



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:30 AM UTC

PDB ID : 4ENP / pdb_00004enp
Title : Structure of E530A variant E. coli KatE
Authors : Loewen, P.C.; Jha, V.
Deposited on : 2012-04-13
Resolution : 1.50 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

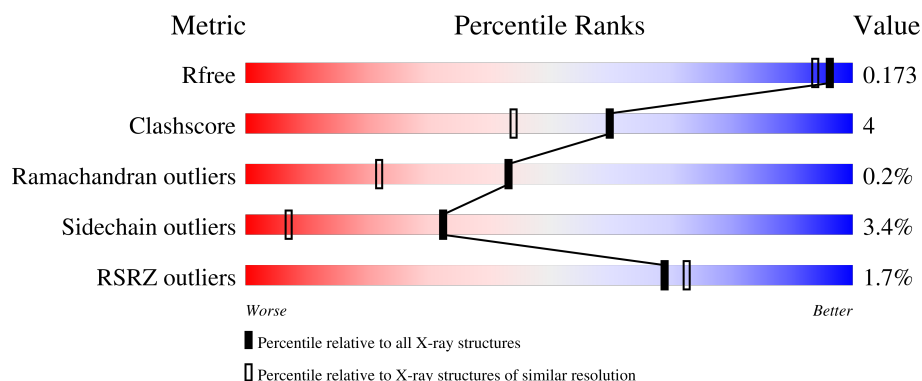
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	4037 (1.50-1.50)
Clashscore	190562	4235 (1.50-1.50)
Ramachandran outliers	187476	4153 (1.50-1.50)
Sidechain outliers	187428	4150 (1.50-1.50)
RSRZ outliers	180081	4039 (1.50-1.50)

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	753	% 84% 10% ...
1	B	753	2% 81% 13% ...
1	C	753	3% 81% 13% ...
1	D	753	% 81% 14% ...

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26715 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.

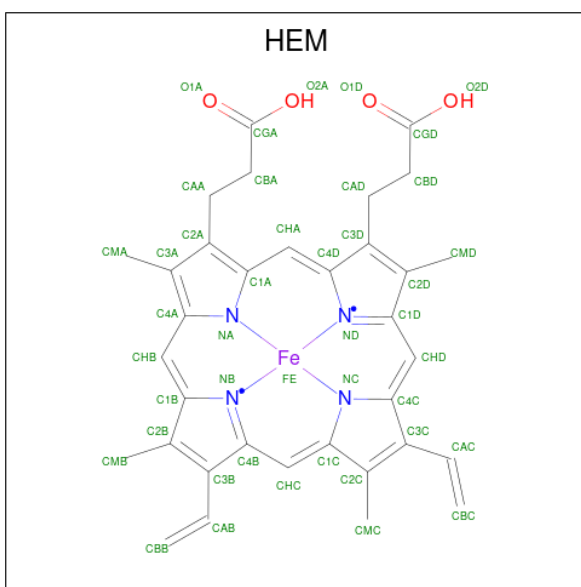
- Molecule 1 is a protein called Catalase HP11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	17	0
			5825	3699	1018	1096	12			
1	B	726	Total	C	N	O	S	0	11	0
			5789	3673	1012	1092	12			
1	C	726	Total	C	N	O	S	0	12	0
			5796	3677	1016	1091	12			
1	D	726	Total	C	N	O	S	0	11	0
			5789	3674	1015	1088	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	530	ALA	GLU	engineered mutation	UNP P21179
B	530	ALA	GLU	engineered mutation	UNP P21179
C	530	ALA	GLU	engineered mutation	UNP P21179
D	530	ALA	GLU	engineered mutation	UNP P21179

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



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

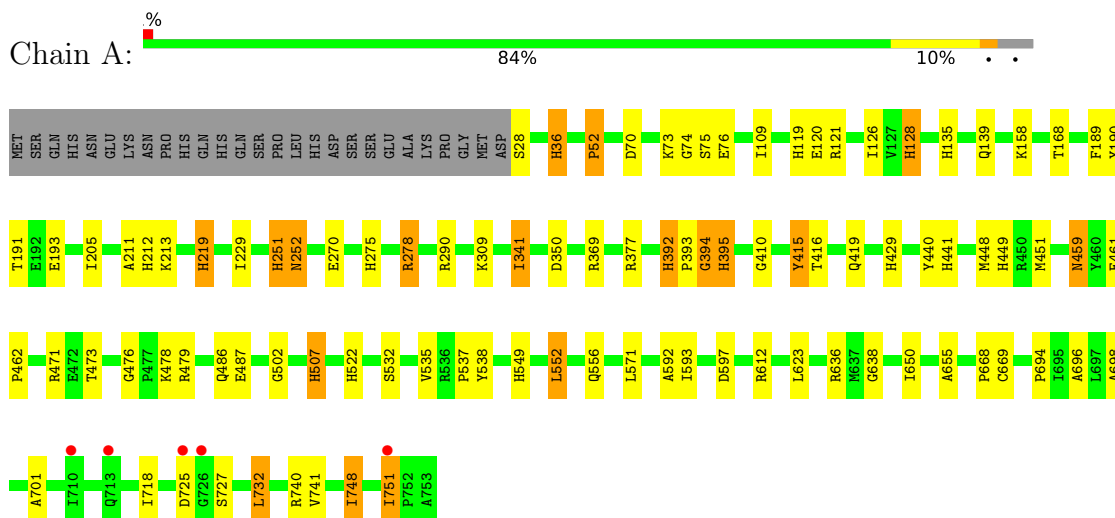
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	874	Total O 874 874	0	0
3	B	776	Total O 776 776	0	0
3	C	808	Total O 808 808	0	0
3	D	886	Total O 886 886	0	0

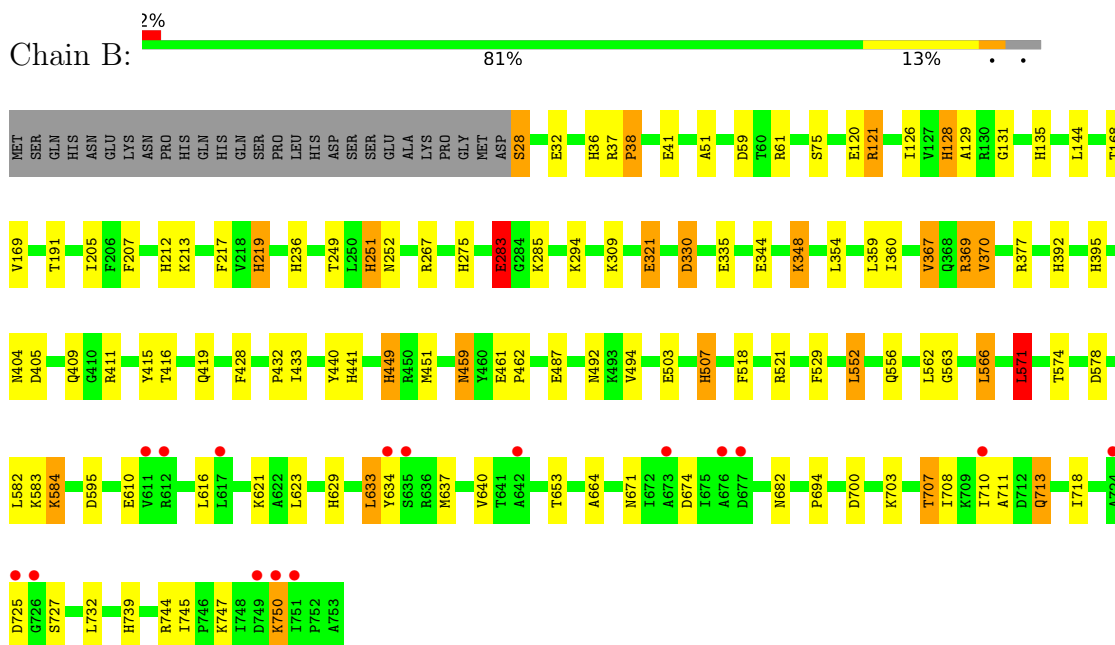
3 Residue-property plots [i](#)

