



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:52 PM UTC

PDB ID : 5SXW / pdb_00005sxw
Title : Crystal structure of the E198A variant of catalase-peroxidase KatG of Burkholderia pseudomallei
Authors : Loewen, P.C.
Deposited on : 2016-08-10
Resolution : 1.60 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

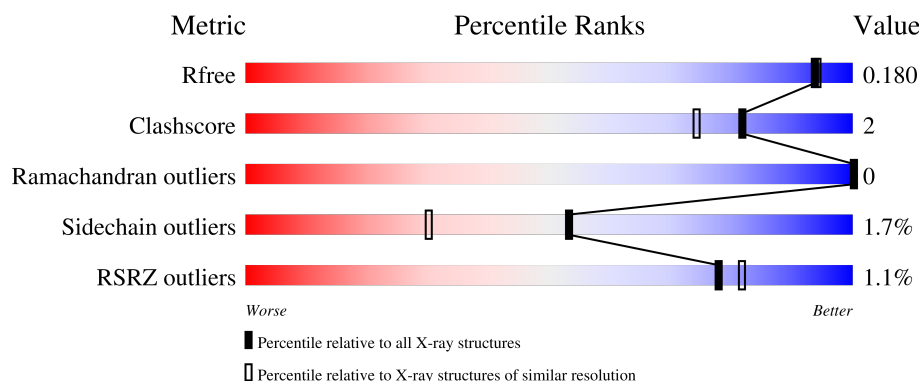
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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
5	PO4	A	804	-	X	-	-
5	PO4	B	805	-	X	-	-

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 13056 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.

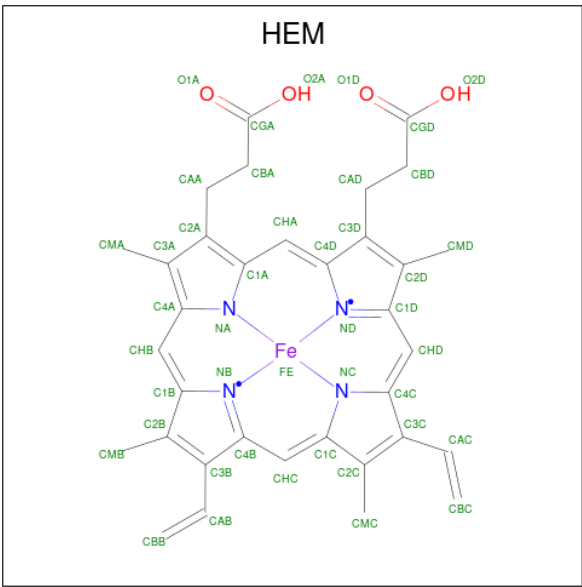
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	6	0
			5526	3490	984	1038	14			
1	B	714	Total	C	N	O	S	0	8	0
			5538	3496	986	1042	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	ALA	GLU	engineered mutation	UNP Q3JNW6
B	198	ALA	GLU	engineered mutation	UNP Q3JNW6

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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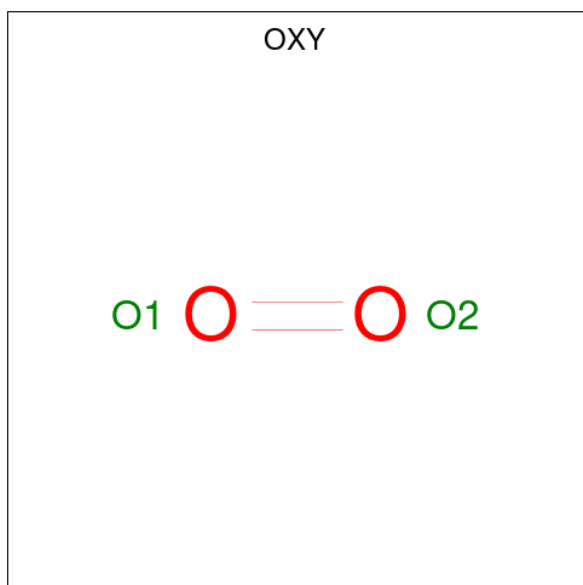
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

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

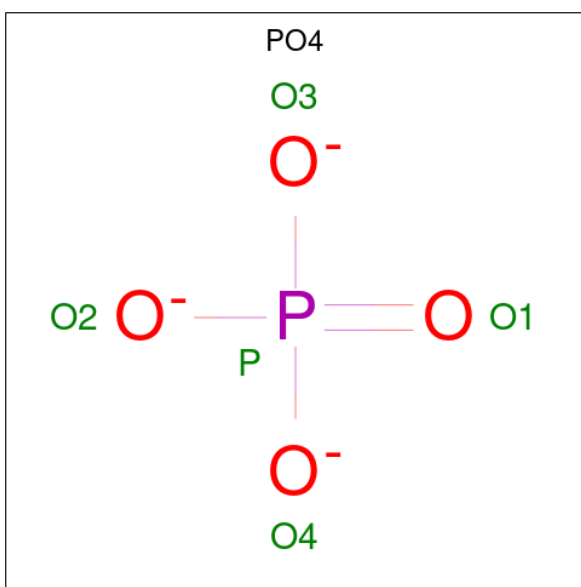
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na		
			1	1	0	0
3	B	1	Total	Na		
			1	1	0	0

- Molecule 4 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



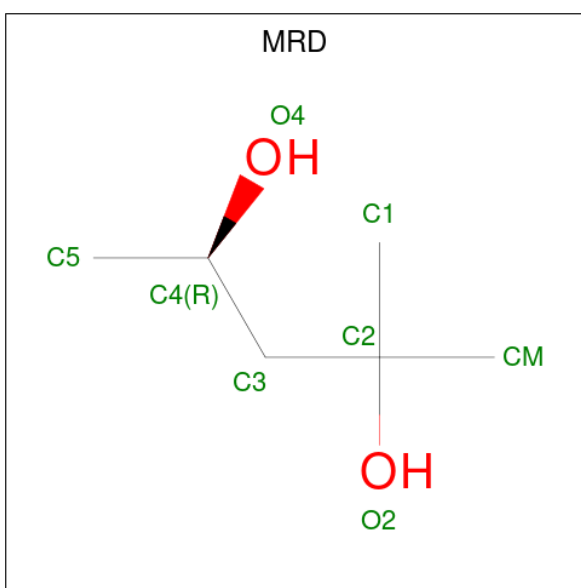
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O		
			2	2	0	0
4	B	1	Total	O		
			2	2	0	0

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



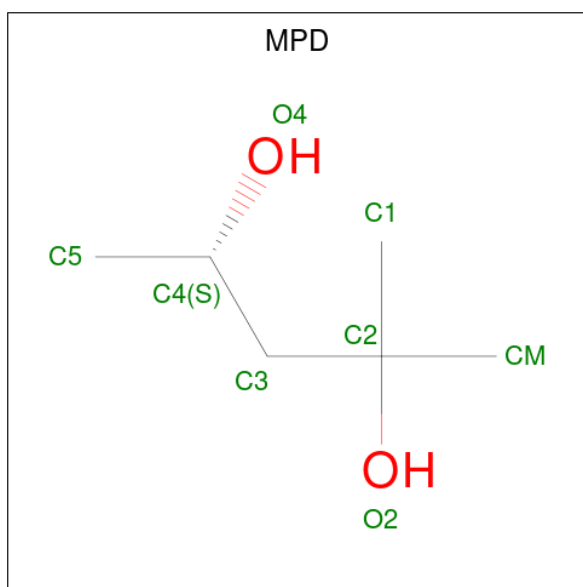
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (CCD ID: MRD) (formula: C₆H₁₄O₂).



