174.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.88 20.00 – 1.88	Depositor EDS
% Data completeness (in resolution range)	98.4 (20.00-1.88) 98.8 (20.00-1.88)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 1.88Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.140 , 0.170 0.153 , 0.179	Depositor DCC
R_{free} test set	8300 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.9	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.6	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	12427	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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: HEM, NA, PO4, NIZ, CL, MPD

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	1.76	64/5706 (1.1%)	1.27	15/7756 (0.2%)
1	B	1.73	70/5684 (1.2%)	1.33	24/7728 (0.3%)
All	All	1.74	134/11390 (1.2%)	1.30	39/15484 (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	B	0	1

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	GLY	N-CA	11.78	1.61	1.45
1	A	63	GLY	N-CA	11.66	1.59	1.45
1	B	681	ASP	CA-C	9.83	1.63	1.52
1	A	285	HIS	C-O	9.63	1.34	1.23
1	A	544	GLN	CD-NE2	9.61	1.53	1.33
1	B	285	HIS	C-O	8.74	1.33	1.23
1	B	694	GLU	CA-C	8.57	1.63	1.52
1	A	448	ASP	C-O	8.36	1.27	1.23
1	A	255	ARG	CD-NE	8.32	1.57	1.46
1	A	725	GLN	N-CA	8.27	1.56	1.46
1	A	448	ASP	N-CA	8.11	1.52	1.46
1	A	679	ALA	N-CA	7.98	1.55	1.46
1	A	40	ARG	N-CA	7.88	1.56	1.46
1	B	64	LYS	C-O	-7.88	1.13	1.24
1	B	592	ALA	CA-C	-7.76	1.42	1.52
1	B	532	ARG	CD-NE	-7.67	1.35	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	448	ASP	CA-CB	7.63	1.58	1.52
1	A	532	ARG	NE-CZ	-7.60	1.24	1.33
1	B	372	PRO	CA-C	-7.58	1.43	1.52
1	A	278	GLY	N-CA	7.27	1.54	1.45
1	B	746	ASP	C-O	-7.22	1.14	1.24
1	A	429	GLY	C-O	-7.19	1.14	1.24
1	B	679	ALA	N-CA	7.09	1.54	1.46
1	B	612	PRO	CA-C	6.98	1.61	1.52
1	B	512	ASP	CG-OD2	6.88	1.38	1.25
1	A	377	PRO	C-O	-6.84	1.14	1.24
1	B	333	THR	CA-C	6.80	1.60	1.52
1	A	70	GLN	CD-OE1	6.77	1.36	1.23
1	A	573	PRO	CA-C	6.71	1.60	1.52
1	A	681	ASP	CA-C	6.70	1.59	1.52
1	A	692	THR	CA-C	-6.63	1.43	1.52
1	B	591	MET	SD-CE	-6.63	1.62	1.79
1	A	91	SER	C-O	-6.59	1.16	1.23
1	B	63	GLY	C-O	6.57	1.31	1.23
1	A	47	LEU	CB-CG	-6.49	1.40	1.53
1	B	212	SER	CA-C	6.48	1.61	1.53
1	B	69	ALA	CA-C	-6.47	1.44	1.52
1	A	453	VAL	C-O	-6.43	1.16	1.24
1	A	570	VAL	CA-C	-6.39	1.45	1.52
1	A	532	ARG	CD-NE	-6.32	1.37	1.46
1	A	40	ARG	CD-NE	6.31	1.55	1.46
1	A	199	ASP	C-O	6.30	1.31	1.23
1	B	479	GLN	CA-C	6.27	1.60	1.52
1	A	680	ALA	N-CA	6.26	1.54	1.46
1	B	442	GLU	CA-C	6.26	1.61	1.52
1	B	125	GLY	C-O	6.24	1.30	1.24
1	B	448	ASP	C-O	6.20	1.26	1.23
1	B	572	VAL	C-O	-6.18	1.17	1.24
1	B	532	ARG	NE-CZ	-6.17	1.26	1.33
1	B	529	GLU	CG-CD	6.16	1.67	1.52
1	B	335	THR	N-CA	-6.13	1.39	1.46
1	A	102	TYR	N-CA	6.12	1.54	1.46
1	A	396	PRO	CA-CB	6.12	1.62	1.53
1	B	365	LYS	N-CA	6.12	1.53	1.46
1	B	534	ALA	CA-C	6.11	1.60	1.52
1	A	311	SER	CA-C	6.10	1.59	1.52
1	A	64	LYS	C-O	-6.09	1.16	1.24
1	A	40	ARG	NE-CZ	6.08	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	47	LEU	CB-CG	-6.06	1.41	1.53
1	A	746	ASP	C-O	-5.96	1.16	1.24
1	B	619	ASP	CG-OD1	-5.95	1.14	1.25
1	A	595	GLU	C-O	-5.91	1.16	1.24
1	A	443	VAL	CA-C	-5.88	1.45	1.52
1	A	619	ASP	CG-OD1	-5.88	1.14	1.25
1	A	612	PRO	CA-C	5.87	1.59	1.52
1	B	92	GLN	C-O	5.87	1.30	1.23
1	B	443	VAL	CA-C	-5.87	1.45	1.52
1	A	82	ARG	CZ-NH2	-5.86	1.25	1.33
1	B	299	ALA	CA-C	-5.85	1.45	1.52
1	B	229	LEU	N-CA	5.83	1.53	1.45
1	B	627	SER	N-CA	5.80	1.53	1.45
1	B	85	HIS	CA-C	5.80	1.60	1.52
1	A	725	GLN	CD-NE2	5.80	1.45	1.33
1	A	299	ALA	CA-C	-5.79	1.45	1.52
1	B	643	ALA	N-CA	-5.77	1.38	1.46
1	A	712	LEU	CA-C	5.77	1.60	1.52
1	A	480	LEU	CA-C	5.74	1.60	1.52
