



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2023 – 11:53 PM EDT

PDB ID : 5KSG
Title : Crystal structure of the W153F variant of catalase-peroxidase from *B. pseudomallei* treated with isoniazid
Authors : Loewen, P.C.
Deposited on : 2016-07-08
Resolution : 1.62 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

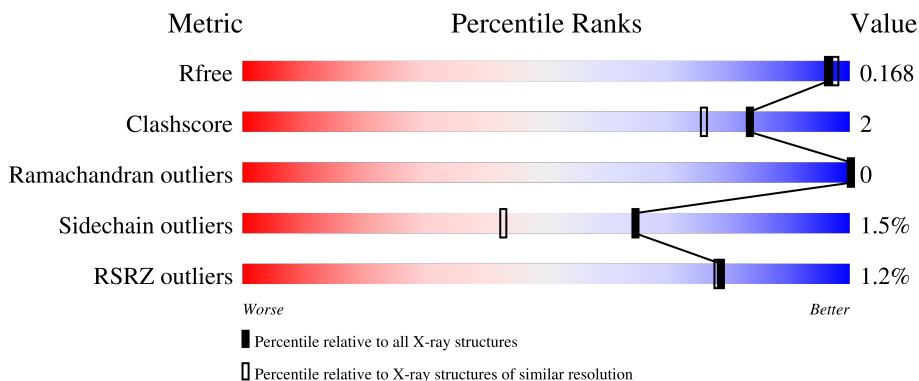
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 1.62 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}	130704	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (1.64-1.60)

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	 82% 13% ..
1	B	728	 83% 13% ..

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PO4	B	806	-	X	-	-
8	NIZ	B	809	-	X	-	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 12995 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
			Total	C	N	O	S			
1	A	713	Total 5570	C 3517	N 994	O 1045	S 14	0	9	0
1	B	714	Total 5590	C 3527	N 998	O 1051	S 14	0	10	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	PHE	TRP	engineered mutation	UNP Q3JNW6
B	153	PHE	TRP	engineered mutation	UNP Q3JNW6

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



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

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

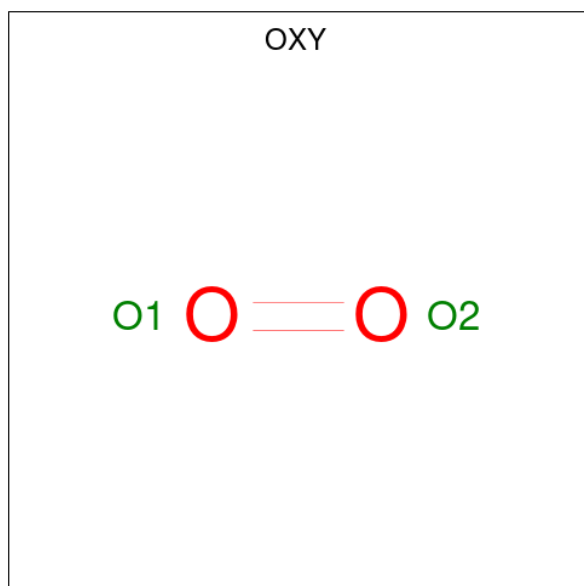
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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 (three-letter code: 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 (three-letter code: OXY) (formula: O₂).



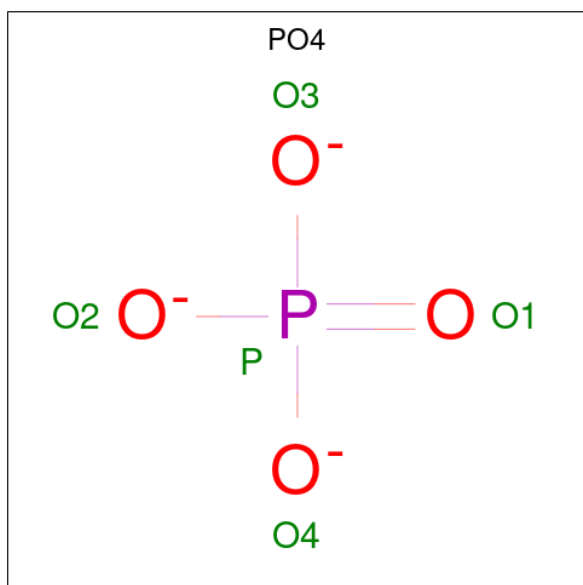
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			2	2		
5	A	1	Total	O	0	0
			2	2		

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

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



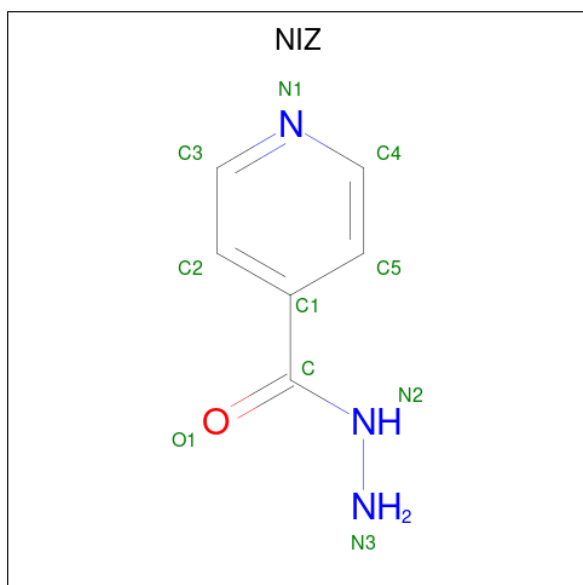
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	B	1	Total O P 5 4 1	0	0

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



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

- Molecule 8 is pyridine-4-carbohydrazide (three-letter code: NIZ) (formula: C₆H₇N₃O).



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

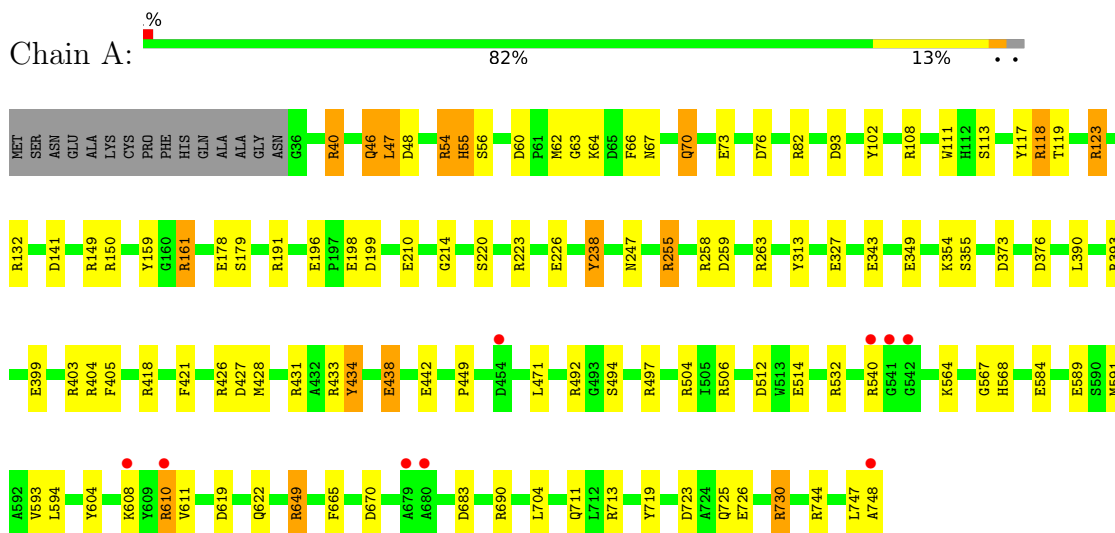
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	844	Total	O	0	0
			844	844		
9	B	841	Total	O	0	0
			841	841		