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

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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

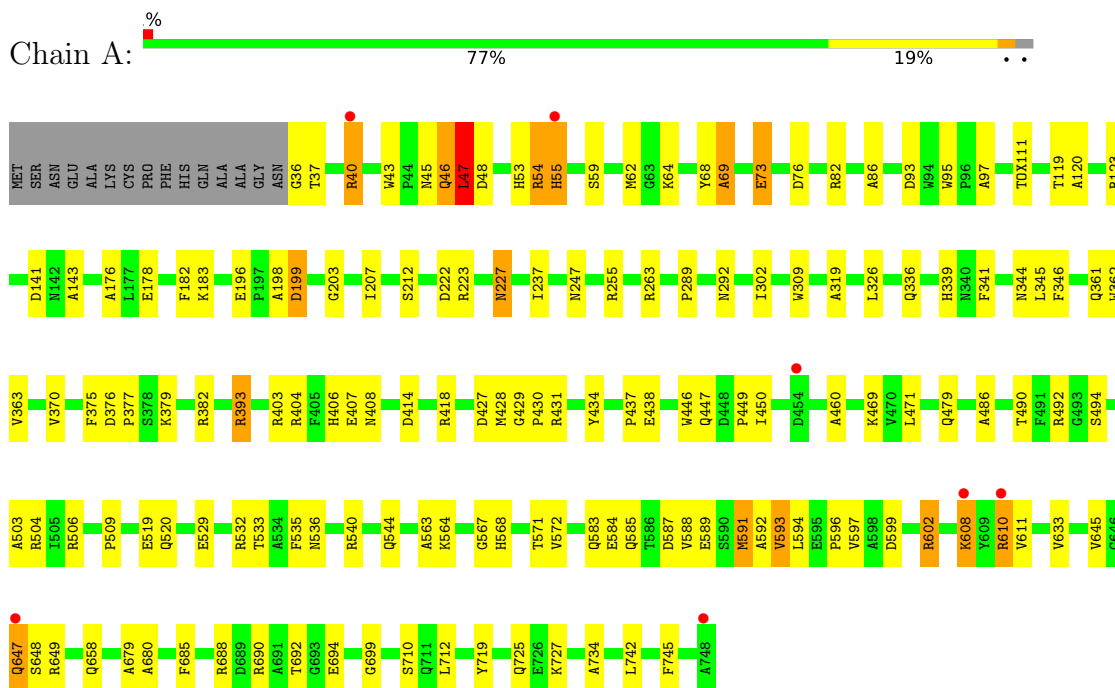
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	955	Total	O	0	0
			955	955		
8	B	911	Total	O	0	0
			911	911		

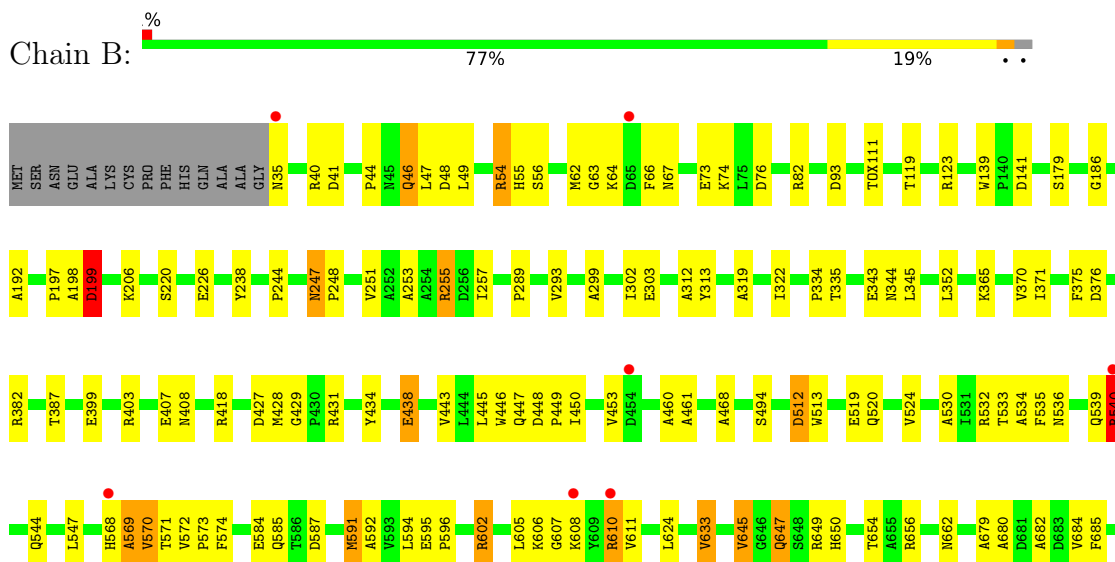
3 Residue-property plots

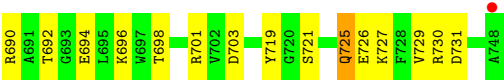
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	100.34Å 116.02Å 174.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.60 20.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-1.60) 99.9 (20.00-1.60)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.59 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.143 , 0.169 0.158 , 0.180	Depositor DCC
R_{free} test set	13409 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	17.8	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13056	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 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	2.03	118/5666 (2.1%)	1.71	66/7701 (0.9%)
1	B	2.03	123/5688 (2.2%)	1.65	75/7732 (1.0%)
All	All	2.03	241/11354 (2.1%)	1.68	141/15433 (0.9%)

