



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2024 – 01:26 AM EST

PDB ID : 5KQ6
Title : Crystal structure of the A359D variant of catalase-peroxidase from *B. pseudo-mallei*
Authors : Loewen, P.C.
Deposited on : 2016-07-05
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 : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 1.21
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.004 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

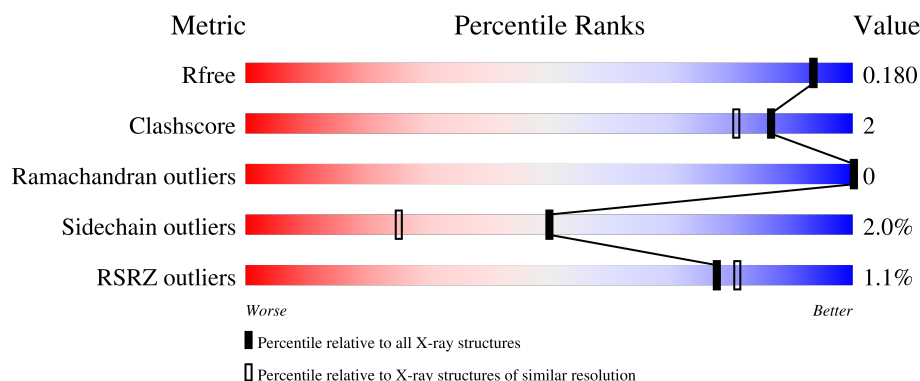
1 Overall quality at a glance

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}	164625	6077 (1.64-1.60)
Clashscore	180529	6617 (1.64-1.60)
Ramachandran outliers	177936	6498 (1.64-1.60)
Sidechain outliers	177891	6497 (1.64-1.60)
RSRZ outliers	164620	6075 (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	
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
6	PO4	B	805	-	X	-	-

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12835 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.

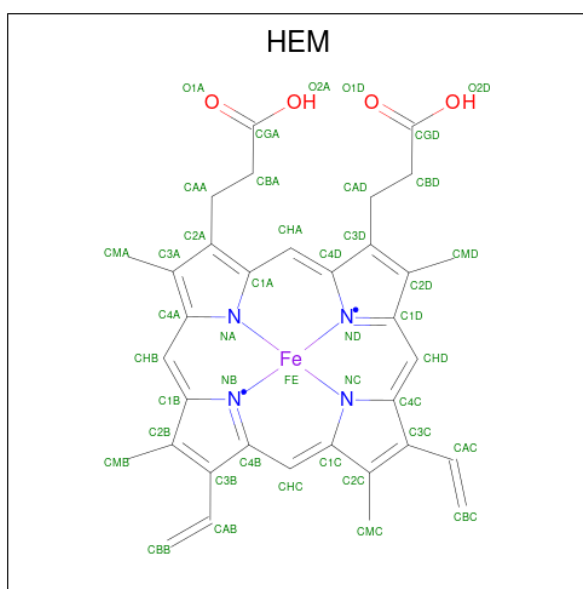
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	8	0
			5568	3512	992	1050	14			
1	B	713	Total	C	N	O	S	0	7	0
			5552	3504	986	1048	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	359	ASP	ALA	engineered mutation	UNP Q3JNW6
B	359	ASP	ALA	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
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

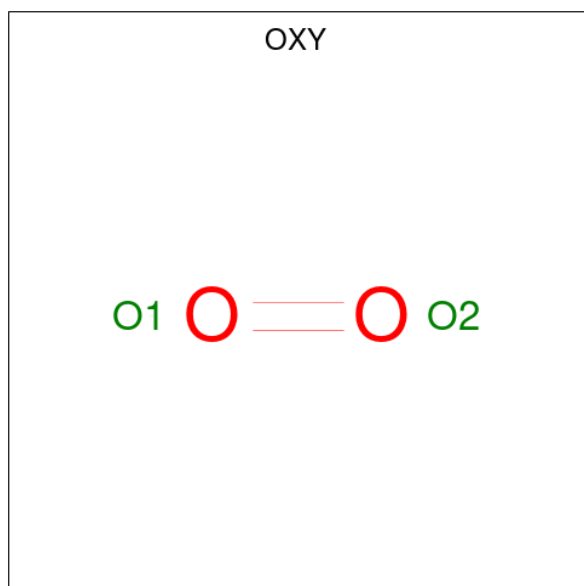
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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 (three-letter code: CL) (formula: Cl).

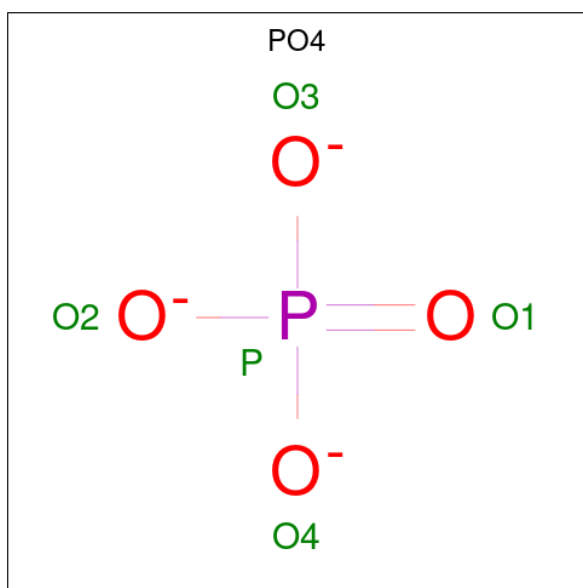
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl		
			1	1	0	0
4	B	1	Total	Cl		
			1	1	0	0

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



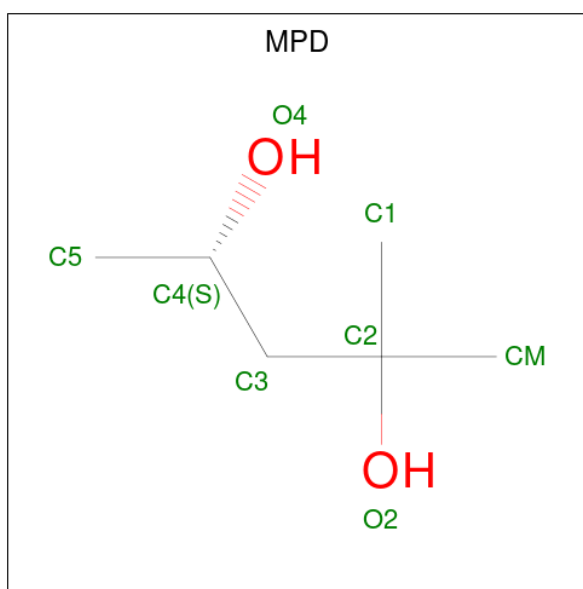
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O		
			2	2	0	0
5	B	1	Total	O		
			2	2	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: 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 (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



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

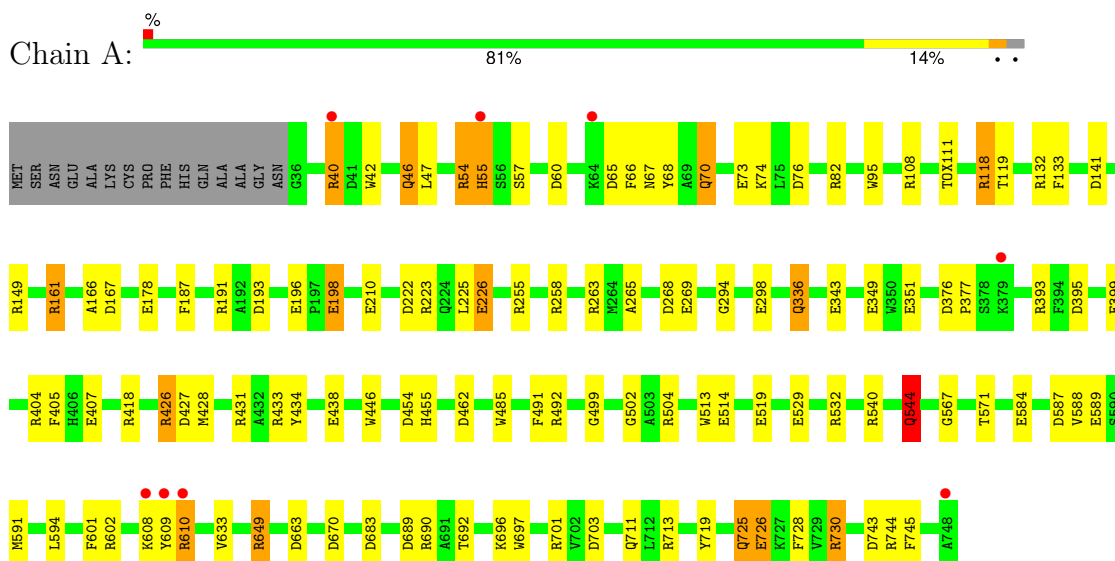
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	794	Total O 794 794	0	0
8	B	785	Total O 785 785	0	0

