



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 12:29 PM UTC

PDB ID : 5KSG / pdb_00005ksg
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	:	4-5-2 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

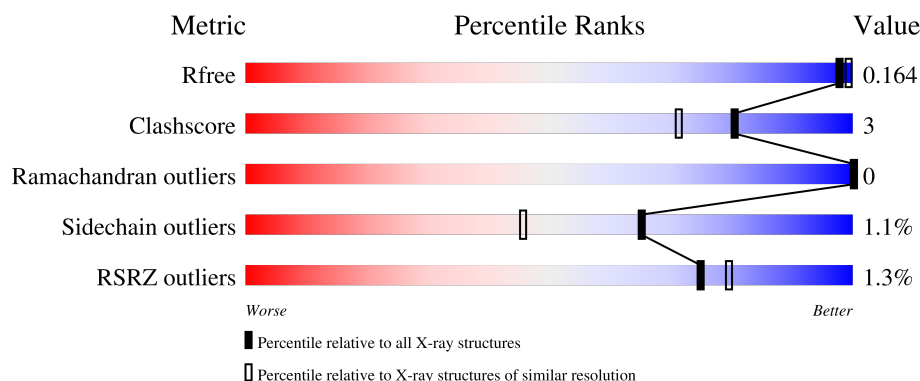
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.62 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}	180053	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (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	 80% 16% ..
1	B	728	 78% 18% ..

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
1	A	713	Total	C	N	O	S	0	9	0
			5570	3517	994	1045	14			
1	B	714	Total	C	N	O	S	0	10	0
			5590	3527	998	1051	14			

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 (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	A	1	Total	O		
			2	2	0	0

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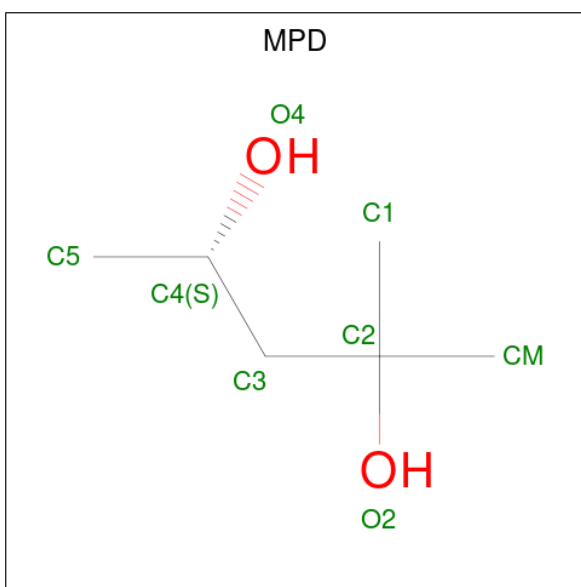
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	O	0	0
			2	2		
5	B	1	Total	O	0	0
			2	2		

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



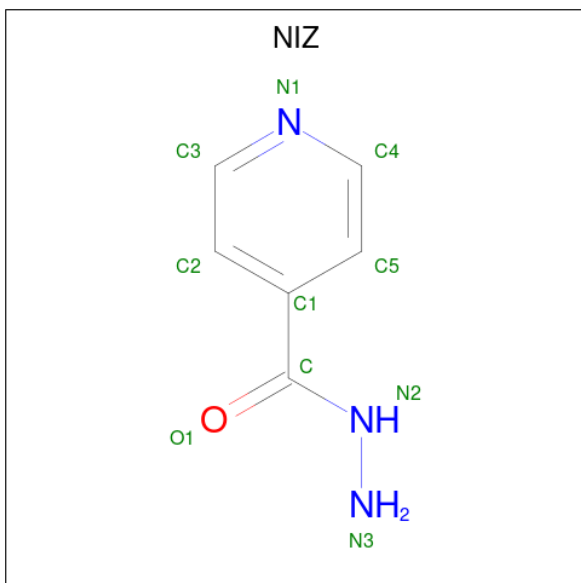
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		

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



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		

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.

Chain A:

Label	Color
L747	Green
A748	Yellow
A669	Green
V570	Green
T571	Yellow
Q583	Green
E584	Yellow
Q585	Yellow
T586	Green
D587	Green
V588	Green
E589	Green
S590	Green
M591	Orange
A592	Yellow
V593	Yellow
L594	Yellow
E595	Yellow
P596	Yellow
D599	Green
K608	Yellow
Y609	Green
R610	Orange
V611	Orange
E614	Yellow
K620	Yellow
A621	Green
Q622	Yellow
G636	Yellow
Q647	Green
S648	Green
R649	Yellow
R656	Yellow
E657	Yellow
Q658	Yellow
D663	Yellow
K676	Yellow
A679	Yellow
T692	Yellow
Q711	Orange
L712	Green
R713	Yellow
A716	Yellow
Q725	Yellow
E726	Yellow
P729	Orange
D376	Yellow
P377	Yellow
R382	Yellow
D414	Yellow
R418	Yellow
R426	Yellow
M427	Green
G429	Yellow
P430	Yellow
R431	Yellow
A432	Yellow
R433	Yellow
Y434	Orange
L435	Yellow
E438	Orange
A441	Yellow
E442	Green
V443	Yellow
D448	Yellow
P449	Yellow
D454	Green
L471	Yellow
T476	Yellow
V477	Yellow
L480	Yellow
G493	Yellow
S494	Yellow
R504	Yellow
D512	Yellow
E519	Yellow
Q520	Yellow
L525	Yellow
E529	Yellow
R532	Yellow
R540	Orange
Q544	Yellow
G567	Orange
H569	Orange
W139	Yellow
F140	Green
D141	Yellow
F153	Yellow
R161	Yellow
D193	Yellow
E198	Yellow
D199	Yellow
W202	Yellow
K206	Yellow
L207	Yellow
S212	Yellow
G213	Green
G214	Yellow
E218	Yellow
R219	Green
S220	Yellow
L225	Yellow
Y238	Yellow
N247	Yellow
R255	Yellow
M266	Yellow
N292	Yellow
S311	Yellow
A312	Green
Y313	Yellow
R314	Green
T315	Yellow
L326	Yellow
T333	Yellow
Q336	Yellow
E343	Yellow
N344	Green
L345	Yellow
Q361	Yellow
M362	Green
V363	Yellow
V370	Yellow
MET	Grey
SER	Grey
ASN	Grey
GLU	Grey
ALA	Grey
LYS	Grey
CYS	Grey
PRO	Grey
PHE	Grey
HIS	Grey
GLN	Grey
ALA	Grey
GLY	Grey
ASN	Grey
G36	Green
Q46	Orange
L47	Yellow
D48	Yellow
L49	Green
S50	Yellow
R54	Yellow
H55	Orange
S56	Yellow
S57	Yellow
M62	Yellow
G63	Yellow
K64	Yellow
D65	Green
F66	Yellow
N67	Yellow
Y68	Yellow
A69	Green
Q70	Orange
A71	Yellow
K74	Yellow
A79	Yellow
R82	Yellow
H85	Yellow
Q92	Yellow
G103	Yellow
W111	Yellow
T119	Orange
A120	Yellow
R123	Orange
G127	Yellow

Chain B:

