



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 3, 2026 – 09:03 AM EDT

PDB ID : 5WHS / pdb_00005whs
Title : Crystal structure of the catalase-peroxidase from *Neurospora crassa* at 2.6 Å
Authors : Diaz-Vilchis, A.; Vega-Garcia, V.; Rudino-Pinera, E.; Hansberg, W.
Deposited on : 2017-07-18
Resolution : 2.60 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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

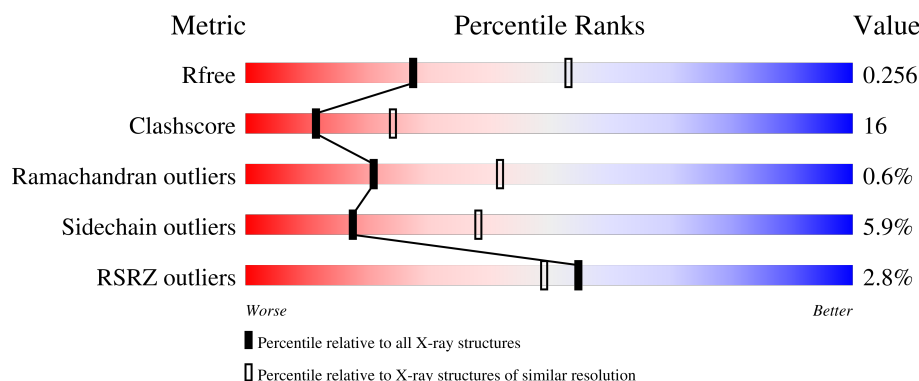
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

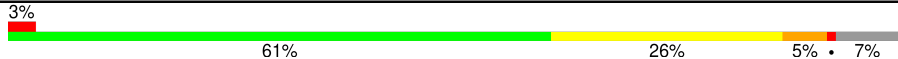
The reported resolution of this entry is 2.60 Å.

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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	768	
1	B	768	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11962 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	0	0
			5597	3555	977	1053	12			
1	B	713	Total	C	N	O	S	0	0	0
			5597	3555	977	1053	12			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	expression tag	UNP Q8X182
A	-13	ARG	-	expression tag	UNP Q8X182
A	-12	GLY	-	expression tag	UNP Q8X182
A	-11	SER	-	expression tag	UNP Q8X182
A	-10	HIS	-	expression tag	UNP Q8X182
A	-9	HIS	-	expression tag	UNP Q8X182
A	-8	HIS	-	expression tag	UNP Q8X182
A	-7	HIS	-	expression tag	UNP Q8X182
A	-6	HIS	-	expression tag	UNP Q8X182
A	-5	HIS	-	expression tag	UNP Q8X182
A	-4	GLY	-	expression tag	UNP Q8X182
A	-3	SER	-	expression tag	UNP Q8X182
A	-2	ALA	-	expression tag	UNP Q8X182
A	-1	CYS	-	expression tag	UNP Q8X182
A	0	GLU	-	expression tag	UNP Q8X182
A	1	LEU	-	expression tag	UNP Q8X182
A	2	SER	-	expression tag	UNP Q8X182
A	3	GLU	-	expression tag	UNP Q8X182
A	4	CYS	-	expression tag	UNP Q8X182
A	5	PRO	-	expression tag	UNP Q8X182
A	6	VAL	-	expression tag	UNP Q8X182
A	742	LYS	-	expression tag	UNP Q8X182
A	743	GLN	-	expression tag	UNP Q8X182
A	744	GLU	-	expression tag	UNP Q8X182
A	745	GLY	-	expression tag	UNP Q8X182

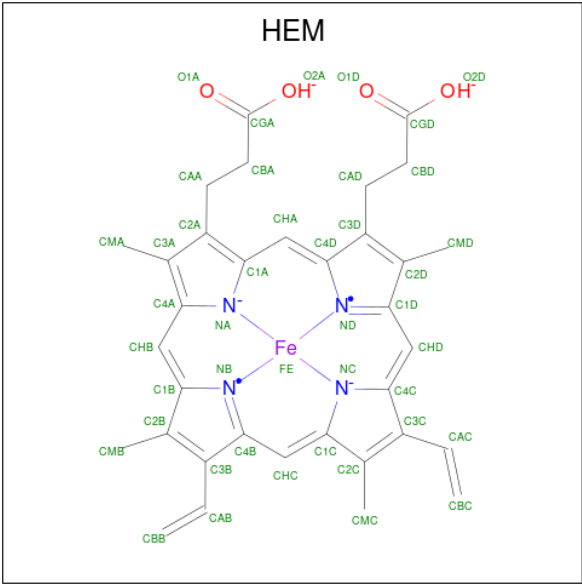
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Chain	Residue	Modelled	Actual	Comment	Reference
A	746	ARG	-	expression tag	UNP Q8X182
A	747	GLY	-	expression tag	UNP Q8X182
A	748	GLN	-	expression tag	UNP Q8X182
A	749	ASN	-	expression tag	UNP Q8X182
A	750	ALA	-	expression tag	UNP Q8X182
A	751	PRO	-	expression tag	UNP Q8X182
A	752	LYS	-	expression tag	UNP Q8X182
A	753	LEU	-	expression tag	UNP Q8X182
B	-14	MET	-	expression tag	UNP Q8X182
B	-13	ARG	-	expression tag	UNP Q8X182
B	-12	GLY	-	expression tag	UNP Q8X182
B	-11	SER	-	expression tag	UNP Q8X182
B	-10	HIS	-	expression tag	UNP Q8X182
B	-9	HIS	-	expression tag	UNP Q8X182
B	-8	HIS	-	expression tag	UNP Q8X182
B	-7	HIS	-	expression tag	UNP Q8X182
B	-6	HIS	-	expression tag	UNP Q8X182
B	-5	HIS	-	expression tag	UNP Q8X182
B	-4	GLY	-	expression tag	UNP Q8X182
B	-3	SER	-	expression tag	UNP Q8X182
B	-2	ALA	-	expression tag	UNP Q8X182
B	-1	CYS	-	expression tag	UNP Q8X182
B	0	GLU	-	expression tag	UNP Q8X182
B	1	LEU	-	expression tag	UNP Q8X182
B	2	SER	-	expression tag	UNP Q8X182
B	3	GLU	-	expression tag	UNP Q8X182
B	4	CYS	-	expression tag	UNP Q8X182
B	5	PRO	-	expression tag	UNP Q8X182
B	6	VAL	-	expression tag	UNP Q8X182
B	742	LYS	-	expression tag	UNP Q8X182
B	743	GLN	-	expression tag	UNP Q8X182
B	744	GLU	-	expression tag	UNP Q8X182
B	745	GLY	-	expression tag	UNP Q8X182
B	746	ARG	-	expression tag	UNP Q8X182
B	747	GLY	-	expression tag	UNP Q8X182
B	748	GLN	-	expression tag	UNP Q8X182
B	749	ASN	-	expression tag	UNP Q8X182
B	750	ALA	-	expression tag	UNP Q8X182
B	751	PRO	-	expression tag	UNP Q8X182
B	752	LYS	-	expression tag	UNP Q8X182
B	753	LEU	-	expression tag	UNP Q8X182

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

C₃₄H₃₂FeN₄O₄).



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

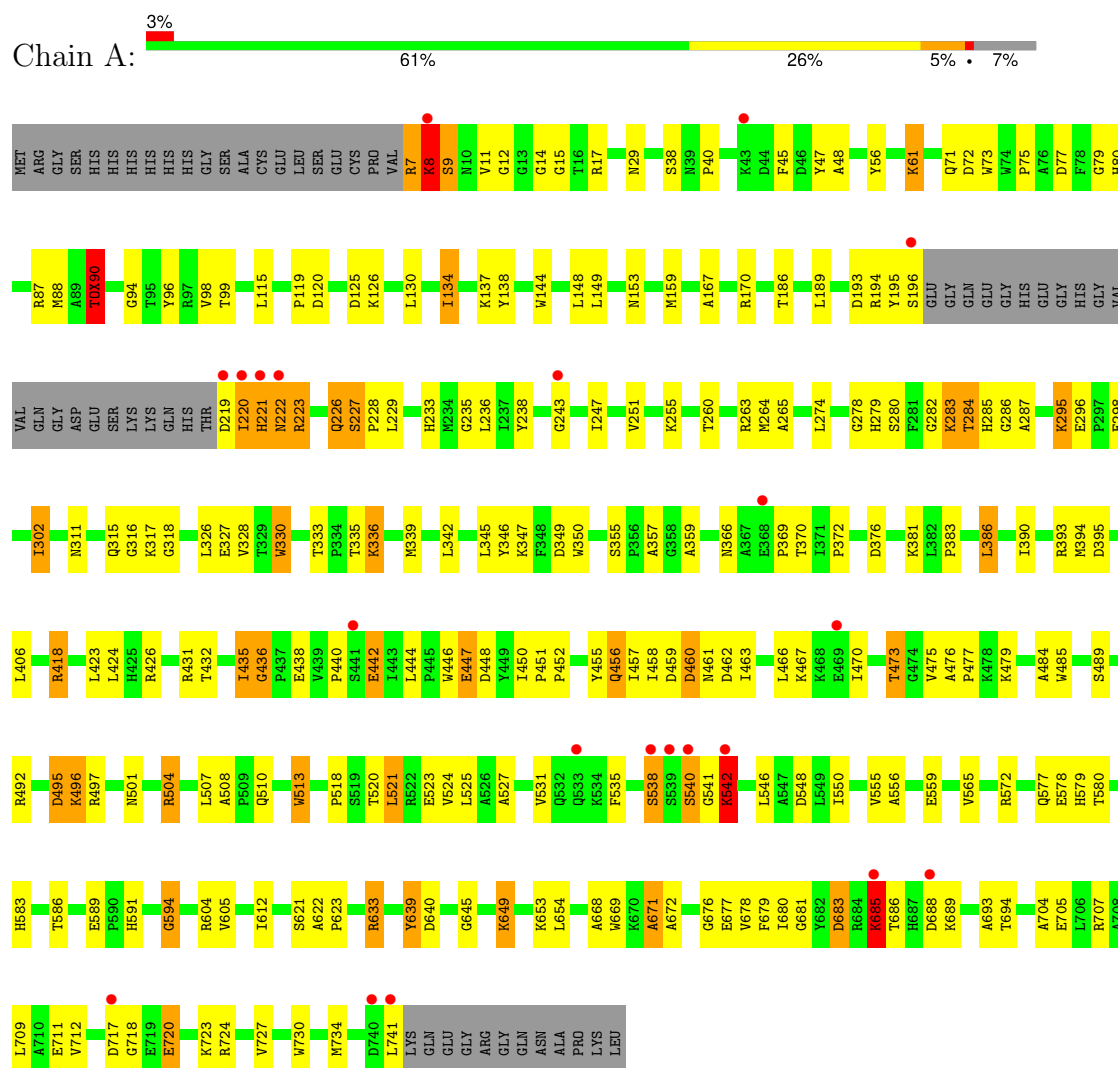
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	314	Total	O	0	0
			314	314		
3	B	368	Total	O	0	0
			368	368		