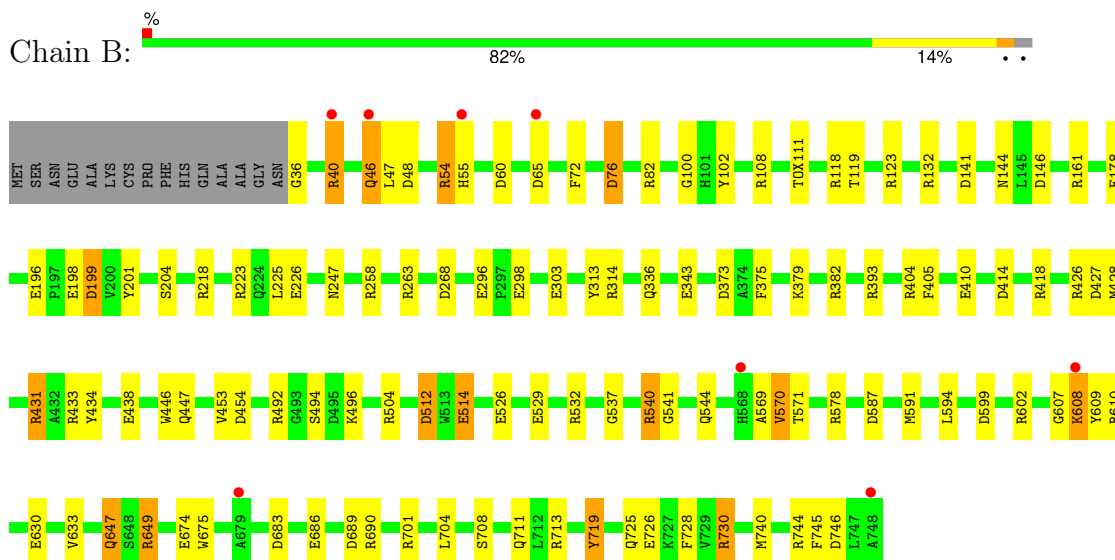
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Catalase-peroxidase



• Molecule 1: Catalase-peroxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.58Å 115.79Å 174.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.80 – 1.62 47.80 – 1.62	Depositor EDS
% Data completeness (in resolution range)	97.5 (47.80-1.62) 97.5 (47.80-1.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 1.62Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.144 , 0.170 0.158 , 0.180	Depositor DCC
R_{free} test set	12728 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.5	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	12835	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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, CL, PO4, MPD, OXY, TOX, NA

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	1.68	79/5696 (1.4%)	1.53	91/7740 (1.2%)
1	B	1.64	61/5683 (1.1%)	1.50	80/7724 (1.0%)
All	All	1.66	140/11379 (1.2%)	1.52	171/15464 (1.1%)