Label	Value
RET	0.02
SER	0.00
ASN	0.00
GLU	0.00
P197	0.00
ALA	0.00
LYS	0.00
CYS	0.00
PRO	0.00
PHE	0.00
HIS	0.00
GLN	0.00
ALA	0.00
GLY	0.00
N35	0.00
G36	0.00
T37	0.00
W43	0.00
Q46	0.00
L47	0.00
D48	0.00
L49	0.00
R54	0.00
H55	0.00
S56	0.00
S57	0.00
L58	0.00
N62	0.00
G63	0.00
K64	0.00
D65	0.00
F66	0.00
N67	0.00
E73	0.00
K74	0.00
R82	0.00
L105	0.00
W111	0.00
T119	0.00
R123	0.00
G127	0.00
D141	0.00
A148	0.00
F153	0.00
E179	0.00
S179	0.00
E196	0.00
P197	0.00
E198	0.00
D199	0.00
S204	0.00
E205	0.00
K206	0.00
S220	0.00
R223	0.00
E226	0.00
Q233	0.00
Y238	0.00
V251	0.00
R255	0.00
R263	0.00
P289	0.00
V293	0.00
A299	0.00
S311	0.00
A312	0.00
T315	0.00
E327	0.00
W330	0.00
T333	0.00
E343	0.00
H344	0.00
L345	0.00
E351	0.00
L352	0.00
S355	0.00
P356	0.00
Q361	0.00
Y362	0.00
V363	0.00
A364	0.00
K365	0.00
D376	0.00
R382	0.00
P393	0.00
T394	0.00
R403	0.00
N408	0.00
F412	0.00
R418	0.00
R426	0.00
Q429	0.00
P430	0.00
R431	0.00
A432	0.00
R433	0.00
Y434	0.00
P437	0.00
V443	0.00
L444	0.00
L445	0.00
W446	0.00
Q447	0.00
D448	0.00
P449	0.00
L450	0.00
V453	0.00
D454	0.00
H455	0.00
P456	0.00
L457	0.00
A461	0.00
A468	0.00
L471	0.00
Q479	0.00
D512	0.00
Q517	0.00
P518	0.00
E519	0.00
I531	0.00
R532	0.00
T533	0.00
A534	0.00
F535	0.00
R540	0.00
G541	0.00
V545	0.00
C556	0.00
Q561	0.00
K564	0.00
H568	0.00
A569	0.00
V570	0.00
T571	0.00
V572	0.00
M591	0.00
A592	0.00
V593	0.00
L594	0.00
E595	0.00
P596	0.00
R602	0.00
L605	0.00
K606	0.00
G607	0.00
K608	0.00
P612	0.00
D619	0.00
Q622	0.00
S627	0.00
V633	0.00
Q647	0.00
S648	0.00
R649	0.00
T654	0.00
E657	0.00
D662	0.00
D663	0.00
A679	0.00
A680	0.00
D681	0.00
A682	0.00
E686	0.00
G687	0.00
E688	0.00



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 96.54 – 1.62	Depositor EDS
% Data completeness (in resolution range)	99.9 (96.54-1.62) 99.9 (96.54-1.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 1.62Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.135 , 0.159 (Not available) , 0.164	Depositor DCC
R_{free} test set	12876 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	17.4	Xtriage
Anisotropy	0.340	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.9	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	12995	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage'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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CL, HEM, OXY, MPD, PO4, NIZ

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	1.90	96/5726 (1.7%)	1.59	50/7781 (0.6%)
1	B	1.90	115/5743 (2.0%)	1.59	52/7804 (0.7%)
All	All	1.90	211/11469 (1.8%)	1.59	102/15585 (0.7%)