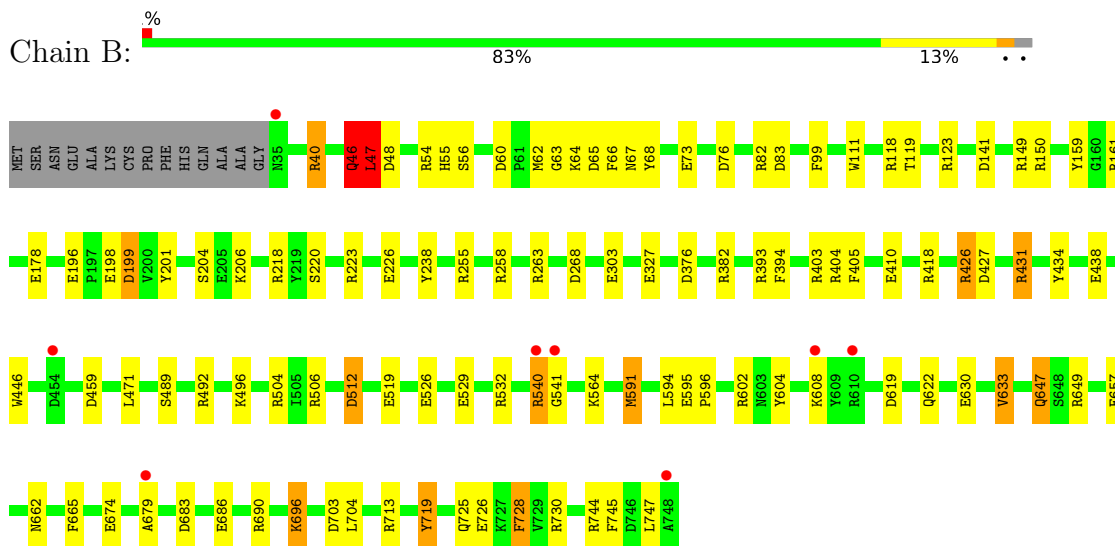
3 Residue-property plots

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	100.67Å 115.93Å 174.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.54 – 1.62 48.36 – 1.62	Depositor EDS
% Data completeness (in resolution range)	99.9 (96.54-1.62) 99.9 (48.36-1.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 1.62Å)	Xtrriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.135 , 0.159 0.146 , 0.168	Depositor DCC
R_{free} test set	12875 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtrriage
Anisotropy	0.340	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 53.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12995	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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, NIZ, CL, NA, PO4, OXY, 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	1.59	59/5726 (1.0%)	1.71	109/7781 (1.4%)
1	B	1.58	58/5743 (1.0%)	1.58	103/7804 (1.3%)
All	All	1.58	117/11469 (1.0%)	1.65	212/15585 (1.4%)

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	4
1	B	0	8
All	All	0	12

All (117) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	532	ARG	CZ-NH1	-12.97	1.16	1.33
1	A	589	GLU	CD-OE2	11.46	1.38	1.25
1	B	726	GLU	CD-OE2	11.15	1.38	1.25
1	A	198	GLU	CD-OE1	10.02	1.36	1.25
1	B	726	GLU	CG-CD	9.96	1.66	1.51
1	B	719	TYR	CD2-CE2	9.85	1.54	1.39
1	B	327	GLU	CD-OE2	9.67	1.36	1.25
1	B	198	GLU	CD-OE1	9.41	1.36	1.25
1	B	532	ARG	CD-NE	-9.21	1.30	1.46
1	B	63	GLY	N-CA	9.13	1.59	1.46
1	B	602	ARG	CZ-NH2	-8.79	1.21	1.33
1	B	196	GLU	CG-CD	8.71	1.65	1.51
1	B	327	GLU	CD-OE1	8.63	1.35	1.25
1	A	438	GLU	CG-CD	8.56	1.64	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	584	GLU	CG-CD	8.54	1.64	1.51
1	A	56	SER	CB-OG	-8.32	1.31	1.42
1	A	589	GLU	CD-OE1	8.26	1.34	1.25
1	A	161[A]	ARG	CZ-NH2	-8.14	1.22	1.33
1	A	161[B]	ARG	CZ-NH2	-8.14	1.22	1.33
1	A	63	GLY	N-CA	7.96	1.57	1.46
1	A	343	GLU	CD-OE1	7.95	1.34	1.25
1	B	410	GLU	CG-CD	7.92	1.63	1.51
1	B	686	GLU	CG-CD	7.85	1.63	1.51
1	A	196	GLU	CG-CD	7.82	1.63	1.51
1	B	512	ASP	CG-OD2	7.80	1.43	1.25
1	B	410	GLU	CD-OE2	7.77	1.34	1.25
1	B	178	GLU	CD-OE2	7.72	1.34	1.25
1	A	434	TYR	CB-CG	-7.67	1.40	1.51
1	B	719	TYR	CZ-OH	7.59	1.50	1.37
1	B	82	ARG	CZ-NH2	-7.56	1.23	1.33
1	A	199	ASP	C-O	7.53	1.37	1.23
1	A	196	GLU	CB-CG	-7.42	1.38	1.52
1	A	102	TYR	CE2-CZ	-7.42	1.28	1.38
1	A	512	ASP	CB-CG	7.40	1.67	1.51
1	A	73	GLU	CG-CD	7.36	1.62	1.51
1	B	540	ARG	C-O	7.35	1.37	1.23
1	A	46	GLN	CG-CD	7.33	1.68	1.51
1	A	748	ALA	N-CA	7.33	1.61	1.46
1	B	196	GLU	CB-CG	-7.01	1.38	1.52
1	A	82	ARG	CZ-NH2	-6.86	1.24	1.33
1	A	327	GLU	CD-OE2	6.85	1.33	1.25
1	A	431	ARG	CZ-NH1	6.82	1.42	1.33
1	B	226	GLU	CG-CD	6.76	1.62	1.51
1	B	204	SER	CA-CB	6.71	1.63	1.52
1	A	313	TYR	CE2-CZ	6.63	1.47	1.38
1	B	526	GLU	CG-CD	6.62	1.61	1.51
1	A	442	GLU	CD-OE2	-6.60	1.18	1.25
1	A	494	SER	CA-CB	-6.55	1.43	1.52
1	B	434	TYR	CE2-CZ	-6.53	1.30	1.38
1	B	541	GLY	C-O	6.48	1.34	1.23
1	B	730	ARG	CZ-NH2	6.45	1.41	1.33
1	A	438	GLU	CD-OE1	-6.45	1.18	1.25
1	B	223	ARG	CG-CD	-6.44	1.35	1.51
1	A	567	GLY	CA-C	-6.43	1.41	1.51
1	A	584	GLU	CD-OE2	6.39	1.32	1.25
1	B	728	PHE	CG-CD1	-6.36	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	647	GLN	CG-CD	6.35	1.65	1.51
1	A	428	MET	CG-SD	-6.32	1.64	1.81
1	A	589	GLU	CG-CD	6.26	1.61	1.51
1	A	327	GLU	CD-OE1	6.23	1.32	1.25
1	B	633[A]	VAL	CB-CG2	-6.20	1.39	1.52
1	B	633[B]	VAL	CB-CG2	-6.20	1.39	1.52
1	A	159	TYR	CD1-CE1	-6.17	1.30	1.39
1	A	540	ARG	C-O	6.09	1.34	1.23
1	B	46	GLN	C-O	6.05	1.34	1.23
1	B	201	TYR	CE1-CZ	-6.05	1.30	1.38
1	A	47	LEU	CB-CG	-6.02	1.35	1.52
1	B	438	GLU	CG-CD	6.01	1.60	1.51
1	A	70	GLN	CG-CD	5.91	1.64	1.51
1	A	719	TYR	CZ-OH	5.88	1.47	1.37
1	B	489	SER	CB-OG	-5.87	1.34	1.42
1	B	178	GLU	CD-OE1	-5.79	1.19	1.25
1	B	630	GLU	CD-OE2	5.78	1.32	1.25
1	B	47	LEU	CB-CG	-5.78	1.35	1.52
1	A	226	GLU	CG-CD	5.76	1.60	1.51
1	A	113	SER	CB-OG	5.76	1.49	1.42
1	A	161[A]	ARG	CG-CD	5.73	1.66	1.51
1	A	161[B]	ARG	CG-CD	5.73	1.66	1.51
1	B	595	GLU	CD-OE2	5.69	1.31	1.25
1	B	56	SER	CB-OG	-5.68	1.34	1.42
1	B	255[A]	ARG	CZ-NH1	-5.68	1.25	1.33
1	B	255[B]	ARG	CZ-NH1	-5.68	1.25	1.33
1	A	532	ARG	CD-NE	-5.67	1.36	1.46
1	B	526	GLU	CD-OE1	-5.64	1.19	1.25
1	B	434	TYR	CG-CD2	-5.60	1.31	1.39
1	A	247	ASN	CG-ND2	-5.59	1.18	1.32
1	A	255[A]	ARG	CZ-NH2	-5.58	1.25	1.33
1	A	255[B]	ARG	CZ-NH2	-5.58	1.25	1.33
1	B	619	ASP	CG-OD1	-5.55	1.12	1.25
1	B	446	TRP	CZ2-CH2	-5.55	1.26	1.37
1	B	679	ALA	N-CA	5.48	1.57	1.46
1	A	399	GLU	CD-OE2	5.46	1.31	1.25
1	A	179	SER	CB-OG	-5.42	1.35	1.42
1	A	514	GLU	CG-CD	5.42	1.60	1.51
1	A	210	GLU	CD-OE2	5.40	1.31	1.25
1	B	54	ARG	C-O	5.32	1.33	1.23
1	B	674	GLU	CG-CD	5.30	1.59	1.51
1	B	541	GLY	C-N	-5.28	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214	GLY	CA-C	-5.24	1.43	1.51
1	B	496	LYS	CE-NZ	-5.23	1.35	1.49
1	A	220	SER	CB-OG	-5.22	1.35	1.42
1	A	178	GLU	CG-CD	5.21	1.59	1.51
1	A	161[A]	ARG	NE-CZ	5.19	1.39	1.33
1	A	161[B]	ARG	NE-CZ	5.19	1.39	1.33
1	B	68	TYR	CG-CD1	-5.18	1.32	1.39
1	B	434	TYR	CG-CD1	-5.18	1.32	1.39
1	B	220	SER	N-CA	5.17	1.56	1.46
1	A	223	ARG	CG-CD	-5.16	1.39	1.51
1	A	355	SER	CA-CB	5.13	1.60	1.52
1	A	67	ASN	CG-OD1	-5.10	1.12	1.24
1	B	73	GLU	CD-OE2	5.09	1.31	1.25
1	A	418	ARG	CZ-NH1	-5.09	1.26	1.33
1	A	343	GLU	CG-CD	5.08	1.59	1.51
1	A	564	LYS	CD-CE	5.07	1.64	1.51
1	B	159	TYR	CE1-CZ	-5.06	1.31	1.38
1	B	199	ASP	C-O	5.01	1.32	1.23
1	B	226	GLU	CB-CG	-5.01	1.42	1.52