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	2
All	All	0	6

All (241) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	571	THR	CA-C	-15.55	1.34	1.52
1	A	532	ARG	CD-NE	-15.13	1.25	1.46
1	A	255	ARG	CD-NE	13.03	1.64	1.46
1	A	725	GLN	CD-NE2	11.78	1.57	1.33
1	B	591	MET	SD-CE	-11.49	1.50	1.79
1	A	199	ASP	C-O	10.93	1.36	1.23
1	B	73	GLU	CD-OE2	10.75	1.45	1.25
1	B	532	ARG	NE-CZ	-9.35	1.22	1.33
1	B	199	ASP	C-O	9.32	1.35	1.23
1	B	63	GLY	N-CA	9.28	1.57	1.45
1	B	512	ASP	CG-OD2	9.21	1.42	1.25
1	B	370	VAL	N-CA	-9.20	1.36	1.46
1	B	572	VAL	N-CA	-9.07	1.37	1.46
1	B	54	ARG	CA-C	-8.65	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	363	VAL	C-O	8.43	1.32	1.24
1	B	446	TRP	N-CA	-8.42	1.35	1.46
1	B	540	ARG	C-O	8.38	1.34	1.23
1	A	53	HIS	CD2-NE2	-8.22	1.28	1.37
1	A	532	ARG	CZ-NH2	-8.17	1.22	1.33
1	A	336	GLN	CG-CD	8.10	1.72	1.52
1	B	703	ASP	N-CA	-8.10	1.36	1.46
1	A	438	GLU	CD-OE2	7.99	1.40	1.25
1	A	47	LEU	CB-CG	-7.89	1.37	1.53
1	B	679	ALA	N-CA	7.86	1.56	1.46
1	A	519	GLU	N-CA	7.85	1.56	1.46
1	B	46	GLN	CG-CD	7.84	1.71	1.52
1	B	371	ILE	N-CA	7.81	1.56	1.46
1	B	571	THR	C-N	7.81	1.40	1.32
1	B	684	VAL	CA-CB	-7.81	1.44	1.54
1	B	725	GLN	CD-OE1	7.76	1.38	1.23
1	B	596	PRO	C-O	7.75	1.30	1.24
1	A	588	VAL	N-CA	-7.74	1.36	1.46
1	A	408	ASN	C-O	7.67	1.33	1.24
1	B	730	ARG	CZ-NH2	7.67	1.43	1.33
1	A	203	GLY	C-O	7.65	1.29	1.23
1	B	606	LYS	N-CA	7.62	1.55	1.46
1	B	376	ASP	N-CA	7.55	1.55	1.46
1	A	183	LYS	CA-CB	7.53	1.63	1.53
1	A	692	THR	CA-C	-7.52	1.42	1.52
1	A	567	GLY	CA-C	-7.49	1.41	1.51
1	A	568	HIS	CA-CB	-7.45	1.41	1.53
1	B	299	ALA	CA-C	-7.42	1.42	1.52
1	A	494	SER	CA-CB	-7.32	1.42	1.53
1	B	289	PRO	N-CA	-7.21	1.38	1.47
1	A	54	ARG	CA-C	-7.19	1.43	1.53
1	A	289	PRO	CA-CB	7.18	1.63	1.53
1	B	448	ASP	C-O	7.15	1.27	1.23
1	A	255	ARG	NE-CZ	7.09	1.40	1.33
1	A	536	ASN	CA-C	6.98	1.62	1.52
1	B	345	LEU	CA-C	6.97	1.61	1.52
1	A	178	GLU	C-O	6.92	1.32	1.24
1	B	572	VAL	CA-CB	6.89	1.62	1.54
1	B	694	GLU	CA-C	6.82	1.61	1.52
1	A	692	THR	N-CA	6.75	1.54	1.46
1	A	43	TRP	CA-CB	6.70	1.60	1.53
1	B	47	LEU	CB-CG	-6.69	1.40	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	587	ASP	CA-C	-6.68	1.44	1.52
1	A	431	ARG	CD-NE	6.65	1.55	1.46
1	B	46	GLN	N-CA	6.65	1.54	1.45
1	B	197	PRO	N-CA	-6.63	1.39	1.47
1	B	453	VAL	C-O	-6.62	1.16	1.24
1	A	532	ARG	CA-C	6.62	1.61	1.52
1	B	343	GLU	C-O	6.62	1.31	1.24
1	B	248	PRO	CA-C	-6.55	1.46	1.53
1	A	688	ARG	CA-C	-6.53	1.44	1.52
1	B	49	LEU	CB-CG	-6.51	1.40	1.53
1	B	534	ALA	CA-CB	-6.50	1.43	1.53
1	B	445	LEU	CA-C	-6.48	1.43	1.52
1	B	418	ARG	CZ-NH1	-6.47	1.23	1.32
1	A	647	GLN	CG-CD	6.47	1.68	1.52
1	A	596	PRO	C-O	6.46	1.29	1.24
1	A	734	ALA	C-O	6.42	1.31	1.24
1	B	35	ASN	CA-C	6.42	1.66	1.52
1	B	434	TYR	CA-C	-6.41	1.44	1.52
1	B	407	GLU	N-CA	6.40	1.54	1.46
1	A	506	ARG	C-O	6.38	1.32	1.24
1	B	592	ALA	CA-C	-6.38	1.44	1.52
1	A	593	VAL	CA-CB	6.37	1.62	1.54
1	A	414	ASP	CG-OD1	-6.34	1.13	1.25
1	A	602	ARG	CZ-NH2	-6.34	1.25	1.33
1	A	339	HIS	N-CA	-6.33	1.38	1.46
1	A	176	ALA	N-CA	6.30	1.53	1.46
1	B	67	ASN	CA-C	6.30	1.60	1.52
1	B	220	SER	N-CA	6.29	1.53	1.45
1	A	222	ASP	CA-C	6.28	1.60	1.53
1	B	530	ALA	CA-C	6.28	1.60	1.52
1	B	387	THR	CA-C	-6.28	1.44	1.52
1	A	437	PRO	N-CA	-6.26	1.39	1.47
1	A	725	GLN	CG-CD	6.26	1.67	1.52
1	B	547	LEU	N-CA	-6.26	1.38	1.46
1	A	597	VAL	N-CA	-6.20	1.38	1.46
1	A	520	GLN	CD-OE1	6.19	1.35	1.23
1	A	745	PHE	N-CA	-6.16	1.38	1.46
1	B	568	HIS	CA-C	6.13	1.60	1.52
1	A	95	TRP	N-CA	6.12	1.54	1.46
1	A	591	MET	SD-CE	-6.11	1.64	1.79
1	B	680	ALA	N-CA	6.10	1.53	1.46
1	B	647	GLN	CG-CD	6.10	1.67	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	ARG	N-CA	6.09	1.53	1.46
1	A	535	PHE	CA-CB	6.09	1.62	1.53
1	A	434	TYR	CA-C	-6.09	1.44	1.52
1	B	197	PRO	C-O	6.09	1.30	1.23
1	B	524	VAL	CA-CB	6.08	1.61	1.54
1	A	532	ARG	NE-CZ	-6.08	1.26	1.33
1	A	376	ASP	N-CA	6.06	1.53	1.46
1	B	344	ASN	N-CA	-6.06	1.39	1.46
1	B	447	GLN	CA-C	6.03	1.62	1.52
1	A	362	TRP	CA-C	-6.02	1.45	1.52
1	B	447	GLN	N-CA	-6.02	1.37	1.46
1	A	479	GLN	C-N	-6.01	1.25	1.33
1	B	512	ASP	CB-CG	6.00	1.67	1.52
1	A	490	THR	N-CA	-5.99	1.38	1.46
1	B	443	VAL	CA-C	-5.97	1.45	1.52
1	B	624	LEU	N-CA	-5.97	1.38	1.46
1	B	382	ARG	CA-C	5.95	1.60	1.53
1	A	247	ASN	CG-ND2	-5.93	1.20	1.33
1	B	226	GLU	C-O	5.93	1.31	1.23
1	B	574	PHE	C-O	5.92	1.30	1.23