1	B	233	GLN	N-CA	5.74	1.53	1.45
1	B	227	ASN	CA-C	-5.70	1.47	1.53
1	B	40	ARG	N-CA	5.70	1.53	1.46
1	A	682	ALA	N-CA	5.69	1.53	1.46
1	B	377	PRO	C-O	-5.68	1.16	1.24
1	B	293	VAL	C-O	-5.62	1.17	1.24
1	A	694	GLU	CA-C	5.61	1.60	1.52
1	B	448	ASP	CA-CB	5.59	1.56	1.52
1	B	111	TRP	CA-C	5.53	1.59	1.52
1	B	728	PHE	CA-C	5.52	1.59	1.52
1	A	671	MET	CA-C	5.50	1.60	1.52
1	A	109	MET	N-CA	5.50	1.52	1.46
1	A	431	ARG	CD-NE	5.50	1.53	1.46
1	B	265	ALA	CA-C	-5.50	1.45	1.52
1	B	605	LEU	C-O	-5.43	1.17	1.23
1	B	703	ASP	N-CA	-5.43	1.40	1.46
1	B	596	PRO	CA-C	-5.43	1.44	1.52
1	A	179	SER	C-O	-5.42	1.17	1.24
1	B	540	ARG	C-O	5.39	1.30	1.23
1	B	82	ARG	CZ-NH2	-5.36	1.26	1.33
1	B	508	ALA	CA-C	5.35	1.58	1.53
1	B	598	ALA	C-O	-5.34	1.18	1.24
1	A	729	VAL	C-O	5.34	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	658	GLN	CD-OE1	-5.31	1.13	1.23
1	B	634	LEU	CA-C	5.30	1.59	1.52
1	A	299	ALA	C-O	-5.30	1.16	1.24
1	A	587	ASP	C-O	5.30	1.30	1.24
1	A	111	TRP	CA-CB	5.27	1.61	1.53
1	A	249	ASP	CA-C	5.26	1.59	1.52
1	B	364	ALA	CA-CB	-5.26	1.46	1.53
1	A	42	TRP	C-O	-5.25	1.17	1.24
1	A	45	ASN	C-O	-5.22	1.16	1.23
1	B	324	SER	C-O	-5.22	1.17	1.24
1	A	101	HIS	CA-C	5.20	1.58	1.52
1	A	728	PHE	N-CA	-5.19	1.40	1.46
1	B	537	GLY	N-CA	5.18	1.52	1.45
1	B	692	THR	CA-C	-5.17	1.45	1.52
1	A	238	TYR	CA-C	5.17	1.57	1.52
1	B	413	ALA	N-CA	-5.14	1.40	1.46
1	B	222	ASP	CA-C	5.14	1.59	1.53
1	B	537	GLY	C-O	-5.14	1.17	1.24
1	A	213	GLY	C-O	-5.13	1.17	1.24
1	B	296	GLU	CA-CB	5.13	1.61	1.53
1	B	327	GLU	CD-OE1	5.13	1.35	1.25
1	B	519	GLU	CA-CB	5.10	1.61	1.53
1	B	74	LYS	C-O	-5.09	1.17	1.24
1	A	494	SER	CA-C	5.09	1.59	1.52
1	B	532	ARG	CZ-NH2	-5.08	1.26	1.33
1	B	102	TYR	N-CA	5.07	1.53	1.46
1	A	255	ARG	NE-CZ	5.07	1.38	1.33
1	B	65	ASP	CA-C	5.04	1.59	1.52
1	B	448	ASP	CG-OD1	5.03	1.34	1.25
1	A	500	ALA	N-CA	5.03	1.52	1.46
1	A	532	ARG	CA-C	5.02	1.59	1.52
1	B	461	ALA	C-O	-5.01	1.18	1.24
1	A	529	GLU	CA-C	5.00	1.59	1.52
1	B	494	SER	CA-C	5.00	1.59	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	ARG	NE-CZ-NH2	-8.50	111.55	119.20
1	B	382	ARG	CG-CD-NE	-7.98	94.44	112.00
1	B	532	ARG	NE-CZ-NH2	-7.51	112.44	119.20
1	A	55	HIS	CB-CA-C	7.35	122.79	111.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	MET	CA-C-N	-7.27	112.51	120.44
1	A	62	MET	C-N-CA	-7.27	112.51	120.44
1	B	622	GLN	CG-CD-NE2	-7.18	105.63	116.40
1	B	255	ARG	NE-CZ-NH2	-6.93	112.97	119.20
1	B	62	MET	CA-C-N	-6.63	112.44	121.06
1	B	62	MET	C-N-CA	-6.63	112.44	121.06
1	B	93	ASP	N-CA-C	6.45	119.13	111.71
1	B	55	HIS	CB-CA-C	6.29	121.15	111.39
1	B	255	ARG	NE-CZ-NH1	6.29	127.79	121.50
1	B	382	ARG	NE-CZ-NH2	-6.26	113.56	119.20
1	A	48	ASP	N-CA-C	6.16	118.73	108.20
1	B	633[A]	VAL	CG1-CB-CG2	-5.96	97.69	110.80
1	B	633[B]	VAL	CG1-CB-CG2	-5.96	97.69	110.80
1	B	40	ARG	N-CA-CB	5.92	119.33	110.22
1	A	47	LEU	N-CA-CB	-5.89	101.16	110.06
1	A	47	LEU	N-CA-C	-5.80	101.04	110.20
1	B	450	ILE	CB-CA-C	-5.65	104.65	110.13
1	B	47	LEU	N-CA-C	-5.64	101.28	110.20
1	B	692	THR	N-CA-C	5.63	120.43	113.50
1	B	608	LYS	CB-CG-CD	5.51	123.97	111.30
1	A	419	ALA	N-CA-C	5.50	117.27	111.28
1	B	255	ARG	CG-CD-NE	-5.46	99.99	112.00
1	A	450	ILE	CB-CA-C	-5.45	104.47	110.52
1	A	382	ARG	CG-CD-NE	-5.36	100.21	112.00
1	A	532	ARG	CG-CD-NE	-5.31	100.31	112.00
1	A	265	ALA	N-CA-C	5.25	118.99	112.58
1	B	532	ARG	CG-CD-NE	-5.23	100.49	112.00
1	A	445	LEU	N-CA-C	5.18	117.60	111.33
1	B	63	GLY	O-C-N	-5.17	116.76	122.60
1	A	40	ARG	CB-CG-CD	5.15	123.15	111.30
1	B	48	ASP	N-CA-C	5.14	117.00	108.20
1	B	597	VAL	N-CA-C	5.12	119.27	111.89
1	A	330	TRP	N-CA-C	5.12	117.98	111.69
1	B	726	GLU	CG-CD-OE2	5.09	130.11	118.40
1	B	46	GLN	N-CA-C	-5.03	104.22	110.41