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

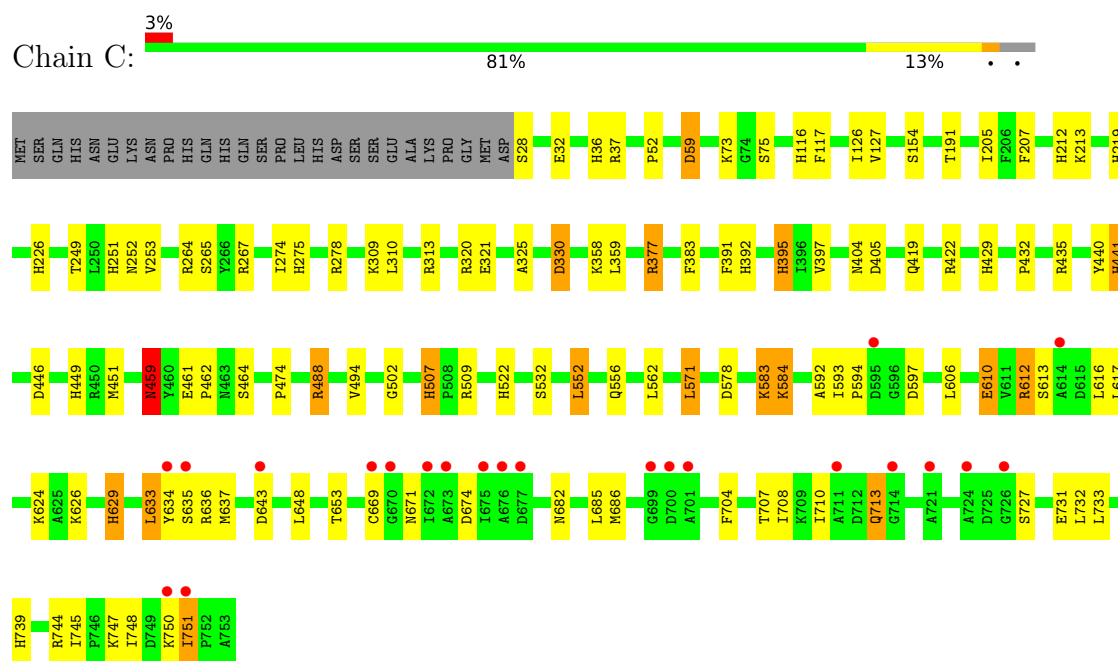
• Molecule 1: Catalase HP11



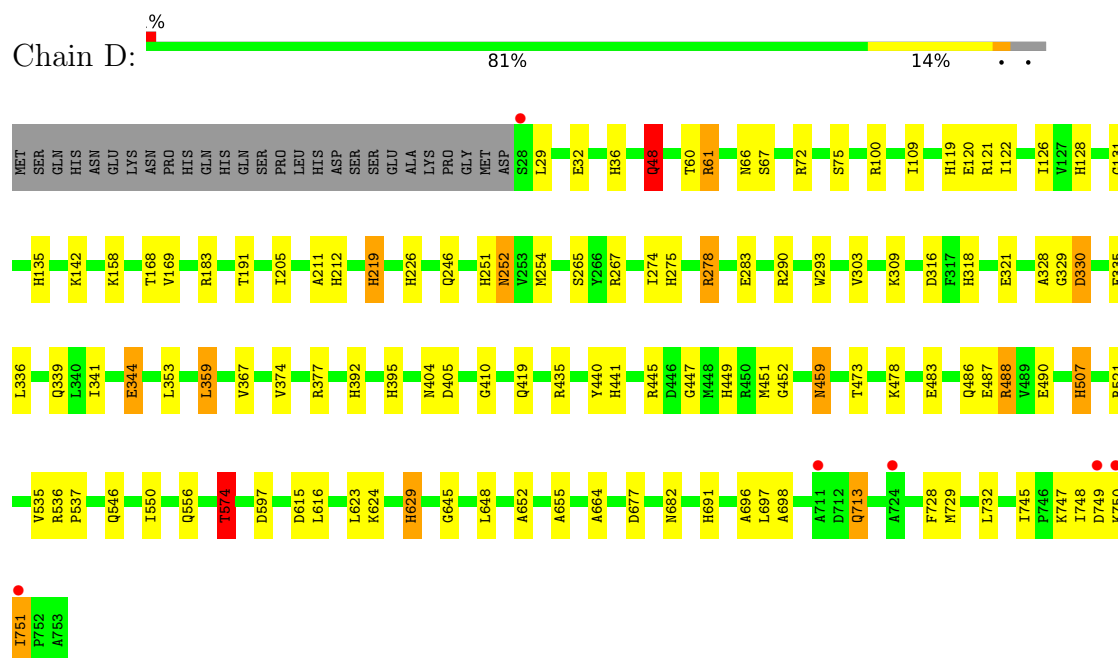
• Molecule 1: Catalase HP11



• Molecule 1: Catalase HP11



- Molecule 1: Catalase HP11



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.33Å 133.11Å 122.74Å 90.00° 109.41° 90.00°	Depositor
Resolution (Å)	35.24 – 1.50 35.24 – 1.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (35.24-1.50) 99.9 (35.24-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 1.50Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.138 , 0.162 (Not available) , 0.173	Depositor DCC
R_{free} test set	22572 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	13.1	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	26715	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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