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 (211) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	532	ARG	CZ-NH1	-11.83	1.16	1.32
1	A	199	ASP	C-O	11.48	1.37	1.24
1	B	532	ARG	CD-NE	-11.05	1.30	1.46
1	B	63	GLY	N-CA	10.76	1.59	1.45
1	B	540	ARG	C-O	10.51	1.37	1.23
1	B	512	ASP	CG-OD2	9.44	1.43	1.25
1	A	63	GLY	N-CA	9.31	1.57	1.45
1	A	47	LEU	CB-CG	-9.18	1.35	1.53
1	B	602	ARG	CZ-NH2	-9.10	1.21	1.33
1	B	679	ALA	N-CA	9.05	1.57	1.46
1	B	443	VAL	CA-C	-8.90	1.41	1.52
1	B	47	LEU	CB-CG	-8.83	1.35	1.53
1	A	46	GLN	N-CA	8.68	1.56	1.45
1	B	46	GLN	C-O	8.65	1.34	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	540	ARG	C-O	8.64	1.34	1.23
1	B	220	SER	N-CA	8.60	1.56	1.45
1	A	448	ASP	C-O	8.51	1.27	1.23
1	B	453	VAL	C-O	-8.25	1.14	1.24
1	B	363	VAL	C-O	8.21	1.32	1.24
1	B	82	ARG	CZ-NH2	-7.87	1.23	1.33
1	B	376	ASP	N-CA	7.84	1.56	1.46
1	A	748	ALA	N-CA	7.77	1.61	1.46
1	A	449	PRO	C-O	-7.66	1.15	1.23
1	B	596	PRO	C-N	-7.64	1.24	1.33
1	B	199	ASP	C-O	7.61	1.32	1.23
1	B	606	LYS	N-CA	7.48	1.55	1.46
1	B	54	ARG	C-O	7.22	1.33	1.23
1	A	82	ARG	CZ-NH2	-7.17	1.24	1.33
1	B	408	ASN	CA-CB	-7.06	1.44	1.53
1	A	567	GLY	CA-C	-7.05	1.41	1.51
1	A	432	ALA	N-CA	-6.91	1.37	1.46
1	A	247	ASN	CG-ND2	-6.85	1.18	1.33
1	A	57	SER	CA-C	6.82	1.62	1.52
1	B	541	GLY	C-N	-6.82	1.23	1.33
1	B	49	LEU	CB-CG	-6.80	1.39	1.53
1	A	589	GLU	CD-OE2	6.79	1.38	1.25
1	A	532	ARG	CD-NE	-6.75	1.36	1.46
1	B	619	ASP	CG-OD1	-6.72	1.12	1.25
1	A	449	PRO	CA-C	6.68	1.61	1.52
1	B	179	SER	C-O	6.66	1.31	1.24
1	B	457	LEU	C-O	6.64	1.32	1.23
1	B	67	ASN	CA-C	6.63	1.60	1.52
1	B	726	GLU	CD-OE2	6.61	1.38	1.25
1	A	494	SER	CA-CB	-6.59	1.43	1.53
1	B	591	MET	SD-CE	-6.59	1.63	1.79
1	A	676	LYS	CA-C	-6.55	1.45	1.52
1	B	382	ARG	CA-C	6.55	1.61	1.53
1	A	431	ARG	CZ-NH1	6.54	1.42	1.32
1	A	692	THR	CA-C	-6.54	1.44	1.52
1	A	220	SER	N-CA	6.53	1.54	1.45
1	B	688	ARG	CA-C	-6.53	1.44	1.52
1	A	448	ASP	N-CA	6.52	1.51	1.46
1	A	636	GLY	C-N	-6.52	1.26	1.33
1	B	365	LYS	N-CA	6.51	1.54	1.46
1	B	343	GLU	C-O	6.50	1.31	1.24
1	B	461	ALA	CA-C	6.45	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	588	VAL	N-CA	-6.44	1.38	1.46
1	A	71	ALA	CA-C	-6.44	1.44	1.52
1	B	312	ALA	N-CA	6.44	1.54	1.46
1	B	692	THR	CA-C	-6.42	1.44	1.52
1	B	682	ALA	CA-C	6.42	1.61	1.52
1	A	428	MET	CG-SD	-6.41	1.64	1.80
1	A	679	ALA	N-CA	6.38	1.54	1.46
1	A	529	GLU	CA-C	6.38	1.61	1.52
1	A	46	GLN	CG-CD	6.35	1.68	1.52
1	A	448	ASP	CA-CB	6.34	1.57	1.52
1	A	207	ILE	N-CA	-6.33	1.38	1.46
1	B	437	PRO	CA-C	-6.29	1.44	1.52
1	A	218	ARG	N-CA	-6.29	1.37	1.46
1	A	370	VAL	CA-C	6.29	1.60	1.52
1	B	204	SER	CA-C	-6.26	1.44	1.52
1	A	586	THR	C-O	6.25	1.31	1.24
1	B	746	ASP	CA-C	-6.22	1.43	1.52
1	A	441	ALA	N-CA	6.17	1.54	1.46
1	B	430	PRO	CA-CB	-6.15	1.45	1.53
1	B	730	ARG	CZ-NH2	6.14	1.41	1.33
1	B	605	LEU	CB-CG	-6.10	1.41	1.53
1	A	512	ASP	CB-CG	6.10	1.67	1.52
1	B	531	ILE	CA-C	-6.07	1.45	1.52
1	B	719	TYR	CZ-OH	6.05	1.50	1.38
1	B	596	PRO	N-CA	6.04	1.53	1.47
1	B	251	VAL	CA-C	-6.04	1.45	1.52
1	A	544	GLN	CA-C	6.03	1.59	1.52
1	B	57	SER	CA-C	6.02	1.60	1.52
1	B	63	GLY	C-O	6.01	1.31	1.23
1	A	292	ASN	CA-C	6.00	1.61	1.52
1	B	568	HIS	CA-C	5.99	1.59	1.52
1	A	198	GLU	CD-OE1	5.96	1.36	1.25
1	B	726	GLU	CG-CD	5.93	1.66	1.52
1	B	315	THR	CA-C	5.92	1.60	1.52
1	A	382	ARG	CA-C	5.91	1.60	1.53
1	A	214	GLY	CA-C	-5.90	1.43	1.51
1	B	468	ALA	CA-C	-5.90	1.45	1.52
1	A	435	LEU	N-CA	-5.89	1.38	1.45
1	B	55	HIS	CA-CB	5.89	1.62	1.53
1	B	444	LEU	N-CA	-5.85	1.38	1.46
1	B	694	GLU	CA-C	5.84	1.60	1.52
1	A	376	ASP	N-CA	5.82	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	541	GLY	C-O	5.82	1.34	1.23
1	B	204	SER	CA-CB	5.79	1.63	1.53
1	A	326	LEU	CA-C	-5.79	1.45	1.52
1	B	327	GLU	CD-OE2	5.76	1.36	1.25
1	A	311	SER	CA-C	5.73	1.59	1.52
1	A	55	HIS	N-CA	-5.70	1.38	1.46
1	A	67	ASN	CG-OD1	-5.69	1.12	1.23
1	B	355	SER	CA-CB	5.69	1.60	1.53
1	A	74	LYS	CA-C	5.66	1.60	1.52
1	B	545	VAL	C-O	5.66	1.30	1.24
1	B	105	LEU	CA-C	5.65	1.60	1.52
1	A	56	SER	CA-C	-5.65	1.45	1.53
1	B	46	GLN	N-CA	5.64	1.52	1.45
1	B	572	VAL	CA-C	5.63	1.57	1.52
1	B	299	ALA	CA-C	-5.62	1.45	1.52
1	A	599	ASP	CA-C	-5.62	1.47	1.53
1	B	198	GLU	CD-OE1	5.61	1.36	1.25
1	A	85	HIS	C-O	5.59	1.30	1.24
1	A	614	GLU	CA-C	-5.58	1.45	1.52
1	B	352	LEU	CA-C	-5.58	1.45	1.52
1	A	225	LEU	CA-C	-5.57	1.45	1.52
1	A	611	VAL	CA-C	5.54	1.58	1.52
1	B	223	ARG	CG-CD	-5.53	1.35	1.52
1	B	461	ALA	C-O	-5.53	1.17	1.24
1	B	535	PHE	CA-C	-5.52	1.45	1.52
1	A	620	LYS	N-CA	5.51	1.53	1.46
1	B	681	ASP	CA-C	5.51	1.58	1.52
1	B	446	TRP	CZ2-CH2	-5.50	1.26	1.37
1	B	74	LYS	N-CA	-5.49	1.38	1.46
1	B	233	GLN	CA-C	5.49	1.59	1.52
1	B	556	CYS	C-O	5.49	1.30	1.24
1	A	525	LEU	CA-C	5.48	1.59	1.52
1	A	430	PRO	CA-CB	-5.47	1.46	1.53
1	B	531	ILE	C-O	5.45	1.30	1.24
1	B	412	PHE	N-CA	5.45	1.52	1.46
1	A	519	GLU	C-O	5.44	1.30	1.24
1	B	647	GLN	CG-CD	5.44	1.65	1.52
1	A	658	GLN	CD-OE1	-5.44	1.13	1.23
1	A	68	TYR	N-CA	5.44	1.53	1.46
1	B	692	THR	CA-CB	-5.43	1.45	1.53
1	A	153	PHE	C-O	-5.43	1.19	1.24
1	B	178	GLU	C-O	5.42	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	37	THR	C-O	5.42	1.30	1.24
1	B	517	GLN	N-CA	5.41	1.53	1.46
1	B	449	PRO	CA-C	5.41	1.59	1.52
1	A	193	ASP	C-O	5.41	1.30	1.23
1	A	519	GLU	N-CA	5.40	1.53	1.46
1	B	448	ASP	CA-CB	-5.40	1.49	1.52
1	A	313	TYR	C-N	5.39	1.41	1.33
1	A	74	LYS	N-CA	-5.39	1.38	1.46
1	B	429	GLY	C-N	-5.39	1.26	1.33
1	B	561	GLN	CA-C	5.37	1.59	1.52
1	B	743	ASP	C-O	5.36	1.30	1.24
1	A	56	SER	CB-OG	-5.36	1.31	1.42
1	A	414	ASP	CG-OD1	-5.35	1.15	1.25
1	B	627	SER	N-CA	5.34	1.52	1.45
1	A	120	ALA	CA-CB	-5.34	1.45	1.53
1	A	596	PRO	C-N	-5.32	1.26	1.33
1	B	418	ARG	N-CA	5.30	1.52	1.46
1	B	453	VAL	CA-C	5.30	1.59	1.52
1	B	450	ILE	CA-C	5.29	1.57	1.52
1	A	570	VAL	CA-CB	5.29	1.64	1.55
1	A	476	THR	CA-C	5.28	1.60	1.53
1	B	432	ALA	N-CA	-5.27	1.39	1.46
1	B	364	ALA	CA-CB	-5.27	1.45	1.53
1	A	363	VAL	C-O	5.25	1.29	1.24
1	A	716	ALA	C-O	5.25	1.30	1.24
1	B	64	LYS	CA-CB	5.25	1.61	1.53
1	A	591	MET	SD-CE	-5.24	1.66	1.79
1	A	434	TYR	CB-CG	-5.23	1.40	1.51
1	A	79	ALA	N-CA	-5.23	1.40	1.46
1	B	612	PRO	CA-C	5.22	1.59	1.52
1	A	92	GLN	CD-NE2	-5.22	1.22	1.33
1	B	333	THR	C-N	-5.21	1.29	1.34
1	A	139	TRP	CA-C	-5.21	1.47	1.53
1	A	570	VAL	CA-C	-5.19	1.46	1.52
1	A	571	THR	CA-C	5.19	1.59	1.52
1	B	196	GLU	CG-CD	5.19	1.65	1.52
1	A	480	LEU	CA-C	5.19	1.59	1.52
1	A	585	GLN	CD-OE1	5.18	1.33	1.23
1	B	689	ASP	CG-OD2	-5.17	1.15	1.25
1	B	455	HIS	CA-CB	-5.17	1.47	1.53
1	A	336	GLN	CD-NE2	5.17	1.44	1.33
1	B	293	VAL	CA-CB	-5.17	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	289	PRO	N-CA	-5.17	1.40	1.47
1	B	384	THR	CA-C	5.17	1.59	1.52
1	B	719	TYR	CD2-CE2	5.16	1.54	1.38
1	B	327	GLU	CD-OE1	5.16	1.35	1.25
1	A	377	PRO	C-O	-5.15	1.17	1.24
1	A	418	ARG	NE-CZ	5.15	1.38	1.33
1	B	606	LYS	CA-C	-5.14	1.46	1.52
1	B	657[A]	GLU	CA-C	5.13	1.59	1.52
1	B	657[B]	GLU	CA-C	5.13	1.59	1.52
1	B	697	TRP	CA-C	-5.11	1.46	1.52
1	B	431	ARG	CZ-NH2	-5.10	1.26	1.33
1	A	438	GLU	CG-CD	5.10	1.64	1.52
1	A	584	GLU	CG-CD	5.09	1.64	1.52
1	B	734	ALA	CA-C	5.07	1.59	1.52
1	B	564	LYS	N-CA	5.07	1.52	1.46
1	B	571	THR	N-CA	5.07	1.52	1.46
1	A	647	GLN	CA-CB	5.07	1.61	1.53
1	B	255[A]	ARG	CZ-NH1	-5.06	1.25	1.32
1	B	255[B]	ARG	CZ-NH1	-5.06	1.25	1.32
1	A	443	VAL	CA-C	-5.06	1.46	1.52
1	A	663	ASP	CA-C	5.05	1.59	1.52
1	A	70	GLN	CG-CD	5.04	1.64	1.52
1	B	43	TRP	CA-CB	5.03	1.60	1.53
1	A	656	ARG	CA-CB	-5.02	1.46	1.53
1	A	449	PRO	N-CA	-5.02	1.41	1.47
1	A	315	THR	C-O	-5.01	1.17	1.24
1	A	103	GLY	N-CA	5.01	1.52	1.45
1	B	479	GLN	C-O	-5.01	1.18	1.24
1	A	343	GLU	N-CA	5.00	1.52	1.46