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	622	GLN	Sidechain

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	5539	0	5374	18	0
1	B	5525	0	5356	26	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	32	0	56	3	0
5	B	32	0	56	4	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	20	0	14	4	0
7	B	20	0	14	6	0
8	A	576	0	0	6	0
8	B	583	0	0	6	0
All	All	12427	0	10930	50	0

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

All (50) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:622:GLN:NE2	7:B:809:NIZ:O1	2.07	0.88
5:A:805:MPD:O2	5:A:805:MPD:H53	1.80	0.80
1:B:119[B]:THR:HG23	8:B:1093:HOH:O	1.80	0.79
1:B:119[B]:THR:HG22	1:B:593:VAL:HG21	1.69	0.75
1:B:178:GLU:OE1	8:B:903:HOH:O	2.07	0.71
1:A:649:ARG:NH2	8:A:905:HOH:O	2.28	0.67
5:B:804:MPD:H53	5:B:804:MPD:H11	1.76	0.66
1:B:119[B]:THR:HG21	8:B:1435:HOH:O	1.95	0.66
7:B:810:NIZ:H4	8:B:1072:HOH:O	1.98	0.64
1:A:647:GLN:HG3	8:A:1212:HOH:O	1.99	0.62
1:B:360:HIS:ND1	8:B:906:HOH:O	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ARG:HG3	8:A:1337:HOH:O	2.07	0.55
1:B:622:GLN:HE21	7:B:809:NIZ:H5	1.73	0.54
5:B:804:MPD:H53	5:B:804:MPD:C1	2.39	0.53
7:A:810:NIZ:H4	8:A:1059:HOH:O	2.09	0.52
1:B:633[A]:VAL:HG22	1:B:719:TYR:CZ	2.45	0.52
1:B:662:ASN:H	1:B:725:GLN:HE22	1.57	0.51
1:A:40:ARG:HD2	1:B:40:ARG:CZ	2.40	0.51
1:A:111:TRP:HE1	7:A:810:NIZ:H7	1.60	0.50
1:A:683:ASP:HA	8:A:903:HOH:O	2.12	0.49
1:A:633[B]:VAL:CG2	1:A:719:TYR:CZ	2.98	0.47
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.97	0.47
1:A:625:THR:HG22	7:A:809:NIZ:H4	1.96	0.47
1:B:564:LYS:HG3	5:B:807:MPD:HM3	1.96	0.47
1:A:682:ALA:O	8:A:903:HOH:O	2.20	0.46
1:A:112:HIS:NE2	7:A:810:NIZ:N2	2.64	0.46
5:B:804:MPD:C1	5:B:804:MPD:C5	2.94	0.46
1:A:247:ASN:HD22	1:A:248:PRO:HD2	1.80	0.45
1:A:111:TRP:HZ3	1:A:238:TYR:HH	1.60	0.45
1:B:633[A]:VAL:HG22	1:B:719:TYR:CE2	2.52	0.44
1:B:696:LYS:HE2	8:B:942:HOH:O	2.18	0.44
5:A:805:MPD:O2	5:A:805:MPD:C5	2.46	0.43
1:B:112:HIS:NE2	7:B:810:NIZ:N3	2.66	0.43
1:B:284:THR:HG22	2:B:801:HEM:HAA1	2.01	0.43
1:B:112:HIS:NE2	7:B:810:NIZ:N2	2.66	0.43
1:A:649:ARG:HA	1:A:649:ARG:HD2	1.73	0.42
1:B:426[B]:ARG:HA	1:B:426[B]:ARG:HD2	1.88	0.42
1:A:405:PHE:HB3	1:A:412:PHE:HB2	2.00	0.42
1:B:673:THR:OG1	1:B:696:LYS:HE3	2.18	0.42
1:B:568:HIS:ND1	1:B:726:GLU:OE1	2.44	0.42
1:B:112:HIS:CE1	7:B:810:NIZ:C	3.02	0.42
1:B:405:PHE:HB3	1:B:412:PHE:HB2	2.02	0.42
1:A:111:TRP:CD1	1:A:112:HIS:HD2	2.38	0.42
5:A:804:MPD:H4	5:A:804:MPD:HM2	1.63	0.42
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.20	0.41
1:A:40:ARG:HD2	1:B:40:ARG:NE	2.35	0.41
1:A:144:ASN:HA	1:A:146:ASP:OD1	2.19	0.41
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	2.02	0.41
1:B:111:TRP:CD1	1:B:112:HIS:HD2	2.39	0.40
1:B:428:MET:O	1:B:433:ARG:HD3	2.21	0.40

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	718/728 (99%)	706 (98%)	12 (2%)	0	100	100
1	B	716/728 (98%)	706 (99%)	10 (1%)	0	100	100
All	All	1434/1456 (98%)	1412 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	556/560 (99%)	550 (99%)	6 (1%)	65	56
1	B	554/560 (99%)	544 (98%)	10 (2%)	51	38
All	All	1110/1120 (99%)	1094 (99%)	16 (1%)	59	48

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

Mol	Chain	Res	Type
1	A	40	ARG
1	A	64	LYS
1	A	302	ILE
1	A	379	LYS
1	A	647	GLN
1	A	649	ARG
1	B	46	GLN
1	B	64	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	73	GLU
1	B	379	LYS
1	B	410	GLU
1	B	540	ARG
1	B	608	LYS
1	B	633[A]	VAL
1	B	633[B]	VAL
1	B	696	LYS