1	A	571	THR	CA-C	5.92	1.59	1.52
1	A	679	ALA	N-CA	5.89	1.53	1.46
1	A	97	ALA	C-O	5.89	1.30	1.24
1	A	289	PRO	N-CA	-5.88	1.40	1.47
1	B	448	ASP	N-CA	5.88	1.50	1.46
1	A	648	SER	CA-C	-5.88	1.45	1.52
1	B	682	ALA	CA-C	5.86	1.60	1.52
1	A	460	ALA	C-O	5.84	1.30	1.24
1	A	120	ALA	N-CA	5.79	1.53	1.46
1	B	179	SER	C-O	5.77	1.30	1.24
1	A	540	ARG	C-O	5.75	1.31	1.23
1	B	731	ASP	N-CA	-5.75	1.39	1.46
1	B	403	ARG	CZ-NH1	-5.74	1.24	1.32
1	B	74	LYS	N-CA	-5.72	1.38	1.46
1	B	244	PRO	CA-CB	-5.71	1.46	1.53
1	B	656	ARG	NE-CZ	-5.71	1.26	1.33
1	A	438	GLU	CD-OE1	-5.70	1.14	1.25
1	A	196	GLU	CG-CD	5.69	1.66	1.52
1	B	654	THR	N-CA	-5.69	1.38	1.45
1	A	382	ARG	CA-C	5.68	1.59	1.53
1	B	62	MET	C-N	-5.67	1.24	1.33
1	B	82	ARG	CZ-NH2	-5.67	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	182	PHE	C-O	-5.67	1.17	1.24
1	B	257	ILE	CA-CB	5.64	1.61	1.54
1	A	393	ARG	N-CA	5.64	1.53	1.46
1	B	656	ARG	C-O	5.63	1.29	1.23
1	A	227	ASN	CA-C	-5.63	1.47	1.53
1	B	606	LYS	CA-C	-5.62	1.45	1.52
1	A	123	ARG	CZ-NH2	5.62	1.40	1.33
1	B	139	TRP	CA-C	-5.58	1.47	1.53
1	B	602	ARG	CZ-NH2	-5.58	1.26	1.33
1	B	535	PHE	CA-C	-5.58	1.45	1.52
1	B	399	GLU	CA-C	-5.57	1.45	1.52
1	A	564	LYS	C-O	5.57	1.30	1.24
1	B	539	GLN	C-O	-5.56	1.16	1.23
1	B	584	GLU	CA-CB	-5.55	1.44	1.53
1	B	701	ARG	C-O	5.54	1.30	1.24
1	A	36	GLY	N-CA	5.54	1.54	1.45
1	B	73	GLU	CG-CD	5.54	1.65	1.52
1	B	532	ARG	CA-CB	-5.53	1.44	1.53
1	B	647	GLN	CA-CB	5.53	1.61	1.53
1	A	207	ILE	CA-C	5.53	1.59	1.52
1	B	313	TYR	C-N	5.53	1.41	1.33
1	B	656	ARG	CD-NE	5.52	1.53	1.46
1	B	536	ASN	CA-C	5.51	1.60	1.52
1	B	685	PHE	N-CA	-5.50	1.39	1.45
1	B	461	ALA	CA-C	5.49	1.59	1.52
1	A	486	ALA	CA-C	-5.48	1.45	1.52
1	B	352	LEU	CA-C	-5.48	1.45	1.52
1	B	726	GLU	CD-OE2	5.47	1.35	1.25
1	B	533	THR	C-N	-5.46	1.26	1.33
1	B	692	THR	CA-CB	-5.44	1.45	1.53
1	A	572	VAL	CA-CB	5.43	1.61	1.54
1	B	573	PRO	CA-C	5.43	1.59	1.52
1	A	370	VAL	C-O	-5.43	1.17	1.24
1	A	418	ARG	CZ-NH1	-5.42	1.25	1.32
1	B	293	VAL	CA-C	-5.41	1.46	1.52
1	A	212	SER	CA-C	5.41	1.59	1.52
1	B	721	SER	CA-CB	-5.41	1.44	1.53
1	B	446	TRP	CD2-CE2	5.38	1.50	1.41
1	A	536	ASN	C-N	-5.37	1.27	1.33
1	A	428	MET	C-N	-5.37	1.25	1.33
1	A	727	LYS	C-N	-5.36	1.27	1.33
1	B	47	LEU	CA-C	5.36	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	ASN	CA-C	5.34	1.60	1.52
1	B	335	THR	N-CA	-5.34	1.40	1.46
1	A	680	ALA	N-CA	5.33	1.52	1.46
1	B	645	VAL	CA-CB	-5.33	1.48	1.54
1	A	377	PRO	C-O	-5.33	1.17	1.24
1	A	207	ILE	N-CA	-5.32	1.40	1.46
1	A	339	HIS	CD2-NE2	5.32	1.43	1.37
1	A	45	ASN	C-O	-5.32	1.16	1.24
1	A	685	PHE	N-CA	-5.31	1.39	1.46
1	A	341	PHE	CA-CB	5.29	1.61	1.53
1	A	82	ARG	CZ-NH2	-5.27	1.26	1.33
1	A	223	ARG	C-O	5.26	1.30	1.23
1	B	468	ALA	C-O	5.24	1.30	1.24
1	B	587	ASP	C-O	5.24	1.29	1.24
1	A	336	GLN	CD-OE1	5.22	1.33	1.23
1	A	699	GLY	N-CA	5.21	1.50	1.45
1	A	302	ILE	CB-CG1	-5.21	1.43	1.53
1	B	494	SER	N-CA	5.21	1.52	1.46
1	B	725	GLN	N-CA	5.21	1.52	1.46
1	B	192	ALA	N-CA	5.19	1.52	1.45
1	A	725	GLN	CD-OE1	5.18	1.33	1.23
1	A	255	ARG	CG-CD	5.18	1.68	1.52
1	B	334	PRO	C-O	5.17	1.31	1.24
1	B	607	GLY	N-CA	5.17	1.50	1.45
1	B	73	GLU	CA-CB	5.17	1.62	1.53
1	A	446	TRP	CD1-NE1	-5.17	1.26	1.37
1	A	563	ALA	N-CA	-5.14	1.40	1.46
1	A	658	GLN	CD-OE1	-5.13	1.13	1.23
1	B	56	SER	C-O	5.12	1.30	1.23
1	B	532	ARG	N-CA	-5.12	1.40	1.46
1	A	427	ASP	CA-C	-5.11	1.45	1.52
1	B	647	GLN	CA-C	5.11	1.60	1.53
1	B	44	PRO	C-N	-5.10	1.26	1.33
1	A	302	ILE	C-O	5.09	1.30	1.24
1	A	404	ARG	NE-CZ	-5.09	1.27	1.33
1	A	533	THR	C-N	-5.09	1.27	1.33
1	B	570	VAL	CA-CB	-5.09	1.50	1.55
1	B	365	LYS	N-CA	5.08	1.52	1.46
1	A	59	SER	C-O	-5.07	1.17	1.24
1	A	430	PRO	CA-CB	-5.07	1.46	1.53
1	A	450	ILE	N-CA	5.07	1.51	1.46
1	A	319	ALA	CA-C	-5.07	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	535	PHE	CA-C	-5.06	1.46	1.52
1	A	68	TYR	N-CA	5.06	1.52	1.46
1	A	503	ALA	C-O	5.06	1.30	1.23
1	B	251	VAL	CA-CB	5.06	1.60	1.54
1	A	584	GLU	C-O	-5.06	1.17	1.24
1	B	322	ILE	N-CA	-5.05	1.39	1.46
1	B	605	LEU	CB-CG	-5.04	1.43	1.53
1	A	223	ARG	CG-CD	-5.03	1.37	1.52
1	A	199	ASP	N-CA	5.02	1.53	1.46
1	A	712	LEU	N-CA	-5.02	1.39	1.46
1	A	599	ASP	CA-C	-5.02	1.47	1.53
1	B	408	ASN	CA-CB	-5.02	1.47	1.53
1	B	429	GLY	C-N	-5.01	1.27	1.33
1	A	694	GLU	CA-C	5.01	1.59	1.52
1	A	418	ARG	NE-CZ	5.01	1.38	1.33
1	B	513	TRP	CA-C	-5.00	1.46	1.52
1	B	41	ASP	N-CA	-5.00	1.40	1.46