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	1.67	56/6023 (0.9%)	1.41	19/8188 (0.2%)
1	B	1.61	42/5972 (0.7%)	1.37	22/8119 (0.3%)
1	C	1.63	44/5984 (0.7%)	1.41	16/8134 (0.2%)
1	D	1.70	69/5976 (1.2%)	1.43	22/8123 (0.3%)
All	All	1.65	211/23955 (0.9%)	1.40	79/32564 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (211) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	441	HIS	ND1-CE1	11.50	1.44	1.32
1	A	392	HIS	ND1-CE1	9.64	1.42	1.32
1	D	392	HIS	ND1-CE1	9.57	1.42	1.32
1	B	370	VAL	CA-CB	9.12	1.66	1.54
1	D	682	ASN	N-CA	-9.08	1.35	1.46
1	C	59	ASP	CG-OD1	8.83	1.42	1.25
1	C	116	HIS	ND1-CE1	8.78	1.41	1.32
1	C	419	GLN	CD-NE2	8.74	1.51	1.33
1	D	419	GLN	CD-OE1	8.68	1.40	1.23
1	A	377	ARG	CZ-NH1	8.66	1.44	1.32
1	D	251	HIS	ND1-CE1	8.59	1.41	1.32
1	D	751	ILE	CA-C	8.51	1.58	1.52
1	B	739	HIS	CG-CD2	8.48	1.45	1.35
1	B	419	GLN	CD-NE2	8.46	1.51	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	549	HIS	ND1-CE1	8.38	1.41	1.32
1	C	522	HIS	CG-CD2	8.06	1.44	1.35
1	A	419	GLN	CD-OE1	8.04	1.38	1.23
1	D	329	GLY	C-O	7.92	1.34	1.24
1	B	633	LEU	C-O	-7.79	1.14	1.23
1	D	652	ALA	CA-C	-7.74	1.43	1.52
1	D	419	GLN	CA-CB	7.69	1.66	1.53
1	A	623	LEU	C-O	7.64	1.33	1.24
1	B	392	HIS	ND1-CE1	7.57	1.40	1.32
1	D	441	HIS	ND1-CE1	7.50	1.40	1.32
1	B	212	HIS	ND1-CE1	7.45	1.40	1.32
1	A	549	HIS	CG-CD2	7.43	1.44	1.35
1	C	59	ASP	CB-CG	7.42	1.70	1.52
1	D	341	ILE	N-CA	7.37	1.51	1.45
1	B	441	HIS	ND1-CE1	7.36	1.40	1.32
1	D	507	HIS	ND1-CE1	7.25	1.39	1.32
1	A	696	ALA	N-CA	7.18	1.55	1.46
1	D	395	HIS	ND1-CE1	7.14	1.39	1.32
1	D	341	ILE	CA-CB	-7.09	1.49	1.54
1	B	128	HIS	ND1-CE1	7.07	1.39	1.32
1	A	275	HIS	CG-CD2	7.04	1.43	1.35
1	D	655	ALA	C-O	7.01	1.32	1.24
1	B	275	HIS	ND1-CE1	7.00	1.39	1.32
1	A	592	ALA	N-CA	6.98	1.55	1.46
1	D	507	HIS	CE1-NE2	6.93	1.39	1.32
1	C	419	GLN	CD-OE1	6.92	1.36	1.23
1	A	395	HIS	ND1-CE1	6.91	1.39	1.32
1	A	419	GLN	CD-NE2	6.86	1.47	1.33
1	D	435	ARG	NE-CZ	6.84	1.40	1.33
1	D	377	ARG	CZ-NH1	6.73	1.42	1.32
1	C	392	HIS	ND1-CE1	6.66	1.39	1.32
1	C	36	HIS	CE1-NE2	6.65	1.39	1.32
1	A	638	GLY	N-CA	6.58	1.52	1.45
1	C	395	HIS	ND1-CE1	6.57	1.39	1.32
1	D	452	GLY	C-O	6.51	1.30	1.24
1	D	275	HIS	ND1-CE1	6.50	1.39	1.32
1	D	419	GLN	CD-NE2	6.49	1.46	1.33
1	B	236	HIS	ND1-CE1	6.45	1.39	1.32
1	C	739	HIS	N-CA	6.40	1.54	1.46
1	C	127	VAL	C-O	6.35	1.30	1.23
1	B	37	ARG	CA-C	6.31	1.59	1.52
1	C	419	GLN	N-CA	6.28	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	36	HIS	CE1-NE2	6.24	1.38	1.32
1	D	336	LEU	N-CA	6.21	1.53	1.46
1	B	494	VAL	C-O	6.20	1.30	1.23
1	C	441	HIS	ND1-CE1	6.18	1.38	1.32
1	C	633	LEU	C-O	-6.17	1.16	1.23
1	C	116	HIS	CG-CD2	6.14	1.42	1.35
1	A	655	ALA	C-O	6.12	1.31	1.24
1	D	359	LEU	N-CA	6.12	1.52	1.45
1	D	219	HIS	CG-CD2	6.05	1.42	1.35
1	C	212	HIS	ND1-CE1	6.05	1.38	1.32
1	C	226	HIS	ND1-CE1	6.01	1.38	1.32
1	D	483	GLU	CA-C	-6.01	1.45	1.52
1	A	275	HIS	CE1-NE2	5.97	1.38	1.32
1	D	131	GLY	N-CA	5.97	1.51	1.45
1	D	48	GLN	C-O	-5.95	1.18	1.24
1	C	275	HIS	ND1-CE1	5.94	1.38	1.32
1	A	507	HIS	CE1-NE2	5.94	1.38	1.32
1	D	629	HIS	CE1-NE2	5.93	1.38	1.32
1	A	522	HIS	ND1-CE1	5.93	1.38	1.32
1	A	668	PRO	N-CA	5.92	1.53	1.46
1	C	507	HIS	CE1-NE2	5.90	1.38	1.32
1	A	251	HIS	ND1-CE1	5.88	1.38	1.32
1	D	212	HIS	ND1-CE1	5.86	1.38	1.32
1	A	741	VAL	N-CA	5.86	1.53	1.46
1	A	193	GLU	N-CA	5.85	1.52	1.46
1	A	189	PHE	N-CA	5.85	1.53	1.46
1	B	419	GLN	CD-OE1	5.82	1.34	1.23
1	C	358	LYS	C-O	5.82	1.31	1.24
1	B	131	GLY	N-CA	5.81	1.51	1.45
1	C	419	GLN	CA-CB	5.79	1.62	1.53
1	B	37	ARG	CZ-NH2	5.79	1.41	1.33
1	B	219	HIS	CG-CD2	5.78	1.42	1.35
1	A	219	HIS	ND1-CE1	5.78	1.38	1.32
1	C	397	VAL	N-CA	5.78	1.51	1.46
1	C	459	ASN	CG-OD1	5.77	1.34	1.23
1	B	507	HIS	CE1-NE2	5.75	1.38	1.32
1	A	732	LEU	C-O	5.75	1.30	1.24
1	D	303	VAL	CA-C	-5.75	1.45	1.52
1	B	360	ILE	C-O	-5.74	1.17	1.24
1	D	36	HIS	CE1-NE2	5.74	1.38	1.32
1	D	751	ILE	CA-CB	5.73	1.58	1.54
1	A	419	GLN	CA-CB	5.72	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	72	ARG	C-O	5.72	1.30	1.23
1	A	593	ILE	N-CA	5.71	1.50	1.46
1	D	729	MET	C-O	5.71	1.30	1.24
1	B	623	LEU	N-CA	5.70	1.53	1.46
1	D	697	LEU	CA-C	5.69	1.59	1.52
1	B	409	GLN	CA-CB	5.68	1.62	1.53
1	A	135	HIS	N-CA	5.65	1.52	1.45
1	A	135	HIS	CG-CD2	5.64	1.42	1.35
1	A	429	HIS	ND1-CE1	5.64	1.38	1.32
1	D	445	ARG	CZ-NH2	5.63	1.40	1.33
1	D	550	ILE	C-O	5.63	1.29	1.23
1	C	253	VAL	CA-C	5.62	1.59	1.52
1	D	135	HIS	CE1-NE2	5.61	1.38	1.32
1	D	316	ASP	N-CA	5.60	1.52	1.46
1	A	212	HIS	ND1-CE1	5.59	1.38	1.32
1	D	29	LEU	N-CA	5.59	1.53	1.45
1	D	122	ILE	CA-CB	5.58	1.59	1.55
1	D	339	GLN	N-CA	5.57	1.53	1.46
1	C	592	ALA	N-CA	5.57	1.53	1.46
1	C	459	ASN	CA-CB	5.57	1.60	1.53
1	B	36	HIS	ND1-CE1	5.54	1.38	1.32
1	B	283	GLU	CA-C	-5.53	1.45	1.52
1	A	486	GLN	CA-CB	5.52	1.59	1.52
1	C	429	HIS	ND1-CE1	5.52	1.38	1.32
1	D	374	VAL	N-CA	5.50	1.52	1.46
1	D	367	VAL	C-O	5.50	1.29	1.24
1	D	473	THR	C-N	5.49	1.39	1.33
1	D	447	GLY	N-CA	5.48	1.51	1.45
1	C	494	VAL	N-CA	5.44	1.52	1.46
1	B	529	PHE	N-CA	5.44	1.52	1.46
1	D	623	LEU	N-CA	5.43	1.52	1.46
1	B	492	ASN	CG-ND2	-5.43	1.21	1.33
1	D	183	ARG	CD-NE	5.43	1.53	1.46
1	D	252	ASN	CG-OD1	5.42	1.33	1.23
1	C	265	SER	CB-OG	-5.41	1.31	1.42
1	A	698	ALA	N-CA	5.40	1.52	1.46
1	A	251	HIS	CG-CD2	5.38	1.41	1.35
1	A	52	PRO	CA-CB	5.38	1.60	1.53
1	C	154	SER	N-CA	5.37	1.53	1.46
1	B	739	HIS	ND1-CE1	5.36	1.38	1.32
1	D	486	GLN	CD-NE2	-5.35	1.22	1.33
1	D	452	GLY	N-CA	5.35	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	474	PRO	CA-C	5.32	1.57	1.52
1	C	502	GLY	N-CA	5.32	1.53	1.45
1	B	41	GLU	C-O	5.31	1.29	1.24
1	D	328	ALA	N-CA	5.30	1.53	1.46
1	B	518	PHE	N-CA	5.29	1.53	1.46
1	B	521	ARG	CZ-NH1	5.29	1.40	1.32
1	A	650	ILE	C-O	5.29	1.30	1.24
1	D	119	HIS	ND1-CE1	5.29	1.37	1.32
1	C	127	VAL	N-CA	5.29	1.51	1.46
1	D	353	LEU	N-CA	5.28	1.52	1.46
1	C	435	ARG	CA-CB	5.28	1.62	1.53
1	C	464	SER	N-CA	5.28	1.53	1.46
1	A	70	ASP	N-CA	5.28	1.52	1.46
1	B	563	GLY	N-CA	5.27	1.52	1.45
1	B	416	THR	N-CA	5.27	1.52	1.46
1	D	290	ARG	CZ-NH2	5.27	1.40	1.33
1	D	142	LYS	C-O	5.26	1.30	1.23
1	A	597	ASP	C-O	5.26	1.29	1.23
1	B	664	ALA	N-CA	5.25	1.52	1.46
1	D	536	ARG	N-CA	5.24	1.52	1.46
1	C	446	ASP	N-CA	5.24	1.52	1.46
1	B	503	GLU	C-O	5.24	1.29	1.23
1	B	128	HIS	CD2-NE2	5.23	1.43	1.37
1	A	538	TYR	CA-C	5.22	1.59	1.52
1	B	217	PHE	CA-CB	5.21	1.61	1.53
1	B	251	HIS	ND1-CE1	5.21	1.37	1.32
1	D	265	SER	CA-CB	5.20	1.62	1.53
1	A	190	TYR	CA-C	5.20	1.59	1.53
1	B	367	VAL	C-O	5.20	1.29	1.24
1	C	629	HIS	CE1-NE2	5.20	1.37	1.32
1	D	664	ALA	CA-C	-5.19	1.46	1.52
1	A	128	HIS	CG-CD2	5.19	1.41	1.35
1	B	694	PRO	N-CA	5.19	1.53	1.47
1	A	350	ASP	CB-CG	-5.18	1.39	1.52
1	D	226	HIS	CG-ND1	5.17	1.44	1.38
1	A	732	LEU	N-CA	5.17	1.52	1.46
1	A	290	ARG	CZ-NH2	5.17	1.40	1.33
1	D	318	HIS	ND1-CE1	5.16	1.37	1.32
1	A	727	SER	CA-C	5.16	1.59	1.52
1	C	325	ALA	CA-CB	-5.15	1.45	1.53
1	D	60	THR	N-CA	5.15	1.52	1.46
1	D	691	HIS	CG-ND1	-5.15	1.32	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	135	HIS	ND1-CE1	5.14	1.37	1.32
1	D	698	ALA	N-CA	5.13	1.52	1.46
1	A	549	HIS	CE1-NE2	5.13	1.37	1.32
1	C	320	ARG	CZ-NH2	5.13	1.40	1.33
1	D	293	TRP	CD2-CE2	5.13	1.50	1.41
1	A	476	GLY	N-CA	5.11	1.51	1.44
1	C	264	ARG	CA-CB	5.11	1.61	1.53
1	A	36	HIS	CE1-NE2	5.10	1.37	1.32
1	A	502	GLY	N-CA	5.10	1.52	1.45
1	B	38	PRO	C-O	5.08	1.29	1.23
1	A	119	HIS	ND1-CE1	5.07	1.37	1.32
1	A	694	PRO	C-O	5.07	1.29	1.23
1	A	718	ILE	C-O	5.07	1.29	1.24
1	A	252	ASN	CG-OD1	5.07	1.33	1.23
1	B	433	ILE	CA-CB	5.06	1.61	1.54
1	A	473	THR	N-CA	5.05	1.52	1.46
1	C	507	HIS	ND1-CE1	5.05	1.37	1.32
1	D	335	GLU	N-CA	-5.05	1.40	1.46
1	C	212	HIS	CG-ND1	5.05	1.43	1.38
1	A	701	ALA	N-CA	5.05	1.52	1.46
1	D	278	ARG	N-CA	5.04	1.52	1.45
1	A	392	HIS	CG-CD2	-5.04	1.30	1.35
1	A	392	HIS	CG-ND1	5.03	1.43	1.38
1	C	395	HIS	CG-CD2	5.03	1.41	1.35
1	D	251	HIS	CE1-NE2	5.03	1.37	1.32
1	B	595	ASP	N-CA	5.02	1.50	1.46
1	D	67[A]	SER	N-CA	5.02	1.52	1.46
1	D	67[B]	SER	N-CA	5.02	1.52	1.46
1	C	422	ARG	CA-CB	5.00	1.61	1.53