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	85	HIS
1	A	247	ASN
1	A	336	GLN
1	A	339	HIS
1	A	568	HIS
1	A	737	ASN
1	B	46	GLN
1	B	406	HIS
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 20 ligands modelled in this entry, 4 are monoatomic - leaving 16 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	NIZ	A	809	-	10,10,10	3.66	6 (60%)	12,12,12	2.28	7 (58%)
6	PO4	A	807	-	4,4,4	0.62	0	6,6,6	1.63	2 (33%)
2	HEM	A	801	1,7	50,50,50	1.69	12 (24%)	67,82,82	1.34	10 (14%)
5	MPD	B	805	-	7,7,7	0.89	1 (14%)	9,10,10	1.79	3 (33%)
5	MPD	B	806	-	7,7,7	0.72	0	9,10,10	1.38	2 (22%)
5	MPD	A	805	-	7,7,7	0.78	0	9,10,10	1.85	3 (33%)
5	MPD	A	806	-	7,7,7	1.63	1 (14%)	9,10,10	1.35	1 (11%)
7	NIZ	B	810	-	10,10,10	5.14	8 (80%)	12,12,12	4.53	10 (83%)
5	MPD	A	804	-	7,7,7	1.22	1 (14%)	9,10,10	2.12	3 (33%)
6	PO4	B	808	-	4,4,4	1.17	0	6,6,6	1.14	1 (16%)
5	MPD	A	808	-	7,7,7	0.74	0	9,10,10	2.10	3 (33%)
7	NIZ	B	809	-	10,10,10	2.17	3 (30%)	12,12,12	3.70	6 (50%)
7	NIZ	A	810	2	10,10,10	4.57	6 (60%)	12,12,12	3.75	9 (75%)
5	MPD	B	804	-	7,7,7	1.38	1 (14%)	9,10,10	4.13	6 (66%)
5	MPD	B	807	-	7,7,7	1.17	0	9,10,10	1.21	1 (11%)
2	HEM	B	801	1	50,50,50	1.62	10 (20%)	67,82,82	1.60	16 (23%)

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	NIZ	A	809	-	-	0/6/6/6	0/1/1/1
7	NIZ	B	810	-	-	0/6/6/6	0/1/1/1
2	HEM	A	801	1,7	-	3/14/54/54	-
5	MPD	B	805	-	-	4/5/5/5	-
5	MPD	B	806	-	-	3/5/5/5	-
5	MPD	A	805	-	-	3/5/5/5	-
5	MPD	A	806	-	-	4/5/5/5	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MPD	A	804	-	-	4/5/5/5	-
5	MPD	A	808	-	-	4/5/5/5	-
7	NIZ	B	809	-	-	0/6/6/6	0/1/1/1
7	NIZ	A	810	2	-	0/6/6/6	0/1/1/1
5	MPD	B	804	-	-	2/5/5/5	-
5	MPD	B	807	-	-	5/5/5/5	-
2	HEM	B	801	1	-	3/14/54/54	-

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	810	NIZ	C-N2	9.13	1.43	1.33
7	A	810	NIZ	C-N2	8.79	1.42	1.33
7	B	810	NIZ	C2-C1	7.21	1.50	1.39
7	B	810	NIZ	C5-C1	7.19	1.50	1.39
7	A	810	NIZ	C5-C1	6.97	1.50	1.39
7	A	809	NIZ	C-N2	6.48	1.40	1.33
7	A	810	NIZ	C2-C1	5.95	1.48	1.39
7	B	810	NIZ	N3-N2	5.85	1.50	1.41
7	A	809	NIZ	C2-C1	5.75	1.48	1.39
7	A	810	NIZ	N3-N2	5.15	1.49	1.41
7	A	809	NIZ	C5-C1	5.09	1.47	1.39
2	B	801	HEM	FE-NB	4.70	2.09	1.94
7	B	809	NIZ	C5-C1	4.52	1.46	1.39
7	A	809	NIZ	C4-N1	4.13	1.45	1.33
2	A	801	HEM	C3B-C4B	4.12	1.52	1.44
2	B	801	HEM	C4B-NB	-4.11	1.30	1.38
2	B	801	HEM	C1B-NB	-4.06	1.33	1.40
7	B	810	NIZ	O1-C	3.98	1.32	1.23
2	A	801	HEM	FE-NC	3.91	2.08	1.95
7	B	810	NIZ	C4-N1	3.61	1.43	1.33
5	A	806	MPD	C1-C2	3.55	1.62	1.52
7	B	809	NIZ	C4-N1	3.46	1.43	1.33
2	A	801	HEM	FE-NA	3.07	2.05	1.95
2	A	801	HEM	C4D-ND	-2.95	1.35	1.40
7	A	810	NIZ	C3-N1	2.87	1.41	1.33
5	B	804	MPD	O2-C2	-2.81	1.37	1.44
2	B	801	HEM	FE-NC	2.79	2.04	1.95
7	A	809	NIZ	N3-N2	-2.79	1.37	1.41
7	A	810	NIZ	C4-N1	2.78	1.41	1.33
2	A	801	HEM	CHB-C4A	2.70	1.45	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	810	NIZ	C3-N1	2.68	1.41	1.33
2	A	801	HEM	C2A-C3A	-2.65	1.32	1.38
2	B	801	HEM	O1D-CGD	2.53	1.30	1.22
2	A	801	HEM	FE-NB	2.51	2.02	1.94
2	B	801	HEM	C3B-C4B	2.51	1.49	1.44
2	B	801	HEM	CMB-C2B	2.49	1.55	1.50
7	B	810	NIZ	C5-C4	2.49	1.43	1.38
2	B	801	HEM	CHD-C1D	-2.45	1.33	1.39
2	A	801	HEM	O1D-CGD	2.32	1.29	1.22
7	A	809	NIZ	C2-C3	2.30	1.43	1.38
5	A	804	MPD	C5-C4	2.29	1.61	1.51
7	B	809	NIZ	N3-N2	-2.27	1.38	1.41
2	B	801	HEM	CBA-CGA	2.20	1.55	1.50
2	A	801	HEM	C1A-NA	-2.19	1.35	1.39
2	A	801	HEM	CMD-C2D	2.16	1.55	1.50
2	B	801	HEM	C1A-NA	2.13	1.43	1.39
2	A	801	HEM	C1D-C2D	2.05	1.48	1.44
2	A	801	HEM	O1A-CGA	2.04	1.28	1.22
5	B	805	MPD	O2-C2	-2.03	1.39	1.44