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	ARG	NE-CZ-NH2	-26.92	94.97	119.20
1	A	532	ARG	NE-CZ-NH1	19.64	141.14	121.50
1	A	532	ARG	CD-NE-CZ	13.04	142.65	124.40
1	B	46	GLN	N-CA-C	-10.77	94.55	110.48
1	A	46	GLN	N-CA-C	-9.70	96.13	110.48
1	B	54	ARG	CG-CD-NE	-8.60	93.09	112.00
1	A	46	GLN	CA-CB-CG	8.28	130.66	114.10
1	A	198	ALA	CA-C-N	-8.23	110.31	123.23
1	A	198	ALA	C-N-CA	-8.23	110.31	123.23
1	B	48	ASP	N-CA-C	8.15	122.92	107.75
1	B	572	VAL	O-C-N	8.10	128.98	121.61
1	A	47	LEU	N-CA-CB	-8.09	98.16	110.04
1	B	199	ASP	CA-C-O	-7.99	112.45	121.39
1	B	571	THR	CA-C-N	-7.75	115.91	123.04
1	B	571	THR	C-N-CA	-7.75	115.91	123.04
1	A	596	PRO	CB-CA-C	7.72	118.36	111.87
1	A	438	GLU	CG-CD-OE1	-7.52	101.10	118.40
1	B	569	ALA	N-CA-C	-7.50	99.38	110.48
1	A	429	GLY	O-C-N	7.49	129.25	121.77
1	B	375	PHE	O-C-N	7.32	129.86	122.10
1	B	345	LEU	O-C-N	7.27	129.83	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	MET	CA-C-N	-7.27	112.31	120.53
1	B	62	MET	C-N-CA	-7.27	112.31	120.53
1	A	592	ALA	N-CA-C	7.19	120.03	111.33
1	A	571	THR	OG1-CB-CG2	-6.86	95.59	109.30
1	A	492	ARG	NE-CZ-NH2	-6.79	113.09	119.20
1	B	680	ALA	N-CA-C	6.76	118.65	111.28
1	A	86	ALA	N-CA-C	6.75	118.64	111.28
1	B	82	ARG	NE-CZ-NH2	-6.75	113.13	119.20
1	B	445	LEU	O-C-N	-6.68	114.40	122.22
1	B	47	LEU	N-CA-CB	-6.66	100.25	110.04
1	B	624	LEU	N-CA-C	6.64	121.23	113.20
1	B	73	GLU	CG-CD-OE2	6.61	133.60	118.40
1	B	46	GLN	CA-CB-CG	6.57	127.23	114.10
1	A	196	GLU	O-C-N	6.55	125.90	121.71
1	B	591	MET	CA-C-O	6.54	127.49	119.97
1	B	428	MET	CA-CB-CG	-6.50	101.10	114.10
1	B	46	GLN	O-C-N	-6.49	115.63	122.96
1	B	35	ASN	CB-CA-C	6.44	122.33	110.10
1	B	54	ARG	CA-C-N	-6.32	113.64	122.74
1	B	54	ARG	C-N-CA	-6.32	113.64	122.74
1	B	438	GLU	CG-CD-OE1	-6.31	103.89	118.40
1	A	326	LEU	O-C-N	-6.28	116.02	123.06
1	A	345	LEU	O-C-N	6.28	128.78	122.12
1	A	47	LEU	CA-C-O	-6.20	114.98	121.55
1	B	730	ARG	NE-CZ-NH1	-6.17	115.33	121.50
1	A	46	GLN	CA-C-O	6.05	128.43	121.47
1	B	198	ALA	CA-C-N	-6.00	113.88	122.77
1	B	198	ALA	C-N-CA	-6.00	113.88	122.77
1	B	312	ALA	N-CA-C	-5.98	105.75	113.16
1	B	303	GLU	N-CA-C	5.96	119.65	112.38
1	B	572	VAL	CA-C-O	-5.94	115.33	119.19
1	B	66	PHE	CA-C-N	-5.92	114.46	122.86
1	B	66	PHE	C-N-CA	-5.92	114.46	122.86
1	A	742	LEU	CA-C-O	-5.91	114.29	120.55
1	A	544	GLN	O-C-N	5.87	129.94	123.25
1	B	319	ALA	N-CA-C	5.87	119.26	111.75
1	B	255[A]	ARG	O-C-N	5.85	128.32	122.12
1	B	255[B]	ARG	O-C-N	5.85	128.32	122.12
1	A	62	MET	CA-C-N	-5.84	114.07	120.44
1	A	62	MET	C-N-CA	-5.84	114.07	120.44
1	B	727	LYS	O-C-N	5.84	128.31	122.12
1	B	47	LEU	CA-C-O	-5.83	115.37	121.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	450	ILE	CB-CA-C	-5.78	104.53	110.13
1	B	46	GLN	CB-CG-CD	5.76	122.39	112.60
1	A	649	ARG	CB-CG-CD	-5.75	98.08	111.30
1	B	123	ARG	NE-CZ-NH1	5.70	127.20	121.50
1	B	596	PRO	CB-CA-C	5.69	116.65	111.87
1	A	55	HIS	CB-CA-C	5.69	120.21	111.39
1	B	76	ASP	OD1-CG-OD2	5.68	136.53	122.90
1	A	429	GLY	CA-C-N	-5.64	114.15	119.85
1	A	429	GLY	C-N-CA	-5.64	114.15	119.85
1	A	255	ARG	CD-NE-CZ	5.64	132.29	124.40
1	A	344	ASN	O-C-N	-5.61	115.75	122.15
1	B	247[A]	ASN	N-CA-C	-5.61	101.44	109.24
1	B	247[B]	ASN	N-CA-C	-5.61	101.44	109.24
1	B	427	ASP	OD1-CG-OD2	5.59	136.32	122.90
1	A	404	ARG	NE-CZ-NH1	5.59	127.09	121.50
1	A	450	ILE	N-CA-CB	-5.57	105.65	111.61
1	B	585	GLN	O-C-N	-5.56	115.22	122.39
1	B	690	ARG	NE-CZ-NH2	5.56	124.20	119.20
1	A	680	ALA	N-CA-C	5.55	117.33	111.28
1	A	362	TRP	O-C-N	-5.55	115.98	123.19
1	B	450	ILE	CA-C-O	-5.54	116.07	119.51
1	A	529	GLU	N-CA-C	-5.52	105.34	111.36
1	B	570	VAL	CA-C-O	-5.52	116.32	120.96
1	A	237	ILE	N-CA-C	5.52	115.61	110.42
1	B	76	ASP	CB-CG-OD2	-5.51	105.72	118.40
1	A	587	ASP	O-C-N	-5.50	115.20	122.57
1	A	46	GLN	O-C-N	-5.50	116.75	122.96
1	A	438	GLU	CB-CG-CD	-5.49	103.27	112.60
1	A	690	ARG	NE-CZ-NH1	-5.46	116.04	121.50
1	B	382	ARG	O-C-N	5.46	127.53	121.53
1	B	449	PRO	O-C-N	5.43	129.74	123.06
1	A	196	GLU	CA-C-O	-5.43	115.51	120.50
1	B	595	GLU	O-C-N	5.43	126.13	121.30
1	B	429	GLY	O-C-N	5.42	127.19	121.77
1	A	263	ARG	NE-CZ-NH2	-5.42	114.33	119.20
1	B	434	TYR	CD1-CG-CD2	-5.39	110.01	118.10
1	A	447	GLN	CA-C-N	-5.38	117.94	123.10
1	A	447	GLN	C-N-CA	-5.38	117.94	123.10
1	A	37	THR	CA-C-O	-5.37	114.93	121.05
1	A	212	SER	O-C-N	5.36	129.41	122.81
1	A	406	HIS	N-CA-CB	-5.36	102.23	110.16
1	A	449	PRO	O-C-N	5.33	129.61	123.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	ALA	N-CA-C	-5.32	105.49	111.28
1	B	570	VAL	O-C-N	5.31	127.59	122.97
1	A	48	ASP	N-CA-C	5.31	118.08	107.62
1	A	583	GLN	O-C-N	5.29	127.73	122.12
1	A	692	THR	N-CA-C	5.29	120.00	113.50
1	A	292	ASN	N-CA-C	5.28	118.82	112.38
1	B	46	GLN	CG-CD-NE2	5.28	124.32	116.40
1	B	248	PRO	N-CA-C	5.26	119.58	112.48
1	B	450	ILE	N-CA-CB	-5.23	106.83	112.37
1	B	729	VAL	O-C-N	-5.21	116.81	121.91
1	A	199	ASP	CA-C-N	-5.20	116.39	123.10
1	A	199	ASP	C-N-CA	-5.20	116.39	123.10
1	B	93	ASP	N-CA-C	5.20	118.88	112.54
1	A	69	ALA	N-CA-C	5.19	116.94	111.28
1	A	54	ARG	CG-CD-NE	-5.19	100.59	112.00
1	B	206	LYS	CG-CD-CE	5.18	123.21	111.30
1	A	434	TYR	O-C-N	-5.17	116.57	122.93
1	A	710	SER	N-CA-C	5.17	117.65	111.71
1	B	302	ILE	CB-CA-C	5.15	118.79	112.04
1	B	460	ALA	N-CA-C	5.14	117.79	111.82
1	B	533	THR	CA-C-N	5.14	127.17	120.28
1	B	533	THR	C-N-CA	5.14	127.17	120.28
1	A	375	PHE	O-C-N	5.14	127.54	122.10
1	B	520	GLN	CB-CG-CD	5.08	121.24	112.60
1	A	46	GLN	CB-CA-C	5.07	118.79	109.46
1	A	361	GLN	CA-C-O	-5.07	116.00	121.38
1	A	178	GLU	CA-C-O	-5.06	115.18	120.55
1	A	73	GLU	CB-CG-CD	5.05	121.19	112.60
1	B	434	TYR	CB-CG-CD1	5.05	128.37	120.80
1	A	93	ASP	N-CA-C	5.05	118.70	112.54
1	B	726	GLU	CG-CD-OE2	5.03	129.97	118.40
1	B	445	LEU	CA-C-O	5.02	125.78	120.10
1	B	692	THR	N-CA-C	5.02	119.68	113.50
1	A	199	ASP	CA-C-O	-5.01	114.94	121.11
1	B	434	TYR	O-C-N	-5.00	116.78	122.93
1	A	431	ARG	NE-CZ-NH2	5.00	123.70	119.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	A	393	ARG	Sidechain
1	A	47	LEU	Mainchain
1	A	471	LEU	Mainchain
1	B	199	ASP	Mainchain
1	B	438	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	5526	0	5342	23	0
1	B	5538	0	5348	26	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	2	0	0	0	0
4	B	2	0	0	1	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	8	0	14	2	0
7	A	8	0	14	2	0
7	B	8	0	14	1	0
8	A	955	0	0	11	2
8	B	911	0	0	12	2
All	All	13056	0	10792	55	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 (55) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:ALA:O	1:B:570:VAL:HG23	1.63	0.99
1:A:119[B]:THR:HG21	8:A:1227:HOH:O	1.67	0.94
1:B:119[B]:THR:HG21	8:B:1263:HOH:O	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:GLN:OE1	8:B:901:HOH:O	1.88	0.90
1:B:431:ARG:HD2	8:B:1576:HOH:O	1.78	0.83
1:A:589:GLU:HG2	8:A:1552:HOH:O	1.79	0.82
1:B:569:ALA:O	1:B:570:VAL:CG2	2.29	0.80
1:B:431:ARG:CD	8:B:1576:HOH:O	2.29	0.77
1:B:610:ARG:HD3	1:B:611:VAL:HG23	1.74	0.70
6:A:805:MRD:O4	6:A:805:MRD:H1C2	1.93	0.68
1:A:610:ARG:HD3	1:A:611:VAL:HG23	1.76	0.67
1:A:633[B]:VAL:CG2	1:A:719:TYR:CZ	2.77	0.67
1:A:76:ASP:OD1	8:A:903:HOH:O	2.12	0.66
1:B:512:ASP:OD1	8:B:902:HOH:O	2.14	0.65
1:B:647:GLN:HG2	8:B:1043:HOH:O	1.97	0.65
1:B:255[B]:ARG:NH2	8:B:907:HOH:O	2.28	0.62
1:B:512:ASP:HB2	8:B:1460:HOH:O	2.00	0.62
1:A:647:GLN:HG2	8:A:1101:HOH:O	2.01	0.61
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.85	0.60
1:A:407:GLU:HG2	8:A:1547:HOH:O	2.02	0.59
1:B:54:ARG:HG3	1:B:199:ASP:OD2	2.07	0.54
1:A:585:GLN:NE2	8:A:911:HOH:O	2.40	0.54
1:B:591:MET:SD	1:B:594:LEU:HD12	2.48	0.54
1:B:662:ASN:H	1:B:725:GLN:HE22	1.57	0.53
6:A:805:MRD:O4	6:A:805:MRD:C1	2.57	0.53
4:B:803:OXY:O2	8:B:903:HOH:O	2.19	0.51
1:B:519:GLU:OE1	8:B:904:HOH:O	2.19	0.50
1:A:69:ALA:O	1:A:73:GLU:HG3	2.12	0.49
1:A:591:MET:SD	1:A:594:LEU:HD12	2.53	0.49
1:A:504:ARG:HD2	8:A:1062:HOH:O	2.13	0.48
7:A:806:MPD:HM2	8:A:1605:HOH:O	2.14	0.47
1:A:633[B]:VAL:HG23	1:A:719:TYR:CE1	2.49	0.47
1:A:593:VAL:HG13	8:A:922:HOH:O	2.14	0.47
1:A:633[B]:VAL:CG2	1:A:719:TYR:CE1	2.98	0.47
7:B:804:MPD:O4	7:B:804:MPD:H11	2.15	0.46
1:A:509:PRO:HD2	1:A:591:MET:HG2	1.98	0.46
1:A:54:ARG:HB3	1:A:55:HIS:CD2	2.51	0.46
1:B:569:ALA:C	1:B:570:VAL:HG23	2.38	0.45
1:B:591:MET:HB2	1:B:591:MET:HE2	1.70	0.45
1:B:633[A]:VAL:CG2	1:B:719:TYR:CE1	3.01	0.44
1:B:186:GLY:HA2	8:B:911:HOH:O	2.17	0.44
1:A:633[B]:VAL:HG21	1:A:719:TYR:CZ	2.51	0.43
1:A:47:LEU:HB2	8:A:908:HOH:O	2.18	0.43
1:B:247[A]:ASN:ND2	8:B:929:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:650:HIS:HD2	1:B:698:THR:OG1	2.01	0.43
1:A:591:MET:HE2	1:A:591:MET:HB2	1.79	0.43
1:A:602:ARG:HB3	1:A:645:VAL:HG23	2.01	0.42
1:A:143:ALA:HA	1:A:309:TRP:CH2	2.54	0.42
1:A:346:PHE:CZ	1:A:403:ARG:HG2	2.55	0.41
7:A:806:MPD:C1	8:A:1091:HOH:O	2.68	0.41
1:B:54:ARG:HB3	1:B:55:HIS:CD2	2.56	0.41
1:B:602:ARG:HB3	1:B:645:VAL:HG23	2.02	0.41
1:A:608:LYS:HD3	1:A:608:LYS:HA	1.91	0.41
1:B:540:ARG:CZ	1:B:540:ARG:HA	2.51	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:1330:HOH:O	8:B:1223:HOH:O[2_444]	2.03	0.17
8:A:1547:HOH:O	8:B:1138:HOH:O[2_444]	2.08	0.12