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	2

All (140) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	407	GLU	CD-OE1	12.16	1.39	1.25
1	A	544	GLN	CD-OE1	12.02	1.50	1.24
1	B	196	GLU	CB-CG	-10.34	1.32	1.52
1	A	434	TYR	CB-CG	-10.26	1.36	1.51
1	A	343	GLU	CD-OE1	9.91	1.36	1.25
1	B	438	GLU	CD-OE2	9.87	1.36	1.25
1	A	407	GLU	CG-CD	9.69	1.66	1.51
1	A	196	GLU	CB-CG	-9.53	1.34	1.52
1	B	410	GLU	CG-CD	9.51	1.66	1.51
1	B	512	ASP	CG-OD2	8.62	1.45	1.25
1	B	161[A]	ARG	CZ-NH1	8.47	1.44	1.33
1	B	161[B]	ARG	CZ-NH1	8.47	1.44	1.33
1	B	726	GLU	CD-OE2	8.24	1.34	1.25
1	B	532	ARG	CZ-NH1	-8.21	1.22	1.33
1	A	434	TYR	CE1-CZ	-8.16	1.27	1.38
1	A	198	GLU	CD-OE1	8.03	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	46	GLN	CG-CD	7.99	1.69	1.51
1	A	73	GLU	CG-CD	7.85	1.63	1.51
1	A	725	GLN	CG-CD	7.82	1.69	1.51
1	A	349	GLU	CD-OE2	-7.79	1.17	1.25
1	B	410	GLU	CD-OE2	7.57	1.33	1.25
1	B	100	GLY	N-CA	-7.46	1.34	1.46
1	A	454	ASP	CB-CG	7.43	1.67	1.51
1	B	512	ASP	CB-CG	7.42	1.67	1.51
1	B	418	ARG	CZ-NH2	-7.37	1.23	1.33
1	B	446	TRP	CD2-CE2	7.37	1.50	1.41
1	A	210	GLU	CD-OE1	-7.29	1.17	1.25
1	B	725	GLN	CD-NE2	7.22	1.50	1.32
1	B	532	ARG	CD-NE	-7.22	1.34	1.46
1	B	226	GLU	CG-CD	7.21	1.62	1.51
1	A	589[A]	GLU	CD-OE2	7.14	1.33	1.25
1	A	589[B]	GLU	CD-OE2	7.14	1.33	1.25
1	A	589[A]	GLU	CD-OE1	7.08	1.33	1.25
1	A	589[B]	GLU	CD-OE1	7.08	1.33	1.25
1	B	82	ARG	CZ-NH2	-7.03	1.24	1.33
1	A	434	TYR	CD1-CE1	7.03	1.49	1.39
1	A	711	GLN	CD-NE2	-6.99	1.15	1.32
1	B	226	GLU	CB-CG	-6.93	1.39	1.52
1	B	196	GLU	CG-CD	6.93	1.62	1.51
1	B	541	GLY	C-O	6.92	1.34	1.23
1	A	584	GLU	CG-CD	6.90	1.62	1.51
1	B	426	ARG	CZ-NH2	6.84	1.42	1.33
1	B	540	ARG	C-O	6.82	1.36	1.23
1	A	46	GLN	CG-CD	6.80	1.66	1.51
1	B	343	GLU	CD-OE2	6.71	1.33	1.25
1	B	102	TYR	CG-CD1	-6.63	1.30	1.39
1	B	675	TRP	CZ3-CH2	-6.59	1.29	1.40
1	A	692	THR	CB-CG2	-6.58	1.30	1.52
1	B	544	GLN	CD-NE2	6.56	1.49	1.32
1	B	434	TYR	CE2-CZ	-6.46	1.30	1.38
1	A	82	ARG	CZ-NH2	-6.45	1.24	1.33
1	B	726	GLU	CG-CD	6.44	1.61	1.51
1	B	453	VAL	C-O	-6.39	1.11	1.23
1	A	728	PHE	CG-CD2	-6.28	1.29	1.38
1	B	496	LYS	CE-NZ	-6.21	1.33	1.49
1	B	686	GLU	CD-OE2	-6.05	1.19	1.25
1	A	584	GLU	CD-OE2	6.04	1.32	1.25
1	B	178	GLU	CG-CD	6.04	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	584	GLU	CD-OE1	5.99	1.32	1.25
1	A	67	ASN	CG-ND2	-5.99	1.17	1.32
1	A	426[A]	ARG	CZ-NH2	5.98	1.40	1.33
1	A	426[B]	ARG	CZ-NH2	5.98	1.40	1.33
1	A	42	TRP	CZ3-CH2	5.97	1.49	1.40
1	B	204	SER	CA-CB	5.92	1.61	1.52
1	B	494	SER	CB-OG	5.87	1.49	1.42
1	A	399	GLU	CD-OE2	5.83	1.32	1.25
1	A	226	GLU	CG-CD	5.82	1.60	1.51
1	B	434	TYR	CG-CD2	-5.82	1.31	1.39
1	A	428	MET	CG-SD	-5.81	1.66	1.81
1	A	745	PHE	CE2-CZ	5.79	1.48	1.37
1	A	161	ARG	CD-NE	-5.77	1.36	1.46
1	A	210	GLU	CD-OE2	5.75	1.31	1.25
1	A	697	TRP	CD1-NE1	-5.71	1.28	1.38
1	B	72	PHE	CG-CD1	-5.70	1.30	1.38
1	A	377	PRO	C-O	-5.70	1.11	1.23
1	B	647	GLN	CG-CD	5.70	1.64	1.51
1	B	223	ARG	CZ-NH1	5.70	1.40	1.33
1	B	434	TYR	CB-CG	-5.66	1.43	1.51
1	B	132	ARG	CZ-NH1	5.64	1.40	1.33
1	A	434	TYR	CG-CD1	-5.58	1.31	1.39
1	B	719	TYR	CD1-CE1	5.58	1.47	1.39
1	A	95	TRP	CG-CD1	-5.55	1.28	1.36
1	A	74	LYS	N-CA	-5.52	1.35	1.46
1	B	746	ASP	CB-CG	5.51	1.63	1.51
1	A	513	TRP	CE2-CZ2	-5.50	1.30	1.39
1	A	649	ARG	CZ-NH1	5.48	1.40	1.33
1	B	711	GLN	CD-NE2	-5.47	1.19	1.32
1	A	726[A]	GLU	CG-CD	5.46	1.60	1.51
1	A	726[B]	GLU	CG-CD	5.46	1.60	1.51
1	A	438	GLU	CD-OE2	5.46	1.31	1.25
1	B	529	GLU	CG-CD	5.46	1.60	1.51
1	A	703	ASP	CG-OD2	5.45	1.37	1.25
1	A	602	ARG	CZ-NH2	-5.45	1.25	1.33
1	A	298	GLU	CG-CD	5.44	1.60	1.51
1	A	343	GLU	CB-CG	-5.43	1.41	1.52
1	A	446	TRP	NE1-CE2	-5.43	1.30	1.37
1	B	674	GLU	CG-CD	5.42	1.60	1.51
1	B	514	GLU	CD-OE1	-5.41	1.19	1.25
1	A	532	ARG	CZ-NH1	-5.39	1.26	1.33
1	A	519	GLU	CD-OE1	5.38	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	708	SER	CA-CB	5.36	1.60	1.52
1	B	46	GLN	CD-OE1	5.36	1.35	1.24
1	A	294	GLY	C-O	5.35	1.32	1.23
1	B	36	GLY	N-CA	5.35	1.54	1.46
1	B	609	TYR	CG-CD2	5.35	1.46	1.39
1	A	76	ASP	CB-CG	5.34	1.62	1.51
1	A	196	GLU	CG-CD	5.34	1.59	1.51
1	B	602	ARG	CZ-NH2	-5.32	1.26	1.33
1	A	567	GLY	CA-C	-5.31	1.43	1.51
1	A	514	GLU	CD-OE1	-5.30	1.19	1.25
1	A	351	GLU	C-O	5.30	1.33	1.23
1	A	502	GLY	CA-C	-5.30	1.43	1.51
1	A	588	VAL	N-CA	-5.29	1.35	1.46
1	A	57	SER	CB-OG	5.28	1.49	1.42
1	A	198	GLU	CG-CD	5.28	1.59	1.51
1	A	540	ARG	C-O	5.28	1.33	1.23
1	A	485	TRP	CG-CD1	-5.25	1.29	1.36
1	B	740	MET	CA-CB	-5.24	1.42	1.53
1	A	269	GLU	CD-OE2	-5.24	1.19	1.25
1	B	247	ASN	CB-CG	5.23	1.63	1.51
1	A	187	PHE	CE1-CZ	5.22	1.47	1.37
1	A	499	GLY	C-O	5.22	1.31	1.23
1	A	376	ASP	CB-CG	5.21	1.62	1.51
1	A	609	TYR	CG-CD2	5.19	1.45	1.39
1	A	711	GLN	CD-OE1	5.17	1.35	1.24
1	A	70	GLN	CG-CD	5.16	1.62	1.51
1	A	336[A]	GLN	CG-CD	5.11	1.62	1.51
1	A	336[B]	GLN	CG-CD	5.11	1.62	1.51
1	A	462	ASP	CA-CB	-5.09	1.42	1.53
1	A	434	TYR	CE2-CZ	-5.09	1.31	1.38
1	B	336	GLN	CG-CD	5.09	1.62	1.51
1	A	529	GLU	CD-OE1	-5.06	1.20	1.25
1	B	298	GLU	CD-OE2	5.04	1.31	1.25
1	A	68	TYR	CG-CD1	-5.04	1.32	1.39
1	A	178	GLU	CD-OE1	-5.03	1.20	1.25
1	B	526	GLU	CG-CD	5.03	1.59	1.51
1	B	201	TYR	CG-CD2	-5.02	1.32	1.39
1	B	537	GLY	N-CA	5.02	1.53	1.46
1	B	418	ARG	CZ-NH1	-5.02	1.26	1.33
1	B	296	GLU	CD-OE1	5.00	1.31	1.25