All (212) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255[A]	ARG	NE-CZ-NH2	-31.84	104.38	120.30
1	A	255[B]	ARG	NE-CZ-NH2	-31.84	104.38	120.30
1	A	255[A]	ARG	NE-CZ-NH1	24.22	132.41	120.30
1	A	255[B]	ARG	NE-CZ-NH1	24.22	132.41	120.30
1	A	161[A]	ARG	NE-CZ-NH1	19.84	130.22	120.30
1	A	161[B]	ARG	NE-CZ-NH1	19.84	130.22	120.30
1	B	263	ARG	NE-CZ-NH2	-15.72	112.44	120.30
1	B	161[A]	ARG	NE-CZ-NH2	-15.13	112.73	120.30
1	B	161[B]	ARG	NE-CZ-NH2	-15.13	112.73	120.30
1	A	649	ARG	NE-CZ-NH2	-13.41	113.60	120.30
1	B	123	ARG	NE-CZ-NH2	-13.23	113.68	120.30
1	B	123	ARG	NE-CZ-NH1	13.19	126.89	120.30
1	A	123	ARG	NE-CZ-NH1	12.96	126.78	120.30
1	A	713	ARG	NE-CZ-NH1	12.45	126.52	120.30
1	B	719	TYR	CB-CG-CD1	-12.24	113.65	121.00
1	B	713	ARG	NE-CZ-NH1	12.18	126.39	120.30
1	A	713	ARG	NE-CZ-NH2	-11.80	114.40	120.30
1	B	405	PHE	CB-CG-CD1	11.70	128.99	120.80
1	B	744	ARG	NE-CZ-NH1	11.54	126.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	ARG	NE-CZ-NH2	-11.37	114.61	120.30
1	B	199	ASP	CB-CG-OD2	-11.20	108.22	118.30
1	A	730	ARG	NE-CZ-NH1	11.19	125.89	120.30
1	A	40	ARG	NE-CZ-NH1	11.17	125.89	120.30
1	A	149	ARG	NE-CZ-NH1	11.16	125.88	120.30
1	B	40	ARG	NE-CZ-NH1	11.09	125.85	120.30
1	A	48	ASP	CB-CG-OD1	10.96	128.16	118.30
1	B	48	ASP	CB-CG-OD1	10.87	128.08	118.30
1	B	744	ARG	NE-CZ-NH2	-10.87	114.87	120.30
1	B	619	ASP	CB-CG-OD1	-10.83	108.56	118.30
1	B	268	ASP	CB-CG-OD1	10.69	127.92	118.30
1	A	532	ARG	NE-CZ-NH2	-10.63	114.99	120.30
1	B	683	ASP	CB-CG-OD2	-10.57	108.78	118.30
1	A	150	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	B	512	ASP	CB-CG-OD1	-10.23	109.09	118.30
1	A	46	GLN	CA-CB-CG	10.23	135.91	113.40
1	A	123	ARG	NE-CZ-NH2	-10.19	115.21	120.30
1	B	686	GLU	OE1-CD-OE2	9.93	135.21	123.30
1	B	393	ARG	NE-CZ-NH2	-9.93	115.34	120.30
1	A	404	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	B	263	ARG	NE-CZ-NH1	9.69	125.14	120.30
1	A	118	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	A	405	PHE	CB-CG-CD2	-9.62	114.07	120.80
1	A	497	ARG	NE-CZ-NH2	-9.43	115.58	120.30
1	B	649	ARG	NE-CZ-NH2	-9.21	115.69	120.30
1	A	434	TYR	CB-CG-CD1	9.19	126.51	121.00
1	A	60	ASP	CB-CG-OD1	9.04	126.43	118.30
1	B	690	ARG	NE-CZ-NH2	9.02	124.81	120.30
1	B	149	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	A	263	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	B	713	ARG	NE-CZ-NH2	-8.83	115.89	120.30
1	A	532	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	A	66	PHE	CB-CG-CD1	-8.41	114.91	120.80
1	B	719	TYR	CG-CD2-CE2	-8.40	114.58	121.30
1	A	118	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	B	150	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	A	744	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	B	82	ARG	NE-CZ-NH2	-8.19	116.21	120.30
1	B	46	GLN	CA-CB-CG	8.08	131.17	113.40
1	A	60	ASP	CB-CG-OD2	-8.07	111.04	118.30
1	A	719	TYR	CB-CG-CD1	-8.03	116.18	121.00
1	A	259	ASP	CB-CG-OD2	-8.01	111.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	405	PHE	CB-CG-CD1	7.93	126.35	120.80
1	A	730	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	B	541	GLY	N-CA-C	-7.81	93.58	113.10
1	A	263	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	B	40	ARG	NE-CZ-NH2	-7.63	116.49	120.30
1	A	161[A]	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	A	161[B]	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	A	73	GLU	OE1-CD-OE2	-7.57	114.22	123.30
1	B	726	GLU	CG-CD-OE2	7.56	133.41	118.30
1	B	492	ARG	NE-CZ-NH1	7.55	124.08	120.30
1	B	405	PHE	CB-CG-CD2	-7.50	115.55	120.80
1	A	54	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	48	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	A	117	TYR	CB-CG-CD1	-7.39	116.57	121.00
1	B	161[A]	ARG	CD-NE-CZ	7.39	133.94	123.60
1	B	161[B]	ARG	CD-NE-CZ	7.39	133.94	123.60
1	A	108	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	492	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	B	459	ASP	CB-CG-OD1	7.34	124.91	118.30
1	B	427	ASP	CB-CG-OD2	-7.32	111.71	118.30
1	B	258	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	B	218	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	B	504	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	B	76	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	B	529[A]	GLU	OE1-CD-OE2	-7.09	114.79	123.30
1	B	529[B]	GLU	OE1-CD-OE2	-7.09	114.79	123.30
1	B	434	TYR	CB-CG-CD1	7.09	125.25	121.00
1	A	404	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	A	670	ASP	CB-CG-OD2	-6.99	112.01	118.30
1	B	404	ARG	NE-CZ-NH2	-6.91	116.84	120.30
1	B	719	TYR	CD1-CG-CD2	6.88	125.47	117.90
1	A	258	ARG	NE-CZ-NH2	-6.85	116.88	120.30
1	A	255[A]	ARG	CD-NE-CZ	6.84	133.17	123.60
1	A	255[B]	ARG	CD-NE-CZ	6.84	133.17	123.60
1	B	730	ARG	NE-CZ-NH1	-6.83	116.89	120.30
1	A	76	ASP	CB-CG-OD2	-6.76	112.21	118.30
1	A	434	TYR	CZ-CE2-CD2	6.76	125.89	119.80
1	B	62	MET	C-N-CA	-6.69	108.24	122.30
1	B	60	ASP	CB-CG-OD1	6.69	124.32	118.30
1	A	719	TYR	CD1-CE1-CZ	-6.62	113.84	119.80
1	A	719	TYR	CG-CD2-CE2	-6.62	116.00	121.30
1	A	393	ARG	NE-CZ-NH2	-6.51	117.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	GLU	OE1-CD-OE2	6.49	131.09	123.30
1	A	421	PHE	CB-CG-CD2	-6.46	116.28	120.80
1	A	649	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	161[A]	ARG	CG-CD-NE	6.43	125.31	111.80
1	A	161[B]	ARG	CG-CD-NE	6.43	125.31	111.80
1	B	506	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	B	602	ARG	NE-CZ-NH1	-6.41	117.10	120.30