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	715/728 (98%)	705 (99%)	10 (1%)	0	100	100
1	B	718/728 (99%)	707 (98%)	11 (2%)	0	100	100
All	All	1433/1456 (98%)	1412 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	553/559 (99%)	544 (98%)	9 (2%)	55	33
1	B	555/559 (99%)	544 (98%)	11 (2%)	48	24
All	All	1108/1118 (99%)	1088 (98%)	20 (2%)	53	28

All (20) 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	141	ASP
1	A	227	ASN
1	A	379	LYS
1	A	469	LYS
1	A	608	LYS
1	A	610	ARG
1	B	40	ARG
1	B	46	GLN
1	B	64	LYS
1	B	141	ASP
1	B	540	ARG
1	B	608	LYS
1	B	610	ARG
1	B	633[A]	VAL
1	B	633[B]	VAL
1	B	649	ARG
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	247	ASN
1	A	520	GLN

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Mol	Chain	Res	Type
1	B	46	GLN
1	B	520	GLN
1	B	544	GLN
1	B	650	HIS
1	B	725	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	14,17,18	1.74	4 (28%)	12,23,25	2.00	4 (33%)
1	TOX	A	111[A]	2	14,17,18	1.34	3 (21%)	12,23,25	2.33	4 (33%)
1	TOX	B	111[B]	-	14,17,18	1.74	4 (28%)	12,23,25	2.00	4 (33%)
1	TOX	A	111[B]	-	14,17,18	1.34	3 (21%)	12,23,25	2.33	4 (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
1	TOX	B	111[A]	2	-	2/5/8/10	0/2/2/2
1	TOX	A	111[A]	2	-	2/5/8/10	0/2/2/2
1	TOX	B	111[B]	-	-	2/5/8/10	0/2/2/2
1	TOX	A	111[B]	-	-	2/5/8/10	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111[A]	TOX	CZ2-CE2	-3.18	1.34	1.39
1	B	111[B]	TOX	CZ2-CE2	-3.18	1.34	1.39
1	B	111[A]	TOX	O1-NE1	-2.98	1.35	1.39
1	B	111[B]	TOX	O1-NE1	-2.98	1.35	1.39
1	B	111[A]	TOX	O-C	2.70	1.30	1.20
1	B	111[B]	TOX	O-C	2.70	1.30	1.20
1	A	111[A]	TOX	CE3-CD2	-2.57	1.36	1.39
1	A	111[B]	TOX	CE3-CD2	-2.57	1.36	1.39
1	B	111[A]	TOX	CD2-CG	2.38	1.47	1.44
1	B	111[B]	TOX	CD2-CG	2.38	1.47	1.44
1	A	111[A]	TOX	CE2-NE1	-2.22	1.35	1.39
1	A	111[B]	TOX	CE2-NE1	-2.22	1.35	1.39
1	A	111[A]	TOX	CH2-CZ2	-2.09	1.35	1.38
1	A	111[B]	TOX	CH2-CZ2	-2.09	1.35	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111[A]	TOX	CZ2-CE2-CD2	-5.39	115.94	121.95
1	A	111[B]	TOX	CZ2-CE2-CD2	-5.39	115.94	121.95
1	B	111[A]	TOX	CZ2-CE2-NE1	4.36	136.31	129.37
1	B	111[B]	TOX	CZ2-CE2-NE1	4.36	136.31	129.37
1	A	111[A]	TOX	CE2-CD2-CG	-3.62	104.06	107.39
1	A	111[B]	TOX	CE2-CD2-CG	-3.62	104.06	107.39
1	A	111[A]	TOX	CZ2-CE2-NE1	3.09	134.30	129.37
1	A	111[B]	TOX	CZ2-CE2-NE1	3.09	134.30	129.37
1	B	111[A]	TOX	CD2-CG-CD1	-2.68	103.91	106.34
1	B	111[B]	TOX	CD2-CG-CD1	-2.68	103.91	106.34
1	A	111[A]	TOX	CE3-CD2-CE2	2.64	122.28	119.24
1	A	111[B]	TOX	CE3-CD2-CE2	2.64	122.28	119.24
1	B	111[A]	TOX	CE3-CD2-CG	-2.38	130.30	133.85
1	B	111[B]	TOX	CE3-CD2-CG	-2.38	130.30	133.85
1	B	111[A]	TOX	CZ3-CE3-CD2	-2.06	116.08	119.80
1	B	111[B]	TOX	CZ3-CE3-CD2	-2.06	116.08	119.80

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

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Mol	Chain	Res	Type	Atoms
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 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	$\# Z > 2$
4	OXY	B	803	-	1,1,1	1.25	0	-		
7	MPD	A	806	-	7,7,7	1.75	2 (28%)	9,10,10	1.16	1 (11%)
5	PO4	B	805	-	4,4,4	1.94	1 (25%)	6,6,6	2.63	3 (50%)
7	MPD	B	804	-	7,7,7	0.70	0	9,10,10	2.06	4 (44%)
2	HEM	B	801	1	50,50,50	1.52	9 (18%)	67,82,82	1.33	8 (11%)
4	OXY	A	803	-	1,1,1	0.71	0	-		
2	HEM	A	801	1	50,50,50	1.46	7 (14%)	67,82,82	1.57	17 (25%)
5	PO4	A	804	-	4,4,4	2.20	2 (50%)	6,6,6	3.35	3 (50%)
6	MRD	A	805	-	7,7,7	0.76	0	9,10,10	1.74	4 (44%)

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	-	-	1/5/5/5	-
7	MPD	B	804	-	-	3/5/5/5	-
2	HEM	B	801	1	-	2/14/54/54	-
2	HEM	A	801	1	-	3/14/54/54	-
6	MRD	A	805	-	-	1/5/5/5	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	FE-NB	4.42	2.08	1.94
2	B	801	HEM	C1B-NB	-4.13	1.33	1.40
2	B	801	HEM	FE-NB	3.63	2.06	1.94
7	A	806	MPD	O2-C2	3.56	1.53	1.44
5	A	804	PO4	P-O4	-3.33	1.44	1.54
5	B	805	PO4	P-O3	-3.20	1.45	1.54
2	A	801	HEM	FE-NA	3.15	2.05	1.95
2	B	801	HEM	C4A-NA	2.92	1.45	1.39
2	B	801	HEM	FE-ND	2.72	2.03	1.94
5	A	804	PO4	P-O1	2.53	1.56	1.50
2	A	801	HEM	C1D-C2D	2.52	1.49	1.44
2	B	801	HEM	C2A-C3A	-2.50	1.32	1.38
2	A	801	HEM	C1A-NA	-2.50	1.34	1.39
2	A	801	HEM	C4A-NA	-2.37	1.35	1.39
2	A	801	HEM	O1A-CGA	2.30	1.29	1.22
2	A	801	HEM	C1B-NB	-2.29	1.36	1.40
2	B	801	HEM	CMB-C2B	2.28	1.55	1.50
2	B	801	HEM	C1D-C2D	2.25	1.49	1.44
2	B	801	HEM	CHC-C1C	2.17	1.42	1.38
2	B	801	HEM	C1A-NA	-2.16	1.35	1.39
7	A	806	MPD	C3-C2	-2.12	1.47	1.54