3 Residue-property plots [i](#)

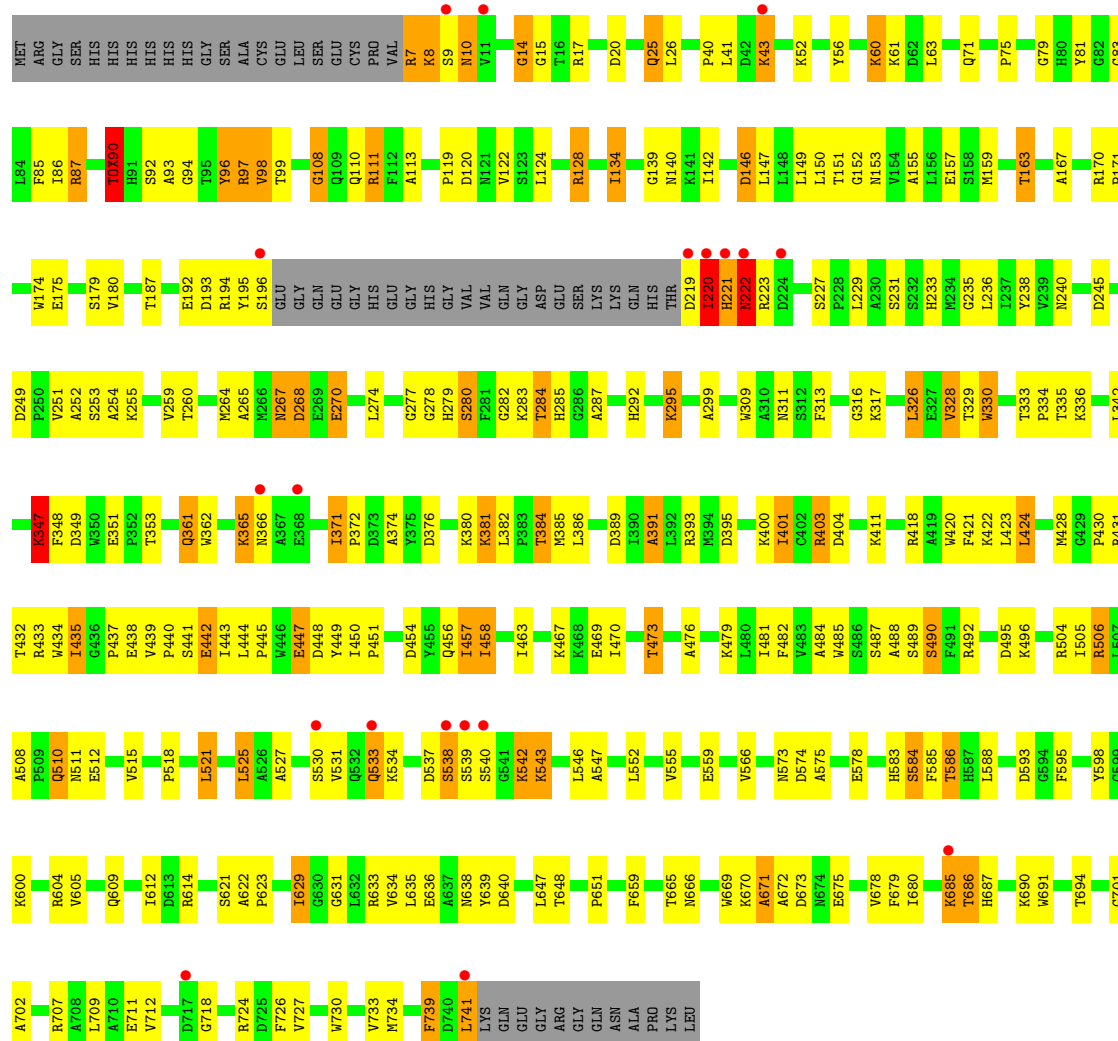
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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	71.81Å 142.35Å 183.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	112.38 – 2.60 112.38 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (112.38-2.60) 99.9 (112.38-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.209 , 0.254 0.212 , 0.256	Depositor DCC
R_{free} test set	2000 reflections (3.41%)	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11962	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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: HEM, TOX

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	1.51	38/5734 (0.7%)	1.12	32/7791 (0.4%)
1	B	1.81	95/5734 (1.7%)	1.31	59/7791 (0.8%)
All	All	1.67	133/11468 (1.2%)	1.22	91/15582 (0.6%)

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	1
1	B	0	1
All	All	0	2

All (133) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	97	ARG	C-O	-7.77	1.15	1.23
1	A	718	GLY	C-O	-7.49	1.17	1.24
1	A	285	HIS	C-O	-7.36	1.15	1.24
1	A	9	SER	C-O	-7.27	1.15	1.23
1	B	142	ILE	C-O	-7.17	1.16	1.24
1	B	96	TYR	C-O	-7.12	1.15	1.23
1	B	171	PRO	C-O	-7.12	1.14	1.24
1	A	369	PRO	C-O	-7.03	1.18	1.24
1	B	724	ARG	C-O	-6.76	1.16	1.24
1	B	380	LYS	C-O	-6.76	1.15	1.23
1	B	268	ASP	C-O	-6.56	1.16	1.24
1	A	653	LYS	C-O	-6.54	1.16	1.24
1	B	450	ILE	N-CA	-6.53	1.40	1.46
1	B	108	GLY	C-O	-6.51	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	63	LEU	C-O	-6.45	1.16	1.24
1	B	401	ILE	C-O	-6.34	1.16	1.24
1	B	153	ASN	C-O	-6.33	1.16	1.24
1	B	317	LYS	C-O	-6.33	1.16	1.23
1	B	86	ILE	C-O	-6.31	1.16	1.24
1	B	482	PHE	C-O	-6.31	1.16	1.24
1	B	718	GLY	C-O	-6.31	1.16	1.23
1	B	435	ILE	C-O	-6.28	1.17	1.24
1	B	111	ARG	C-O	-6.21	1.15	1.24
1	A	649	LYS	C-O	-6.18	1.16	1.24
1	B	673	ASP	C-O	-6.17	1.19	1.24
1	A	442	GLU	C-O	-6.17	1.16	1.23
1	B	612	ILE	C-O	-6.15	1.16	1.24
1	B	71	GLN	C-O	-6.09	1.16	1.23
1	B	328	VAL	C-O	-6.07	1.17	1.24
1	B	255	LYS	C-O	-6.05	1.16	1.24
1	B	694	THR	C-O	-6.05	1.15	1.24
1	B	361	GLN	C-O	-5.97	1.17	1.23
1	B	518	PRO	C-O	-5.93	1.16	1.24
1	A	612	ILE	C-O	-5.92	1.17	1.24
1	B	441	SER	C-O	-5.92	1.16	1.24
1	A	455	TYR	CA-C	-5.90	1.45	1.52
1	B	573	ASN	C-O	-5.89	1.16	1.23
1	B	638	ASN	C-O	-5.87	1.16	1.24
1	A	580	THR	CA-C	-5.86	1.46	1.53
1	B	267	ASN	C-O	-5.84	1.17	1.23
1	B	443	ILE	C-O	-5.82	1.17	1.24
1	B	253	SER	C-O	-5.80	1.17	1.24
1	B	609	GLN	C-O	-5.80	1.16	1.24
1	B	92	SER	N-CA	-5.79	1.39	1.46
1	B	525	LEU	C-O	-5.79	1.17	1.24
1	A	418	ARG	C-O	-5.78	1.17	1.24
1	B	574	ASP	C-O	-5.77	1.16	1.23
1	B	593	ASP	C-O	-5.75	1.17	1.23
1	A	723	LYS	C-O	-5.73	1.17	1.24
1	B	87	ARG	C-O	-5.73	1.17	1.24
1	A	386	LEU	C-O	-5.72	1.16	1.23
1	B	152	GLY	C-O	-5.72	1.17	1.24
1	B	134	ILE	C-O	-5.72	1.17	1.24
1	B	75	PRO	C-O	-5.71	1.17	1.23
1	A	565	VAL	C-O	-5.70	1.17	1.24
1	A	477	PRO	C-O	-5.67	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	HIS	C-O	-5.67	1.17	1.23
1	A	71	GLN	C-O	-5.66	1.17	1.23
1	A	621	SER	C-O	-5.65	1.16	1.23
1	B	79	GLY	C-O	-5.63	1.16	1.24
1	A	720	GLU	C-O	-5.62	1.17	1.24
1	B	342	LEU	C-O	-5.60	1.17	1.24
1	B	442	GLU	C-O	-5.60	1.17	1.24
1	B	270	GLU	C-O	-5.59	1.16	1.24
1	B	99	THR	C-O	-5.59	1.17	1.24
1	B	128	ARG	C-O	-5.57	1.17	1.24
1	B	347	LYS	C-O	-5.57	1.17	1.24
1	B	140	ASN	C-O	-5.56	1.16	1.24
1	B	584	SER	CA-C	-5.56	1.45	1.52
1	B	61	LYS	C-O	-5.55	1.17	1.24
1	B	585	PHE	C-O	-5.53	1.16	1.24
1	A	153	ASN	C-O	-5.51	1.17	1.24
1	A	705	GLU	C-O	-5.51	1.17	1.24
1	B	336	LYS	C-O	-5.50	1.17	1.23
1	B	420	TRP	C-O	-5.49	1.17	1.24
1	B	403	ARG	C-O	-5.47	1.17	1.24
1	B	421	PHE	C-O	-5.47	1.17	1.24
1	B	60	LYS	C-O	-5.46	1.17	1.24
1	A	134	ILE	C-O	-5.45	1.17	1.24
1	B	98	VAL	C-O	-5.45	1.16	1.24
1	B	546	LEU	C-O	-5.44	1.17	1.24
1	B	496	LYS	C-O	-5.43	1.15	1.23
1	B	479	LYS	C-O	-5.42	1.17	1.24
1	B	422	LYS	C-O	-5.39	1.17	1.24
1	B	702	ALA	C-O	-5.39	1.16	1.23
1	A	283	LYS	C-O	-5.38	1.18	1.23
1	B	85	PHE	C-O	-5.38	1.17	1.24
1	A	676	GLY	C-O	-5.37	1.17	1.24
1	A	724	ARG	C-O	-5.37	1.17	1.24
1	A	226	GLN	C-O	-5.34	1.17	1.23
1	B	155	ALA	C-O	-5.33	1.17	1.24
1	B	174	TRP	C-O	-5.31	1.17	1.24
1	A	315	GLN	C-O	-5.31	1.17	1.24
1	A	535	PHE	N-CA	-5.27	1.39	1.46
1	A	504	ARG	C-O	-5.26	1.17	1.24
1	B	490	SER	C-O	-5.24	1.17	1.24
1	B	329	THR	C-O	-5.22	1.18	1.24
1	B	543	LYS	C-O	-5.21	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	673	ASP	CA-C	-5.20	1.46	1.53
1	A	683	ASP	C-O	-5.20	1.17	1.23
1	B	146	ASP	C-O	-5.18	1.17	1.24
1	B	333	THR	C-O	-5.18	1.18	1.24
1	B	179	SER	C-O	-5.18	1.17	1.24
1	B	552	LEU	C-O	-5.17	1.17	1.24
1	A	436	GLY	C-N	5.16	1.38	1.33
1	A	484	ALA	C-O	-5.16	1.18	1.24
1	B	449	TYR	N-CA	-5.14	1.39	1.46
1	B	385	MET	C-O	-5.14	1.17	1.23
1	B	621	SER	C-O	-5.14	1.17	1.23
1	A	521	LEU	N-CA	-5.14	1.40	1.46
1	B	437	PRO	C-O	-5.14	1.17	1.24
1	A	513	TRP	C-O	-5.10	1.17	1.24
1	B	588	LEU	C-O	-5.10	1.16	1.23
1	B	353	THR	N-CA	-5.10	1.40	1.46
1	B	584	SER	C-O	-5.08	1.18	1.24
1	A	523	GLU	N-CA	-5.08	1.40	1.46
1	B	484	ALA	C-O	-5.08	1.18	1.24
1	B	521	LEU	N-CA	-5.07	1.40	1.46
1	B	424	LEU	C-O	-5.07	1.17	1.24
1	A	654	LEU	C-O	-5.06	1.17	1.24
1	A	435	ILE	C-O	-5.06	1.17	1.23
1	B	259	VAL	N-CA	-5.06	1.40	1.46
1	B	180	VAL	C-O	-5.05	1.18	1.24
1	B	374	ALA	C-O	-5.05	1.17	1.24
1	B	547	ALA	C-O	-5.05	1.18	1.24
1	A	594	GLY	C-O	-5.04	1.17	1.24
1	B	150	LEU	C-O	-5.04	1.17	1.24
1	B	487	SER	C-O	-5.04	1.18	1.24
1	A	518	PRO	C-O	-5.04	1.17	1.24
1	B	393	ARG	C-O	-5.03	1.17	1.24
1	B	227	SER	C-O	-5.02	1.17	1.23
1	B	659	PHE	C-O	-5.01	1.18	1.24
1	B	391	ALA	C-O	-5.01	1.17	1.24