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	GLN	CA-CB-CG	10.90	135.91	114.10
1	B	595	GLU	O-C-N	10.24	130.42	121.30
1	A	46	GLN	N-CA-C	-9.76	96.08	110.52
1	B	596	PRO	CB-CA-C	9.32	119.70	111.87
1	B	62	MET	CA-C-N	-8.99	108.24	121.01
1	B	62	MET	C-N-CA	-8.99	108.24	121.01
1	A	62	MET	CA-C-N	-8.67	109.78	121.06
1	A	62	MET	C-N-CA	-8.67	109.78	121.06
1	B	541	GLY	N-CA-C	-8.61	93.58	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	GLN	CA-CB-CG	8.54	131.17	114.10
1	B	595	GLU	CA-C-O	-8.42	111.84	119.75
1	A	592	ALA	N-CA-C	7.95	119.94	111.28
1	B	46	GLN	N-CA-C	-7.79	99.00	110.52
1	B	46	GLN	CB-CG-CD	-7.76	99.42	112.60
1	A	47	LEU	N-CA-CB	-7.59	98.75	110.29
1	A	596	PRO	CB-CA-C	7.54	118.26	111.40
1	B	47	LEU	N-CA-CB	-7.53	98.84	110.29
1	B	263	ARG	NE-CZ-NH2	-7.51	112.44	119.20
1	B	57	SER	N-CA-C	-7.42	104.10	113.01
1	A	127	GLY	N-CA-C	7.35	122.76	114.67
1	A	57	SER	N-CA-C	-7.18	104.40	113.01
1	B	54	ARG	N-CA-C	-7.04	101.05	110.55
1	A	432	ALA	CA-C-O	6.86	127.78	119.49
1	B	206	LYS	CG-CD-CE	6.79	126.92	111.30
1	B	46	GLN	CB-CA-C	6.77	121.68	109.83
1	A	55	HIS	CB-CA-C	6.65	121.70	111.39
1	B	596	PRO	O-C-N	-6.62	118.03	122.73
1	B	432	ALA	CA-C-O	6.60	127.47	119.49
1	A	449	PRO	O-C-N	6.53	131.09	123.06
1	B	726	GLU	CG-CD-OE2	6.53	133.41	118.40
1	B	345	LEU	O-C-N	6.51	129.02	122.12
1	A	429	GLY	O-C-N	6.40	128.17	121.77
1	A	568	HIS	CA-CB-CG	-6.29	107.51	113.80
1	B	592	ALA	N-CA-C	6.27	118.92	111.33
1	B	127	GLY	N-CA-C	6.23	121.53	114.67
1	B	690	ARG	NE-CZ-NH2	6.23	124.81	119.20
1	A	649	ARG	NE-CZ-NH2	-6.23	113.60	119.20
1	B	47	LEU	CA-C-O	-6.21	114.32	121.47
1	B	123	ARG	NE-CZ-NH2	-6.13	113.68	119.20
1	A	370	VAL	CA-C-N	-6.08	117.44	123.04
1	A	370	VAL	C-N-CA	-6.08	117.44	123.04
1	B	55	HIS	CB-CA-C	6.06	120.79	111.39
1	A	544	GLN	O-C-N	6.05	130.15	123.25
1	B	429	GLY	O-C-N	6.03	127.80	121.77
1	A	361	GLN	CA-C-O	-5.99	114.90	121.31
1	A	345	LEU	O-C-N	5.92	128.40	122.12
1	B	382	ARG	O-C-N	5.89	128.01	121.53
1	A	584	GLU	CB-CG-CD	5.85	122.54	112.60
1	B	570	VAL	CA-C-O	5.83	126.54	120.36
1	A	66	PHE	CA-C-O	5.76	127.62	121.16
1	B	654	THR	O-C-N	5.71	129.78	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	351	GLU	CB-CG-CD	-5.70	102.91	112.60
1	B	432	ALA	N-CA-C	5.69	119.33	112.38
1	A	70	GLN	CA-CB-CG	5.69	125.48	114.10
1	A	46	GLN	CA-C-O	5.69	128.43	121.72
1	A	692	THR	N-CA-C	5.69	120.49	113.50
1	B	361	GLN	CA-C-O	-5.67	115.35	121.36
1	A	595	GLU	O-C-N	5.67	126.34	121.30
1	B	532	ARG	CG-CD-NE	-5.63	99.61	112.00
1	B	663	ASP	O-C-N	-5.60	116.18	122.12
1	A	382	ARG	O-C-N	5.58	127.67	121.53
1	B	153	PHE	CA-C-N	-5.49	112.95	119.05
1	B	153	PHE	C-N-CA	-5.49	112.95	119.05
1	A	493	GLY	O-C-N	5.47	130.39	122.68
1	A	520	GLN	CA-C-O	5.44	126.32	120.55
1	B	311	SER	O-C-N	5.44	129.71	123.29
1	B	123	ARG	NE-CZ-NH1	5.39	126.89	121.50
1	A	48	ASP	N-CA-C	5.38	118.22	107.62
1	A	50	SER	N-CA-C	-5.38	105.81	112.38
1	A	711	GLN	OE1-CD-NE2	5.37	127.97	122.60
1	A	311	SER	O-C-N	5.37	129.62	123.29
1	A	202	TRP	CA-C-O	5.35	125.61	119.35
1	A	333	THR	O-C-N	5.33	125.55	121.23
1	A	713	ARG	NE-CZ-NH2	-5.33	114.40	119.20
1	A	50	SER	CA-CB-OG	-5.31	100.48	111.10
1	B	356	PRO	O-C-N	-5.30	115.14	122.24
1	A	206	LYS	CG-CD-CE	5.29	123.47	111.30
1	A	123	ARG	NE-CZ-NH1	5.28	126.78	121.50
1	B	58	LEU	CA-C-O	-5.27	115.28	120.82
1	A	571	THR	OG1-CB-CG2	-5.26	98.79	109.30
1	B	434	TYR	CA-CB-CG	5.24	123.33	113.90
1	A	432	ALA	O-C-N	-5.23	115.59	122.39
1	A	47	LEU	N-CA-C	-5.20	102.78	110.48
1	A	477	VAL	N-CA-C	-5.16	104.94	110.36
1	B	512	ASP	CA-CB-CG	5.16	117.76	112.60
1	B	692	THR	N-CA-C	5.15	119.83	113.50
1	A	529	GLU	N-CA-C	-5.14	105.86	111.82
1	B	686	GLU	OE1-CD-OE2	5.13	135.21	122.90
1	A	433	ARG	NE-CZ-NH2	-5.09	114.61	119.20
1	B	686	GLU	CG-CD-OE2	-5.09	106.69	118.40
1	B	148	ALA	CA-C-O	5.09	126.16	120.82
1	A	438	GLU	CG-CD-OE1	-5.08	106.71	118.40
1	A	212	SER	O-C-N	5.07	128.69	122.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	GLU	N-CA-CB	5.07	117.45	109.69
1	A	583	GLN	O-C-N	5.06	127.49	122.12
1	B	330	TRP	CA-C-O	-5.06	114.62	120.24
1	B	445	LEU	O-C-N	-5.06	116.75	122.12
1	B	533	THR	CA-C-O	-5.06	115.51	120.82
1	B	197	PRO	CA-C-O	-5.03	115.61	121.34
1	B	710	SER	N-CA-C	5.03	117.66	111.82
1	A	713	ARG	NE-CZ-NH1	5.02	126.52	121.50
1	A	46	GLN	O-C-N	-5.00	117.34	122.94