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	512	ASP	CB-CG-OD1	-14.00	105.70	118.30
1	A	161	ARG	NE-CZ-NH1	13.95	127.27	120.30
1	B	161[A]	ARG	NE-CZ-NH2	-13.31	113.64	120.30
1	B	161[B]	ARG	NE-CZ-NH2	-13.31	113.64	120.30
1	A	108	ARG	NE-CZ-NH1	12.49	126.55	120.30
1	B	427	ASP	CB-CG-OD2	-12.43	107.11	118.30
1	B	123	ARG	NE-CZ-NH2	-12.09	114.25	120.30
1	A	649	ARG	NE-CZ-NH2	-12.03	114.29	120.30
1	B	649	ARG	NE-CZ-NH2	-11.71	114.44	120.30
1	A	649	ARG	NE-CZ-NH1	11.69	126.15	120.30
1	A	713	ARG	NE-CZ-NH1	11.59	126.10	120.30
1	A	255[A]	ARG	NE-CZ-NH2	-11.37	114.61	120.30
1	A	255[B]	ARG	NE-CZ-NH2	-11.37	114.61	120.30
1	A	504	ARG	NE-CZ-NH2	-10.97	114.81	120.30
1	A	149	ARG	NE-CZ-NH1	10.81	125.70	120.30
1	B	108	ARG	NE-CZ-NH1	10.60	125.60	120.30
1	A	431	ARG	NE-CZ-NH2	10.58	125.59	120.30
1	A	431	ARG	NE-CZ-NH1	-10.58	115.01	120.30
1	A	161	ARG	NE-CZ-NH2	-10.40	115.10	120.30
1	A	730	ARG	NE-CZ-NH1	10.29	125.44	120.30
1	A	40	ARG	NE-CZ-NH1	10.19	125.39	120.30
1	A	376	ASP	CB-CG-OD2	-10.09	109.22	118.30
1	A	434	TYR	CB-CG-CD1	9.92	126.95	121.00
1	B	40	ARG	NE-CZ-NH1	9.61	125.10	120.30
1	B	393	ARG	NE-CZ-NH2	-9.59	115.51	120.30
1	A	492	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	B	60	ASP	CB-CG-OD2	-9.40	109.84	118.30
1	B	76	ASP	CB-CG-OD2	-9.38	109.86	118.30
1	B	82	ARG	NE-CZ-NH1	9.23	124.92	120.30
1	A	60	ASP	CB-CG-OD2	-9.16	110.06	118.30
1	B	263	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	B	649	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	B	454	ASP	CB-CG-OD1	8.98	126.38	118.30
1	A	744	ARG	NE-CZ-NH2	-8.95	115.82	120.30
1	A	405	PHE	CB-CG-CD1	-8.89	114.58	120.80
1	A	407	GLU	OE1-CD-OE2	-8.81	112.73	123.30
1	A	744	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	A	713	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	B	108	ARG	NE-CZ-NH2	-8.69	115.95	120.30
1	A	258	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	A	407	GLU	CG-CD-OE1	8.59	135.48	118.30
1	B	744	ARG	NE-CZ-NH2	-8.57	116.01	120.30
1	A	404	ARG	NE-CZ-NH1	8.54	124.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	ASP	CB-CG-OD2	-8.38	110.75	118.30
1	B	514	GLU	OE1-CD-OE2	-8.34	113.29	123.30
1	B	428	MET	CA-CB-CG	-8.28	99.22	113.30
1	A	149	ARG	NE-CZ-NH2	-8.17	116.21	120.30
1	A	690	ARG	NE-CZ-NH1	-8.15	116.23	120.30
1	B	404	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	A	426[A]	ARG	NE-CZ-NH1	-8.01	116.30	120.30
1	A	426[B]	ARG	NE-CZ-NH1	-8.01	116.30	120.30
1	B	713	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	A	54	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	B	690	ARG	NE-CZ-NH2	7.86	124.23	120.30
1	B	123	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	B	504	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	B	268	ASP	CB-CG-OD1	7.79	125.31	118.30
1	B	196	GLU	OE1-CD-OE2	-7.77	113.97	123.30
1	B	434	TYR	CB-CG-CD1	7.75	125.65	121.00
1	A	602	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	A	690	ARG	NE-CZ-NH2	7.71	124.16	120.30
1	B	730	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	191	ARG	NE-CZ-NH2	-7.67	116.46	120.30
1	A	587	ASP	CB-CG-OD1	7.63	125.17	118.30
1	B	683	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	A	703	ASP	CB-CG-OD1	7.36	124.92	118.30
1	A	683	ASP	CB-CG-OD1	7.31	124.88	118.30
1	B	730	ARG	NE-CZ-NH2	-7.31	116.65	120.30
1	B	433	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	A	258	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	60	ASP	CB-CG-OD1	6.98	124.58	118.30
1	A	210	GLU	OE1-CD-OE2	-6.98	114.93	123.30
1	A	434	TYR	CZ-CE2-CD2	6.84	125.96	119.80
1	B	201	TYR	CB-CG-CD1	-6.81	116.91	121.00
1	B	540	ARG	NE-CZ-NH2	-6.81	116.89	120.30
1	B	541	GLY	N-CA-C	-6.81	96.07	113.10
1	A	263	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	A	745	PHE	CB-CG-CD1	-6.77	116.06	120.80
1	A	663	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	A	532	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	73	GLU	OE1-CD-OE2	-6.64	115.33	123.30
1	A	76	ASP	CB-CG-OD2	-6.64	112.33	118.30
1	A	68	TYR	CB-CG-CD2	-6.56	117.06	121.00
1	B	46	GLN	CA-CB-CG	6.56	127.84	113.40
1	A	689	ASP	CB-CG-OD2	-6.55	112.41	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	512	ASP	CB-CG-OD2	6.54	124.19	118.30
1	B	701	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	258	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	433	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	418	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	532	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	82	ARG	NE-CZ-NH1	6.39	123.50	120.30
1	B	431	ARG	NE-CZ-NH1	-6.39	117.10	120.30
1	B	587	ASP	CB-CG-OD1	6.37	124.03	118.30
1	B	570	VAL	CG1-CB-CG2	-6.35	100.74	110.90
1	A	393	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	704	LEU	CB-CG-CD2	6.26	121.64	111.00
1	B	201	TYR	CB-CG-CD2	6.24	124.75	121.00
1	A	540	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	A	268	ASP	CB-CG-OD2	-6.23	112.70	118.30
1	A	433	ARG	NE-CZ-NH1	6.23	123.41	120.30
1	A	40	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	670	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	B	492	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	46	GLN	CA-CB-CG	6.11	126.85	113.40
1	A	395	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	226	GLU	OE1-CD-OE2	-6.09	115.99	123.30
1	A	66	PHE	CG-CD2-CE2	-6.08	114.12	120.80
1	A	701	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	132	ARG	NE-CZ-NH2	6.05	123.33	120.30
1	B	223	ARG	CA-CB-CG	-6.05	100.08	113.40
1	B	314	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	A	601	PHE	CB-CG-CD2	6.01	125.01	120.80
1	B	438	GLU	OE1-CD-OE2	5.99	130.48	123.30
1	B	492	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	B	744	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	B	60	ASP	CB-CG-OD1	5.93	123.64	118.30
1	B	218	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	414	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	118	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	A	427	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	B	434	TYR	CA-CB-CG	5.76	124.35	113.40
1	B	630	GLU	OE1-CD-OE2	-5.75	116.41	123.30
1	B	404	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	225	LEU	CB-CG-CD2	-5.73	101.27	111.00
1	A	55	HIS	CB-CA-C	5.65	121.70	110.40
1	B	405	PHE	CB-CG-CD1	-5.62	116.87	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	434	TYR	CZ-CE2-CD2	5.61	124.84	119.80
1	B	578	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	588	VAL	CG1-CB-CG2	5.59	119.84	110.90
1	A	571	THR	OG1-CB-CG2	-5.56	97.20	110.00
1	B	373	ASP	CB-CG-OD1	5.56	123.31	118.30
1	B	313	TYR	CB-CG-CD1	-5.56	117.66	121.00
1	B	427	ASP	OD1-CG-OD2	5.54	133.83	123.30
1	B	47	LEU	N-CA-CB	-5.53	99.35	110.40
1	A	504	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	118	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	418	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	222	ASP	CB-CG-OD1	5.46	123.22	118.30
1	B	48	ASP	CB-CG-OD1	5.46	123.22	118.30
1	B	303	GLU	OE1-CD-OE2	-5.45	116.77	123.30
1	B	683	ASP	CB-CG-OD1	5.44	123.19	118.30
1	A	743	ASP	CB-CG-OD1	5.43	123.18	118.30
1	A	108	ARG	NH1-CZ-NH2	-5.41	113.45	119.40
1	B	314	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	B	199	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	B	689	ASP	CB-CG-OD1	5.38	123.14	118.30
1	B	382	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	A	47	LEU	N-CA-CB	-5.34	99.73	110.40
1	A	601	PHE	CB-CG-CD1	-5.33	117.07	120.80
1	B	599	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	B	225	LEU	CB-CG-CD2	-5.31	101.97	111.00
1	A	730	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	728	PHE	CB-CG-CD1	-5.26	117.12	120.80
1	B	745	PHE	CB-CG-CD1	-5.25	117.12	120.80
1	A	167	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	B	726	GLU	CG-CD-OE2	5.24	128.77	118.30
1	A	405	PHE	CB-CG-CD2	5.21	124.45	120.80
1	B	375	PHE	CB-CG-CD1	-5.19	117.17	120.80
1	B	713	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	68	TYR	CG-CD2-CE2	-5.16	117.17	121.30
1	B	40	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	376	ASP	OD1-CG-OD2	5.11	133.02	123.30
1	A	491	PHE	CB-CG-CD1	-5.11	117.22	120.80
1	A	728	PHE	CD1-CE1-CZ	-5.08	114.00	120.10
1	A	193	ASP	CB-CG-OD1	-5.08	113.73	118.30
1	A	133	PHE	CB-CG-CD2	5.06	124.34	120.80
1	A	82	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	166	ALA	CB-CA-C	5.04	117.67	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	405	PHE	CB-CG-CD2	5.03	124.32	120.80
1	A	670	ASP	CB-CG-OD1	5.00	122.81	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	199	ASP	Mainchain
1	B	514	GLU	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	5568	0	5365	15	0
1	B	5552	0	5353	20	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	1	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	1	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	24	0	42	7	0
7	B	8	0	14	2	0
8	A	794	0	0	7	2
8	B	785	0	0	10	2
All	All	12835	0	10834	45	2