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	809	NIZ	C1-C-N2	9.44	126.80	116.33
7	B	810	NIZ	C3-C2-C1	-7.52	110.83	119.05
5	B	804	MPD	O2-C2-CM	-7.08	85.91	107.99
5	B	804	MPD	O2-C2-C3	-6.97	83.21	109.27
7	A	810	NIZ	C1-C-N2	6.83	123.91	116.33
7	B	810	NIZ	C1-C-N2	6.64	123.70	116.33
7	A	810	NIZ	O1-C-C1	-6.54	107.95	120.90
7	B	810	NIZ	O1-C-C1	-6.43	108.16	120.90
7	B	810	NIZ	C5-C1-C2	5.54	125.62	118.57
7	B	810	NIZ	C-N2-N3	-5.22	113.32	121.50
5	B	804	MPD	O4-C4-C3	-5.07	91.17	111.35
7	B	809	NIZ	O1-C-N2	-4.96	116.50	122.46
5	A	804	MPD	O4-C4-C3	-4.64	92.90	111.35
7	A	810	NIZ	O1-C-N2	4.54	127.92	122.46
7	B	810	NIZ	O1-C-N2	4.08	127.36	122.46
2	A	801	HEM	CHC-C4B-NB	4.02	128.75	124.42
5	A	808	MPD	O2-C2-C3	-3.93	94.57	109.27
7	A	810	NIZ	C5-C1-C2	3.88	123.50	118.57
2	B	801	HEM	CHC-C4B-NB	3.60	128.30	124.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	804	MPD	CM-C2-C3	3.58	125.63	110.20
7	A	810	NIZ	C3-C2-C1	-3.54	115.18	119.05
7	B	809	NIZ	C5-C4-N1	-3.49	117.64	123.60
7	B	809	NIZ	C5-C1-C2	3.49	123.01	118.57
7	A	809	NIZ	C2-C3-N1	-3.48	117.66	123.60
5	A	808	MPD	CM-C2-C1	-3.47	102.85	110.63
7	B	809	NIZ	C3-C2-C1	-3.47	115.26	119.05
5	B	805	MPD	O2-C2-C3	-3.42	96.46	109.27
5	A	805	MPD	O2-C2-CM	-3.40	97.39	107.99
7	A	809	NIZ	C4-C5-C1	-3.33	115.41	119.05
2	B	801	HEM	C3B-C2B-C1B	-3.25	103.97	106.41
7	B	810	NIZ	C4-C5-C1	-3.23	115.52	119.05
7	A	810	NIZ	C4-N1-C3	3.12	124.01	116.86
7	A	809	NIZ	O1-C-C1	-3.03	114.89	120.90
2	A	801	HEM	O1A-CGA-CBA	-2.94	113.75	123.09
2	B	801	HEM	CAA-CBA-CGA	-2.90	105.96	113.67
2	B	801	HEM	O1D-CGD-CBD	-2.90	113.91	123.09
2	B	801	HEM	C4A-NA-C1A	-2.87	101.14	105.82
2	A	801	HEM	C3D-C4D-ND	2.87	113.32	110.17
2	A	801	HEM	CAA-CBA-CGA	-2.80	106.24	113.67
5	A	804	MPD	O4-C4-C5	2.78	121.43	109.45
7	A	809	NIZ	C4-N1-C3	2.77	123.20	116.86
2	B	801	HEM	CAC-C3C-C4C	-2.77	118.21	124.82
5	B	804	MPD	CM-C2-C1	2.75	116.78	110.63
6	A	807	PO4	O3-P-O1	-2.71	101.37	110.95
7	A	810	NIZ	C4-C5-C1	-2.68	116.12	119.05
5	A	805	MPD	O2-C2-C1	2.67	116.32	107.99
2	B	801	HEM	O2A-CGA-CBA	2.67	122.44	114.00
7	A	809	NIZ	C-N2-N3	2.67	125.69	121.50
5	B	806	MPD	O2-C2-C1	-2.64	99.77	107.99
5	A	806	MPD	CM-C2-C1	2.62	116.48	110.63
7	B	810	NIZ	C5-C1-C	-2.61	112.15	120.60
5	B	805	MPD	CM-C2-C3	2.59	121.36	110.20
2	A	801	HEM	CMA-C3A-C2A	2.57	131.08	125.62
5	A	808	MPD	O2-C2-CM	2.53	115.86	107.99
2	B	801	HEM	CMB-C2B-C3B	2.52	134.52	128.43
7	A	810	NIZ	C5-C4-N1	-2.44	119.44	123.60
2	B	801	HEM	CMC-C2C-C1C	2.44	129.02	124.73
5	B	807	MPD	O2-C2-C1	-2.44	100.39	107.99
2	B	801	HEM	C3B-C4B-NB	-2.43	107.72	109.47
2	A	801	HEM	C4B-C3B-C2B	-2.43	105.05	107.28
2	B	801	HEM	CMB-C2B-C1B	-2.40	121.28	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	809	NIZ	C1-C-N2	2.36	118.95	116.33
7	A	810	NIZ	C-N2-N3	2.31	125.13	121.50
5	B	805	MPD	O2-C2-C1	-2.31	100.78	107.99
6	B	808	PO4	O4-P-O3	2.31	115.09	107.91
2	A	801	HEM	O2A-CGA-CBA	2.28	121.19	114.00
7	B	810	NIZ	C5-C4-N1	-2.27	119.73	123.60
2	A	801	HEM	CAD-C3D-C4D	2.26	128.63	124.70
5	A	805	MPD	O4-C4-C3	-2.24	102.43	111.35
2	B	801	HEM	CBD-CAD-C3D	2.24	118.73	112.53
2	B	801	HEM	CHD-C4C-C3C	2.24	128.98	125.21
7	B	809	NIZ	O1-C-C1	-2.23	116.47	120.90
5	B	804	MPD	O4-C4-C5	2.18	118.84	109.45
2	B	801	HEM	C3C-C2C-C1C	-2.13	105.03	107.05
5	A	804	MPD	O2-C2-C1	2.11	114.57	107.99
5	B	806	MPD	O4-C4-C3	-2.11	102.97	111.35
2	A	801	HEM	C4D-C3D-C2D	-2.10	103.83	106.89
7	B	810	NIZ	C2-C3-N1	2.06	127.11	123.60
2	B	801	HEM	CAD-C3D-C4D	2.04	128.25	124.70
2	A	801	HEM	CMB-C2B-C1B	-2.03	121.86	125.03
7	A	809	NIZ	O1-C-N2	2.02	124.89	122.46
2	B	801	HEM	C1B-NB-C4B	2.01	107.58	105.21
6	A	807	PO4	O4-P-O3	2.00	114.15	107.91