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	751	ILE	CB-CA-C	9.68	119.52	110.13
1	A	377	ARG	NE-CZ-NH2	-9.03	111.08	119.20
1	D	751	ILE	CA-C-O	8.91	125.04	119.51
1	C	37	ARG	NE-CZ-NH2	-8.18	111.83	119.20
1	D	278	ARG	NE-CZ-NH1	-7.73	113.77	121.50
1	D	278	ARG	NE-CZ-NH2	7.49	125.94	119.20
1	C	330	ASP	CB-CA-C	-7.13	101.43	112.12
1	D	615	ASP	N-CA-C	-7.11	103.46	111.07
1	C	419	GLN	CB-CA-C	7.00	124.12	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	419	GLN	CB-CA-C	6.93	123.98	110.67
1	B	415	TYR	CA-C-O	-6.92	113.09	120.42
1	D	61	ARG	NE-CZ-NH2	6.77	125.29	119.20
1	A	751	ILE	N-CA-CB	6.74	116.35	110.08
1	C	278	ARG	NE-CZ-NH1	-6.68	114.82	121.50
1	A	748	ILE	N-CA-C	6.66	120.37	111.44
1	C	37	ARG	CB-CG-CD	-6.66	95.99	111.30
1	D	109	ILE	N-CA-C	-6.49	104.53	110.82
1	A	341	ILE	CA-C-O	6.45	123.30	119.94
1	A	636	ARG	NE-CZ-NH2	6.33	124.90	119.20
1	B	129	ALA	CA-C-O	-6.30	112.98	120.10
1	D	645	GLY	N-CA-C	6.29	123.39	115.21
1	B	574	THR	CA-C-N	6.14	124.14	119.66
1	B	574	THR	C-N-CA	6.14	124.14	119.66
1	A	377	ARG	NH1-CZ-NH2	5.84	126.89	119.30
1	D	751	ILE	N-CA-C	5.84	114.55	107.61
1	B	640	VAL	N-CA-C	-5.83	100.67	108.96
1	D	344	GLU	CA-CB-CG	5.76	125.61	114.10
1	B	377	ARG	CG-CD-NE	-5.73	99.40	112.00
1	C	745	ILE	O-C-N	5.72	124.08	120.42
1	B	745	ILE	CA-C-N	-5.66	113.84	119.56
1	B	745	ILE	C-N-CA	-5.66	113.84	119.56
1	C	509	ARG	NE-CZ-NH2	5.63	124.27	119.20
1	A	109	ILE	N-CA-C	-5.59	105.39	110.82
1	C	59	ASP	CA-CB-CG	-5.59	107.01	112.60
1	B	354	LEU	CD1-CG-CD2	5.57	123.06	110.80
1	D	748	ILE	N-CA-C	5.54	118.01	111.09
1	B	370	VAL	CB-CA-C	-5.54	106.19	111.06
1	B	377	ARG	NE-CZ-NH1	-5.49	116.01	121.50
1	C	321	GLU	CB-CG-CD	-5.49	103.27	112.60
1	D	377	ARG	CG-CD-NE	-5.46	99.98	112.00
1	A	394	GLY	N-CA-C	-5.45	108.18	115.32
1	A	415	TYR	CA-C-O	-5.42	114.68	120.42
1	C	278	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	A	740	ARG	NE-CZ-NH2	-5.39	114.35	119.20
1	A	278	ARG	NE-CZ-NH2	5.39	124.05	119.20
1	B	330	ASP	CB-CA-C	-5.37	104.06	112.12
1	D	169	VAL	CB-CA-C	-5.31	106.39	111.44
1	B	727	SER	CA-C-N	5.31	127.65	120.38
1	B	727	SER	C-N-CA	5.31	127.65	120.38
1	D	745	ILE	CA-C-N	-5.28	113.47	119.28
1	D	745	ILE	C-N-CA	-5.28	113.47	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	330	ASP	CB-CA-C	-5.27	104.21	112.12
1	C	391	PHE	CA-C-O	-5.27	115.12	120.71
1	A	419	GLN	CB-CA-C	5.26	120.77	110.67
1	D	574	THR	CB-CA-C	5.25	116.98	109.26
1	C	635	SER	N-CA-C	5.25	118.95	112.54
1	C	383	PHE	CA-CB-CG	-5.25	108.55	113.80
1	A	74	GLY	N-CA-C	-5.23	105.13	112.66
1	D	246	GLN	O-C-N	-5.23	116.72	121.17
1	D	100	ARG	CB-CA-C	-5.21	103.05	111.28
1	A	139	GLN	O-C-N	5.20	125.49	121.85
1	A	471	ARG	NE-CZ-NH1	-5.19	116.31	121.50
1	D	344	GLU	CG-CD-OE1	-5.18	106.47	118.40
1	D	749	ASP	N-CA-C	5.18	117.60	111.33
1	A	270	GLU	CA-C-N	5.17	125.75	122.18
1	A	270	GLU	C-N-CA	5.17	125.75	122.18
1	B	348	LYS	CA-CB-CG	-5.15	103.79	114.10
1	C	37	ARG	CG-CD-NE	-5.15	100.66	112.00
1	A	592	ALA	N-CA-C	-5.15	105.79	111.71
1	B	169	VAL	CB-CA-C	-5.13	106.57	111.44
1	B	449[A]	HIS	CA-C-O	-5.12	114.42	120.57
1	B	449[B]	HIS	CA-C-O	-5.12	114.42	120.57
1	A	229	ILE	N-CA-C	-5.10	105.01	109.19
1	B	36	HIS	N-CA-C	-5.09	106.58	112.89
1	B	419	GLN	CB-CA-C	5.08	120.92	110.31
1	B	571	LEU	N-CA-C	-5.05	107.06	113.18
1	B	744	ARG	NE-CZ-NH2	5.03	123.73	119.20
1	C	377	ARG	CB-CG-CD	5.03	122.86	111.30
1	C	613	SER	N-CA-C	5.01	117.40	111.33

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	121	ARG	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	5825	0	5671	47	0
1	B	5789	0	5618	67	0
1	C	5796	0	5631	60	0
1	D	5789	0	5632	46	0
2	A	43	0	30	0	0
2	B	43	0	30	3	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
3	A	874	0	0	14	0
3	B	776	0	0	16	0
3	C	808	0	0	22	0
3	D	886	0	0	18	0
All	All	26715	0	22672	197	0

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 4.