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	447	GLU	N-CA-C	10.98	123.33	111.36
1	B	447	GLU	N-CA-C	9.33	122.64	111.82
1	A	330	TRP	N-CA-C	8.12	121.68	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	636	GLU	N-CA-C	7.39	121.87	111.52
1	A	639	TYR	N-CA-C	7.21	120.98	111.75
1	A	395	ASP	N-CA-C	-7.19	101.02	109.93
1	B	287	ALA	N-CA-C	7.00	119.76	111.71
1	B	395	ASP	N-CA-C	-6.97	101.29	110.07
1	B	113	ALA	C-N-CD	6.96	135.92	120.60
1	A	376	ASP	CA-C-N	-6.95	112.73	120.45
1	A	376	ASP	C-N-CA	-6.95	112.73	120.45
1	A	221	HIS	N-CA-C	-6.89	103.77	111.28
1	B	10	ASN	N-CA-C	6.74	125.16	110.80
1	B	685	LYS	CA-C-N	6.73	129.84	120.29
1	B	685	LYS	C-N-CA	6.73	129.84	120.29
1	B	330	TRP	N-CA-C	6.68	120.64	112.23
1	B	371	ILE	N-CA-C	6.65	115.90	108.05
1	B	222	ASN	N-CA-C	6.61	121.19	111.87
1	B	372	PRO	N-CA-C	6.59	121.85	111.38
1	B	221	HIS	N-CA-C	-6.55	105.20	113.72
1	B	508	ALA	C-N-CD	6.49	134.87	120.60
1	A	251	VAL	N-CA-CB	6.46	118.10	110.55
1	B	282	GLY	N-CA-C	6.43	123.98	112.02
1	B	349	ASP	N-CA-C	-6.36	99.34	109.76
1	B	295	LYS	N-CA-C	6.31	119.39	110.23
1	B	671	ALA	N-CA-C	-6.27	101.20	110.48
1	B	518	PRO	N-CA-C	6.27	122.11	113.65
1	B	639	TYR	N-CA-C	6.26	119.76	111.75
1	B	511	ASN	CA-C-N	-6.26	112.73	122.37
1	B	511	ASN	C-N-CA	-6.26	112.73	122.37
1	B	25	GLN	N-CA-C	6.25	119.52	110.28
1	A	704	ALA	N-CA-C	6.16	118.79	111.71
1	A	282	GLY	N-CA-C	6.15	123.46	112.02
1	B	249	ASP	CA-C-N	-6.06	113.57	119.87
1	B	249	ASP	C-N-CA	-6.06	113.57	119.87
1	A	671	ALA	N-CA-C	-6.05	101.53	110.48
1	B	284	THR	N-CA-C	-5.97	101.36	109.95
1	B	14	GLY	N-CA-C	5.92	122.26	112.66
1	A	284	THR	N-CA-C	-5.85	101.53	109.95
1	A	302	ILE	N-CA-C	5.85	118.36	111.05
1	A	366	ASN	N-CA-C	5.84	117.74	110.91
1	B	229	LEU	N-CA-C	5.82	118.67	110.23
1	B	512	GLU	N-CA-C	-5.82	104.73	112.94
1	B	484	ALA	N-CA-C	-5.81	105.03	111.36
1	B	94	GLY	N-CA-C	5.78	125.09	115.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	505	ILE	N-CA-C	-5.78	103.95	112.04
1	B	334	PRO	N-CA-C	5.77	121.34	113.84
1	A	45	PHE	N-CA-C	5.76	119.17	110.64
1	B	686	THR	N-CA-C	5.72	117.59	111.36
1	B	63	LEU	CA-C-N	5.71	128.99	120.31
1	B	63	LEU	C-N-CA	5.71	128.99	120.31
1	B	180	VAL	CB-CA-C	-5.71	103.83	110.91
1	A	295	LYS	N-CA-C	5.70	118.06	110.53
1	A	339	MET	N-CA-C	5.70	119.55	112.59
1	A	75	PRO	N-CA-C	5.67	120.23	111.21
1	A	484	ALA	N-CA-C	-5.67	105.18	111.36
1	A	318	GLY	CA-C-N	-5.62	113.97	120.04
1	A	318	GLY	C-N-CA	-5.62	113.97	120.04
1	A	350	TRP	N-CA-C	5.60	118.86	109.95
1	B	376	ASP	CA-C-N	-5.53	113.98	120.12
1	B	376	ASP	C-N-CA	-5.53	113.98	120.12
1	B	140	ASN	N-CA-C	5.43	119.02	112.93
1	A	685	LYS	N-CA-C	5.38	117.23	111.36
1	A	372	PRO	N-CA-C	5.37	120.64	111.68
1	B	651	PRO	CB-CA-C	-5.37	104.88	111.64
1	B	81	TYR	N-CA-C	5.33	120.73	113.37
1	A	450	ILE	CA-C-N	-5.30	114.92	120.38
1	A	450	ILE	C-N-CA	-5.30	114.92	120.38
1	B	739	PHE	N-CA-C	-5.29	106.34	112.89
1	B	476	ALA	CA-C-N	-5.28	114.65	119.82
1	B	476	ALA	C-N-CA	-5.28	114.65	119.82
1	B	451	PRO	CA-C-N	-5.26	114.30	119.92
1	B	451	PRO	C-N-CA	-5.26	114.30	119.92
1	B	61	LYS	CA-C-N	5.24	127.30	120.28
1	B	61	LYS	C-N-CA	5.24	127.30	120.28
1	B	328	VAL	N-CA-C	5.24	115.66	108.12
1	B	240	ASN	CA-C-N	-5.22	114.32	120.12
1	B	240	ASN	C-N-CA	-5.22	114.32	120.12
1	A	349	ASP	N-CA-C	-5.21	101.77	110.17
1	A	222	ASN	N-CA-C	5.20	116.87	108.34
1	B	718	GLY	N-CA-C	5.19	124.65	115.61
1	A	591	HIS	N-CA-C	-5.19	105.24	112.45
1	A	542	LYS	N-CA-C	5.16	117.14	109.25
1	B	326	LEU	O-C-N	-5.16	116.66	123.21
1	B	510	GLN	N-CA-C	5.15	117.64	111.71
1	B	691	TRP	N-CA-C	5.14	116.11	108.86
1	A	29	ASN	N-CA-C	5.13	116.87	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	ALA	N-CA-C	5.11	118.66	112.23
1	B	41	LEU	N-CA-C	5.06	117.06	110.43
1	B	445	PRO	N-CA-C	5.04	120.16	113.86
1	B	93	ALA	N-CA-C	5.01	117.63	111.82

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	90	TOX	Mainchain
1	B	90	TOX	Mainchain

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	5597	0	5411	201	0
1	B	5597	0	5411	163	0
2	A	43	0	30	6	0
2	B	43	0	30	8	0
3	A	314	0	0	12	2
3	B	368	0	0	10	2
All	All	11962	0	10882	355	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 16.