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	804	PO4	O3-P-O1	-6.71	87.22	110.95
2	A	801	HEM	CHA-C4D-ND	-4.65	118.62	124.37
5	B	805	PO4	O3-P-O2	4.39	121.57	107.91
5	B	805	PO4	O2-P-O1	-3.76	97.65	110.95
2	A	801	HEM	C3C-C2C-C1C	-3.59	103.65	107.05
5	A	804	PO4	O4-P-O1	3.20	122.27	110.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	804	MPD	O2-C2-C3	-3.19	97.32	109.27
7	B	804	MPD	O4-C4-C5	3.06	122.63	109.45
2	B	801	HEM	CHC-C4B-NB	2.96	127.61	124.42
2	A	801	HEM	C4B-C3B-C2B	-2.83	104.68	107.28
2	A	801	HEM	CAA-CBA-CGA	-2.82	106.18	113.67
6	A	805	MRD	CM-C2-C1	-2.81	104.34	110.63
2	A	801	HEM	C1B-NB-C4B	2.75	108.47	105.21
6	A	805	MRD	O2-C2-CM	2.72	116.48	107.99
7	A	806	MPD	CM-C2-C1	-2.69	104.60	110.63
7	B	804	MPD	C1-C2-C3	2.47	120.86	110.20
2	B	801	HEM	C4D-ND-C1D	2.47	108.13	105.21
2	A	801	HEM	CHC-C1C-C2C	-2.45	120.38	125.49
2	B	801	HEM	C3D-C4D-ND	-2.37	107.57	110.17
5	A	804	PO4	O2-P-O1	2.35	119.25	110.95
2	B	801	HEM	CAA-CBA-CGA	-2.34	107.45	113.67
2	B	801	HEM	C4A-C3A-C2A	2.33	109.49	106.82
2	A	801	HEM	O1D-CGD-CBD	-2.31	115.77	123.09
6	A	805	MRD	C1-C2-C3	2.28	120.02	110.20
6	A	805	MRD	CM-C2-C3	-2.22	100.61	110.20
2	B	801	HEM	CHA-C4D-ND	2.20	127.08	124.37
2	A	801	HEM	O2D-CGD-CBD	2.18	120.89	114.00
2	A	801	HEM	C3B-C2B-C1B	2.17	108.04	106.41
2	A	801	HEM	CMC-C2C-C1C	2.16	128.54	124.73
2	A	801	HEM	CMB-C2B-C1B	-2.15	121.67	125.03
2	B	801	HEM	C1C-CHC-C4B	-2.12	121.51	126.02
2	A	801	HEM	CBD-CAD-C3D	2.12	118.40	112.53
2	A	801	HEM	CHD-C1D-ND	2.11	126.70	124.42
7	B	804	MPD	O2-C2-CM	2.10	114.54	107.99
2	A	801	HEM	C2C-C1C-NC	2.08	113.49	109.64
2	A	801	HEM	O2A-CGA-CBA	2.06	120.50	114.00
2	A	801	HEM	C3D-C4D-ND	2.03	112.40	110.17
2	A	801	HEM	C4A-C3A-C2A	2.03	109.14	106.82
5	B	805	PO4	O4-P-O2	2.02	114.21	107.91
2	B	801	HEM	CAD-CBD-CGD	2.02	119.02	113.67

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	804	MPD	C1-C2-C3-C4
7	B	804	MPD	CM-C2-C3-C4
2	B	801	HEM	CAA-CBA-CGA-O2A

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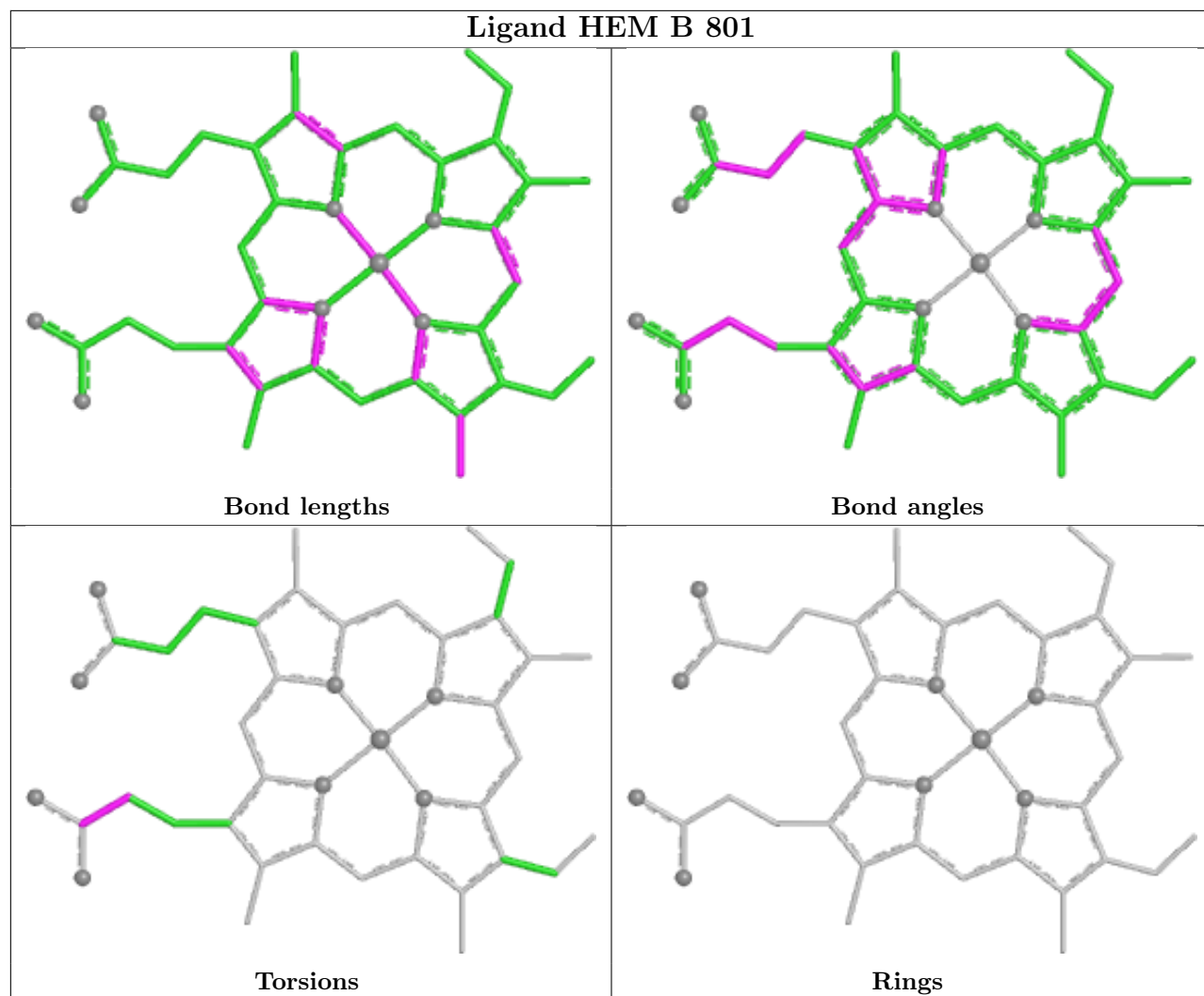
Mol	Chain	Res	Type	Atoms
2	A	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	CAA-CBA-CGA-O1A
7	A	806	MPD	O2-C2-C3-C4
7	B	804	MPD	O2-C2-C3-C4
6	A	805	MRD	C2-C3-C4-O4
2	A	801	HEM	CAD-CBD-CGD-O2D

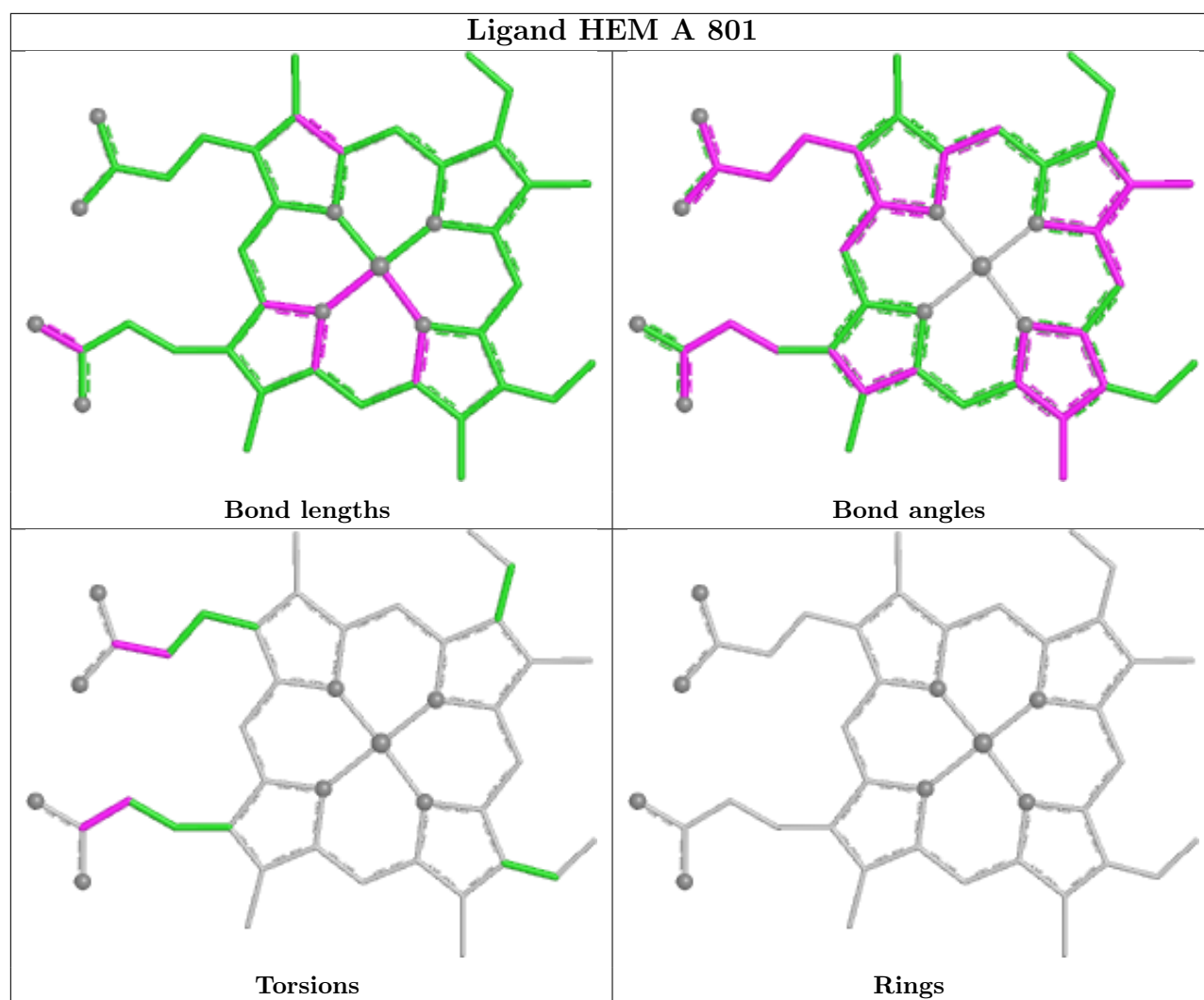
There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	803	OXY	1	0
7	A	806	MPD	2	0
7	B	804	MPD	1	0
6	A	805	MRD	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%)	-0.49	7 (0%) 79 83	8, 17, 34, 81	6 (0%)
1	B	713/728 (97%)	-0.48	8 (1%) 78 82	8, 17, 34, 94	8 (1%)
All	All	1425/1456 (97%)	-0.49	15 (1%) 78 82	8, 17, 34, 94	14 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	4.3
1	B	35	ASN	4.0
1	B	748	ALA	4.0
1	B	610	ARG	3.0
1	B	65	ASP	2.7
1	A	608	LYS	2.4
1	B	568	HIS	2.4
1	A	40	ARG	2.4
1	A	55	HIS	2.3
1	B	540	ARG	2.2
1	A	610	ARG	2.2
1	A	454	ASP	2.1
1	B	454	ASP	2.1
1	A	647	GLN	2.0
1	B	608	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($\text{\AA}^2$)	Q<0.9
1	TOX	B	111[A]	16/17	0.98	0.04	11,12,17,21	1
1	TOX	B	111[B]	16/17	0.98	0.04	11,12,14,21	1
1	TOX	A	111[A]	16/17	0.99	0.03	10,12,16,19	2
1	TOX	A	111[B]	16/17	0.99	0.03	10,12,14,19	2