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	30	0
1	B	5590	0	5405	24	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	12	3
All	All	12995	0	10923	57	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 3.

All (57) 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
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:657[A]:GLU:CD	9:B:922:HOH:O	2.34	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:A:725[A]:GLN:NE2	1:A:726[A]:GLU:CD	2.52	0.67
1:A:725[A]:GLN:CD	1:A:726[A]:GLU:HG3	2.19	0.64
1:B:540:ARG:NE	1:B:540:ARG:HA	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:807:MPD:O4	7:A:807:MPD:HM2	1.96	0.63
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: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:725[B]:GLN:CD	9:A:909:HOH:O	2.57	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: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:A:111:TRP:HZ3	1:A:238:TYR:HH	1.60	0.44
1:B:426[B]:ARG:HA	1:B:426[B]:ARG:HD2	1.86	0.44
1:A:725[A]:GLN:HE21	1:A:726[A]:GLU:CD	2.25	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:B:591:MET:HB2	1:B:591:MET:HE2	1.78	0.42
1:A:266:MET:HE2	1:A:426[A]:ARG:HH11	1.84	0.41
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
1:B:649:ARG:HH22	1:B:657[B]:GLU:CD	2.28	0.40

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	552 (99%)	7 (1%)	61	39
1	B	561/561 (100%)	555 (99%)	6 (1%)	65	46
All	All	1120/1122 (100%)	1107 (99%)	13 (1%)	65	43

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	GLN

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Mol	Chain	Res	Type
1	A	64	LYS
1	A	141	ASP
1	A	161[A]	ARG
1	A	161[B]	ARG
1	A	608	LYS
1	A	610	ARG
1	B	46	GLN
1	B	64	LYS
1	B	74	LYS
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 (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	737	ASN
1	B	406	HIS
1	B	647	GLN
1	B	725	GLN
1	B	737	ASN