All (355) 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:96:TYR:O	1:A:264:MET:HE2	1.36	1.18
1:A:284:THR:OG1	1:A:326:LEU:O	1.62	1.17
1:B:159:MET:HE2	1:B:335:THR:HA	1.19	1.14
1:B:431:ARG:NH2	1:B:440:PRO:O	1.85	1.08
1:A:219:ASP:O	1:A:220:ILE:HG13	1.55	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:ASN:OD1	1:B:270:GLU:HG3	1.56	1.04
1:A:8:LYS:HA	1:A:15:GLY:H	1.21	1.01
1:B:56:TYR:OH	1:B:438:GLU:OE1	1.77	1.00
1:B:7:ARG:HH21	1:B:7:ARG:HG3	1.24	0.99
1:B:96:TYR:O	1:B:264:MET:HE2	1.66	0.95
1:A:467:LYS:NZ	1:A:559:GLU:OE1	1.99	0.95
1:A:633:ARG:HG2	1:A:645:GLY:O	1.67	0.93
1:A:555:VAL:O	1:A:559:GLU:HG3	1.70	0.91
1:B:14:GLY:O	1:B:17:ARG:NH1	2.03	0.91
1:B:159:MET:HE2	1:B:335:THR:CA	1.99	0.91
1:B:284:THR:OG1	1:B:326:LEU:O	1.91	0.89
1:B:220:ILE:HG12	1:B:221:HIS:N	1.88	0.88
1:A:456:GLN:NE2	1:A:542:LYS:CE	2.38	0.87
1:A:479:LYS:HD3	1:A:520:THR:HG23	1.58	0.86
1:A:195:TYR:O	1:A:196:SER:OG	1.94	0.85
1:A:473:THR:CG2	1:A:475:VAL:HG23	2.08	0.83
1:A:431:ARG:HD2	1:A:447:GLU:OE2	1.77	0.81
1:A:219:ASP:O	1:A:220:ILE:CG1	2.28	0.81
1:B:220:ILE:HG23	1:B:222:ASN:H	1.45	0.81
1:B:533:GLN:O	1:B:537:ASP:HB2	1.80	0.81
1:A:456:GLN:NE2	1:A:542:LYS:HE3	1.96	0.81
1:A:7:ARG:NH2	3:A:902:HOH:O	2.13	0.80
1:A:7:ARG:O	1:A:9:SER:N	2.13	0.80
1:A:72:ASP:O	1:A:317:LYS:HE3	1.81	0.80
1:A:9:SER:HB3	1:B:605:VAL:HG22	1.65	0.78
1:A:709:LEU:CD2	1:B:40:PRO:HG3	2.14	0.78
1:A:605:VAL:HG22	1:B:9:SER:HB2	1.66	0.77
1:A:473:THR:HG22	1:A:475:VAL:HG23	1.65	0.77
1:B:98:VAL:HG11	1:B:265:ALA:HB2	1.66	0.76
1:A:8:LYS:HA	1:A:15:GLY:N	2.00	0.76
1:A:672:ALA:HB3	1:A:678:VAL:HG23	1.66	0.76
1:A:14:GLY:O	1:A:17:ARG:NH1	2.17	0.76
1:B:431:ARG:HD2	1:B:447:GLU:OE2	1.86	0.75
1:B:467:LYS:NZ	1:B:559:GLU:OE1	2.19	0.74
1:B:159:MET:CE	1:B:335:THR:HA	2.11	0.73
1:A:685:LYS:HG3	1:A:686:THR:HG23	1.69	0.73
1:A:513:TRP:CE2	1:A:589:GLU:HG3	2.24	0.72
1:A:345:LEU:O	1:A:393:ARG:NH1	2.23	0.72
1:B:470:ILE:O	1:B:473:THR:OG1	2.05	0.72
1:B:506:ARG:NH2	1:B:575:ALA:O	2.18	0.72
1:A:467:LYS:HG2	1:A:556:ALA:HB2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ILE:HG23	1:B:221:HIS:H	1.55	0.72
1:A:418:ARG:NH2	1:A:442:GLU:OE2	2.23	0.71
1:B:8:LYS:HA	1:B:15:GLY:H	1.54	0.71
1:A:456:GLN:HB3	1:A:542:LYS:HG2	1.72	0.71
1:B:17:ARG:O	1:B:20:ASP:HB2	1.91	0.70
1:B:220:ILE:HG12	1:B:221:HIS:H	1.53	0.70
1:A:435:ILE:HG22	1:A:436:GLY:N	2.05	0.70
1:B:7:ARG:HG3	1:B:7:ARG:NH2	1.98	0.70
1:A:38:SER:OG	3:A:901:HOH:O	2.09	0.69
1:A:195:TYR:C	1:A:196:SER:HG	1.98	0.69
1:B:220:ILE:CG1	1:B:221:HIS:H	2.05	0.69
1:A:604:ARG:O	1:B:9:SER:HB3	1.93	0.69
1:B:98:VAL:CG1	1:B:265:ALA:HB2	2.22	0.69
1:A:504:ARG:NH1	1:A:579:HIS:O	2.27	0.68
1:B:7:ARG:HH21	1:B:7:ARG:CG	2.03	0.68
1:B:149:LEU:HD22	1:B:424:LEU:HD22	1.76	0.68
1:B:741:LEU:O	3:B:901:HOH:O	2.12	0.68
1:A:538:SER:C	1:A:540:SER:H	2.01	0.67
1:A:393:ARG:O	1:A:393:ARG:HG2	1.92	0.67
1:A:167:ALA:O	1:A:170:ARG:NH2	2.27	0.67
1:A:40:PRO:HG3	1:B:709:LEU:CD2	2.25	0.67
1:A:456:GLN:NE2	1:A:542:LYS:HE2	2.09	0.67
1:A:685:LYS:HG3	1:A:686:THR:CG2	2.24	0.67
2:B:800:HEM:HBC2	2:B:800:HEM:CMC	2.24	0.67
1:B:220:ILE:HG23	1:B:221:HIS:N	2.09	0.67
1:B:542:LYS:O	1:B:543:LYS:HG2	1.95	0.67
1:A:219:ASP:O	1:A:220:ILE:CB	2.42	0.66
1:A:220:ILE:HG22	1:A:221:HIS:N	2.09	0.66
1:A:467:LYS:CE	1:A:559:GLU:OE1	2.42	0.66
1:A:456:GLN:CD	1:A:542:LYS:HE3	2.20	0.66
1:A:447:GLU:O	1:A:448:ASP:HB2	1.94	0.66
1:A:283:LYS:HE3	1:A:284:THR:O	1.95	0.65
1:A:459:ASP:O	1:A:461:ASN:N	2.30	0.65
1:B:194:ARG:NH1	1:B:231:SER:O	2.29	0.65
2:B:800:HEM:HBC2	2:B:800:HEM:HMC1	1.78	0.65
2:A:800:HEM:HBC2	2:A:800:HEM:CMC	2.27	0.65
1:B:167:ALA:O	1:B:170:ARG:NH2	2.30	0.64
1:A:520:THR:O	1:A:524:VAL:HG23	1.97	0.64
1:A:685:LYS:CG	1:A:686:THR:HG23	2.27	0.64
1:A:456:GLN:HE22	1:A:542:LYS:CE	2.08	0.64
1:A:476:ALA:HB3	1:A:479:LYS:HG3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ARG:CB	1:A:7:ARG:HH21	2.10	0.64
1:A:456:GLN:HE22	1:A:542:LYS:HE3	1.60	0.63
1:A:495:ASP:O	1:A:496:LYS:HB2	1.96	0.63
1:B:537:ASP:C	1:B:539:SER:H	2.07	0.63
1:A:485:TRP:O	1:A:489:SER:HB2	1.98	0.63
2:A:800:HEM:HBC2	2:A:800:HEM:HMC1	1.81	0.63
1:B:504:ARG:NH1	3:B:909:HOH:O	2.31	0.63
1:B:686:THR:O	1:B:687:HIS:HB2	1.97	0.63
1:A:604:ARG:O	1:B:9:SER:CB	2.46	0.62
1:B:690:LYS:HE2	3:B:1221:HOH:O	1.99	0.62
1:A:279:HIS:HB3	1:A:330:TRP:CE2	2.34	0.62
1:A:219:ASP:C	1:A:220:ILE:HG13	2.23	0.62
1:A:243:GLY:HA3	1:A:247:ILE:O	1.99	0.62
1:B:279:HIS:HB3	1:B:330:TRP:CE2	2.35	0.62
1:B:672:ALA:HB3	1:B:678:VAL:HG23	1.80	0.62
1:A:504:ARG:HG2	1:A:507:LEU:HD12	1.82	0.62
1:A:159:MET:HE2	1:A:335:THR:HA	1.82	0.61
1:A:80:HIS:ND1	1:A:159:MET:HE3	2.15	0.61
1:B:555:VAL:O	1:B:559:GLU:HG3	2.01	0.61
1:A:546:LEU:O	1:A:550:ILE:HG13	2.00	0.60
1:A:96:TYR:O	1:A:264:MET:CE	2.31	0.60
1:A:495:ASP:HB3	1:A:497:ARG:HG3	1.84	0.60
1:A:709:LEU:HD22	1:B:40:PRO:HG3	1.82	0.60
1:A:462:ASP:O	1:A:466:LEU:HG	2.02	0.60
1:B:157:GLU:OE2	1:B:163:THR:OG1	2.19	0.60
1:A:223:ARG:NH1	3:A:909:HOH:O	2.34	0.60
1:A:594:GLY:O	1:A:633:ARG:NH2	2.28	0.59
1:A:355:SER:C	1:A:357:ALA:H	2.10	0.59
1:A:189:LEU:O	1:A:233:HIS:ND1	2.30	0.59
1:B:481:ILE:HD13	1:B:635:LEU:HD13	1.84	0.59
1:B:600:LYS:HE3	1:B:675:GLU:OE2	2.03	0.59
1:A:220:ILE:HG22	1:A:222:ASN:H	1.68	0.59
1:A:448:ASP:OD2	1:A:497:ARG:NH1	2.36	0.58
1:A:7:ARG:HH21	1:A:7:ARG:CG	2.16	0.58
1:A:548:ASP:OD1	1:A:572:ARG:HB2	2.03	0.58
1:B:220:ILE:CG1	1:B:221:HIS:N	2.56	0.58
1:A:431:ARG:HH11	1:A:447:GLU:CD	2.12	0.58
1:B:431:ARG:HD2	1:B:447:GLU:CD	2.29	0.57
1:A:284:THR:HB	2:A:800:HEM:HAA2	1.86	0.57
1:B:159:MET:HG2	1:B:335:THR:O	2.04	0.57
1:A:709:LEU:HD23	1:B:40:PRO:HG3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:371:ILE:O	1:B:381:LYS:N	2.35	0.57
1:B:284:THR:HB	2:B:800:HEM:HAA2	1.87	0.57
1:A:521:LEU:O	1:A:525:LEU:HG	2.06	0.56
1:B:195:TYR:O	1:B:196:SER:OG	2.21	0.56
1:B:539:SER:O	1:B:540:SER:HB3	2.04	0.56
1:A:717:ASP:OD1	1:B:139:GLY:HA3	2.06	0.56
1:A:458:ILE:HB	1:A:462:ASP:HB2	1.87	0.56
1:A:444:LEU:CD2	3:A:953:HOH:O	2.54	0.56
1:A:444:LEU:HD22	1:A:446:TRP:HE1	1.70	0.56
1:B:17:ARG:NH1	3:B:915:HOH:O	2.38	0.56
1:A:61:LYS:HE3	3:A:915:HOH:O	2.06	0.55
1:B:25:GLN:HG3	1:B:26:LEU:N	2.21	0.55
1:A:264:MET:O	1:A:426:ARG:NH1	2.39	0.55
1:A:633:ARG:HG2	1:A:645:GLY:C	2.30	0.55
1:A:435:ILE:HG22	1:A:436:GLY:H	1.71	0.55
1:B:260:THR:O	1:B:264:MET:HG3	2.07	0.55
1:B:485:TRP:CZ3	1:B:733:VAL:HG11	2.41	0.55
1:A:671:ALA:HA	1:A:679:PHE:CD1	2.42	0.55
1:A:220:ILE:CG2	1:A:221:HIS:N	2.69	0.55
1:B:488:ALA:C	1:B:490:SER:H	2.13	0.55
1:A:119:PRO:HD2	1:A:235:GLY:HA3	1.89	0.54
1:A:492:ARG:NH2	1:A:495:ASP:OD2	2.40	0.54
1:B:119:PRO:HD2	1:B:235:GLY:HA3	1.89	0.54
1:B:542:LYS:C	1:B:543:LYS:HG2	2.32	0.54
1:A:431:ARG:NH1	1:A:447:GLU:OE1	2.40	0.54
1:A:460:ASP:HA	1:A:463:ILE:HD12	1.89	0.54
1:A:40:PRO:HG3	1:B:709:LEU:HD22	1.89	0.54
1:B:220:ILE:CG2	1:B:221:HIS:H	2.14	0.54
1:A:219:ASP:O	1:A:220:ILE:HB	2.08	0.54
1:A:485:TRP:O	1:A:489:SER:CB	2.55	0.54
1:A:649:LYS:NZ	3:A:916:HOH:O	2.40	0.54
1:A:125:ASP:OD2	1:A:126:LYS:HE3	2.08	0.53
1:A:87:ARG:HD3	3:A:903:HOH:O	2.07	0.53
1:B:403:ARG:HD2	3:B:1156:HOH:O	2.07	0.53
1:B:278:GLY:C	1:B:280:SER:H	2.15	0.53
1:B:559:GLU:HG2	1:B:566:VAL:HG23	1.90	0.53
1:A:435:ILE:CG2	1:A:436:GLY:N	2.72	0.53
1:A:90:TOX:H9	1:A:238:TYR:OH	2.09	0.53
1:B:279:HIS:HB3	1:B:330:TRP:CD2	2.44	0.53
1:A:279:HIS:HB3	1:A:330:TRP:CD2	2.44	0.52
1:A:193:ASP:OD2	1:A:604:ARG:NH2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:THR:O	1:A:264:MET:HG3	2.09	0.52
1:A:296:GLU:OE1	1:A:296:GLU:N	2.33	0.52
1:A:346:TYR:CE1	1:A:393:ARG:HG3	2.45	0.52
1:B:583:HIS:O	1:B:586:THR:HB	2.10	0.51
1:A:683:ASP:OD1	1:A:685:LYS:HG2	2.10	0.51
1:A:479:LYS:HD3	1:A:520:THR:CG2	2.37	0.51
1:B:90:TOX:H8	1:B:423:LEU:HD21	1.93	0.51
1:B:311:ASN:ND2	1:B:316:GLY:HA2	2.25	0.51
1:A:233:HIS:HB2	1:A:236:LEU:HD12	1.92	0.51