All (197) 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:C:313:ARG:HD2	3:C:1684:HOH:O	1.14	1.30
1:B:369:ARG:HD3	3:B:1673:HOH:O	1.44	1.18
1:A:451:MET:HE2	1:C:451:MET:HE2	1.22	1.09
1:B:451:MET:HE2	1:D:451:MET:HE2	1.35	1.08
1:C:267:ARG:HG3	3:C:1553:HOH:O	1.53	1.08
1:B:28:SER:HA	3:B:1624:HOH:O	1.53	1.06
1:C:751:ILE:HB	3:C:1456:HOH:O	1.54	1.05
1:A:341:ILE:HG13	3:A:1750:HOH:O	1.59	1.03
1:D:267:ARG:HG3	3:D:1375:HOH:O	1.59	1.02
1:B:449[A]:HIS:ND1	1:D:449[A]:HIS:CG	1.96	1.00
1:B:449[A]:HIS:CG	1:D:449[A]:HIS:CG	2.37	1.00
1:B:267:ARG:HG3	3:B:1371:HOH:O	1.59	1.00
1:B:449[A]:HIS:CG	1:D:449[A]:HIS:ND1	1.98	0.99
1:A:158:LYS:HE3	3:A:1735:HOH:O	1.64	0.98
1:A:479:ARG:NH2	3:A:1556:HOH:O	2.01	0.94
1:D:321:GLU:HG3	3:D:1434:HOH:O	1.70	0.90
1:B:367:VAL:HG12	1:B:369:ARG:HH12	1.39	0.88
1:B:487:GLU:CD	3:B:1647:HOH:O	2.17	0.87
1:B:369:ARG:HB3	1:B:369:ARG:CZ	1.96	0.87
1:A:126[B]:ILE:HD11	3:D:1009:HOH:O	1.80	0.81
1:C:686:MET:HB3	1:C:751:ILE:HD11	1.62	0.81
1:D:321:GLU:CG	3:D:1434:HOH:O	2.27	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:532[A]:SER:OG	3:A:1685:HOH:O	1.95	0.79
1:C:727:SER:HA	3:C:1523:HOH:O	1.86	0.75
1:A:369[A]:ARG:HH21	1:A:369[A]:ARG:HG3	1.52	0.75
1:B:335:GLU:OE1	1:B:369:ARG:NE	2.21	0.72
1:C:583:LYS:C	3:C:1673:HOH:O	2.32	0.72
1:C:597:ASP:OD2	3:C:1412:HOH:O	2.07	0.72
1:C:488[A]:ARG:HH11	1:C:488[A]:ARG:HG2	1.54	0.72
1:A:309:LYS:HE2	3:A:1688:HOH:O	1.89	0.71
1:A:341:ILE:CG1	3:A:1750:HOH:O	2.29	0.70
1:B:309:LYS:HE2	3:B:1592:HOH:O	1.93	0.69
1:A:73[B]:LYS:CE	3:C:1139:HOH:O	2.41	0.68
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.75	0.68
1:D:309:LYS:HE2	3:D:1732:HOH:O	1.94	0.68
1:D:283:GLU:OE1	3:D:1526:HOH:O	2.14	0.66
1:B:144:LEU:HD11	1:B:370:VAL:HG13	1.77	0.65
1:A:751:ILE:O	1:A:751:ILE:HD12	1.97	0.64
1:D:597:ASP:OD1	3:D:1717:HOH:O	2.15	0.64
1:D:597:ASP:OD2	3:D:1581:HOH:O	2.15	0.64
1:B:283:GLU:HG3	3:B:1676:HOH:O	1.96	0.64
1:C:309:LYS:HE2	3:C:1642:HOH:O	1.98	0.63
1:A:369[A]:ARG:HH21	1:A:369[A]:ARG:CG	2.10	0.63
1:A:126[B]:ILE:CD1	3:D:1009:HOH:O	2.40	0.63
1:D:713:GLN:HB3	3:D:1562:HOH:O	1.99	0.63
1:D:629:HIS:HD2	3:D:1258:HOH:O	1.82	0.63
1:C:532[B]:SER:OG	3:C:1619:HOH:O	2.12	0.61
1:C:395:HIS:HE1	3:C:1628:HOH:O	1.83	0.61
1:A:395:HIS:HE1	3:A:1698:HOH:O	1.83	0.61
1:C:629:HIS:HD2	3:C:1206:HOH:O	1.83	0.61
1:B:610:GLU:O	1:B:610:GLU:HG3	1.99	0.61
1:B:578[B]:ASP:HB2	1:B:582:LEU:O	2.02	0.60
1:B:395:HIS:HE1	3:B:1585:HOH:O	1.84	0.60
1:B:629:HIS:HD2	3:B:1159:HOH:O	1.85	0.60
1:A:278:ARG:HH12	1:A:487[A]:GLU:CD	2.10	0.58
1:C:552:LEU:HD22	1:C:556:GLN:HG3	1.85	0.58
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.83	0.58
1:A:73[B]:LYS:HE2	3:C:1139:HOH:O	2.01	0.58
1:A:36:HIS:CD2	1:A:36:HIS:H	2.22	0.57
1:B:121:ARG:CZ	1:C:126[B]:ILE:HG12	2.35	0.57
1:C:313:ARG:CD	3:C:1684:HOH:O	1.96	0.57
1:A:126[A]:ILE:HD11	1:D:120:GLU:HB2	1.86	0.57
1:C:73:LYS:HD2	3:C:1519:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:583:LYS:O	1:C:584:LYS:HB3	2.05	0.57
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.88	0.56
1:B:552:LEU:HD22	1:B:556:GLN:HG3	1.86	0.56
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.88	0.55
1:B:369:ARG:CZ	1:B:369:ARG:CB	2.77	0.55
1:B:708:ILE:HD12	1:B:710:ILE:HD11	1.89	0.55
1:B:562:LEU:HA	1:C:637:MET:HB2	1.88	0.54
1:B:583:LYS:O	1:B:584:LYS:HB3	2.07	0.54
1:B:428:PHE:HE2	3:B:1586:HOH:O	1.90	0.54
1:B:747:LYS:O	1:B:750:LYS:HD2	2.08	0.53
1:A:28:SER:HB2	3:C:1652:HOH:O	2.08	0.53
2:B:801:HEM:HMC2	2:B:801:HEM:HBC2	1.91	0.53
1:B:634:TYR:O	1:B:653:THR:HA	2.09	0.52
1:A:120:GLU:HB2	1:D:126[A]:ILE:HD11	1.92	0.52
1:A:612:ARG:HE	1:A:669:CYS:HB3	1.75	0.52
1:B:487:GLU:CG	3:B:1647:HOH:O	2.56	0.52
1:C:359:LEU:H	1:C:507:HIS:HD2	1.56	0.52
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.93	0.51
1:B:294:LYS:NZ	3:B:1514:HOH:O	2.39	0.51
1:B:367:VAL:HG12	1:B:369:ARG:NH1	2.19	0.51
1:A:449[B]:HIS:CD2	1:C:449[B]:HIS:CD2	2.99	0.50
1:C:682:ASN:O	1:C:686:MET:HG3	2.11	0.50
1:D:478:LYS:NZ	3:D:1001:HOH:O	2.35	0.50
1:C:643:ASP:OD2	3:C:1589:HOH:O	2.19	0.50
1:B:121:ARG:NH2	1:C:126[B]:ILE:HG12	2.27	0.50
1:D:535:VAL:O	1:D:537:PRO:HD3	2.11	0.50
1:A:552[B]:LEU:HD11	1:A:571:LEU:HD23	1.94	0.49
1:B:487:GLU:HG2	3:B:1647:HOH:O	2.12	0.49
1:B:708:ILE:CD1	1:B:710:ILE:HD11	2.43	0.49
1:B:359:LEU:H	1:B:507:HIS:HD2	1.59	0.49
1:C:28:SER:HA	3:C:1657:HOH:O	2.13	0.49
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.28	0.49
1:D:359:LEU:H	1:D:507:HIS:HD2	1.61	0.48
1:C:744:ARG:HA	1:C:747:LYS:HE2	1.94	0.48
1:A:449[A]:HIS:CG	1:C:449[A]:HIS:CG	2.32	0.48
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.29	0.48
1:C:578[B]:ASP:CG	1:C:583:LYS:HG3	2.39	0.48
1:B:126[B]:ILE:HD12	1:C:117:PHE:CZ	2.48	0.48
1:D:404:ASN:O	1:D:405:ASP:C	2.56	0.48