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 oligosaccharides 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	$\# Z > 2$
8	NIZ	B	809	-	10,10,10	5.48	6 (60%)	12,12,12	3.63	8 (66%)
5	OXY	B	804	-	1,1,1	0.20	0	-		
7	MPD	A	807	-	7,7,7	0.46	0	9,10,10	1.20	1 (11%)
7	MPD	A	808	-	7,7,7	0.78	0	9,10,10	1.05	0
6	PO4	B	806	-	4,4,4	2.58	2 (50%)	6,6,6	3.26	4 (66%)
5	OXY	A	804	-	1,1,1	0.28	0	-		
5	OXY	B	805	-	1,1,1	0.10	0	-		
6	PO4	A	806	-	4,4,4	2.25	1 (25%)	6,6,6	3.19	2 (33%)
2	HEM	B	801	1,9	50,50,50	1.43	10 (20%)	67,82,82	1.34	8 (11%)
2	HEM	A	801	1,9	50,50,50	1.57	9 (18%)	67,82,82	1.72	16 (23%)
7	MPD	B	807	-	7,7,7	0.38	0	9,10,10	1.31	2 (22%)
7	MPD	B	808	-	7,7,7	1.13	0	9,10,10	1.72	3 (33%)
5	OXY	A	805	-	1,1,1	0.17	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
8	NIZ	B	809	-	-	0/6/6/6	0/1/1/1
7	MPD	A	807	-	-	3/5/5/5	-
7	MPD	A	808	-	-	1/5/5/5	-
2	HEM	B	801	1,9	-	3/14/54/54	-
2	HEM	A	801	1,9	-	3/14/54/54	-
7	MPD	B	807	-	-	3/5/5/5	-
7	MPD	B	808	-	-	1/5/5/5	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	809	NIZ	C4-N1	11.27	1.65	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	809	NIZ	C5-C1	8.91	1.52	1.39
8	B	809	NIZ	N3-N2	-6.32	1.32	1.41
8	B	809	NIZ	C-N2	5.23	1.39	1.33
6	A	806	PO4	P-O4	-3.79	1.43	1.54
2	A	801	HEM	C4A-NA	-3.58	1.32	1.39
2	B	801	HEM	FE-NB	3.57	2.05	1.94
6	B	806	PO4	P-O1	3.50	1.58	1.50
8	B	809	NIZ	C5-C4	-3.37	1.32	1.38
8	B	809	NIZ	C2-C1	3.20	1.44	1.39
2	A	801	HEM	FE-NB	3.19	2.04	1.94
2	B	801	HEM	CHB-C1B	3.16	1.44	1.38
2	A	801	HEM	O1A-CGA	3.06	1.32	1.22
2	A	801	HEM	FE-NC	2.99	2.05	1.95
6	B	806	PO4	P-O3	-2.98	1.46	1.54
2	A	801	HEM	C3B-C2B	2.87	1.43	1.37
2	A	801	HEM	C3C-C4C	-2.86	1.41	1.46
2	A	801	HEM	FE-NA	2.76	2.04	1.95
2	B	801	HEM	CBA-CGA	2.53	1.56	1.50
2	B	801	HEM	FE-ND	2.51	2.02	1.94
2	A	801	HEM	FE-ND	2.49	2.02	1.94
2	B	801	HEM	C3C-C4C	-2.44	1.41	1.46
2	B	801	HEM	FE-NC	2.24	2.02	1.95
2	B	801	HEM	CHA-C4D	2.20	1.42	1.38
2	A	801	HEM	CMD-C2D	-2.16	1.46	1.50
2	B	801	HEM	C1B-C2B	-2.05	1.40	1.44
2	B	801	HEM	CMB-C2B	2.02	1.54	1.50
2	B	801	HEM	C4A-C3A	2.01	1.47	1.43

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	809	NIZ	C1-C-N2	7.78	124.96	116.33
8	B	809	NIZ	C5-C4-N1	-6.16	113.09	123.60
6	A	806	PO4	O3-P-O1	-5.84	90.30	110.95
2	A	801	HEM	C4C-C3C-C2C	5.19	111.32	106.81
6	B	806	PO4	O4-P-O3	5.16	123.98	107.91
6	A	806	PO4	O4-P-O1	4.91	128.32	110.95
2	B	801	HEM	C3B-C4B-NB	-4.78	106.03	109.47
2	A	801	HEM	C4B-C3B-C2B	-4.14	103.48	107.28
2	A	801	HEM	C1D-C2D-C3D	-4.11	102.66	106.98
8	B	809	NIZ	C5-C1-C2	3.98	123.63	118.57
6	B	806	PO4	O4-P-O1	-3.92	97.10	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	806	PO4	O3-P-O2	-3.62	96.66	107.91
8	B	809	NIZ	C3-C2-C1	-3.48	115.24	119.05
2	A	801	HEM	C2D-C1D-ND	3.47	113.91	109.90
2	A	801	HEM	C3C-C2C-C1C	-3.43	103.80	107.05
8	B	809	NIZ	O1-C-C1	-3.33	114.29	120.90
2	A	801	HEM	O1A-CGA-CBA	-2.94	113.75	123.09
7	B	808	MPD	O2-C2-CM	2.78	116.65	107.99
2	A	801	HEM	C3B-C2B-C1B	2.60	108.36	106.41
8	B	809	NIZ	C4-C5-C1	2.55	121.84	119.05
2	A	801	HEM	O2A-CGA-CBA	2.54	122.03	114.00
2	A	801	HEM	C1B-NB-C4B	2.52	108.19	105.21
2	B	801	HEM	CMB-C2B-C1B	-2.50	121.13	125.03
8	B	809	NIZ	O1-C-N2	-2.49	119.47	122.46
2	A	801	HEM	O1D-CGD-CBD	-2.46	115.29	123.09
6	B	806	PO4	O4-P-O2	2.45	115.52	107.91
2	A	801	HEM	CMD-C2D-C1D	2.41	128.79	125.03
2	B	801	HEM	CBA-CAA-C2A	2.39	119.13	112.53
2	A	801	HEM	C3B-C4B-NB	2.38	111.18	109.47
7	A	807	MPD	CM-C2-C1	2.36	115.92	110.63
2	A	801	HEM	CHD-C4C-C3C	2.35	129.18	125.21
2	B	801	HEM	CHC-C4B-NB	2.34	126.95	124.42
8	B	809	NIZ	C4-N1-C3	2.28	122.07	116.86
2	A	801	HEM	CAA-CBA-CGA	-2.27	107.64	113.67
7	B	808	MPD	O2-C2-C1	-2.25	100.96	107.99
7	B	808	MPD	C1-C2-C3	-2.23	100.57	110.20
7	B	807	MPD	C1-C2-C3	2.20	119.68	110.20
2	A	801	HEM	CHA-C4D-ND	-2.19	121.66	124.37
2	B	801	HEM	C1D-C2D-C3D	-2.19	104.68	106.98
2	B	801	HEM	CAA-CBA-CGA	-2.18	107.89	113.67
2	A	801	HEM	C4D-ND-C1D	-2.15	102.66	105.21
2	B	801	HEM	CBD-CAD-C3D	2.10	118.34	112.53
2	B	801	HEM	O1A-CGA-CBA	-2.04	116.63	123.09
7	B	807	MPD	CM-C2-C1	-2.01	106.13	110.63

There are no chirality outliers.