1	A	54	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	A	584	GLU	OE1-CD-OE2	-6.39	115.63	123.30
1	A	506	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	512	ASP	CB-CG-OD2	-6.35	112.59	118.30
1	A	433	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	376	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	B	512	ASP	CB-CG-OD2	6.23	123.91	118.30
1	B	696	LYS	CD-CE-NZ	6.20	125.95	111.70
1	A	514	GLU	OE1-CD-OE2	-6.13	115.94	123.30
1	B	703	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	349	GLU	OE1-CD-OE2	6.09	130.61	123.30
1	B	83	ASP	CB-CG-OD2	6.08	123.78	118.30
1	A	108	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	B	683	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	62	MET	C-N-CA	-5.96	109.78	122.30
1	B	719	TYR	CD1-CE1-CZ	-5.88	114.51	119.80
1	A	66	PHE	CG-CD2-CE2	-5.87	114.34	120.80
1	A	47	LEU	N-CA-CB	-5.83	98.75	110.40
1	A	40	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	B	686	GLU	CG-CD-OE2	-5.81	106.69	118.30
1	B	532	ARG	CG-CD-NE	-5.80	99.61	111.80
1	A	438	GLU	CG-CD-OE1	-5.79	106.71	118.30
1	B	47	LEU	N-CA-CB	-5.78	98.84	110.40
1	B	303	GLU	CG-CD-OE1	5.77	129.85	118.30
1	A	161[A]	ARG	CD-NE-CZ	5.77	131.68	123.60
1	A	161[B]	ARG	CD-NE-CZ	5.77	131.68	123.60
1	A	390	LEU	CB-CG-CD2	5.77	120.81	111.00
1	A	704	LEU	CB-CG-CD2	-5.75	101.22	111.00
1	A	161[A]	ARG	NH1-CZ-NH2	-5.74	113.08	119.40
1	A	161[B]	ARG	NH1-CZ-NH2	-5.74	113.08	119.40
1	A	492	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	726	GLU	OE1-CD-OE2	-5.72	116.43	123.30
1	B	704	LEU	CB-CG-CD2	-5.71	101.30	111.00
1	B	161[A]	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	B	161[B]	ARG	NE-CZ-NH1	5.71	123.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	427	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	B	532	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	A	55	HIS	CB-CA-C	5.65	121.70	110.40
1	B	46	GLN	CB-CA-C	5.64	121.68	110.40
1	B	382	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	745	PHE	CG-CD2-CE2	-5.64	114.60	120.80
1	B	564	LYS	CD-CE-NZ	-5.63	98.74	111.70
1	B	418	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	B	434	TYR	CZ-CE2-CD2	5.60	124.84	119.80
1	B	665	PHE	CB-CG-CD2	-5.58	116.90	120.80
1	A	238	TYR	CB-CG-CD2	5.57	124.34	121.00
1	A	438	GLU	OE1-CD-OE2	5.54	129.95	123.30
1	B	427	ASP	OD1-CG-OD2	5.54	133.83	123.30
1	A	604	TYR	CB-CG-CD1	-5.53	117.68	121.00
1	A	198	GLU	CG-CD-OE2	-5.53	107.24	118.30
1	B	728	PHE	CB-CG-CD1	-5.53	116.93	120.80
1	A	46	GLN	N-CA-C	-5.53	96.08	111.00
1	A	619	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	B	431	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	A	70	GLN	CA-CB-CG	5.49	125.48	113.40
1	A	665	PHE	CG-CD1-CE1	-5.47	114.78	120.80
1	B	99	PHE	CB-CG-CD2	-5.47	116.97	120.80
1	A	93	ASP	CB-CG-OD1	5.44	123.20	118.30
1	B	394	PHE	CB-CG-CD2	5.43	124.61	120.80
1	B	591	MET	CG-SD-CE	-5.42	91.52	100.20
1	A	191	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	B	418	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	426[A]	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	426[B]	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	B	745	PHE	CD1-CE1-CZ	-5.39	113.63	120.10
1	A	373	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	82	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	132	ARG	NE-CZ-NH2	5.35	122.98	120.30
1	B	730	ARG	NH1-CZ-NH2	5.35	125.29	119.40
1	B	65	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	B	376	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	B	438	GLU	OE1-CD-OE2	5.34	129.71	123.30
1	B	82	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	683	ASP	CB-CG-OD1	5.27	123.05	118.30
1	A	449	PRO	O-C-N	5.24	131.09	122.70
1	A	723	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	A	434	TYR	CB-CG-CD2	-5.23	117.86	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	258	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	B	434	TYR	CA-CB-CG	5.23	123.33	113.40
1	A	149	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	403	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	55	HIS	CB-CA-C	5.19	120.79	110.40
1	A	690	ARG	NE-CZ-NH1	-5.19	117.71	120.30
1	A	540	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	A	431	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	B	73	GLU	OE1-CD-OE2	5.11	129.44	123.30
1	B	730	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	604	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	B	66	PHE	CD1-CE1-CZ	-5.08	114.01	120.10
1	B	719	TYR	CZ-CE2-CD2	-5.08	115.23	119.80
1	B	532	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	B	196	GLU	OE1-CD-OE2	-5.06	117.23	123.30
1	A	564	LYS	CD-CE-NZ	-5.05	100.08	111.70
1	A	354	LYS	CD-CE-NZ	-5.05	100.08	111.70
1	B	327	GLU	OE1-CD-OE2	-5.03	117.26	123.30
1	B	410	GLU	CG-CD-OE2	5.02	128.34	118.30
1	A	255[A]	ARG	CG-CD-NE	-5.02	101.27	111.80
1	A	255[B]	ARG	CG-CD-NE	-5.02	101.27	111.80
1	B	438	GLU	CG-CD-OE1	-5.01	108.27	118.30
1	B	206	LYS	CG-CD-CE	5.01	126.92	111.90
1	A	82	ARG	NE-CZ-NH1	5.00	122.80	120.30
1	B	649	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	434	TYR	Sidechain
1	A	438	GLU	Sidechain
1	A	471	LEU	Mainchain
1	A	747	LEU	Peptide
1	B	199	ASP	Mainchain
1	B	46	GLN	Mainchain
1	B	47	LEU	Mainchain
1	B	471	LEU	Mainchain
1	B	596	PRO	Mainchain
1	B	67	ASN	Sidechain
1	B	719	TYR	Sidechain
1	B	747	LEU	Mainchain