1:D:158:LYS:HB3	3:D:1761:HOH:O	2.13	0.48
1:D:254:MET:HE3	1:D:254:MET:HB3	1.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.29	0.47
1:B:610:GLU:HB3	1:B:671:ASN:HB2	1.97	0.47
1:C:488[A]:ARG:HH11	1:C:488[A]:ARG:CG	2.24	0.47
1:C:634:TYR:O	1:C:653:THR:HA	2.14	0.47
1:A:126[A]:ILE:CD1	1:D:120:GLU:HB2	2.44	0.47
1:A:556:GLN:NE2	3:A:1492:HOH:O	2.48	0.47
1:B:128:HIS:HA	1:B:168:THR:O	2.15	0.47
1:A:461:GLU:HA	1:A:462:PRO:C	2.40	0.46
1:B:700:ASP:O	1:B:703:LYS:HD3	2.15	0.46
1:B:309:LYS:CE	3:B:1592:HOH:O	2.59	0.46
1:D:61:ARG:NH1	3:D:1715:HOH:O	2.48	0.46
1:C:274:ILE:HD12	2:C:801:HEM:HMB1	1.98	0.46
1:C:624:LYS:HE3	3:C:1471:HOH:O	2.15	0.46
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.51	0.46
1:C:126[B]:ILE:HG22	3:C:1087:HOH:O	2.16	0.46
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.98	0.45
1:D:556:GLN:NE2	3:D:1593:HOH:O	2.49	0.45
1:B:461:GLU:HA	1:B:462:PRO:C	2.40	0.45
1:A:369[A]:ARG:CG	1:A:369[A]:ARG:NH2	2.71	0.45
1:A:748:ILE:O	1:A:751:ILE:HG13	2.17	0.45
1:B:59:ASP:OD2	1:B:61:ARG:NH2	2.50	0.45
1:B:671:ASN:O	1:B:674:ASP:HB3	2.16	0.45
1:A:392:HIS:CD2	1:A:394:GLY:H	2.35	0.45
1:B:207:PHE:O	1:B:249:THR:HA	2.17	0.45
1:B:556:GLN:HA	1:B:566:LEU:HD21	1.98	0.45
1:C:552:LEU:HD21	1:C:571:LEU:HD12	1.99	0.45
1:D:274:ILE:HD12	2:D:801:HEM:HMB1	1.98	0.45
1:A:76:GLU:OE1	3:A:1708:HOH:O	2.21	0.45
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.47	0.45
1:B:120:GLU:HB2	1:C:126[A]:ILE:HD11	1.97	0.45
1:B:359:LEU:HD12	1:B:359:LEU:C	2.41	0.45
1:D:574:THR:HG23	3:D:1303:HOH:O	2.17	0.45
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.46	0.45
1:D:309:LYS:CE	3:D:1732:HOH:O	2.61	0.45
1:C:59:ASP:OD2	3:C:1482:HOH:O	2.20	0.45
1:C:359:LEU:H	1:C:507:HIS:CD2	2.35	0.44
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.33	0.44
1:B:283:GLU:CD	3:B:1546:HOH:O	2.60	0.44
1:D:48:GLN:HE21	1:D:48:GLN:HB3	1.68	0.44
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.26	0.44
1:A:73[A]:LYS:HD3	1:C:441:HIS:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:610:GLU:OE1	1:C:643:ASP:HA	2.18	0.44
1:C:704:PHE:O	1:C:707:THR:HG22	2.18	0.44
1:A:128:HIS:HA	1:A:168:THR:O	2.18	0.44
1:C:727:SER:O	1:C:731:GLU:HG3	2.19	0.43
1:B:294:LYS:NZ	3:B:1645:HOH:O	2.46	0.43
1:C:671:ASN:O	1:C:674:ASP:HB3	2.17	0.43
1:D:696:ALA:HB1	1:D:728:PHE:CZ	2.53	0.43
1:A:251:HIS:CE1	1:A:507:HIS:HB3	2.53	0.43
1:A:448:MET:O	1:A:449[A]:HIS:HB2	2.19	0.43
1:B:449[B]:HIS:CD2	1:D:449[B]:HIS:CD2	3.06	0.43
1:C:126[A]:ILE:CG2	2:C:801:HEM:HMD1	2.48	0.43
1:D:359:LEU:H	1:D:507:HIS:CD2	2.37	0.43
1:A:478:LYS:HE3	3:A:1599:HOH:O	2.19	0.43
1:D:126[A]:ILE:HG22	2:D:801:HEM:HMD1	2.00	0.43
1:B:404:ASN:O	1:B:405:ASP:C	2.62	0.43
1:B:732:LEU:C	1:B:732:LEU:HD13	2.44	0.43
1:C:748:ILE:O	1:C:751:ILE:HG23	2.18	0.43
1:A:309:LYS:CE	3:A:1688:HOH:O	2.57	0.42
1:C:748:ILE:O	1:C:751:ILE:CG2	2.67	0.42
1:B:359:LEU:H	1:B:507:HIS:CD2	2.35	0.42
1:C:207:PHE:O	1:C:249:THR:HA	2.19	0.42
1:D:128:HIS:HA	1:D:168:THR:O	2.19	0.42
1:A:393:PRO:HD2	1:A:415:TYR:CG	2.54	0.42
1:D:61:ARG:HH11	1:D:66:ASN:HA	1.83	0.42
1:D:459:ASN:HD22	1:D:459:ASN:H	1.68	0.42
1:A:52:PRO:HG3	3:C:1138:HOH:O	2.19	0.42
1:B:411:ARG:HG2	2:B:801:HEM:C2C	2.54	0.42
1:C:313:ARG:CG	3:C:1684:HOH:O	2.50	0.42
1:A:341:ILE:CD1	3:A:1750:HOH:O	2.66	0.42
1:B:713:GLN:NE2	1:B:713:GLN:H	2.18	0.42
1:C:404:ASN:O	1:C:405:ASP:C	2.62	0.41
1:D:732:LEU:C	1:D:732:LEU:HD13	2.45	0.41
1:B:38:PRO:HG2	1:B:51:ALA:HB2	2.02	0.41
1:D:126[A]:ILE:CG2	2:D:801:HEM:HMD1	2.50	0.41
1:D:488[A]:ARG:HG2	1:D:488[A]:ARG:HH11	1.85	0.41
1:C:461:GLU:HA	1:C:462:PRO:C	2.44	0.41
1:D:677:ASP:HB2	3:D:1736:HOH:O	2.20	0.41
1:B:126[A]:ILE:CG2	2:B:801:HEM:HMD1	2.50	0.41
1:C:612:ARG:HH11	1:C:669:CYS:HB3	1.85	0.41
1:A:126[A]:ILE:HD12	1:D:121:ARG:HG2	2.02	0.41
3:A:1047:HOH:O	1:C:52:PRO:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:711:ALA:HB1	1:B:713:GLN:HE22	1.85	0.41
1:B:710:ILE:HD13	1:B:718:ILE:HG13	2.03	0.41
1:A:416[B]:THR:HG22	3:A:1016:HOH:O	2.21	0.41
1:C:593:ILE:HA	1:C:594:PRO:HD3	1.94	0.41
1:B:348:LYS:NZ	3:B:1639:HOH:O	2.54	0.41
1:C:251:HIS:CE1	1:C:507:HIS:HB3	2.55	0.41
1:A:535:VAL:O	1:A:537:PRO:HD3	2.22	0.40
1:C:713:GLN:H	1:C:713:GLN:HG3	1.69	0.40
1:A:121:ARG:CZ	1:D:126[B]:ILE:HG12	2.52	0.40
1:B:267:ARG:NE	1:B:321:GLU:OE1	2.52	0.40
1:B:637:MET:HB2	1:C:562:LEU:HA	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	741/753 (98%)	723 (98%)	16 (2%)	2 (0%)	36	17
1	B	735/753 (98%)	712 (97%)	21 (3%)	2 (0%)	36	17
1	C	736/753 (98%)	718 (98%)	17 (2%)	1 (0%)	48	24
1	D	735/753 (98%)	717 (98%)	17 (2%)	1 (0%)	48	24
All	All	2947/3012 (98%)	2870 (97%)	71 (2%)	6 (0%)	43	22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	ASP
1	A	75	SER
1	A	725	ASP
1	C	75	SER