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

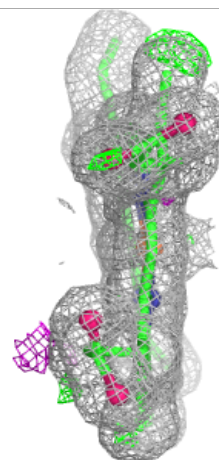
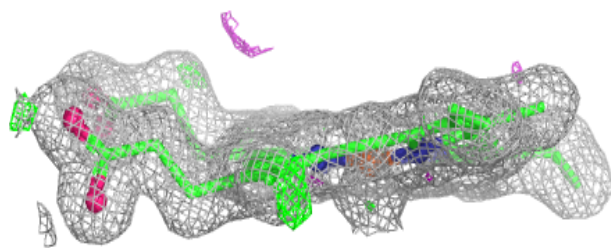
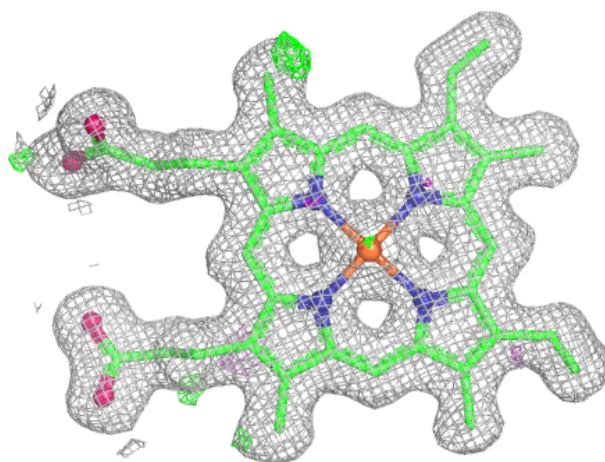
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

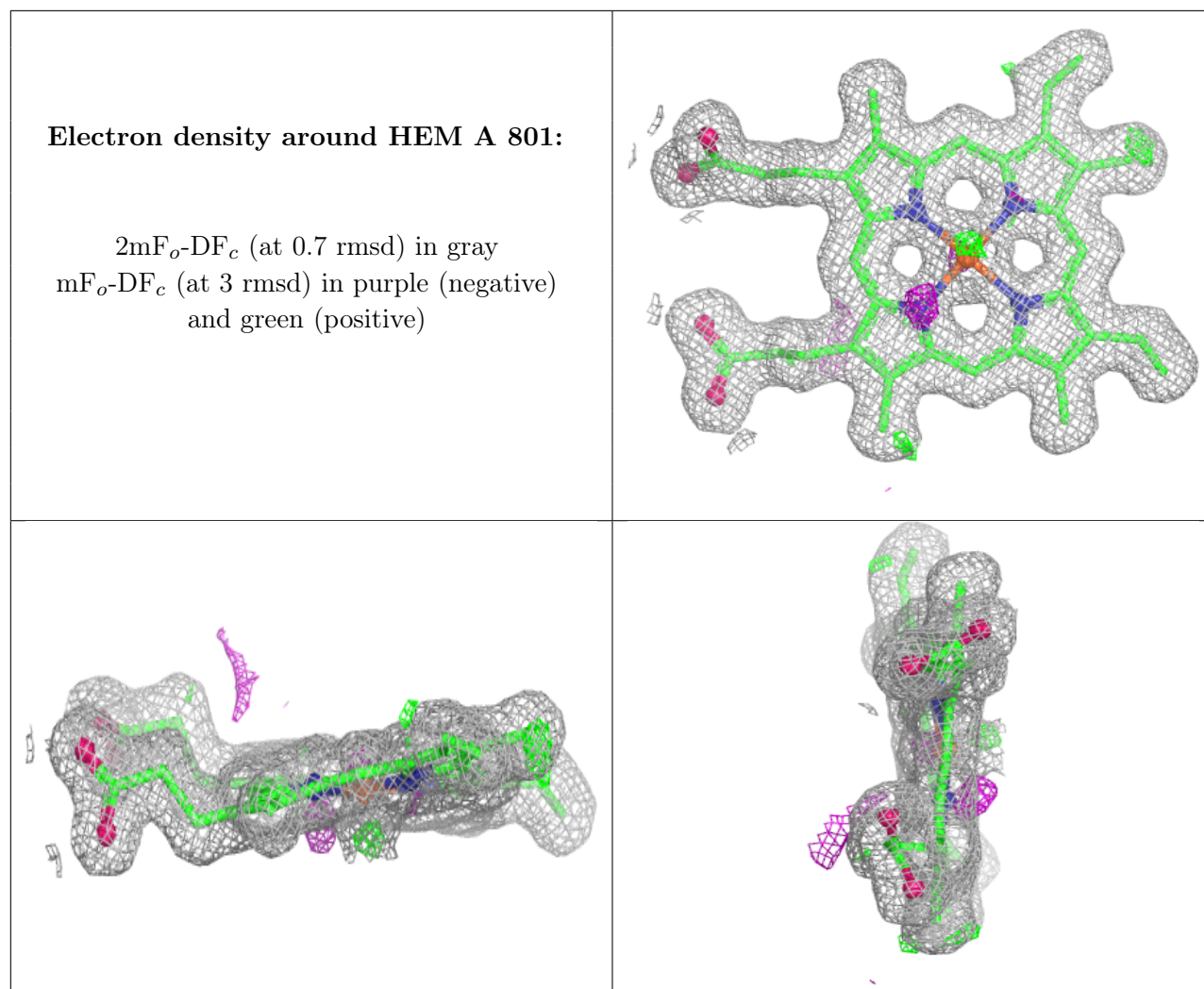
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MPD	B	804	8/8	0.85	0.15	50,53,57,61	0
6	MRD	A	805	8/8	0.88	0.14	45,50,61,62	0
7	MPD	A	806	8/8	0.89	0.11	32,35,46,52	0
4	OXY	A	803	2/2	0.90	0.20	28,28,28,31	0
5	PO4	B	805	5/5	0.92	0.09	37,51,57,63	0
4	OXY	B	803	2/2	0.92	0.18	24,24,24,28	0
5	PO4	A	804	5/5	0.94	0.08	38,42,51,57	0
3	NA	B	802	1/1	0.98	0.06	20,20,20,20	0
3	NA	A	802	1/1	0.98	0.06	18,18,18,18	0
2	HEM	B	801	43/43	0.99	0.04	12,13,15,18	0
2	HEM	A	801	43/43	0.99	0.04	11,13,15,15	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 ⓘ

There are no such residues in this entry.