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:807:MPD:H52	7:A:807:MPD:H11	1.38	1.05
1:A:119[B]:THR:HG21	8:A:1080:HOH:O	1.62	0.97
1:B:569:ALA:O	1:B:570:VAL:HG23	1.65	0.95
1:B:198[A]:GLU:OE1	8:B:901:HOH:O	1.83	0.94
1:B:76:ASP:OD2	8:B:902:HOH:O	1.89	0.89
1:B:119[B]:THR:HG21	8:B:1142:HOH:O	1.77	0.83
1:B:540:ARG:NE	1:B:540:ARG:HA	1.94	0.83
5:B:804:OXY:O2	8:B:903:HOH:O	1.99	0.81
1:B:647:GLN:HG2	8:B:990:HOH:O	1.80	0.80
1:B:65:ASP:HB2	8:B:930:HOH:O	1.80	0.80
1:B:512:ASP:OD1	8:B:904:HOH:O	2.00	0.77
1:B:569:ALA:O	1:B:570:VAL:CG2	2.33	0.75
7:A:808:MPD:O4	7:A:808:MPD:HM2	1.87	0.73
7:A:807:MPD:H11	7:A:807:MPD:C5	2.11	0.71
1:B:431:ARG:CD	8:B:1511:HOH:O	2.39	0.70
1:B:540:ARG:NE	1:B:540:ARG:CA	2.57	0.67
1:B:431:ARG:HD2	8:B:1511:HOH:O	1.98	0.63
1:B:540:ARG:HA	1:B:540:ARG:CZ	2.35	0.56
1:A:633[A]:VAL:CG2	1:A:719:TYR:CZ	2.91	0.53
1:A:696:LYS:NZ	8:A:903:HOH:O	2.32	0.53
1:B:591:MET:SD	1:B:594:LEU:HD12	2.48	0.53
1:A:226:GLU:OE1	1:A:610:ARG:NH2	2.43	0.52
1:A:119[A]:THR:CG2	1:A:265:ALA:HB2	2.39	0.51
1:B:54:ARG:HB3	1:B:55:HIS:CD2	2.48	0.49
7:B:806:MPD:CM	7:B:806:MPD:H52	2.42	0.48
7:B:806:MPD:H52	7:B:806:MPD:HM2	1.96	0.47
7:A:807:MPD:C1	8:A:1165:HOH:O	2.62	0.47
7:A:807:MPD:HM2	8:A:1514:HOH:O	2.15	0.47
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.98	0.46
1:A:726[B]:GLU:HG2	1:A:730:ARG:HH12	1.81	0.46
1:A:426[B]:ARG:HA	1:A:426[B]:ARG:HD2	1.65	0.45
7:A:808:MPD:O4	7:A:808:MPD:CM	2.62	0.44
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.17	0.44
1:A:70:GLN:NE2	8:A:929:HOH:O	2.50	0.44
1:A:591:MET:SD	1:A:594:LEU:HD12	2.58	0.44
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.18	0.43
7:A:807:MPD:H11	8:A:1165:HOH:O	2.18	0.43
1:B:431:ARG:HD3	8:B:1511:HOH:O	2.13	0.43
1:A:54:ARG:HB2	1:A:55:HIS:CD2	2.54	0.43
1:A:336[B]:GLN:HG3	8:A:922:HOH:O	2.19	0.42
1:A:119[A]:THR:HG21	1:A:265:ALA:HB2	2.02	0.42
1:A:198:GLU:HG3	4:A:803:CL:CL	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:GLY:C	1:B:608:LYS:HE2	2.41	0.41
1:A:455:HIS:CE1	1:A:544:GLN:HG3	2.55	0.41
1:A:726[B]:GLU:CG	1:A:730:ARG:HH12	2.34	0.40

All (2) 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)
8:A:1227:HOH:O	8:B:954:HOH:O[2_444]	2.18	0.02
8:A:1538:HOH:O	8:B:1351:HOH:O[4_445]	2.19	0.01

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	717/728 (98%)	704 (98%)	13 (2%)	0	100	100
1	B	716/728 (98%)	704 (98%)	12 (2%)	0	100	100
All	All	1433/1456 (98%)	1408 (98%)	25 (2%)	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	557/561 (99%)	546 (98%)	11 (2%)	50	25
1	B	556/561 (99%)	544 (98%)	12 (2%)	47	22
All	All	1113/1122 (99%)	1090 (98%)	23 (2%)	50	23

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	46	GLN
1	A	118	ARG
1	A	141	ASP
1	A	161	ARG
1	A	223	ARG
1	A	544	GLN
1	A	608	LYS
1	A	610	ARG
1	A	649	ARG
1	A	725	GLN
1	B	40	ARG
1	B	46	GLN
1	B	54	ARG
1	B	118	ARG
1	B	141	ASP
1	B	379	LYS
1	B	571[A]	THR
1	B	571[B]	THR
1	B	608	LYS
1	B	610	ARG
1	B	649	ARG
1	B	730	ARG

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	A	339	HIS
1	B	227	ASN
1	B	406	HIS
1	B	520	GLN
1	B	647	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TOX	B	111[A]	2	11,17,18	2.70	6 (54%)	8,23,25	2.21	2 (25%)
1	TOX	A	111[B]	-	11,17,18	3.08	4 (36%)	8,23,25	0.94	0
1	TOX	B	111[B]	-	11,17,18	2.70	6 (54%)	8,23,25	2.21	2 (25%)
1	TOX	A	111[A]	2	11,17,18	3.08	4 (36%)	8,23,25	0.94	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
1	TOX	B	111[A]	2	-	2/4/8/10	0/2/2/2
1	TOX	A	111[B]	-	-	2/4/8/10	0/2/2/2
1	TOX	B	111[B]	-	-	2/4/8/10	0/2/2/2
1	TOX	A	111[A]	2	-	2/4/8/10	0/2/2/2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111[A]	TOX	CD1-NE1	-8.41	1.31	1.39
1	A	111[B]	TOX	CD1-NE1	-8.41	1.31	1.39
1	B	111[A]	TOX	CZ2-CE2	-5.35	1.30	1.41
1	B	111[B]	TOX	CZ2-CE2	-5.35	1.30	1.41
1	B	111[A]	TOX	CD1-NE1	-4.15	1.35	1.39
1	B	111[B]	TOX	CD1-NE1	-4.15	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111[A]	TOX	CE3-CD2	-3.53	1.35	1.42
1	A	111[B]	TOX	CE3-CD2	-3.53	1.35	1.42
1	B	111[A]	TOX	CD1-CG	-3.42	1.33	1.37
1	B	111[B]	TOX	CD1-CG	-3.42	1.33	1.37
1	B	111[A]	TOX	O-C	2.90	1.31	1.20
1	B	111[B]	TOX	O-C	2.90	1.31	1.20
1	A	111[A]	TOX	O-C	2.70	1.30	1.20
1	A	111[B]	TOX	O-C	2.70	1.30	1.20
1	A	111[A]	TOX	CH2-CZ2	2.52	1.42	1.36
1	A	111[B]	TOX	CH2-CZ2	2.52	1.42	1.36
1	B	111[A]	TOX	CA-N	-2.45	1.41	1.48
1	B	111[B]	TOX	CA-N	-2.45	1.41	1.48
1	B	111[A]	TOX	CH2-CZ3	2.25	1.43	1.38
1	B	111[B]	TOX	CH2-CZ3	2.25	1.43	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111[A]	TOX	CZ3-CE3-CD2	-5.24	113.83	120.91
1	B	111[B]	TOX	CZ3-CE3-CD2	-5.24	113.83	120.91
1	B	111[A]	TOX	CH2-CZ3-CE3	2.44	123.67	120.40
1	B	111[B]	TOX	CH2-CZ3-CE3	2.44	123.67	120.40