All (14) 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

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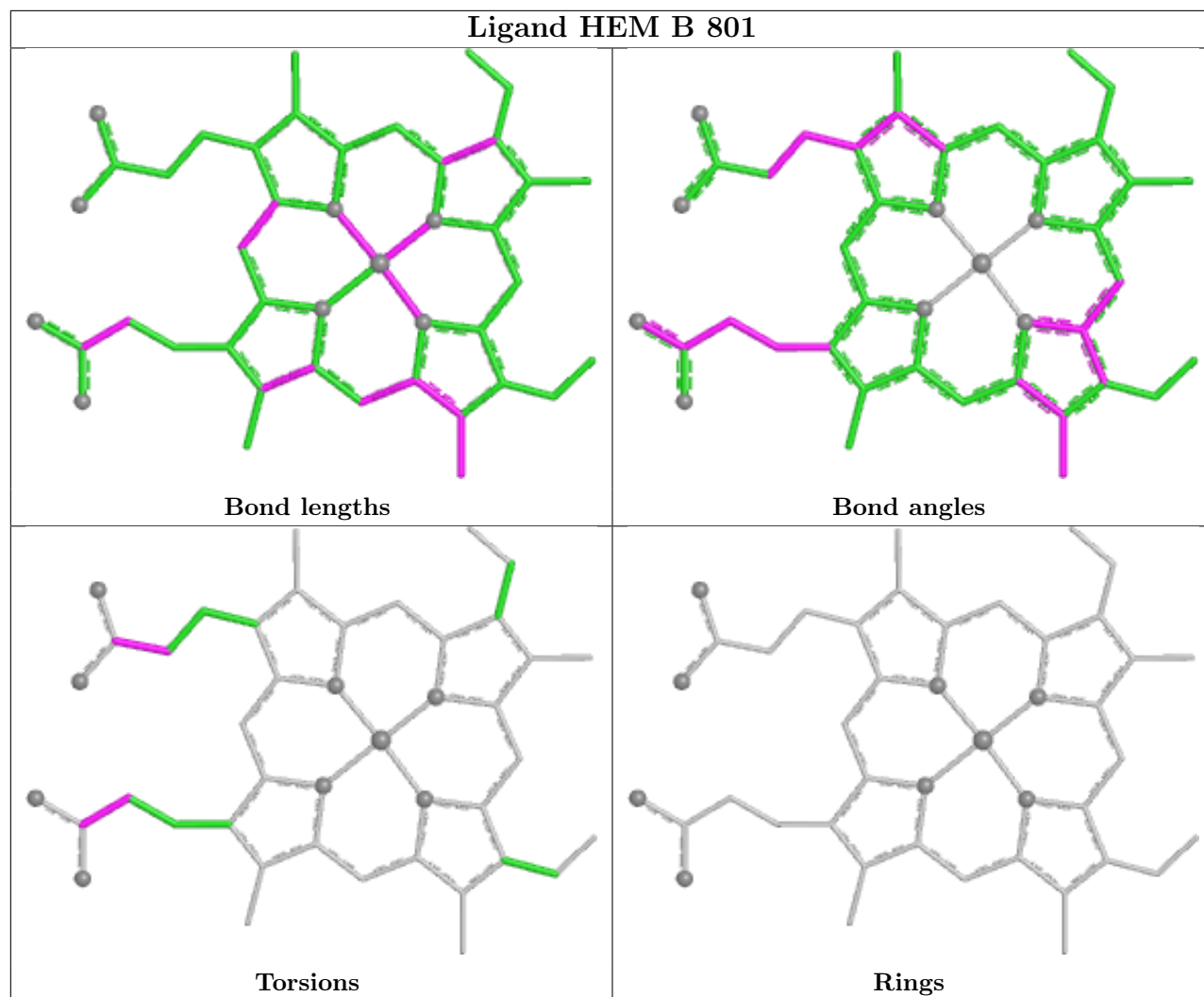
Mol	Chain	Res	Type	Atoms
7	A	808	MPD	O2-C2-C3-C4
2	A	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O1A
7	A	807	MPD	C2-C3-C4-O4
7	A	807	MPD	C1-C2-C3-C4
7	B	807	MPD	CM-C2-C3-C4
2	A	801	HEM	CAD-CBD-CGD-O2D
2	B	801	HEM	CAD-CBD-CGD-O2D

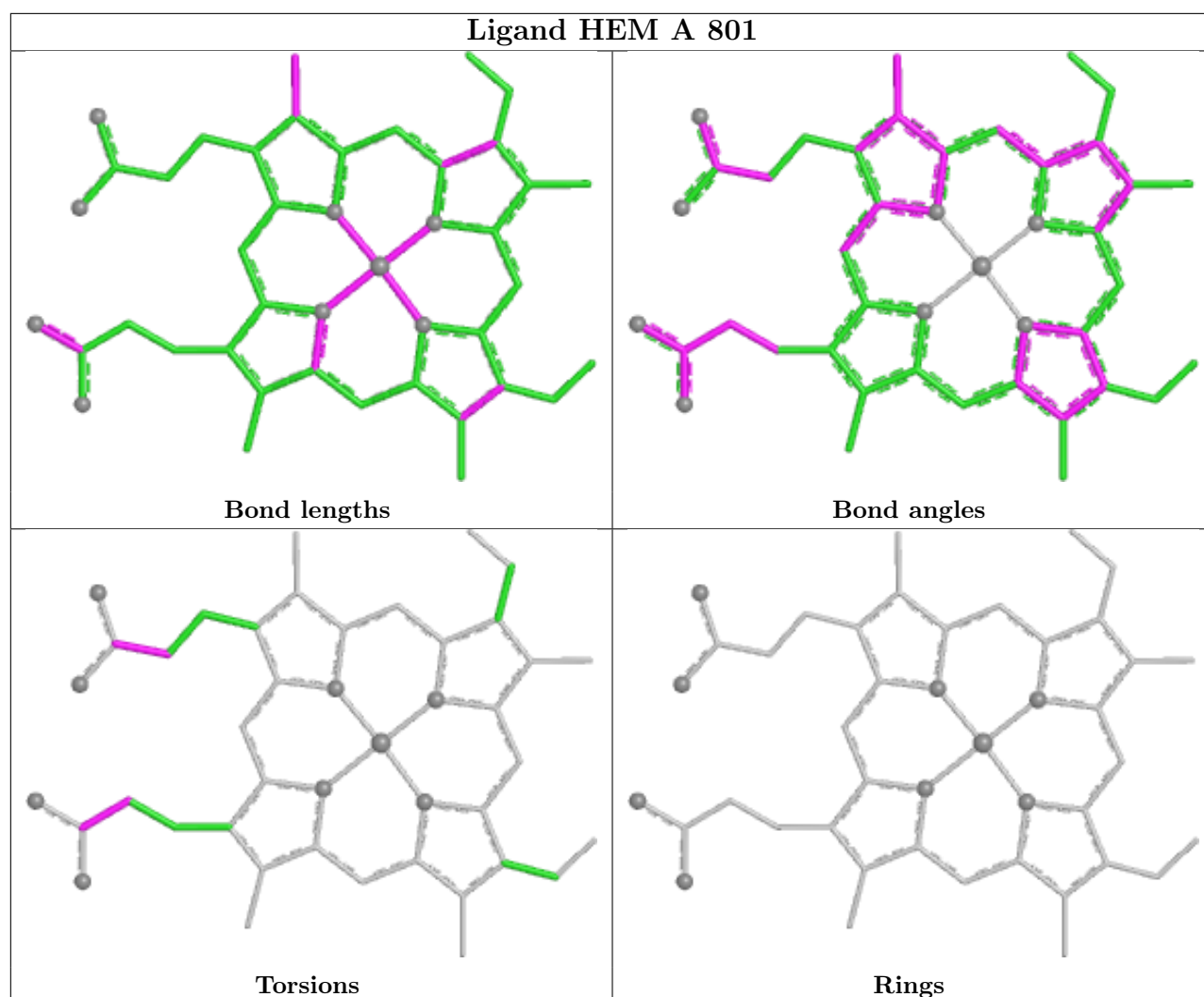
There are no ring outliers.