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Mol	Chain	Res	Type
1	D	75	SER
1	B	75	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	627/635 (99%)	618 (99%)	9 (1%)	59	33
1	B	621/635 (98%)	597 (96%)	24 (4%)	28	5
1	C	622/635 (98%)	591 (95%)	31 (5%)	22	3
1	D	621/635 (98%)	599 (96%)	22 (4%)	32	7
All	All	2491/2540 (98%)	2405 (96%)	86 (4%)	32	7

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	THR
1	A	205	ILE
1	A	213	LYS
1	A	252	ASN
1	A	440	TYR
1	A	459	ASN
1	A	552[A]	LEU
1	A	552[B]	LEU
1	A	732	LEU
1	B	28	SER
1	B	32	GLU
1	B	191	THR
1	B	205	ILE
1	B	213	LYS
1	B	252	ASN
1	B	283	GLU
1	B	285	LYS
1	B	321	GLU
1	B	344	GLU

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Mol	Chain	Res	Type
1	B	369	ARG
1	B	432	PRO
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	566	LEU
1	B	571	LEU
1	B	584	LYS
1	B	616	LEU
1	B	621	LYS
1	B	633	LEU
1	B	707	THR
1	B	713	GLN
1	B	750	LYS
1	C	32	GLU
1	C	191	THR
1	C	205	ILE
1	C	213	LYS
1	C	252	ASN
1	C	310	LEU
1	C	377	ARG
1	C	432	PRO
1	C	440	TYR
1	C	459	ASN
1	C	488[A]	ARG
1	C	488[B]	ARG
1	C	552	LEU
1	C	571	LEU
1	C	583	LYS
1	C	584	LYS
1	C	606	LEU
1	C	610	GLU
1	C	612	ARG
1	C	616	LEU
1	C	617	LEU
1	C	626	LYS
1	C	633	LEU
1	C	636	ARG
1	C	648	LEU
1	C	685	LEU
1	C	713	GLN
1	C	732	LEU

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Mol	Chain	Res	Type
1	C	733	LEU
1	C	750	LYS
1	C	751	ILE
1	D	32	GLU
1	D	48	GLN
1	D	191	THR
1	D	205	ILE
1	D	252	ASN
1	D	344	GLU
1	D	440	TYR
1	D	459	ASN
1	D	488[A]	ARG
1	D	488[B]	ARG
1	D	490	GLU
1	D	521	ARG
1	D	546[A]	GLN
1	D	546[B]	GLN
1	D	574	THR
1	D	616	LEU
1	D	624	LYS
1	D	648	LEU
1	D	713	GLN
1	D	747	LYS
1	D	750	LYS
1	D	751	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	66	ASN
1	A	252	ASN
1	A	419	GLN
1	A	459	ASN
1	A	515	GLN
1	A	556	GLN
1	B	66	ASN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	B	713	GLN

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Mol	Chain	Res	Type
1	C	77	ASN
1	C	139	GLN
1	C	252	ASN
1	C	459	ASN
1	C	507	HIS
1	C	629	HIS
1	D	48	GLN
1	D	246	GLN
1	D	252	ASN
1	D	459	ASN
1	D	507	HIS
1	D	556	GLN
1	D	629	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	A	801	1	50,50,50	1.62	10 (20%)	67,82,82	1.86	20 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	C	801	1	50,50,50	1.71	15 (30%)	67,82,82	2.19	21 (31%)
2	HEM	D	801	1	50,50,50	1.51	6 (12%)	67,82,82	1.57	11 (16%)
2	HEM	B	801	1	50,50,50	1.59	10 (20%)	67,82,82	1.80	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	A	801	1	-	2/14/54/54	-
2	HEM	C	801	1	-	2/14/54/54	-
2	HEM	D	801	1	-	2/14/54/54	-
2	HEM	B	801	1	-	2/14/54/54	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	HEM	FE-NB	4.28	2.08	1.94
2	A	801	HEM	CHB-C1B	4.12	1.46	1.38
2	B	801	HEM	FE-NB	3.74	2.06	1.94
2	B	801	HEM	CHA-C4D	3.59	1.45	1.38
2	C	801	HEM	FE-NB	3.57	2.05	1.94
2	A	801	HEM	C1C-NC	3.42	1.46	1.39
2	D	801	HEM	FE-NA	3.36	2.06	1.95
2	A	801	HEM	FE-NB	3.36	2.05	1.94
2	C	801	HEM	C4A-C3A	3.27	1.50	1.43
2	A	801	HEM	FE-ND	3.20	2.04	1.94
2	B	801	HEM	C4A-C3A	3.17	1.50	1.43
2	D	801	HEM	FE-ND	3.15	2.04	1.94
2	A	801	HEM	O2A-CGA	-3.01	1.20	1.30
2	A	801	HEM	CHD-C1D	2.96	1.45	1.39
2	C	801	HEM	C1D-ND	-2.96	1.33	1.38
2	A	801	HEM	CHA-C4D	2.91	1.44	1.38
2	B	801	HEM	C1C-NC	2.88	1.45	1.39
2	C	801	HEM	C3C-C4C	2.88	1.51	1.46
2	B	801	HEM	C1A-NA	2.82	1.44	1.39
2	B	801	HEM	FE-NC	2.77	2.04	1.95
2	B	801	HEM	CBD-CAD	2.73	1.61	1.51
2	C	801	HEM	O1D-CGD	2.67	1.30	1.22
2	C	801	HEM	CHD-C1D	2.53	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C1D-C2D	-2.53	1.39	1.44
2	C	801	HEM	O2D-CGD	-2.52	1.22	1.30
2	D	801	HEM	CHA-C4D	2.52	1.43	1.38
2	C	801	HEM	CBD-CAD	2.51	1.60	1.51
2	B	801	HEM	FE-ND	2.50	2.02	1.94
2	A	801	HEM	FE-NA	2.43	2.03	1.95
2	C	801	HEM	O2A-CGA	-2.40	1.22	1.30
2	C	801	HEM	CHA-C4D	2.38	1.43	1.38
2	A	801	HEM	C4A-C3A	2.38	1.48	1.43
2	B	801	HEM	CHB-C1B	2.34	1.43	1.38
2	C	801	HEM	C4D-ND	-2.33	1.36	1.40
2	D	801	HEM	C3D-C2D	2.31	1.41	1.36
2	C	801	HEM	CHC-C1C	2.31	1.42	1.38
2	C	801	HEM	FE-ND	2.28	2.01	1.94
2	B	801	HEM	O1D-CGD	2.26	1.29	1.22
2	C	801	HEM	O1A-CGA	2.14	1.29	1.22
2	C	801	HEM	C1C-NC	2.13	1.43	1.39
2	D	801	HEM	CHB-C1B	2.02	1.42	1.38