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	808	MPD	O2-C2-C3-C4
5	A	808	MPD	CM-C2-C3-C4
5	A	808	MPD	C2-C3-C4-C5
5	B	806	MPD	C1-C2-C3-C4
5	B	804	MPD	O2-C2-C3-C4
5	B	807	MPD	C2-C3-C4-O4
5	A	805	MPD	C1-C2-C3-C4
5	A	805	MPD	CM-C2-C3-C4
5	A	808	MPD	C1-C2-C3-C4
5	B	804	MPD	CM-C2-C3-C4
5	B	805	MPD	C1-C2-C3-C4
5	B	805	MPD	CM-C2-C3-C4
5	B	806	MPD	CM-C2-C3-C4
5	B	807	MPD	C1-C2-C3-C4
5	B	807	MPD	CM-C2-C3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	804	MPD	C2-C3-C4-C5
5	A	806	MPD	C2-C3-C4-C5
5	B	805	MPD	C2-C3-C4-C5
5	B	807	MPD	C2-C3-C4-C5
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
5	A	804	MPD	O2-C2-C3-C4
5	A	805	MPD	O2-C2-C3-C4
5	A	806	MPD	O2-C2-C3-C4
5	B	806	MPD	O2-C2-C3-C4
5	B	807	MPD	O2-C2-C3-C4
5	A	804	MPD	C2-C3-C4-O4
5	A	806	MPD	C2-C3-C4-O4
5	B	805	MPD	C2-C3-C4-O4
5	A	804	MPD	C1-C2-C3-C4
5	A	806	MPD	CM-C2-C3-C4
2	A	801	HEM	CAD-CBD-CGD-O2D
2	B	801	HEM	CAD-CBD-CGD-O2D

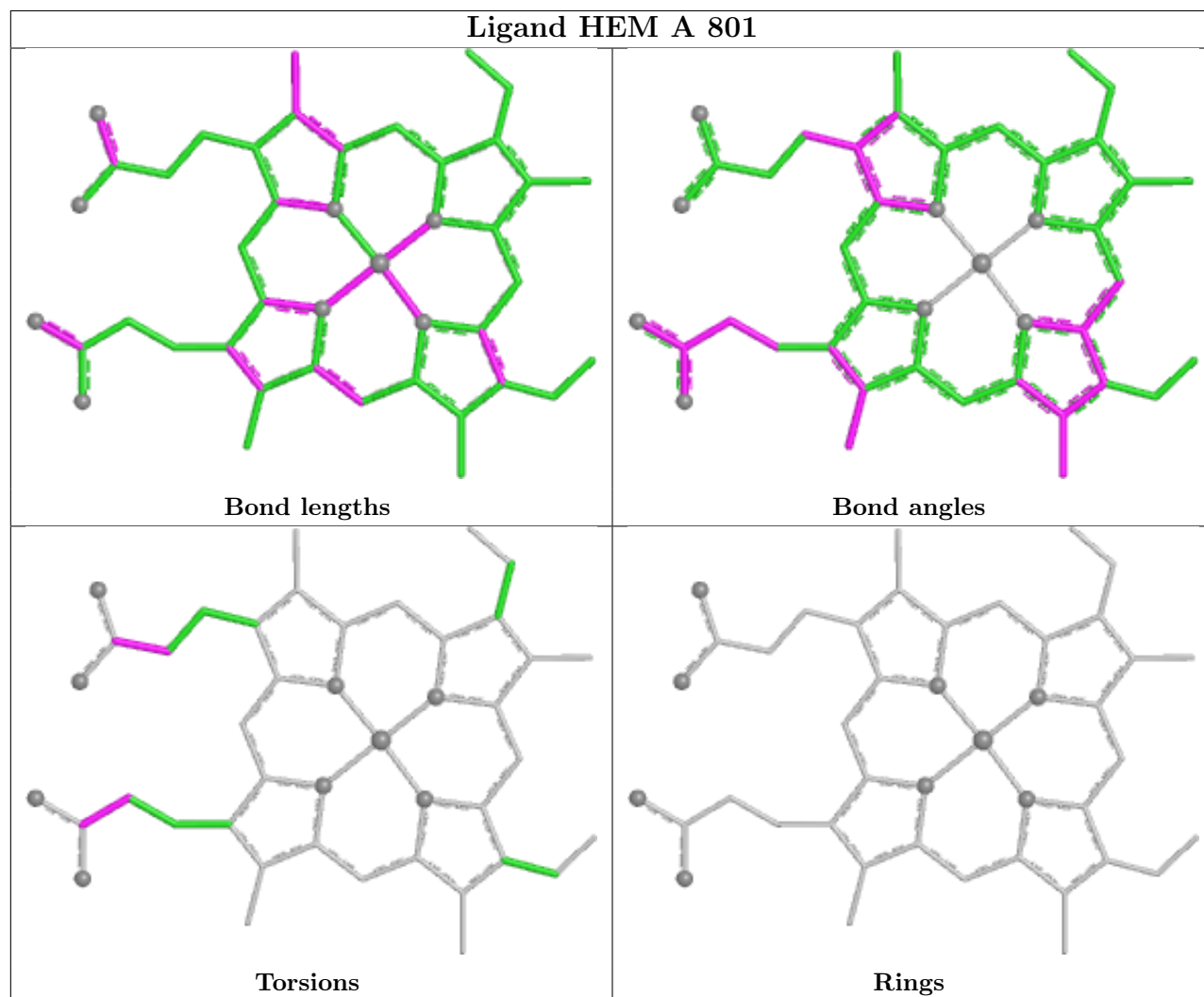
There are no ring outliers.