1:B:521:LEU:O	1:B:525:LEU:HG	2.10	0.51
1:A:278:GLY:C	1:A:280:SER:H	2.17	0.51
1:B:146:ASP:OD1	1:B:170:ARG:HB2	2.11	0.51
1:A:456:GLN:CD	1:A:542:LYS:CE	2.83	0.50
1:B:538:SER:O	1:B:539:SER:OG	2.26	0.50
1:A:326:LEU:HD23	1:A:359:ALA:HB3	1.93	0.50
1:A:393:ARG:HD3	1:A:394:MET:HE3	1.93	0.50
1:B:431:ARG:CD	1:B:447:GLU:OE2	2.57	0.50
1:A:80:HIS:CE1	1:A:159:MET:HE3	2.47	0.50
1:A:311:ASN:ND2	1:A:316:GLY:HA2	2.27	0.50
1:A:677:GLU:O	1:A:694:THR:HA	2.12	0.50
1:B:90:TOX:H9	1:B:238:TYR:OH	2.12	0.50
1:B:454:ASP:OD1	1:B:454:ASP:N	2.43	0.50
1:A:56:TYR:OH	1:A:438:GLU:OE1	2.25	0.50
1:A:459:ASP:O	1:A:462:ASP:N	2.41	0.50
1:B:527:ALA:O	1:B:531:VAL:HG23	2.11	0.49
1:A:40:PRO:HG2	1:B:712:VAL:HG21	1.94	0.49
1:B:510:GLN:NE2	3:B:917:HOH:O	2.45	0.49
1:B:634:VAL:HG12	1:B:648:THR:HB	1.94	0.49
1:A:7:ARG:NH2	1:A:7:ARG:CG	2.74	0.49
1:A:194:ARG:CZ	1:A:229:LEU:HD13	2.43	0.49
1:A:219:ASP:C	1:A:220:ILE:CG1	2.85	0.49
1:A:77:ASP:C	1:A:79:GLY:H	2.20	0.49
1:B:254:ALA:HB2	1:B:391:ALA:HB1	1.94	0.49
1:B:277:GLY:O	1:B:280:SER:HB2	2.12	0.49
1:A:98:VAL:CG1	1:A:265:ALA:HB2	2.43	0.49
1:A:444:LEU:HD22	3:A:953:HOH:O	2.12	0.49
1:B:110:GLN:HG2	1:B:128:ARG:NH1	2.28	0.49
1:A:501:ASN:HA	1:A:572:ARG:HG2	1.95	0.49
1:A:513:TRP:CD2	1:A:589:GLU:HG3	2.48	0.48
1:B:403:ARG:CD	3:B:1156:HOH:O	2.61	0.48
1:A:527:ALA:O	1:A:531:VAL:HG23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:VAL:HG21	1:A:386:LEU:HD23	1.96	0.48
1:B:492:ARG:NH2	1:B:495:ASP:OD2	2.31	0.48
1:A:394:MET:HA	1:A:394:MET:HE2	1.95	0.48
1:A:431:ARG:CD	1:A:447:GLU:OE2	2.56	0.48
1:B:351:GLU:HB3	1:B:365:LYS:HE3	1.95	0.48
1:A:96:TYR:HB2	3:A:938:HOH:O	2.12	0.48
1:A:193:ASP:CG	1:A:604:ARG:HH22	2.21	0.48
2:B:800:HEM:HMC1	2:B:800:HEM:CBC	2.42	0.48
1:A:221:HIS:CE1	1:A:255:LYS:HE3	2.47	0.48
1:A:538:SER:C	1:A:540:SER:N	2.68	0.48
1:B:108:GLY:O	1:B:111:ARG:HG2	2.14	0.48
1:A:355:SER:C	1:A:357:ALA:N	2.68	0.48
1:A:680:ILE:HG23	1:A:689:LYS:HE3	1.95	0.48
1:B:87:ARG:NH2	1:B:120:ASP:O	2.46	0.48
1:B:221:HIS:CE1	1:B:252:ALA:HB2	2.48	0.47
1:B:193:ASP:CG	1:B:604:ARG:HH22	2.22	0.47
1:A:90:TOX:H8	1:A:423:LEU:HD21	1.96	0.47
1:A:195:TYR:CD1	1:A:223:ARG:HB2	2.48	0.47
1:A:326:LEU:HD23	1:A:359:ALA:CB	2.44	0.47
2:A:800:HEM:HMC1	2:A:800:HEM:CBC	2.44	0.47
1:A:98:VAL:HG11	1:A:265:ALA:HB2	1.96	0.47
1:A:508:ALA:H	1:A:577:GLN:HE22	1.63	0.47
1:A:712:VAL:HG21	1:B:40:PRO:HG2	1.96	0.47
1:B:362:TRP:N	1:B:362:TRP:CD1	2.82	0.47
1:B:488:ALA:O	1:B:490:SER:N	2.48	0.47
1:A:221:HIS:HE1	1:A:255:LYS:HE3	1.79	0.47
1:A:456:GLN:OE1	1:A:542:LYS:HE3	2.15	0.47
1:B:671:ALA:HA	1:B:679:PHE:CD2	2.50	0.47
1:A:286:GLY:O	1:A:327:GLU:HG2	2.14	0.46
1:B:122:VAL:HA	1:B:309:TRP:CZ3	2.50	0.46
1:B:647:LEU:N	1:B:647:LEU:HD23	2.30	0.46
1:B:330:TRP:HH2	2:B:800:HEM:CHA	2.27	0.46
1:A:73:TRP:CZ2	1:A:130:LEU:HD23	2.50	0.46
1:B:488:ALA:C	1:B:490:SER:N	2.73	0.46
1:A:583:HIS:O	1:A:586:THR:HG22	2.16	0.46
1:B:640:ASP:OD1	1:B:640:ASP:N	2.49	0.46
1:B:219:ASP:O	1:B:220:ILE:HB	2.15	0.46
1:B:530:SER:O	1:B:534:LYS:HG3	2.16	0.46
1:B:578:GLU:H	1:B:578:GLU:CD	2.24	0.45
1:B:147:LEU:O	1:B:151:THR:OG1	2.27	0.45
1:B:223:ARG:NH1	1:B:245:ASP:OD1	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:HIS:HB2	1:B:236:LEU:HD12	1.97	0.45
1:B:122:VAL:HG22	1:B:309:TRP:CE2	2.51	0.45
1:B:669:TRP:HA	1:B:680:ILE:O	2.15	0.45
1:A:9:SER:OG	1:B:604:ARG:O	2.20	0.45
1:A:87:ARG:NH2	1:A:120:ASP:O	2.50	0.45
1:B:361:GLN:C	1:B:362:TRP:CD1	2.94	0.45
1:B:595:PHE:CD1	1:B:629:ILE:HD12	2.51	0.45
1:A:40:PRO:HG3	1:B:709:LEU:HD23	1.98	0.45
1:A:98:VAL:HG22	1:A:263:ARG:O	2.16	0.45
1:A:126:LYS:NZ	3:A:912:HOH:O	2.40	0.45
1:A:9:SER:HA	3:A:910:HOH:O	2.17	0.45
1:A:333:THR:HB	1:A:336:LYS:HB3	1.98	0.45
1:B:124:LEU:HD23	1:B:124:LEU:HA	1.79	0.45
1:B:431:ARG:HG2	1:B:434:TRP:CZ3	2.52	0.45
1:B:457:ILE:H	1:B:457:ILE:HG12	1.61	0.45
1:A:77:ASP:C	1:A:79:GLY:N	2.74	0.45
1:A:390:ILE:O	1:A:394:MET:HG2	2.17	0.45
1:B:386:LEU:O	1:B:389:ASP:HB2	2.17	0.45
1:A:473:THR:HG22	1:A:475:VAL:H	1.82	0.44
1:B:404:ASP:OD2	1:B:411:LYS:HE2	2.18	0.44
1:B:622:ALA:HB3	1:B:623:PRO:HD3	1.99	0.44
1:B:430:PRO:C	1:B:432:THR:N	2.74	0.44
1:A:298:GLU:OE1	1:B:25:GLN:NE2	2.43	0.44
1:B:418:ARG:NH2	1:B:442:GLU:OE2	2.49	0.44
1:B:515:VAL:HG23	1:B:598:TYR:CG	2.52	0.44
1:A:381:LYS:HE2	3:A:968:HOH:O	2.17	0.44
1:A:577:GLN:O	1:A:577:GLN:HG3	2.17	0.44
1:B:433:ARG:HD3	1:B:739:PHE:CE1	2.53	0.44
1:A:467:LYS:HG2	1:A:556:ALA:CB	2.46	0.44
1:B:295:LYS:HD2	1:B:299:ALA:HB3	1.99	0.44
1:B:43:LYS:HA	1:B:43:LYS:HD3	1.73	0.44
1:A:622:ALA:HB3	1:A:623:PRO:HD3	1.99	0.43
1:B:685:LYS:HG3	3:B:1050:HOH:O	2.18	0.43
1:A:459:ASP:C	1:A:461:ASN:N	2.76	0.43
1:A:11:VAL:HG13	1:A:12:GLY:O	2.18	0.43
1:A:125:ASP:OD1	1:A:125:ASP:N	2.51	0.43
1:A:668:ALA:O	1:A:681:GLY:HA2	2.19	0.43
1:A:669:TRP:HA	1:A:680:ILE:O	2.18	0.43
1:A:220:ILE:CG2	1:A:221:HIS:H	2.32	0.43
1:B:170:ARG:NH1	1:B:424:LEU:O	2.52	0.43
1:B:328:VAL:HG22	1:B:384:THR:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ARG:NH2	1:A:7:ARG:HG3	2.33	0.43
1:A:149:LEU:HG	1:A:424:LEU:HD22	2.01	0.43
2:A:800:HEM:CMC	2:A:800:HEM:CBC	2.97	0.43
1:A:227:SER:HA	1:A:228:PRO:HA	1.71	0.43
1:A:264:MET:O	1:A:265:ALA:HB3	2.19	0.43
1:A:671:ALA:HA	1:A:679:PHE:HD1	1.83	0.42
1:B:52:LYS:HE2	1:B:435:ILE:CG2	2.49	0.42
1:A:470:ILE:O	1:A:473:THR:HB	2.19	0.42
1:A:137:LYS:HD3	1:A:138:TYR:CE1	2.54	0.42
1:A:540:SER:HB3	1:A:541:GLY:H	1.39	0.42
1:B:707:ARG:O	1:B:711:GLU:HG3	2.19	0.42
1:A:296:GLU:H	1:A:296:GLU:CD	2.19	0.42
1:A:431:ARG:NH2	1:A:440:PRO:O	2.52	0.42
1:A:459:ASP:O	1:A:460:ASP:C	2.62	0.42
1:A:707:ARG:O	1:A:711:GLU:HG3	2.19	0.42
1:B:595:PHE:HE2	1:B:614:ARG:HG2	1.85	0.42
1:A:355:SER:O	1:A:357:ALA:N	2.52	0.42
1:B:631:GLY:HA3	1:B:726:PHE:CE2	2.55	0.42
1:B:268:ASP:HB3	1:B:401:ILE:CD1	2.50	0.42
1:A:326:LEU:CD2	1:A:359:ALA:HB1	2.50	0.42
1:A:513:TRP:NE1	1:A:589:GLU:HG3	2.34	0.42
1:B:347:LYS:HE2	1:B:348:PHE:CZ	2.55	0.42
1:B:439:VAL:CG1	1:B:440:PRO:HD2	2.50	0.42
1:B:537:ASP:O	1:B:539:SER:N	2.52	0.42
1:B:295:LYS:HA	1:B:295:LYS:HD3	1.86	0.41
1:B:670:LYS:HB3	3:B:924:HOH:O	2.20	0.41
1:B:292:HIS:CG	1:B:313:PHE:HB2	2.55	0.41
1:B:439:VAL:HG13	1:B:440:PRO:HD2	2.02	0.41
1:B:739:PHE:C	1:B:741:LEU:H	2.28	0.41
1:B:458:ILE:HD12	1:B:463:ILE:CG1	2.50	0.41
1:B:685:LYS:HG3	1:B:685:LYS:H	1.51	0.41
1:A:144:TRP:O	1:A:148:LEU:HG	2.20	0.41
1:A:274:LEU:C	2:A:800:HEM:HMC3	2.45	0.41
1:A:346:TYR:CZ	1:A:393:ARG:HG3	2.56	0.41
1:A:604:ARG:O	1:B:9:SER:HB2	2.20	0.41
1:A:94:GLY:O	1:A:264:MET:HE1	2.20	0.41
1:B:595:PHE:CE1	1:B:629:ILE:HD12	2.55	0.41
1:B:701:GLY:O	1:B:707:ARG:NH1	2.48	0.41
1:B:83:GLY:O	2:B:800:HEM:HBD2	2.21	0.41
1:A:451:PRO:HA	1:A:452:PRO:HD3	1.96	0.41
1:B:458:ILE:HD12	1:B:463:ILE:HG12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:MET:HE2	1:A:88:MET:HB3	1.97	0.41
1:A:159:MET:HE2	1:A:335:THR:CA	2.51	0.41
1:A:730:TRP:CZ2	1:A:734:MET:HE3	2.56	0.41
1:B:726:PHE:CD1	1:B:726:PHE:C	2.98	0.41
1:A:435:ILE:CG2	1:A:436:GLY:H	2.32	0.41
1:A:510:GLN:HG2	1:A:513:TRP:CZ3	2.56	0.41
1:A:678:VAL:HA	1:A:693:ALA:O	2.21	0.41
1:B:274:LEU:C	2:B:800:HEM:HMC3	2.45	0.41
1:B:629:ILE:O	1:B:633:ARG:HG2	2.21	0.41
1:B:739:PHE:C	1:B:741:LEU:N	2.79	0.41
1:A:342:LEU:HB3	1:A:406:LEU:HG	2.04	0.40
1:A:640:ASP:OD1	1:A:640:ASP:N	2.46	0.40
1:B:447:GLU:O	1:B:448:ASP:HB2	2.21	0.40
1:A:47:TYR:O	1:A:48:ALA:C	2.61	0.40
1:B:283:LYS:HG3	1:B:284:THR:O	2.22	0.40
1:B:284:THR:HG22	2:B:800:HEM:CAA	2.51	0.40
1:B:666:ASN:HB3	3:B:1050:HOH:O	2.20	0.40
1:A:467:LYS:HE3	1:A:559:GLU:OE1	2.20	0.40
1:B:559:GLU:HG2	1:B:566:VAL:CG2	2.51	0.40
1:B:730:TRP:CZ2	1:B:734:MET:HE3	2.56	0.40
1:B:295:LYS:HD2	1:B:299:ALA:CB	2.52	0.40
1:B:456:GLN:HB3	1:B:542:LYS:CG	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)
3:A:1179:HOH:O	3:B:949:HOH:O[3_555]	2.14	0.06
3:A:1200:HOH:O	3:B:1177:HOH:O[3_555]	2.15	0.05