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	111[A]	TOX	N-CA-CB-CG
1	A	111[A]	TOX	C-CA-CB-CG
1	A	111[B]	TOX	N-CA-CB-CG
1	A	111[B]	TOX	C-CA-CB-CG
1	B	111[A]	TOX	N-CA-CB-CG
1	B	111[A]	TOX	C-CA-CB-CG
1	B	111[B]	TOX	N-CA-CB-CG
1	B	111[B]	TOX	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	806	-	7,7,7	1.69	1 (14%)	9,10,10	2.86	5 (55%)
6	PO4	B	805	-	4,4,4	2.22	3 (75%)	6,6,6	1.62	2 (33%)
5	OXY	B	804	-	1,1,1	0.62	0	-		
2	HEM	B	801	1	42,50,50	1.93	10 (23%)	46,82,82	2.46	20 (43%)
2	HEM	A	801	1	42,50,50	1.73	12 (28%)	46,82,82	2.16	14 (30%)
7	MPD	A	808	-	7,7,7	0.87	0	9,10,10	2.23	4 (44%)
7	MPD	A	807	-	7,7,7	1.15	1 (14%)	9,10,10	1.94	4 (44%)
5	OXY	A	804	-	1,1,1	0.64	0	-		
7	MPD	B	806	-	7,7,7	1.06	0	9,10,10	1.56	1 (11%)
6	PO4	A	805	-	4,4,4	1.91	1 (25%)	6,6,6	2.18	2 (33%)

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	806	-	-	0/5/5/5	-
2	HEM	B	801	1	-	3/12/54/54	-
2	HEM	A	801	1	-	2/12/54/54	-
7	MPD	A	808	-	-	3/5/5/5	-
7	MPD	A	807	-	-	3/5/5/5	-
7	MPD	B	806	-	-	3/5/5/5	-

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C1B-NB	-5.61	1.30	1.40
2	B	801	HEM	C1B-C2B	-4.23	1.35	1.44
2	B	801	HEM	CHB-C1B	4.06	1.44	1.34
7	A	806	MPD	C5-C4	3.92	1.67	1.51
2	A	801	HEM	C1A-NA	3.77	1.44	1.36
6	A	805	PO4	P-O3	-3.48	1.44	1.54
2	A	801	HEM	CHB-C1B	3.31	1.42	1.34
2	A	801	HEM	CMD-C2D	-3.23	1.44	1.50
2	B	801	HEM	C4A-NA	3.20	1.42	1.36
2	B	801	HEM	CMB-C2B	3.09	1.57	1.50
2	A	801	HEM	C3B-C4B	3.07	1.50	1.44
2	A	801	HEM	C4D-C3D	3.04	1.50	1.45
6	B	805	PO4	P-O2	-3.02	1.45	1.54
2	B	801	HEM	C3D-C2D	2.80	1.42	1.36
2	B	801	HEM	C1D-ND	-2.76	1.33	1.38
2	A	801	HEM	C1B-NB	-2.70	1.35	1.40
2	A	801	HEM	C3C-C4C	2.67	1.45	1.41
2	B	801	HEM	C3B-C2B	-2.59	1.31	1.37
2	A	801	HEM	O1A-CGA	2.57	1.30	1.22
2	A	801	HEM	O1D-CGD	2.56	1.30	1.22
6	B	805	PO4	P-O1	2.42	1.56	1.50
2	B	801	HEM	C3C-C2C	-2.38	1.37	1.40
2	A	801	HEM	C1D-C2D	2.36	1.49	1.44
7	A	807	MPD	O2-C2	2.18	1.50	1.44
2	B	801	HEM	C3C-C4C	-2.17	1.38	1.41
6	B	805	PO4	P-O3	-2.13	1.48	1.54
2	A	801	HEM	FE-NB	2.04	2.09	1.98
2	A	801	HEM	C4A-NA	-2.02	1.32	1.36

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	C3B-C2B-C1B	7.76	112.24	106.41
2	A	801	HEM	C4B-C3B-C2B	-5.71	102.03	107.28
2	B	801	HEM	C3B-C4B-NB	-5.56	105.48	109.47
2	A	801	HEM	C3B-C2B-C1B	5.32	110.41	106.41
7	A	806	MPD	O2-C2-C1	-4.86	92.83	107.99
7	A	806	MPD	O4-C4-C3	-4.40	93.84	111.35
2	A	801	HEM	C4C-CHD-C1D	4.16	128.05	122.56
2	A	801	HEM	C2D-C1D-ND	4.13	114.68	109.90
2	B	801	HEM	CAD-C3D-C4D	4.01	131.69	124.70
2	B	801	HEM	CHA-C4D-ND	3.89	129.20	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	806	MPD	CM-C2-C1	3.83	119.21	110.63
2	B	801	HEM	CMB-C2B-C1B	-3.83	119.05	125.03
7	A	808	MPD	O2-C2-CM	-3.79	96.16	107.99
7	A	807	MPD	CM-C2-C1	-3.77	102.19	110.63
7	A	806	MPD	C5-C4-C3	3.65	128.62	111.67
7	A	808	MPD	CM-C2-C1	3.51	118.48	110.63
2	A	801	HEM	CAA-CBA-CGA	-3.44	104.55	113.83
6	A	805	PO4	O4-P-O1	-3.37	99.03	110.95
2	B	801	HEM	CMA-C3A-C4A	-3.37	123.53	128.46
2	A	801	HEM	CHA-C4D-ND	-3.35	120.22	124.37
2	A	801	HEM	CHD-C1D-ND	-3.31	120.87	124.44
2	A	801	HEM	C1B-NB-C4B	3.13	108.91	105.21
2	B	801	HEM	CBA-CAA-C2A	3.07	117.69	112.54
2	B	801	HEM	C4B-C3B-C2B	-3.05	104.47	107.28
2	B	801	HEM	CMA-C3A-C2A	3.05	130.69	124.94
2	A	801	HEM	C1D-C2D-C3D	-2.88	103.95	106.98
2	B	801	HEM	CAD-C3D-C2D	-2.82	122.58	127.87
2	B	801	HEM	CHC-C4B-NB	2.80	127.45	124.44
6	A	805	PO4	O4-P-O3	-2.76	99.32	107.91
2	B	801	HEM	CHA-C4D-C3D	-2.70	120.26	125.23
2	A	801	HEM	C4D-ND-C1D	-2.69	102.02	105.21
6	B	805	PO4	O2-P-O1	-2.69	101.45	110.95
2	B	801	HEM	C4D-ND-C1D	2.68	108.38	105.21
2	A	801	HEM	CMB-C2B-C1B	-2.60	120.97	125.03
2	B	801	HEM	O1A-CGA-CBA	-2.57	114.94	123.09
2	B	801	HEM	C2C-C3C-C4C	-2.49	105.16	106.90
7	A	808	MPD	O2-C2-C3	2.41	118.27	109.27
7	A	806	MPD	CM-C2-C3	2.37	120.43	110.20
2	B	801	HEM	C4B-CHC-C1C	2.36	125.67	122.56
2	B	801	HEM	CBD-CAD-C3D	2.34	118.99	112.53
6	B	805	PO4	O3-P-O2	2.32	115.12	107.91
7	A	807	MPD	C5-C4-C3	2.31	122.42	111.67
2	A	801	HEM	O1A-CGA-CBA	-2.30	115.80	123.09
7	A	806	MPD	O2-C2-C3	2.28	117.78	109.27
2	A	801	HEM	CBA-CAA-C2A	2.27	116.36	112.54
2	A	801	HEM	O2A-CGA-CBA	2.27	121.16	114.00
2	B	801	HEM	C1B-NB-C4B	2.25	107.87	105.21
2	B	801	HEM	CAD-CBD-CGD	2.23	119.57	113.67
7	A	807	MPD	O4-C4-C5	-2.21	99.96	109.45
2	B	801	HEM	C4C-CHD-C1D	2.16	125.41	122.56
7	A	807	MPD	O4-C4-C3	-2.09	103.04	111.35
7	A	808	MPD	CM-C2-C3	-2.01	101.53	110.20

There are no chirality outliers.