5.2 Too-close contacts [i](#)

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	5570	0	5395	28	0
1	B	5590	0	5405	23	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	4	0	0	0	0
5	B	4	0	0	0	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	16	0	28	3	0
7	B	16	0	28	0	0
8	B	10	0	7	3	0
9	A	844	0	0	11	2
9	B	841	0	0	13	3
All	All	12995	0	10923	54	3

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725[A]:GLN:NE2	1:A:726[A]:GLU:HG3	1.41	1.35
1:A:725[A]:GLN:NE2	1:A:726[A]:GLU:CG	1.99	1.26
1:A:725[A]:GLN:HE22	1:A:726[A]:GLU:CG	1.78	0.91
1:A:119[B]:THR:HG21	9:A:1158:HOH:O	1.72	0.90
7:A:807:MPD:O4	7:A:807:MPD:CM	2.17	0.90
1:B:119[B]:THR:HG21	9:B:1091:HOH:O	1.74	0.87
1:A:725[A]:GLN:HE22	1:A:726[A]:GLU:HG2	1.42	0.83
1:B:622[A]:GLN:OE1	8:B:809:NIZ:O1	1.97	0.83
1:B:647:GLN:HG2	9:B:957:HOH:O	1.79	0.81
1:A:725[A]:GLN:HE21	1:A:726[A]:GLU:HG3	1.47	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:725[A]:GLN:NE2	1:A:726[A]:GLU:HG2	1.98	0.77
1:A:426[A]:ARG:NE	9:A:903:HOH:O	1.67	0.76
7:A:807:MPD:O4	7:A:807:MPD:HM1	1.82	0.76
1:B:426[A]:ARG:NE	9:B:903:HOH:O	1.77	0.72
1:B:46:GLN:NE2	9:B:904:HOH:O	1.97	0.71
1:B:519:GLU:OE1	9:B:905:HOH:O	2.09	0.71
1:A:711:GLN:OE1	9:A:904:HOH:O	2.09	0.70
1:B:47:LEU:O	9:B:906:HOH:O	2.11	0.69
1:B:657[A]:GLU:CD	9:B:922:HOH:O	2.34	0.66
1:B:540:ARG:NE	1:B:540:ARG:HA	2.12	0.64
7:A:807:MPD:O4	7:A:807:MPD:HM2	1.96	0.63
1:A:725[A]:GLN:NE2	1:A:726[A]:GLU:CD	2.52	0.62
1:B:512:ASP:HB2	9:B:1452:HOH:O	2.02	0.60
1:B:512:ASP:OD1	9:B:907:HOH:O	2.15	0.60
1:A:725[A]:GLN:CD	1:A:726[A]:GLU:HG3	2.19	0.60
1:A:568:HIS:CD2	1:A:725[A]:GLN:OE1	2.58	0.56
1:B:662:ASN:H	1:B:725:GLN:HE22	1.52	0.55
1:B:622[A]:GLN:HE22	8:B:809:NIZ:C1	2.20	0.54
1:A:47:LEU:HB2	9:A:953:HOH:O	2.07	0.54
1:B:591:MET:SD	1:B:594:LEU:HD12	2.49	0.54
1:B:403:ARG:NH1	9:B:914:HOH:O	2.38	0.53
1:A:47:LEU:O	9:A:906:HOH:O	2.19	0.51
1:A:255[A]:ARG:NH2	9:A:905:HOH:O	2.11	0.51
1:A:54:ARG:HB2	1:A:55:HIS:CD2	2.46	0.51
1:A:610:ARG:HG2	1:A:611:VAL:N	2.25	0.50
1:A:123:ARG:NH2	1:A:622[B]:GLN:OE1	2.46	0.49
1:A:504:ARG:HD2	9:A:974:HOH:O	2.13	0.49
1:B:622[A]:GLN:HE22	8:B:809:NIZ:C	2.27	0.47
1:A:593:VAL:HG13	9:A:937:HOH:O	2.15	0.47
1:A:54:ARG:CB	1:A:55:HIS:CD2	2.98	0.47
1:B:47:LEU:HB2	9:B:1126:HOH:O	2.14	0.47
1:B:633[B]:VAL:HG12	1:B:728:PHE:CE1	2.50	0.47
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.96	0.46
1:B:426[A]:ARG:NH2	9:B:901:HOH:O	0.62	0.46
1:B:111:TRP:HZ3	1:B:238:TYR:HH	1.60	0.45
1:A:591:MET:SD	1:A:594:LEU:HD12	2.57	0.45
1:B:426[B]:ARG:HA	1:B:426[B]:ARG:HD2	1.86	0.44
1:A:111:TRP:HZ3	1:A:238:TYR:HH	1.61	0.44
1:A:726[B]:GLU:HG2	1:A:730:ARG:NH1	2.33	0.44
1:A:70:GLN:NE2	9:A:930:HOH:O	2.50	0.43
1:A:725[B]:GLN:CD	9:A:909:HOH:O	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:ARG:HD3	9:B:1557:HOH:O	2.20	0.41
1:B:540:ARG:HA	1:B:540:ARG:CZ	2.50	0.41
1:A:426[A]:ARG:CG	9:A:903:HOH:O	2.67	0.41

All (3) 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:1308:HOH:O	9:B:1229:HOH:O[2_444]	1.90	0.30
9:A:1461:HOH:O	9:B:1579:HOH:O[4_445]	2.01	0.19
9:B:1336:HOH:O	9:B:1535:HOH:O[4_445]	2.17	0.03

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	720/728 (99%)	710 (99%)	10 (1%)	0	100	100
1	B	722/728 (99%)	712 (99%)	10 (1%)	0	100	100
All	All	1442/1456 (99%)	1422 (99%)	20 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	559/561 (100%)	549 (98%)	10 (2%)	59	34
1	B	561/561 (100%)	554 (99%)	7 (1%)	71	52
All	All	1120/1122 (100%)	1103 (98%)	17 (2%)	65	43