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	708/768 (92%)	672 (95%)	33 (5%)	3 (0%)	30	51
1	B	708/768 (92%)	682 (96%)	21 (3%)	5 (1%)	18	38
All	All	1416/1536 (92%)	1354 (96%)	54 (4%)	8 (1%)	21	42

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	LYS
1	A	220	ILE
1	A	460	ASP
1	B	220	ILE
1	B	10	ASN
1	B	43	LYS
1	B	538	SER
1	B	489	SER

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	577/621 (93%)	544 (94%)	33 (6%)	18	40
1	B	577/621 (93%)	542 (94%)	35 (6%)	17	37
All	All	1154/1242 (93%)	1086 (94%)	68 (6%)	18	38

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	8	LYS
1	A	61	LYS
1	A	99	THR
1	A	115	LEU
1	A	134	ILE
1	A	186	THR
1	A	223	ARG

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Mol	Chain	Res	Type
1	A	226	GLN
1	A	227	SER
1	A	295	LYS
1	A	302	ILE
1	A	336	LYS
1	A	347	LYS
1	A	370	THR
1	A	383	PRO
1	A	432	THR
1	A	456	GLN
1	A	457	ILE
1	A	473	THR
1	A	495	ASP
1	A	496	LYS
1	A	538	SER
1	A	540	SER
1	A	542	LYS
1	A	578	GLU
1	A	633	ARG
1	A	639	TYR
1	A	685	LYS
1	A	688	ASP
1	A	720	GLU
1	A	727	VAL
1	A	741	LEU
1	B	7	ARG
1	B	8	LYS
1	B	60	LYS
1	B	97	ARG
1	B	134	ILE
1	B	163	THR
1	B	175	GLU
1	B	187	THR
1	B	192	GLU
1	B	220	ILE
1	B	222	ASN
1	B	251	VAL
1	B	280	SER
1	B	347	LYS
1	B	365	LYS
1	B	366	ASN
1	B	381	LYS

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Mol	Chain	Res	Type
1	B	382	LEU
1	B	384	THR
1	B	400	LYS
1	B	428	MET
1	B	444	LEU
1	B	457	ILE
1	B	458	ILE
1	B	469	GLU
1	B	473	THR
1	B	506	ARG
1	B	533	GLN
1	B	542	LYS
1	B	584	SER
1	B	586	THR
1	B	629	ILE
1	B	665	THR
1	B	727	VAL
1	B	741	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	136	GLN
1	A	226	GLN
1	A	305	GLN
1	A	360	ASN
1	A	456	GLN
1	A	577	GLN
1	A	579	HIS
1	A	638	ASN
1	B	221	HIS
1	B	226	GLN
1	B	378	ASN
1	B	408	ASN
1	B	510	GLN
1	B	533	GLN
1	B	560	GLN
1	B	579	HIS
1	B	638	ASN
1	B	666	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	A	90	1	14,17,18	2.27	3 (21%)	12,23,25	1.94	6 (50%)
1	TOX	B	90	1	14,17,18	2.31	4 (28%)	12,23,25	1.83	3 (25%)

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	A	90	1	-	2/5/8/10	0/2/2/2
1	TOX	B	90	1	-	2/5/8/10	0/2/2/2