All (14) torsion outliers are listed below:

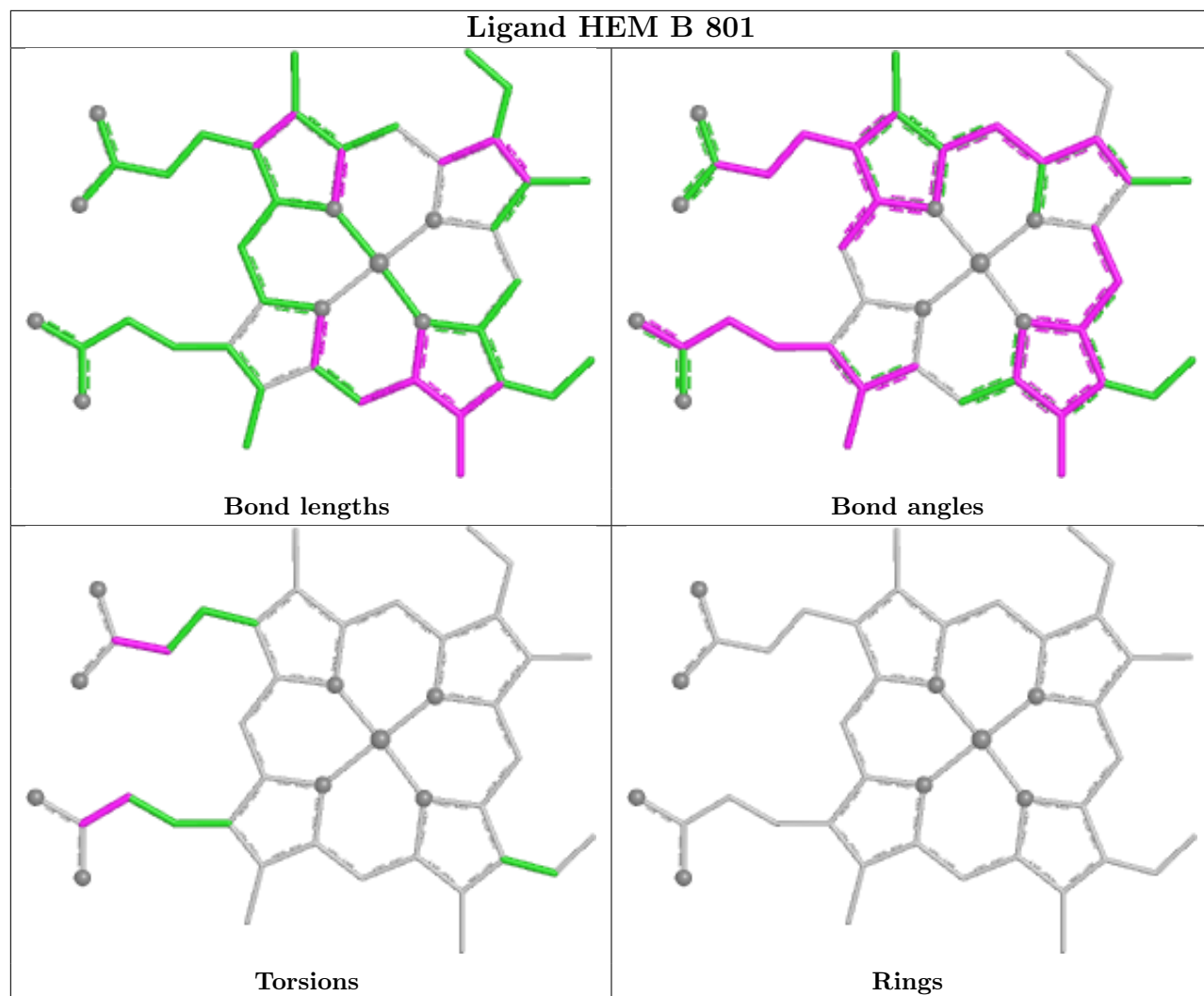
Mol	Chain	Res	Type	Atoms
7	A	807	MPD	C1-C2-C3-C4
7	A	807	MPD	C2-C3-C4-O4
7	A	808	MPD	C2-C3-C4-C5
7	B	806	MPD	O2-C2-C3-C4
7	B	806	MPD	C2-C3-C4-C5
2	B	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	CAA-CBA-CGA-O1A
2	A	801	HEM	CAA-CBA-CGA-O2A
7	A	808	MPD	C2-C3-C4-O4
7	B	806	MPD	C2-C3-C4-O4
7	A	807	MPD	CM-C2-C3-C4
7	A	808	MPD	C1-C2-C3-C4
2	B	801	HEM	CAD-CBD-CGD-O2D

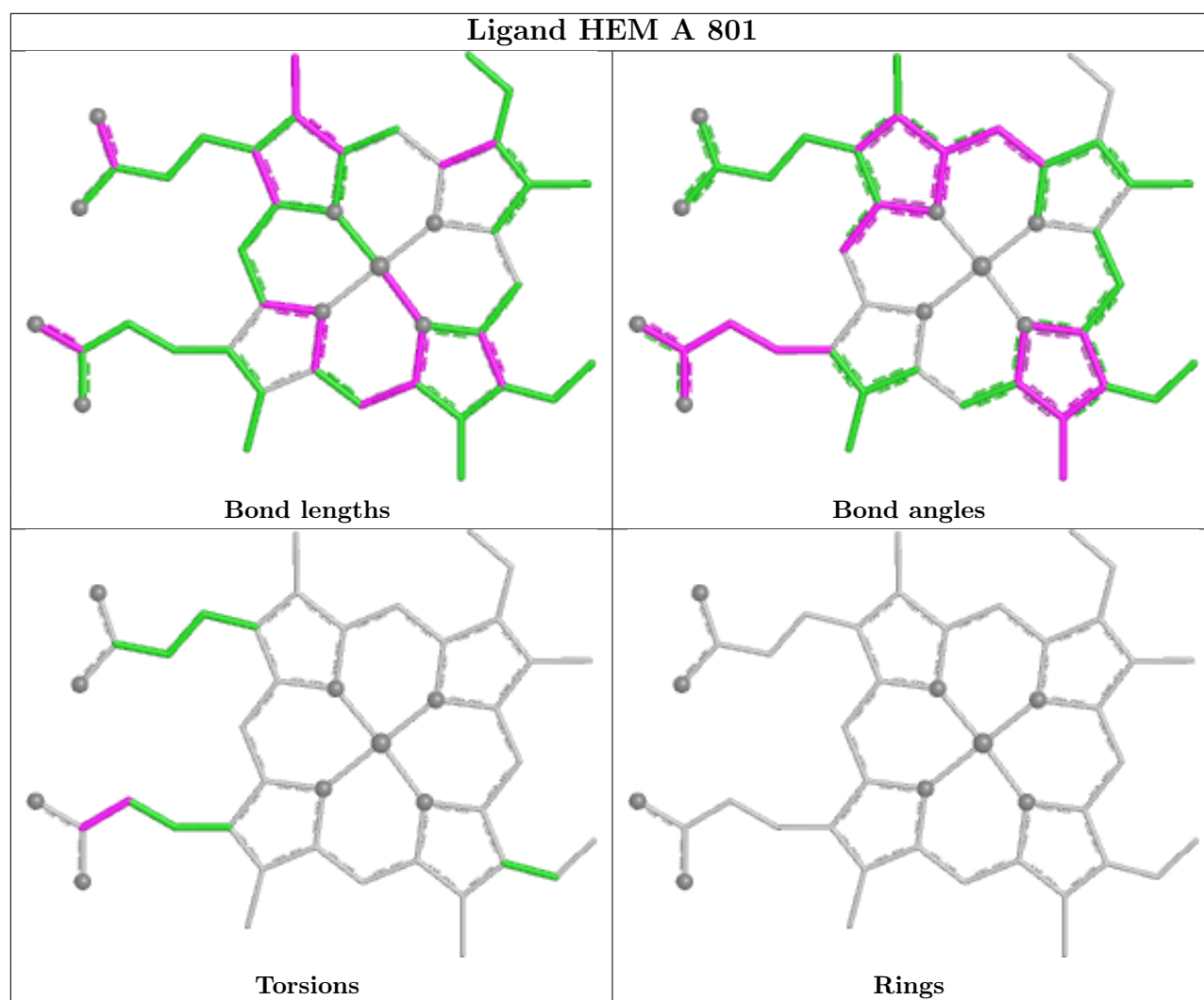
There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	804	OXY	1	0
7	A	808	MPD	2	0
7	A	807	MPD	5	0
7	B	806	MPD	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	712/728 (97%)	-0.41	8 (1%) 77 81	8, 21, 37, 79	7 (0%)
1	B	712/728 (97%)	-0.43	8 (1%) 77 81	8, 20, 38, 90	6 (0%)
All	All	1424/1456 (97%)	-0.42	16 (1%) 77 81	8, 20, 38, 90	13 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	748	ALA	6.0
1	A	748	ALA	5.1
1	B	55	HIS	3.4
1	A	608	LYS	2.9
1	B	40	ARG	2.8
1	A	610	ARG	2.6
1	B	608	LYS	2.5
1	B	65	ASP	2.4
1	B	568	HIS	2.4
1	A	40	ARG	2.3
1	A	379	LYS	2.2
1	B	679	ALA	2.0
1	A	55	HIS	2.0
1	B	46	GLN	2.0
1	A	609	TYR	2.0
1	A	64	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	TOX	A	111[A]	16/17	0.98	0.04	13,15,27,28	1
1	TOX	A	111[B]	16/17	0.98	0.04	13,15,19,27	1
1	TOX	B	111[A]	16/17	0.98	0.04	14,15,24,26	0
1	TOX	B	111[B]	16/17	0.98	0.04	14,15,17,26	1