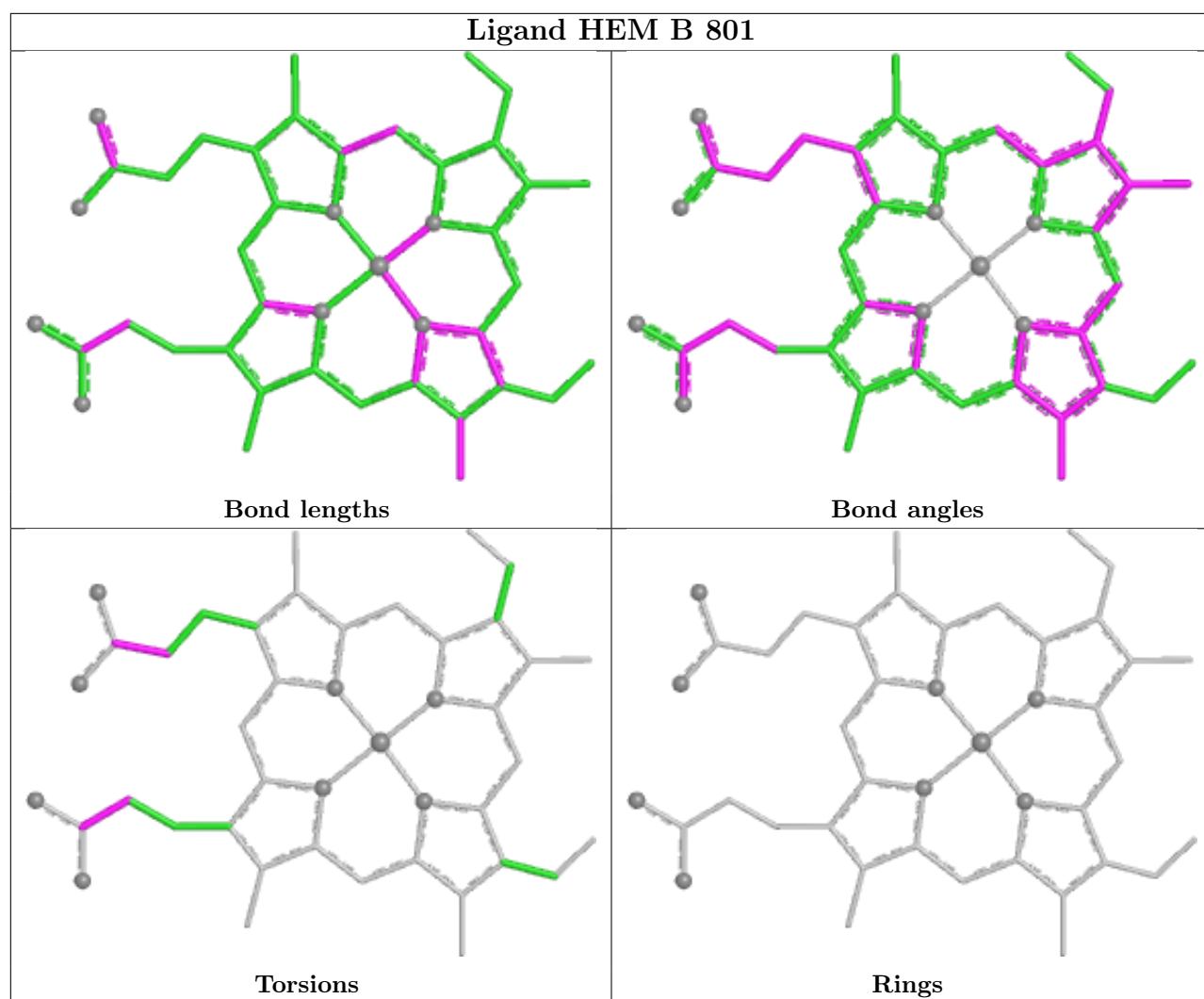
9 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	809	NIZ	1	0
5	A	805	MPD	2	0
7	B	810	NIZ	4	0
5	A	804	MPD	1	0
7	B	809	NIZ	2	0
7	A	810	NIZ	3	0
5	B	804	MPD	3	0
5	B	807	MPD	1	0
2	B	801	HEM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	713/728 (97%)	-0.52	3 (0%) 88 92	11, 26, 47, 79	7 (0%)
1	B	713/728 (97%)	-0.61	5 (0%) 84 88	12, 24, 43, 77	5 (0%)
All	All	1426/1456 (97%)	-0.56	8 (0%) 85 89	11, 25, 45, 79	12 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	55	HIS	3.3
1	B	679	ALA	2.8
1	B	748	ALA	2.8
1	A	55	HIS	2.8
1	A	748	ALA	2.6
1	A	541	GLY	2.4
1	B	40	ARG	2.3
1	B	53	HIS	2.1

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 [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,

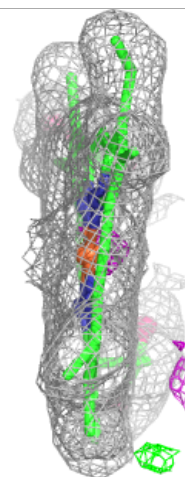
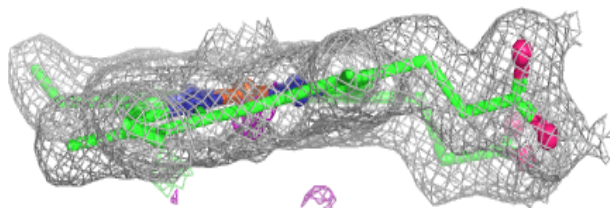
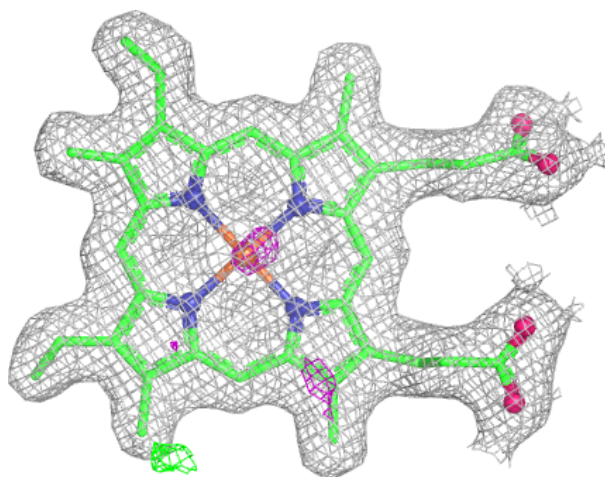
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