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	90	TOX	O-C	5.35	1.40	1.20
1	A	90	TOX	O-C	5.33	1.40	1.20
1	B	90	TOX	O1-NE1	-4.13	1.33	1.39
1	A	90	TOX	O1-NE1	-4.00	1.33	1.39
1	B	90	TOX	CE2-NE1	-3.47	1.33	1.39
1	A	90	TOX	CE2-NE1	-3.31	1.33	1.39
1	B	90	TOX	CE3-CD2	-2.30	1.36	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	90	TOX	CZ2-CE2-NE1	3.92	135.61	129.37
1	B	90	TOX	CZ2-CE2-NE1	3.75	135.35	129.37
1	B	90	TOX	CZ3-CH2-CZ2	-2.86	116.71	120.24
1	A	90	TOX	CZ3-CH2-CZ2	-2.72	116.88	120.24
1	B	90	TOX	CZ2-CE2-CD2	-2.27	119.41	121.95
1	A	90	TOX	CZ2-CE2-CD2	-2.17	119.52	121.95
1	A	90	TOX	CE3-CD2-CE2	2.14	121.70	119.24
1	A	90	TOX	CH2-CZ3-CE3	2.13	122.87	120.24
1	A	90	TOX	CE3-CD2-CG	-2.10	130.72	133.85

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	90	TOX	N-CA-CB-CG
1	A	90	TOX	C-CA-CB-CG
1	B	90	TOX	N-CA-CB-CG
1	B	90	TOX	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	90	TOX	2	0
1	B	90	TOX	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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
2	HEM	B	800	1	50,50,50	1.50	11 (22%)	67,82,82	1.60	13 (19%)
2	HEM	A	800	1	50,50,50	1.50	12 (24%)	67,82,82	1.59	10 (14%)

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
2	HEM	B	800	1	-	4/14/54/54	-
2	HEM	A	800	1	-	4/14/54/54	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	HEM	C1B-NB	-3.80	1.33	1.40
2	B	800	HEM	FE-NB	3.80	2.06	1.94
2	A	800	HEM	FE-NB	3.72	2.06	1.94
2	A	800	HEM	C1B-NB	-3.56	1.34	1.40
2	B	800	HEM	FE-NC	3.39	2.06	1.95
2	A	800	HEM	C4D-ND	-3.38	1.34	1.40
2	B	800	HEM	C4D-ND	-3.26	1.34	1.40
2	A	800	HEM	FE-NC	3.11	2.05	1.95
2	A	800	HEM	C1A-C2A	-2.54	1.39	1.44
2	B	800	HEM	C3C-C4C	-2.52	1.41	1.46
2	B	800	HEM	C4B-NB	-2.49	1.34	1.38
2	A	800	HEM	C4B-NB	-2.44	1.34	1.38
2	B	800	HEM	C1A-NA	-2.39	1.35	1.39
2	A	800	HEM	C1C-C2C	-2.34	1.40	1.45
2	A	800	HEM	C3C-C4C	-2.30	1.42	1.46
2	B	800	HEM	C4C-NC	-2.29	1.35	1.39
2	B	800	HEM	C1C-C2C	-2.23	1.40	1.45
2	A	800	HEM	C4C-NC	-2.21	1.35	1.39
2	A	800	HEM	C3B-C4B	2.18	1.49	1.44
2	A	800	HEM	O2D-CGD	-2.17	1.23	1.30
2	B	800	HEM	O2D-CGD	-2.07	1.24	1.30
2	A	800	HEM	C1A-NA	-2.07	1.35	1.39
2	B	800	HEM	C1A-C2A	-2.01	1.40	1.44

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	HEM	CHC-C4B-NB	5.12	129.94	124.42
2	B	800	HEM	CHC-C4B-NB	4.79	129.57	124.42
2	B	800	HEM	C1B-NB-C4B	4.35	110.35	105.21
2	A	800	HEM	C1B-NB-C4B	4.11	110.08	105.21
2	B	800	HEM	CHB-C1B-NB	3.97	129.28	124.37
2	A	800	HEM	CHB-C1B-NB	3.57	128.78	124.37
2	A	800	HEM	C3B-C4B-NB	-3.34	107.07	109.47
2	B	800	HEM	C3B-C4B-NB	-3.28	107.11	109.47
2	A	800	HEM	CHD-C1D-ND	2.97	127.62	124.42
2	B	800	HEM	CHD-C1D-ND	2.90	127.54	124.42
2	A	800	HEM	C1C-CHC-C4B	-2.84	119.99	126.02
2	B	800	HEM	C1C-CHC-C4B	-2.54	120.61	126.02
2	B	800	HEM	C4A-CHB-C1B	-2.48	120.42	126.25
2	B	800	HEM	C1A-CHA-C4D	-2.40	120.61	126.25
2	B	800	HEM	CHA-C4D-ND	2.34	127.26	124.37
2	A	800	HEM	C4A-CHB-C1B	-2.28	120.89	126.25
2	A	800	HEM	O2D-CGD-CBD	2.24	121.07	114.00
2	A	800	HEM	C1A-CHA-C4D	-2.08	121.35	126.25
2	A	800	HEM	O2A-CGA-CBA	2.07	120.53	114.00
2	B	800	HEM	O2D-CGD-CBD	2.06	120.52	114.00
2	B	800	HEM	O2A-CGA-CBA	2.04	120.46	114.00
2	B	800	HEM	C4D-ND-C1D	2.04	107.62	105.21
2	B	800	HEM	CHB-C1B-C2B	-2.01	121.23	126.95

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	800	HEM	C4B-C3B-CAB-CBB
2	B	800	HEM	C4B-C3B-CAB-CBB
2	A	800	HEM	C2B-C3B-CAB-CBB
2	B	800	HEM	C2B-C3B-CAB-CBB
2	B	800	HEM	CAA-CBA-CGA-O1A
2	A	800	HEM	CAA-CBA-CGA-O1A
2	A	800	HEM	CAA-CBA-CGA-O2A
2	B	800	HEM	CAA-CBA-CGA-O2A

There are no ring outliers.

2 monomers are involved in 14 short contacts:

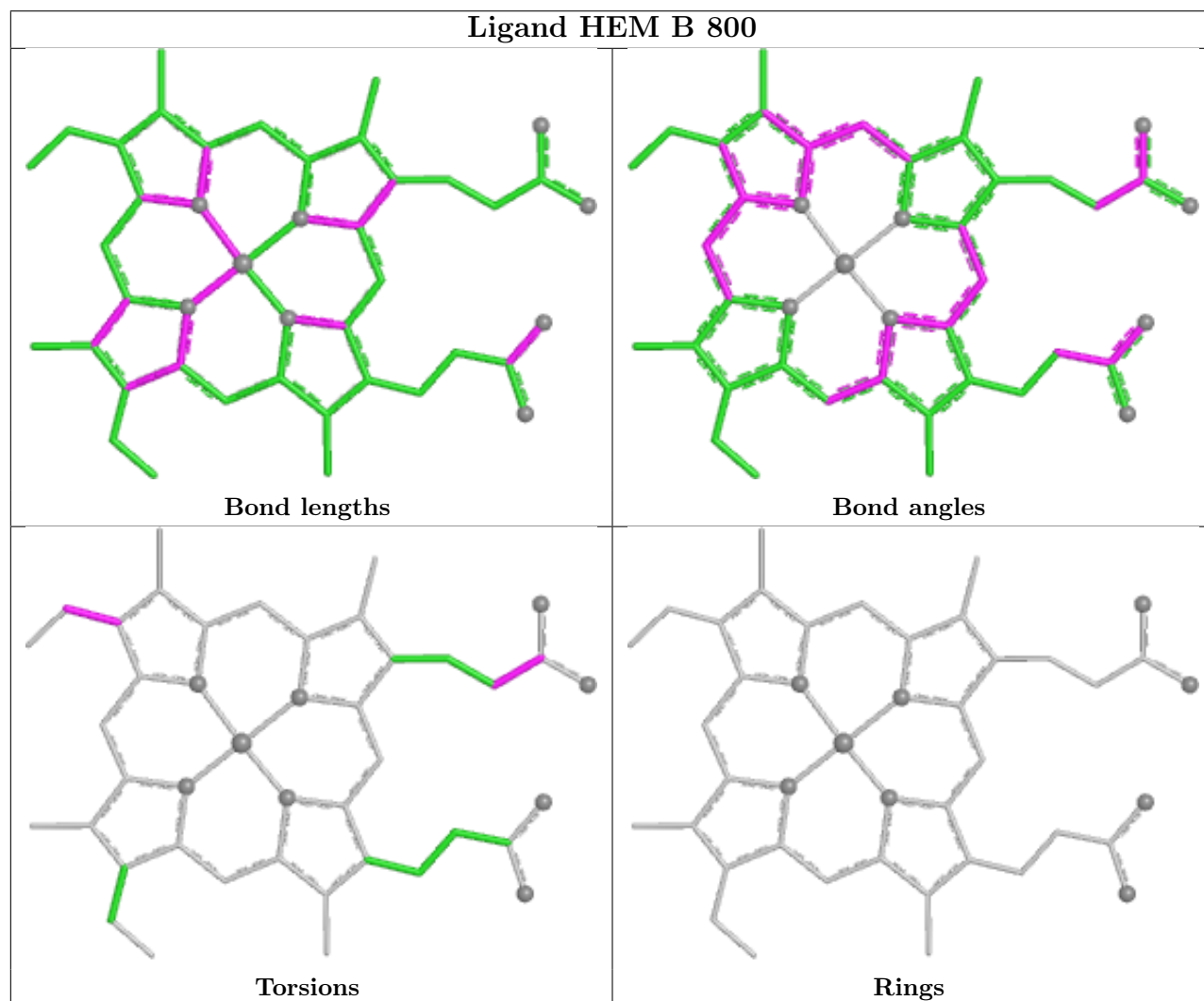
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	800	HEM	8	0