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

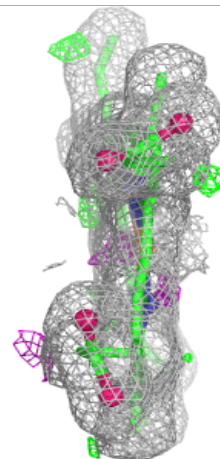
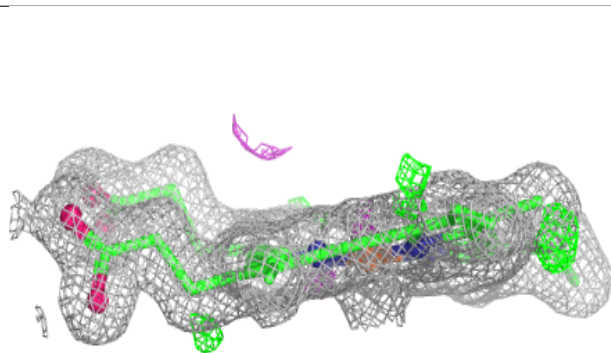
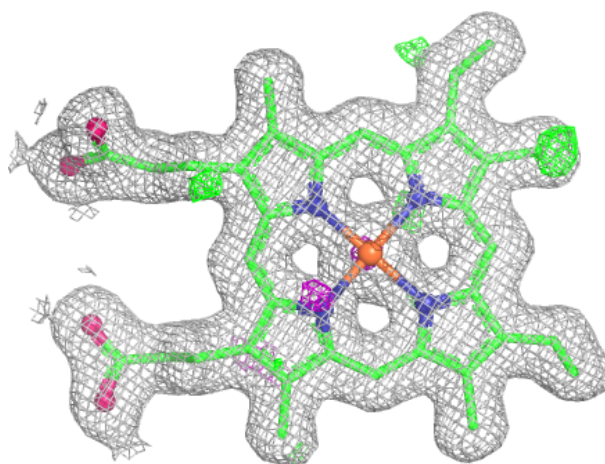
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

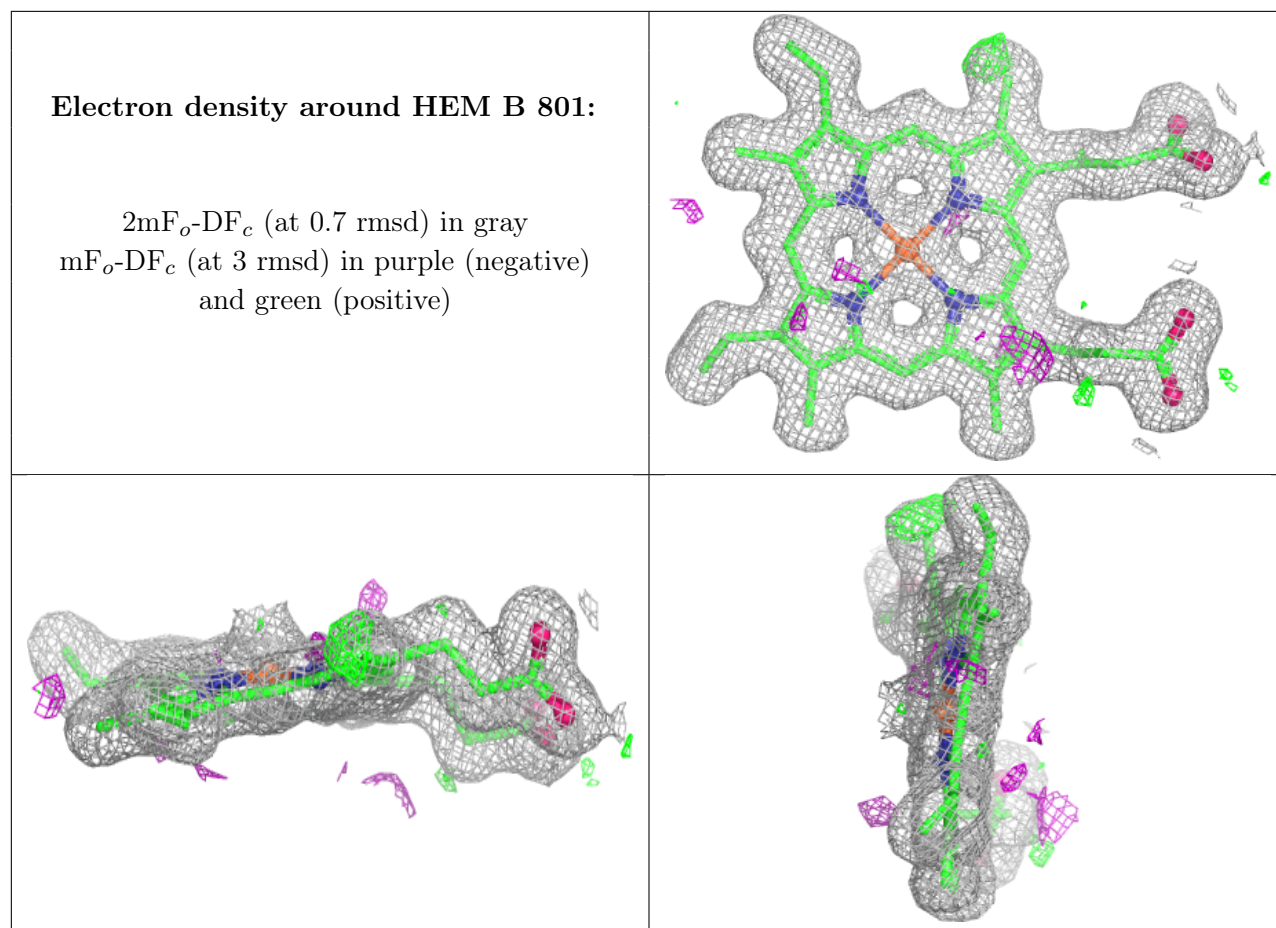
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	MPD	A	806	8/8	0.77	0.27	49,59,62,67	0
7	MPD	B	806	8/8	0.81	0.22	53,55,61,67	0
7	MPD	A	808	8/8	0.83	0.22	57,68,73,73	0
5	OXY	A	804	2/2	0.89	0.28	30,30,30,40	0
7	MPD	A	807	8/8	0.91	0.13	34,40,58,58	0
4	CL	A	803	1/1	0.92	0.12	39,39,39,39	0
6	PO4	A	805	5/5	0.94	0.07	40,44,63,64	0
6	PO4	B	805	5/5	0.94	0.08	40,50,51,63	0
5	OXY	B	804	2/2	0.94	0.21	28,28,28,36	0
2	HEM	A	801	43/43	0.99	0.04	14,16,19,20	0
4	CL	B	803	1/1	0.99	0.08	26,26,26,26	1
2	HEM	B	801	43/43	0.99	0.04	13,15,18,20	0
3	NA	A	802	1/1	0.99	0.04	18,18,18,18	0
3	NA	B	802	1/1	0.99	0.04	18,18,18,18	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.