2 monomers are involved in 6 short contacts:

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

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	713/728 (97%)	-0.43	6 (0%) 82 86	7, 18, 34, 75	9 (1%)
1	B	714/728 (98%)	-0.46	12 (1%) 69 73	7, 17, 34, 67	10 (1%)
All	All	1427/1456 (98%)	-0.44	18 (1%) 75 79	7, 17, 34, 75	19 (1%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	5.4
1	B	748	ALA	4.8
1	B	657[A]	GLU	4.7
1	B	64	LYS	4.0
1	B	541	GLY	2.9
1	B	35	ASN	2.8
1	B	65	ASP	2.8
1	B	46	GLN	2.7
1	B	55	HIS	2.6
1	A	540	ARG	2.5
1	A	610	ARG	2.4
1	A	454	ASP	2.3
1	B	73	GLU	2.2
1	B	540	ARG	2.2
1	B	680	ALA	2.2
1	A	55	HIS	2.1
1	A	119[A]	THR	2.1
1	B	608	LYS	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 ⓘ

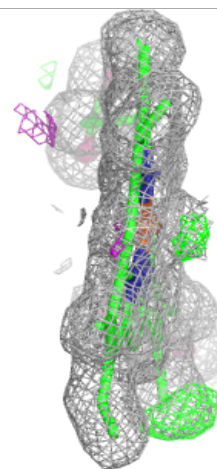
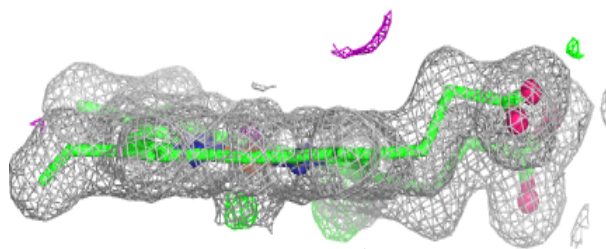
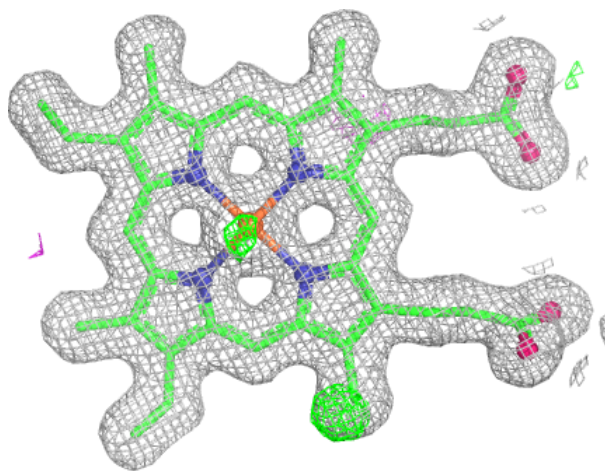
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

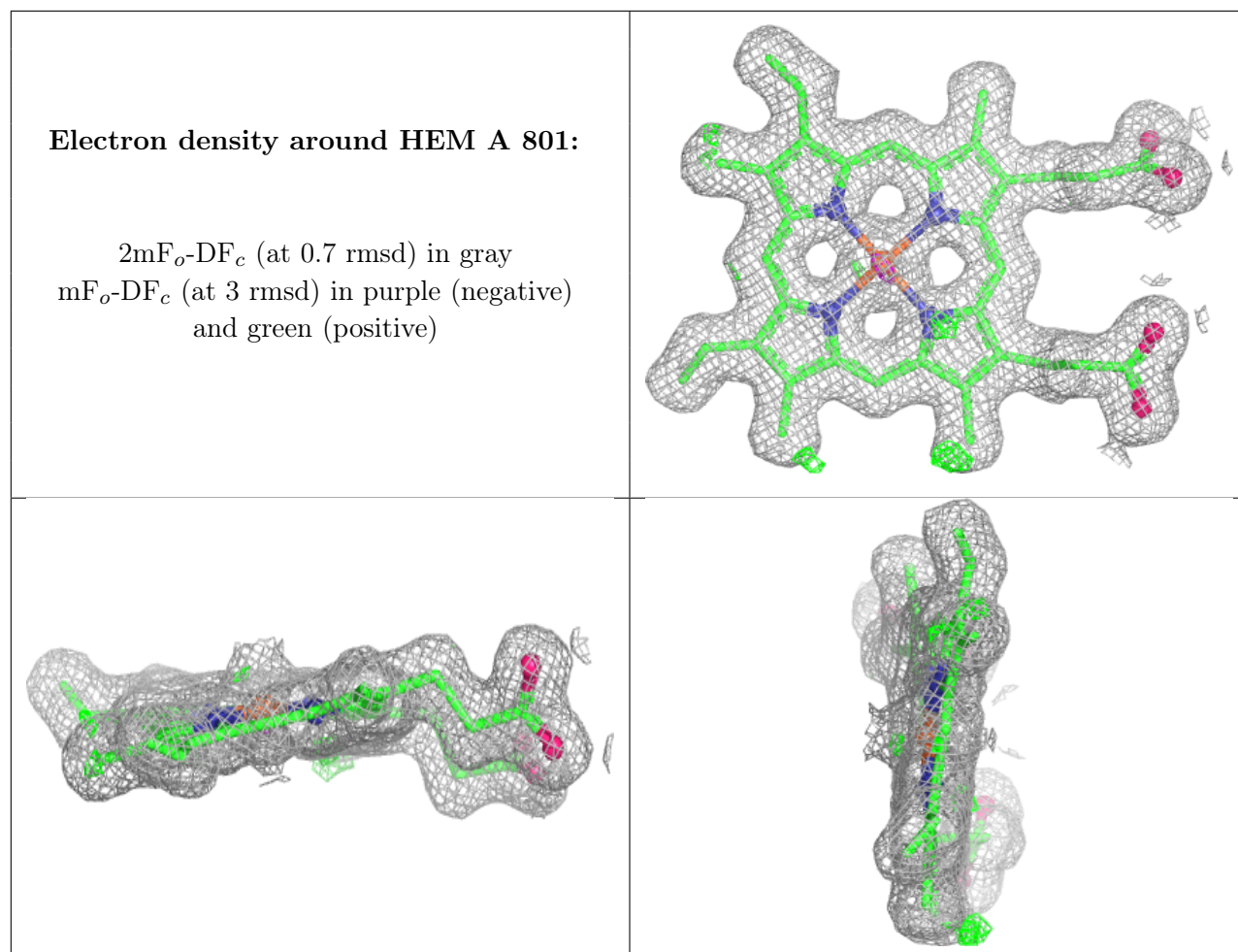
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	NIZ	B	809	10/10	0.85	0.14	23,34,39,40	0
7	MPD	B	807	8/8	0.89	0.18	42,49,57,58	0
7	MPD	A	807	8/8	0.89	0.21	49,57,76,77	0
7	MPD	B	808	8/8	0.90	0.13	34,37,40,46	0
7	MPD	A	808	8/8	0.92	0.12	34,44,52,56	0
6	PO4	B	806	5/5	0.92	0.10	36,50,55,64	0
6	PO4	A	806	5/5	0.93	0.09	34,46,52,54	0
5	OXY	A	805	2/2	0.96	0.10	19,19,19,24	2
5	OXY	B	805	2/2	0.97	0.08	21,21,21,26	2
5	OXY	A	804	2/2	0.97	0.18	24,24,24,28	0
4	CL	A	803	1/1	0.97	0.09	29,29,29,29	0
5	OXY	B	804	2/2	0.97	0.20	21,21,21,26	0
4	CL	B	803	1/1	0.98	0.08	26,26,26,26	0
2	HEM	B	801	43/43	0.99	0.04	11,12,14,15	0
3	NA	A	802	1/1	0.99	0.04	14,14,14,14	0
2	HEM	A	801	43/43	0.99	0.04	10,12,15,16	0
3	NA	B	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.