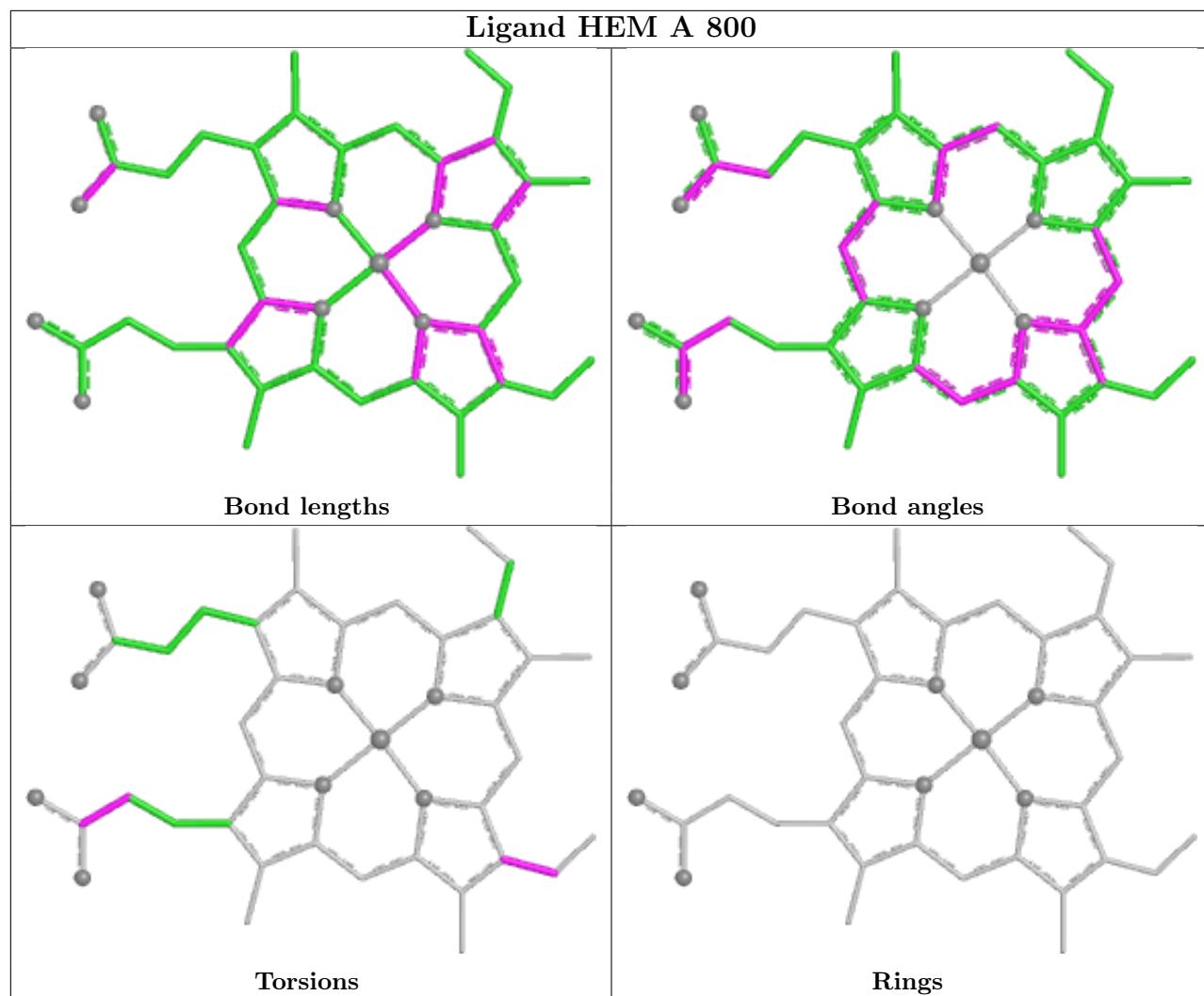
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	HEM	6	0

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

6.1 Protein, DNA and RNA chains

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	712/768 (92%)	0.21	21 (2%) 53 48	14, 29, 49, 91	0
1	B	712/768 (92%)	0.06	19 (2%) 56 50	13, 24, 47, 106	0
All	All	1424/1536 (92%)	0.14	40 (2%) 55 49	13, 27, 48, 106	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	220	ILE	5.5
1	B	538	SER	5.4
1	B	220	ILE	4.8
1	B	539	SER	4.3
1	A	539	SER	4.2
1	A	222	ASN	4.0
1	A	717	ASP	3.8
1	B	221	HIS	3.8
1	A	741	LEU	3.6
1	B	540	SER	3.5
1	B	222	ASN	3.5
1	A	221	HIS	3.4
1	A	538	SER	3.3
1	A	368	GLU	3.1
1	B	685	LYS	3.1
1	A	685	LYS	2.9
1	B	219	ASP	2.8
1	A	441	SER	2.8
1	A	542	LYS	2.7
1	B	43	LYS	2.6
1	A	196	SER	2.6
1	B	741	LEU	2.5
1	A	533	GLN	2.5
1	A	688	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	530	SER	2.4
1	A	540	SER	2.4
1	B	533	GLN	2.4
1	A	43	LYS	2.3
1	A	740	ASP	2.3
1	B	196	SER	2.3
1	A	8	LYS	2.3
1	B	366	ASN	2.3
1	A	243	GLY	2.3
1	A	219	ASP	2.2
1	B	717	ASP	2.2
1	B	9	SER	2.2
1	B	224	ASP	2.1
1	B	368	GLU	2.1
1	A	469	GLU	2.1
1	B	11	VAL	2.1

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(Å ²)	Q<0.9
1	TOX	A	90	16/17	0.94	0.10	21,23,28,33	0
1	TOX	B	90	16/17	0.95	0.09	12,14,19,23	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

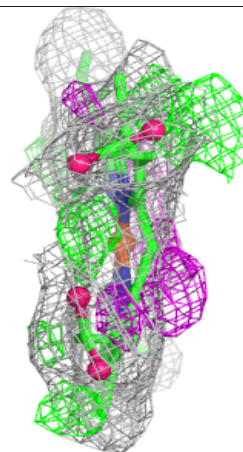
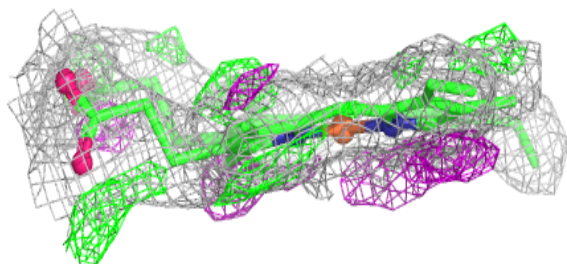
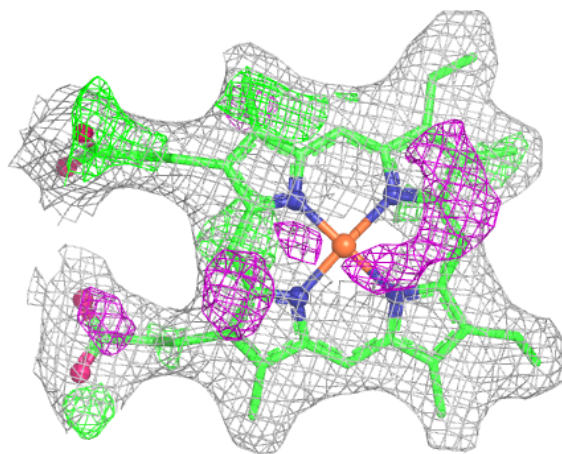
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

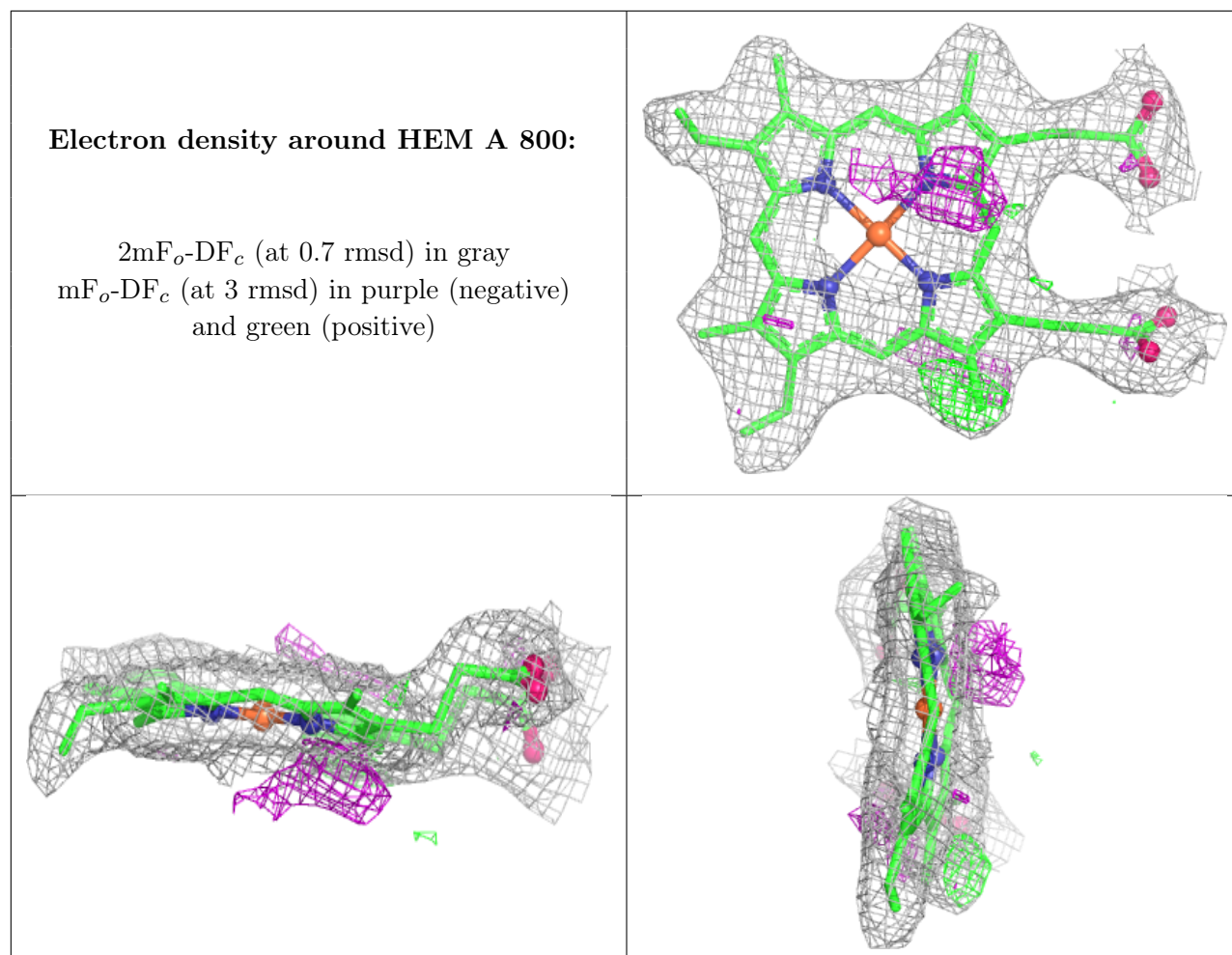
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	B	800	43/43	0.92	0.13	16,18,19,20	0
2	HEM	A	800	43/43	0.93	0.12	22,24,28,31	0

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 800:

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.