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	46	GLN
1	A	64	LYS
1	A	118	ARG
1	A	141	ASP
1	A	161[A]	ARG
1	A	161[B]	ARG
1	A	608	LYS
1	A	610	ARG
1	A	649	ARG
1	B	40	ARG
1	B	46	GLN
1	B	64	LYS
1	B	118	ARG
1	B	141	ASP
1	B	608	LYS
1	B	696	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	247	ASN
1	B	227	ASN
1	B	406	HIS
1	B	544	GLN
1	B	647	GLN
1	B	725	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0.43	0	9,10,10	1.22	1 (11%)
2	HEM	B	801	1,9	41,50,50	1.48	6 (14%)	45,82,82	1.63	13 (28%)
2	HEM	A	801	1,9	41,50,50	1.38	5 (12%)	45,82,82	2.26	20 (44%)
7	MPD	B	808	-	7,7,7	1.10	0	9,10,10	1.65	3 (33%)
5	OXY	A	805	-	1,1,1	0.24	0	-	-	-
6	PO4	A	806	-	4,4,4	2.17	1 (25%)	6,6,6	3.08	2 (33%)
7	MPD	A	808	-	7,7,7	0.74	0	9,10,10	1.07	1 (11%)
7	MPD	B	807	-	7,7,7	0.34	0	9,10,10	1.29	2 (22%)
5	OXY	B	804	-	1,1,1	0.18	0	-	-	-
8	NIZ	B	809	-	10,10,10	5.18	6 (60%)	12,12,12	3.57	8 (66%)
6	PO4	B	806	-	4,4,4	2.48	2 (50%)	6,6,6	3.15	4 (66%)
5	OXY	B	805	-	1,1,1	0.07	0	-	-	-
5	OXY	A	804	-	1,1,1	0.27	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
7	MPD	A	807	-	-	2/5/5/5	-
2	HEM	B	801	1,9	-	3/12/54/54	-
2	HEM	A	801	1,9	-	3/12/54/54	-
7	MPD	B	808	-	-	1/5/5/5	-
7	MPD	A	808	-	-	0/5/5/5	-
8	NIZ	B	809	-	-	0/6/6/6	0/1/1/1
7	MPD	B	807	-	-	2/5/5/5	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	809	NIZ	C4-N1	10.76	1.65	1.33
8	B	809	NIZ	C5-C1	7.95	1.52	1.39
8	B	809	NIZ	N3-N2	-6.12	1.32	1.41
8	B	809	NIZ	C-N2	5.18	1.39	1.33
2	B	801	HEM	CHB-C1B	3.84	1.44	1.35
6	A	806	PO4	P-O4	-3.66	1.43	1.54
6	B	806	PO4	P-O1	3.36	1.58	1.50
8	B	809	NIZ	C5-C4	-3.21	1.32	1.38
2	B	801	HEM	CHA-C4D	3.10	1.42	1.35
2	A	801	HEM	O1A-CGA	3.01	1.32	1.22
8	B	809	NIZ	C2-C1	2.90	1.44	1.39
6	B	806	PO4	P-O3	-2.87	1.46	1.54
2	A	801	HEM	C3B-C2B	2.82	1.43	1.37
2	A	801	HEM	CHA-C4D	2.75	1.42	1.35
2	B	801	HEM	CAA-C2A	-2.68	1.48	1.52
2	B	801	HEM	CBA-CGA	2.52	1.56	1.50
2	A	801	HEM	C3C-C2C	-2.42	1.37	1.40
2	B	801	HEM	C1B-C2B	-2.17	1.40	1.44
2	A	801	HEM	CMD-C2D	-2.10	1.46	1.50
2	B	801	HEM	C2C-C1C	2.05	1.47	1.42

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	809	NIZ	C1-C-N2	7.61	124.96	116.27
2	A	801	HEM	C2C-C3C-C4C	6.33	111.32	106.90
8	B	809	NIZ	C5-C4-N1	-6.05	113.09	123.62
6	A	806	PO4	O3-P-O1	-5.63	90.30	110.89
6	B	806	PO4	O4-P-O3	4.99	123.98	107.97
6	A	806	PO4	O4-P-O1	4.76	128.32	110.89
2	A	801	HEM	C4B-C3B-C2B	-4.58	103.48	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	C4C-CHD-C1D	4.25	128.17	122.56
2	A	801	HEM	C1D-C2D-C3D	-4.09	102.66	106.96
2	B	801	HEM	CBA-CAA-C2A	3.82	119.13	112.62
6	B	806	PO4	O4-P-O1	-3.77	97.10	110.89
8	B	809	NIZ	O1-C-C1	-3.73	114.29	120.94
8	B	809	NIZ	C5-C1-C2	3.54	123.63	118.59
6	B	806	PO4	O3-P-O2	-3.52	96.66	107.97
8	B	809	NIZ	C3-C2-C1	-3.48	115.24	119.05
2	A	801	HEM	C4B-CHC-C1C	3.47	127.14	122.56
2	A	801	HEM	C2D-C1D-ND	3.36	113.91	109.88
2	B	801	HEM	CMC-C2C-C3C	3.33	130.91	124.68
2	B	801	HEM	C4C-CHD-C1D	3.21	126.79	122.56
2	A	801	HEM	C1B-NB-C4B	3.01	108.19	105.07
2	A	801	HEM	O1A-CGA-CBA	-2.90	113.75	123.08
7	B	808	MPD	O2-C2-CM	2.67	116.65	108.08
2	A	801	HEM	CMC-C2C-C3C	2.62	129.57	124.68
2	A	801	HEM	CMA-C3A-C4A	-2.59	124.49	128.46
2	B	801	HEM	CMB-C2B-C1B	-2.57	121.13	125.04
7	A	807	MPD	CM-C2-C1	2.56	115.92	110.57
8	B	809	NIZ	C4-C5-C1	2.56	121.84	119.05
2	A	801	HEM	C3B-C2B-C1B	2.53	108.36	106.49
2	A	801	HEM	O2A-CGA-CBA	2.49	122.03	114.03
2	A	801	HEM	CMD-C2D-C1D	2.47	128.79	125.04
8	B	809	NIZ	O1-C-N2	-2.43	119.47	122.50
2	A	801	HEM	O1D-CGD-CBD	-2.43	115.29	123.08
2	B	801	HEM	C4A-C3A-C2A	-2.40	105.33	107.00
2	B	801	HEM	C1B-NB-C4B	2.37	107.53	105.07
6	B	806	PO4	O4-P-O2	2.35	115.52	107.97
2	A	801	HEM	C4D-ND-C1D	-2.33	102.66	105.07
2	B	801	HEM	CHC-C4B-NB	2.31	126.95	124.43
2	B	801	HEM	CAD-CBD-CGD	2.30	118.56	113.60
2	A	801	HEM	C3C-C4C-NC	-2.26	106.68	110.94
2	B	801	HEM	C4B-C3B-C2B	2.22	108.88	107.11
8	B	809	NIZ	C4-N1-C3	2.22	122.07	116.85
7	B	808	MPD	O2-C2-C1	-2.22	100.96	108.08
2	A	801	HEM	CHA-C4D-ND	-2.21	121.66	124.38
2	A	801	HEM	CAA-CBA-CGA	-2.18	107.64	113.76
2	B	801	HEM	C1D-C2D-C3D	-2.17	104.68	106.96
7	B	807	MPD	CM-C2-C1	-2.13	106.13	110.57
2	A	801	HEM	CMA-C3A-C2A	2.12	128.94	124.94
2	B	801	HEM	CAA-CBA-CGA	-2.09	107.89	113.76
7	B	807	MPD	C1-C2-C3	2.09	119.68	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	808	MPD	CM-C2-C1	-2.09	106.23	110.57
2	B	801	HEM	CBD-CAD-C3D	2.06	118.34	112.63
2	A	801	HEM	CMB-C2B-C1B	-2.05	121.92	125.04
7	B	808	MPD	C1-C2-C3	-2.02	100.57	109.96
2	B	801	HEM	O1A-CGA-CBA	-2.01	116.63	123.08

There are no chirality outliers.