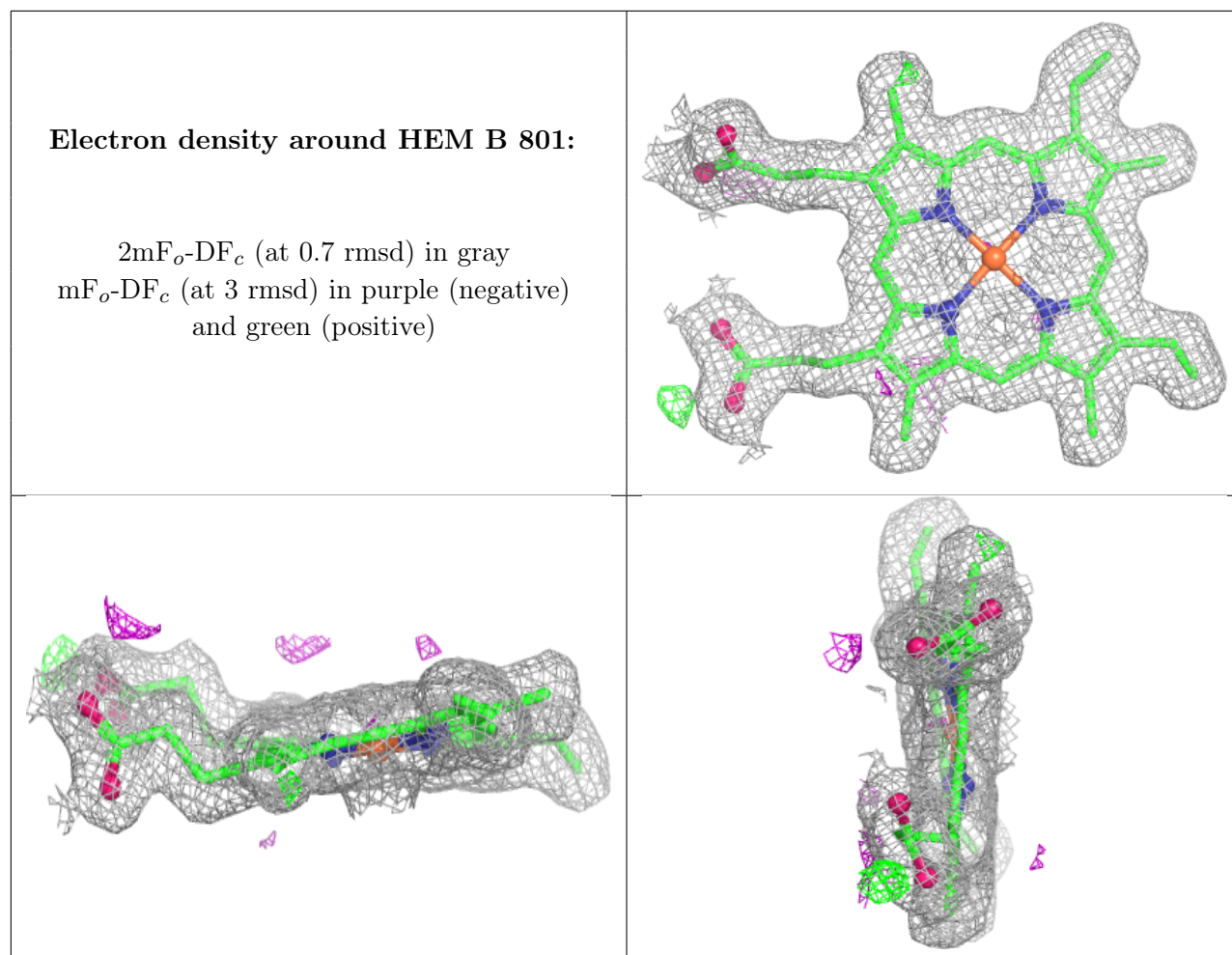
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	NIZ	B	810	10/10	0.75	0.17	37,47,54,58	0
6	PO4	B	808	5/5	0.77	0.10	51,76,92,94	0
7	NIZ	A	810	10/10	0.78	0.17	46,56,61,64	0
5	MPD	A	806	8/8	0.78	0.18	46,65,70,71	0
5	MPD	A	808	8/8	0.81	0.18	59,72,80,81	0
6	PO4	A	807	5/5	0.82	0.10	59,93,95,99	0
5	MPD	A	804	8/8	0.83	0.16	54,57,69,69	0
5	MPD	B	806	8/8	0.84	0.18	47,63,73,76	0
5	MPD	B	804	8/8	0.87	0.15	45,58,67,71	0
7	NIZ	A	809	10/10	0.87	0.12	39,44,52,58	0
5	MPD	B	807	8/8	0.88	0.13	49,58,62,65	0
5	MPD	A	805	8/8	0.90	0.17	56,62,80,81	0
7	NIZ	B	809	10/10	0.91	0.09	32,36,40,41	0
5	MPD	B	805	8/8	0.94	0.09	47,49,53,55	0
3	NA	A	802	1/1	0.99	0.04	21,21,21,21	0
3	NA	B	802	1/1	0.99	0.05	20,20,20,20	0
4	CL	A	803	1/1	0.99	0.04	35,35,35,35	0
4	CL	B	803	1/1	0.99	0.05	30,30,30,30	0
2	HEM	A	801	43/43	0.99	0.04	19,21,25,27	0
2	HEM	B	801	43/43	0.99	0.04	15,19,21,23	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HEM A 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.