All (11) torsion outliers are listed below:

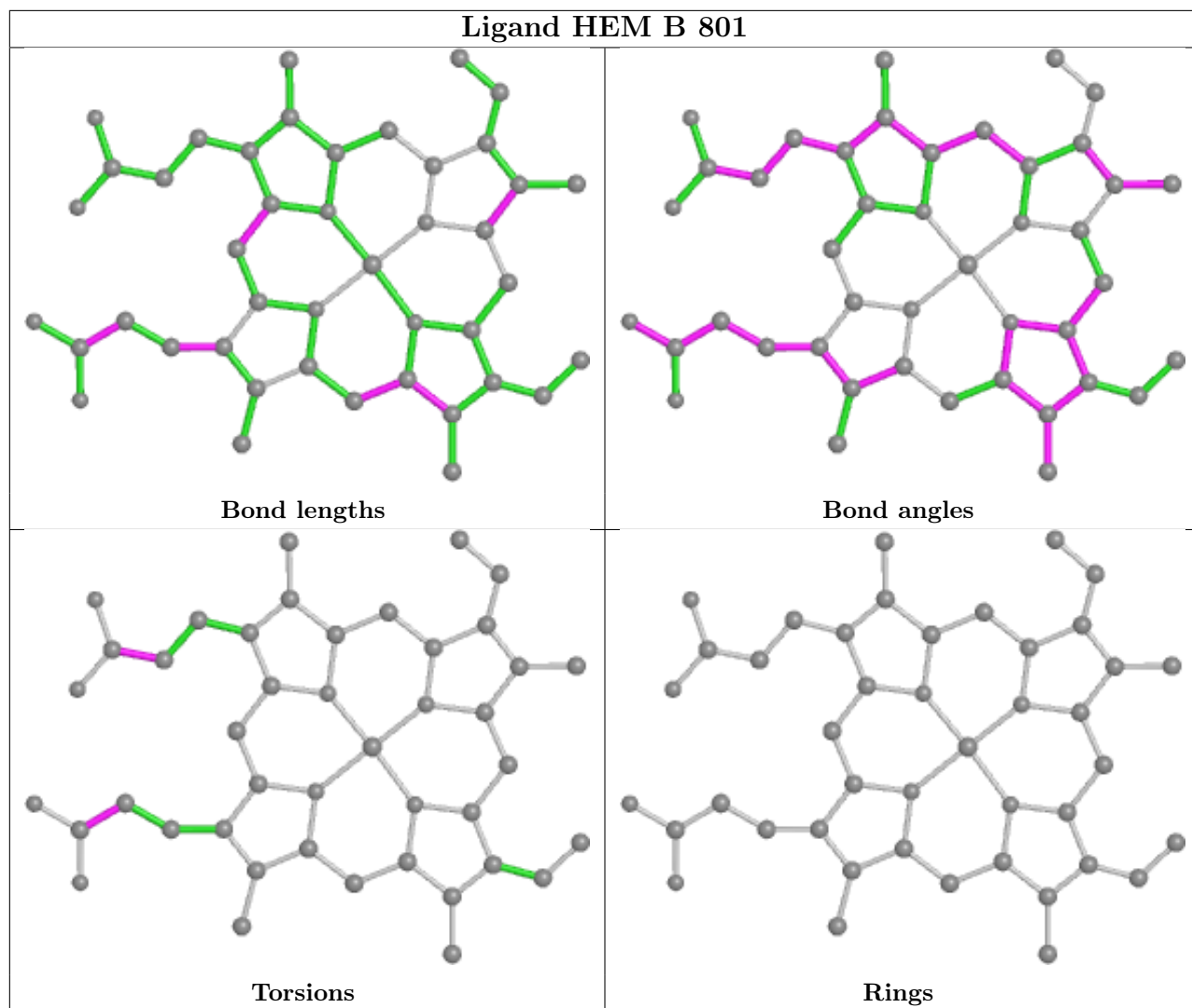
Mol	Chain	Res	Type	Atoms
7	A	807	MPD	CM-C2-C3-C4
7	B	807	MPD	C1-C2-C3-C4
7	B	807	MPD	O2-C2-C3-C4
7	B	808	MPD	O2-C2-C3-C4
2	A	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O1A
2	A	801	HEM	CAD-CBD-CGD-O2D
2	B	801	HEM	CAD-CBD-CGD-O2D
7	A	807	MPD	C2-C3-C4-O4

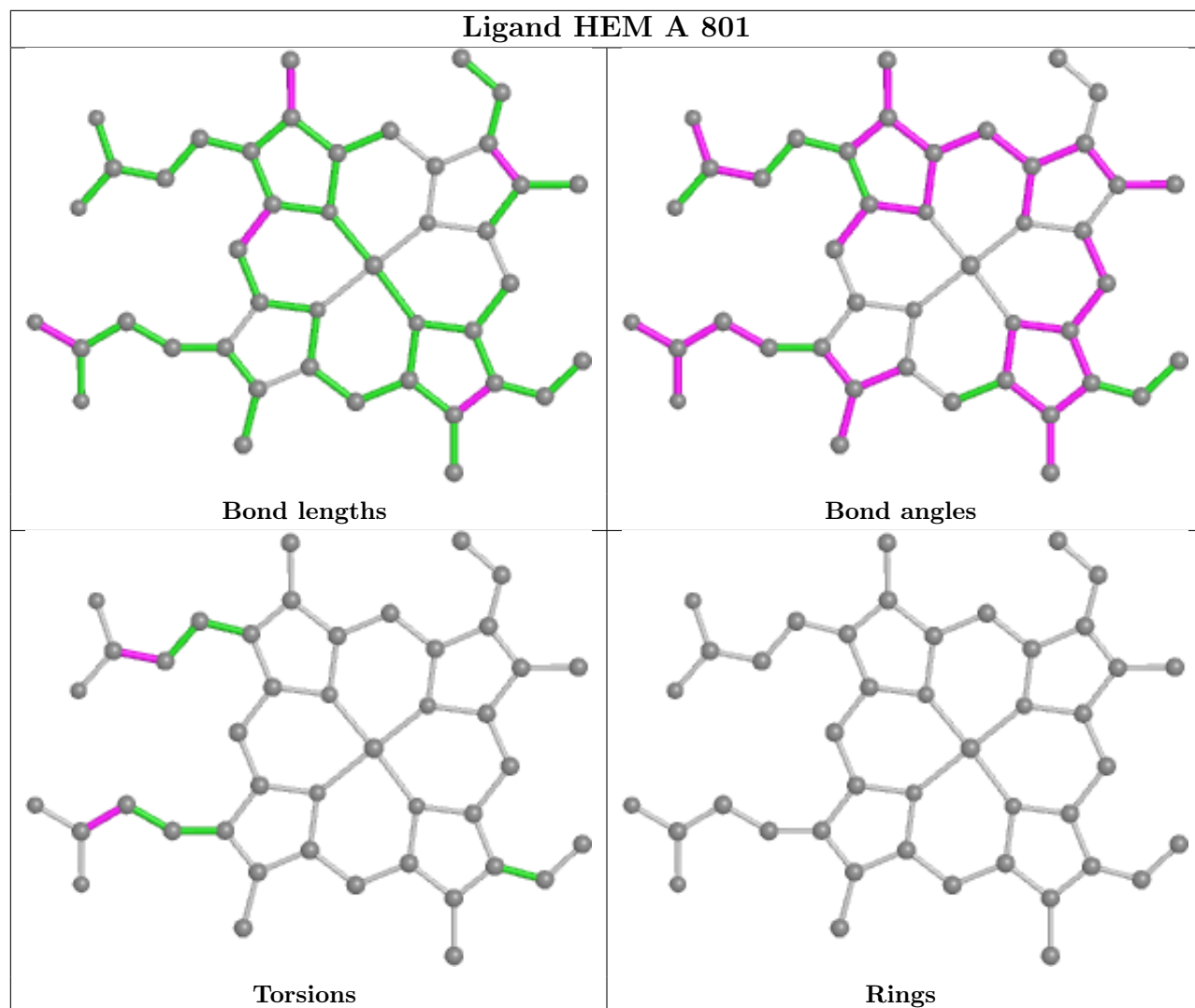
There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	807	MPD	3	0
8	B	809	NIZ	3	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	713/728 (97%)	-0.48	9 (1%) 77 76	11, 18, 34, 75	0
1	B	714/728 (98%)	-0.53	8 (1%) 80 80	11, 17, 34, 67	0
All	All	1427/1456 (98%)	-0.50	17 (1%) 79 78	11, 18, 34, 75	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	540	ARG	4.7
1	A	748	ALA	4.3
1	A	541	GLY	4.0
1	B	540	ARG	3.8
1	A	680	ALA	3.6
1	B	748	ALA	3.5
1	A	679	ALA	3.4
1	A	454	ASP	3.1
1	B	610	ARG	2.7
1	A	610	ARG	2.5
1	B	35	ASN	2.5
1	B	454	ASP	2.4
1	B	679	ALA	2.4
1	B	541	GLY	2.3
1	B	608	LYS	2.3
1	A	542	GLY	2.1
1	A	608	LYS	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 monosaccharides in this entry.

6.4 Ligands [i](#)

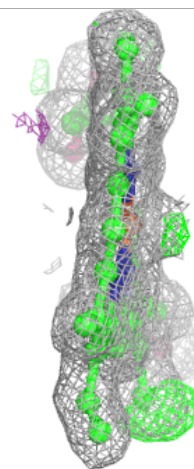
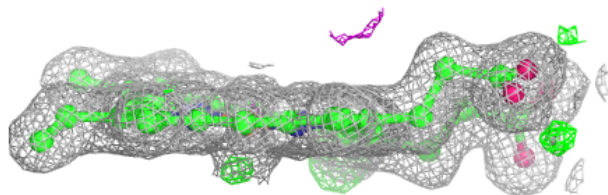
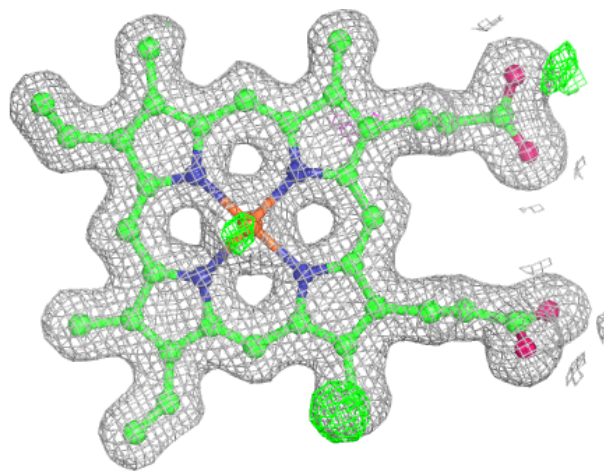
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

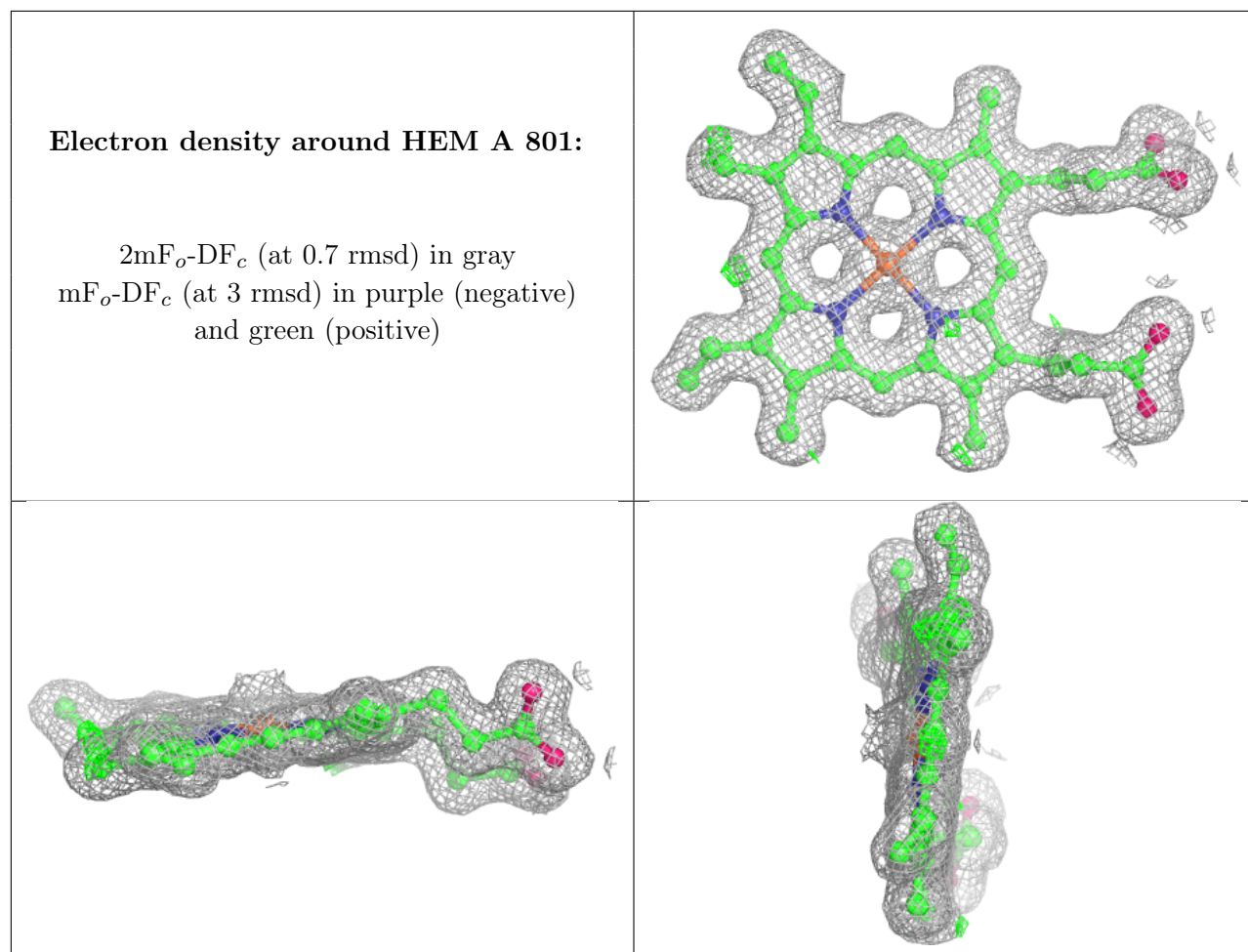
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	NIZ	B	809	10/10	0.83	0.19	23,34,39,40	0
7	MPD	B	808	8/8	0.88	0.10	34,37,40,46	0
7	MPD	B	807	8/8	0.92	0.11	42,49,57,58	0
7	MPD	A	807	8/8	0.93	0.13	49,57,76,77	0
6	PO4	B	806	5/5	0.94	0.21	36,50,55,64	0
7	MPD	A	808	8/8	0.95	0.13	34,44,52,56	0
6	PO4	A	806	5/5	0.95	0.17	34,46,52,54	0
5	OXY	B	805	2/2	0.96	0.12	21,21,21,26	2
5	OXY	A	805	2/2	0.98	0.09	19,19,19,24	2
4	CL	A	803	1/1	0.98	0.05	29,29,29,29	0
5	OXY	A	804	2/2	0.98	0.12	24,24,24,28	0
4	CL	B	803	1/1	0.99	0.05	26,26,26,26	0
2	HEM	B	801	43/43	0.99	0.08	11,12,14,15	0
2	HEM	A	801	43/43	0.99	0.07	10,12,15,16	0
5	OXY	B	804	2/2	0.99	0.10	21,21,21,26	0
3	NA	B	802	1/1	1.00	0.04	14,14,14,14	0
3	NA	A	802	1/1	1.00	0.05	14,14,14,14	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.