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	HEM	C3B-C2B-C1B	-7.13	101.06	106.41
2	B	801	HEM	C3B-C2B-C1B	-6.81	101.30	106.41
2	D	801	HEM	C3B-C2B-C1B	-5.75	102.09	106.41
2	B	801	HEM	C4B-C3B-C2B	5.72	112.53	107.28
2	C	801	HEM	C2D-C1D-ND	5.60	116.38	109.90
2	C	801	HEM	CHD-C1D-C2D	-4.53	117.88	125.03
2	A	801	HEM	CHB-C4A-NA	4.39	131.81	123.86
2	A	801	HEM	CHB-C1B-NB	4.35	129.75	124.37
2	C	801	HEM	C1D-C2D-C3D	-4.27	102.49	106.98
2	C	801	HEM	CBD-CAD-C3D	-4.15	101.06	112.53
2	B	801	HEM	C2B-C1B-NB	4.14	114.60	109.84
2	A	801	HEM	C4A-CHB-C1B	-4.02	116.80	126.25
2	A	801	HEM	C2D-C1D-ND	3.91	114.42	109.90
2	B	801	HEM	C3B-C4B-NB	-3.91	106.66	109.47
2	C	801	HEM	C4B-C3B-C2B	3.90	110.86	107.28
2	D	801	HEM	CBD-CAD-C3D	-3.89	101.77	112.53
2	A	801	HEM	CHB-C4A-C3A	-3.67	116.77	127.43
2	B	801	HEM	CBD-CAD-C3D	-3.66	102.41	112.53
2	A	801	HEM	CHB-C1B-C2B	-3.35	117.43	126.95
2	C	801	HEM	C2B-C1B-NB	3.33	113.67	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	HEM	C2B-C1B-NB	3.30	113.64	109.84
2	C	801	HEM	CHD-C4C-NC	3.22	127.96	124.45
2	A	801	HEM	CBD-CAD-C3D	-3.17	103.76	112.53
2	C	801	HEM	O2D-CGD-CBD	3.17	124.02	114.00
2	D	801	HEM	CAA-CBA-CGA	-3.06	105.55	113.67
2	A	801	HEM	CAA-CBA-CGA	-2.91	105.94	113.67
2	C	801	HEM	CAA-CBA-CGA	-2.86	106.07	113.67
2	C	801	HEM	C2A-C1A-NA	2.81	113.27	110.15
2	A	801	HEM	C3B-C2B-C1B	-2.75	104.34	106.41
2	D	801	HEM	C4B-C3B-C2B	2.74	109.80	107.28
2	B	801	HEM	CAA-CBA-CGA	-2.68	106.57	113.67
2	C	801	HEM	CHB-C1B-C2B	-2.67	119.35	126.95
2	D	801	HEM	C2D-C1D-ND	2.67	112.99	109.90
2	C	801	HEM	C4C-CHD-C1D	-2.62	120.46	126.02
2	C	801	HEM	O1A-CGA-CBA	-2.55	114.99	123.09
2	D	801	HEM	CHD-C4C-C3C	-2.55	120.91	125.21
2	A	801	HEM	C4B-C3B-C2B	2.51	109.59	107.28
2	A	801	HEM	CMA-C3A-C4A	2.51	129.24	125.42
2	A	801	HEM	CAD-C3D-C2D	2.50	132.56	127.87
2	C	801	HEM	CHC-C1C-NC	-2.50	121.73	124.45
2	A	801	HEM	O2D-CGD-O1D	-2.48	116.96	123.33
2	B	801	HEM	O2D-CGD-O1D	-2.46	117.00	123.33
2	D	801	HEM	CBB-CAB-C3B	-2.43	115.39	127.53
2	C	801	HEM	C3D-C4D-ND	2.42	112.83	110.17
2	A	801	HEM	CHC-C4B-NB	-2.42	121.82	124.42
2	C	801	HEM	CMB-C2B-C1B	2.41	128.80	125.03
2	C	801	HEM	O2D-CGD-O1D	-2.37	117.23	123.33
2	A	801	HEM	O1A-CGA-CBA	-2.33	115.70	123.09
2	A	801	HEM	C4C-C3C-C2C	-2.30	104.82	106.81
2	C	801	HEM	C2C-C1C-NC	2.30	113.89	109.64
2	B	801	HEM	C4D-C3D-C2D	-2.29	103.56	106.89
2	A	801	HEM	CMB-C2B-C1B	2.24	128.54	125.03
2	A	801	HEM	C4C-NC-C1C	-2.23	102.19	105.82
2	A	801	HEM	CHC-C4B-C3B	2.23	129.51	125.07
2	D	801	HEM	CAD-C3D-C2D	2.19	131.97	127.87
2	A	801	HEM	C2B-C1B-NB	2.15	112.31	109.84
2	B	801	HEM	CHD-C4C-C3C	-2.14	121.61	125.21
2	B	801	HEM	C2D-C1D-ND	2.11	112.34	109.90
2	C	801	HEM	CHB-C4A-C3A	-2.09	121.36	127.43
2	D	801	HEM	C3C-C2C-C1C	-2.07	105.09	107.05
2	D	801	HEM	CHB-C4A-NA	2.04	127.57	123.86
2	C	801	HEM	CHA-C4D-C3D	-2.03	121.49	125.23

There are no chirality outliers.

All (8) torsion outliers are listed below:

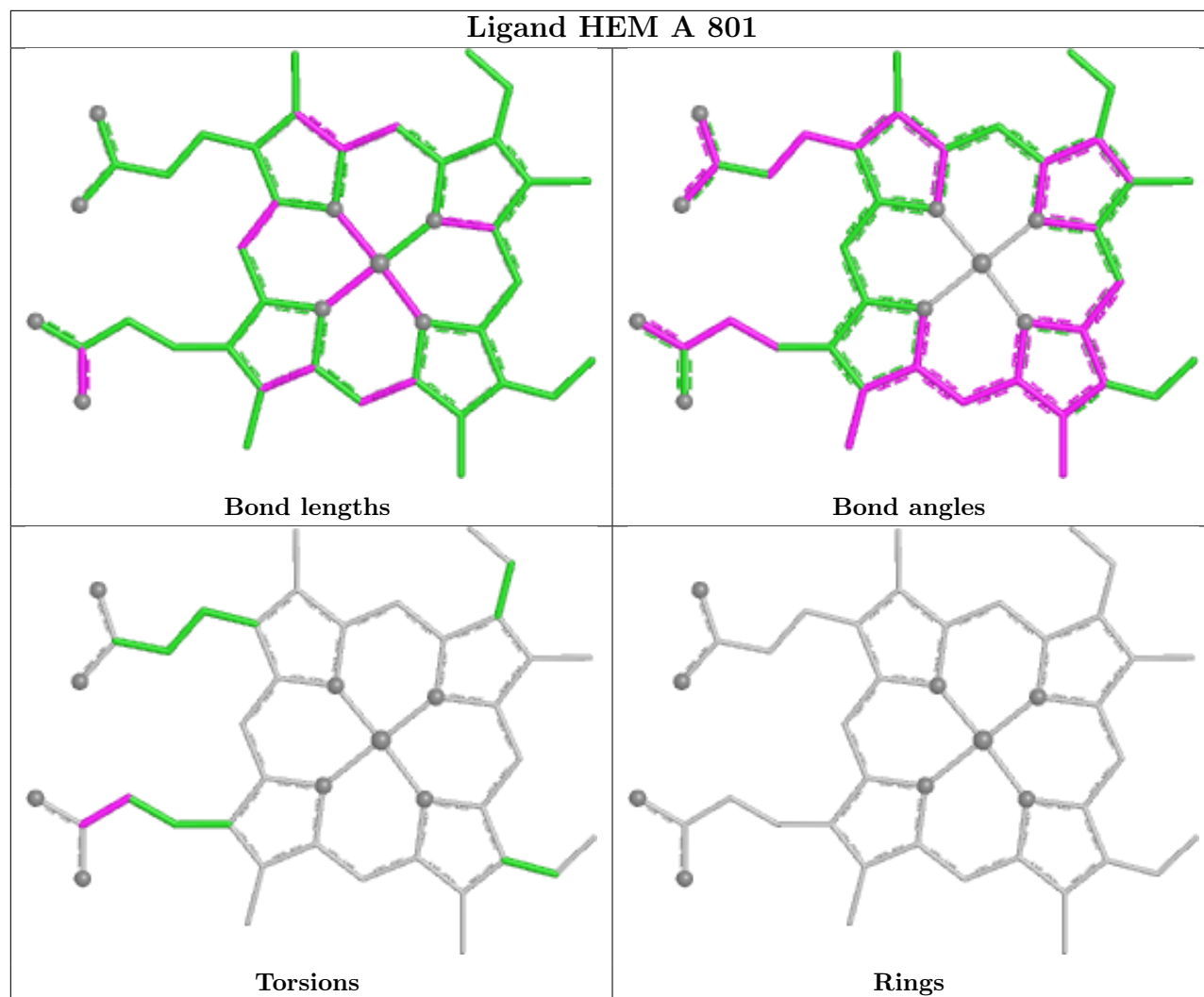
Mol	Chain	Res	Type	Atoms
2	A	801	HEM	CAA-CBA-CGA-O1A
2	A	801	HEM	CAA-CBA-CGA-O2A
2	C	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O2A
2	D	801	HEM	CAA-CBA-CGA-O2A
2	C	801	HEM	CAA-CBA-CGA-O1A
2	D	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	CAA-CBA-CGA-O1A

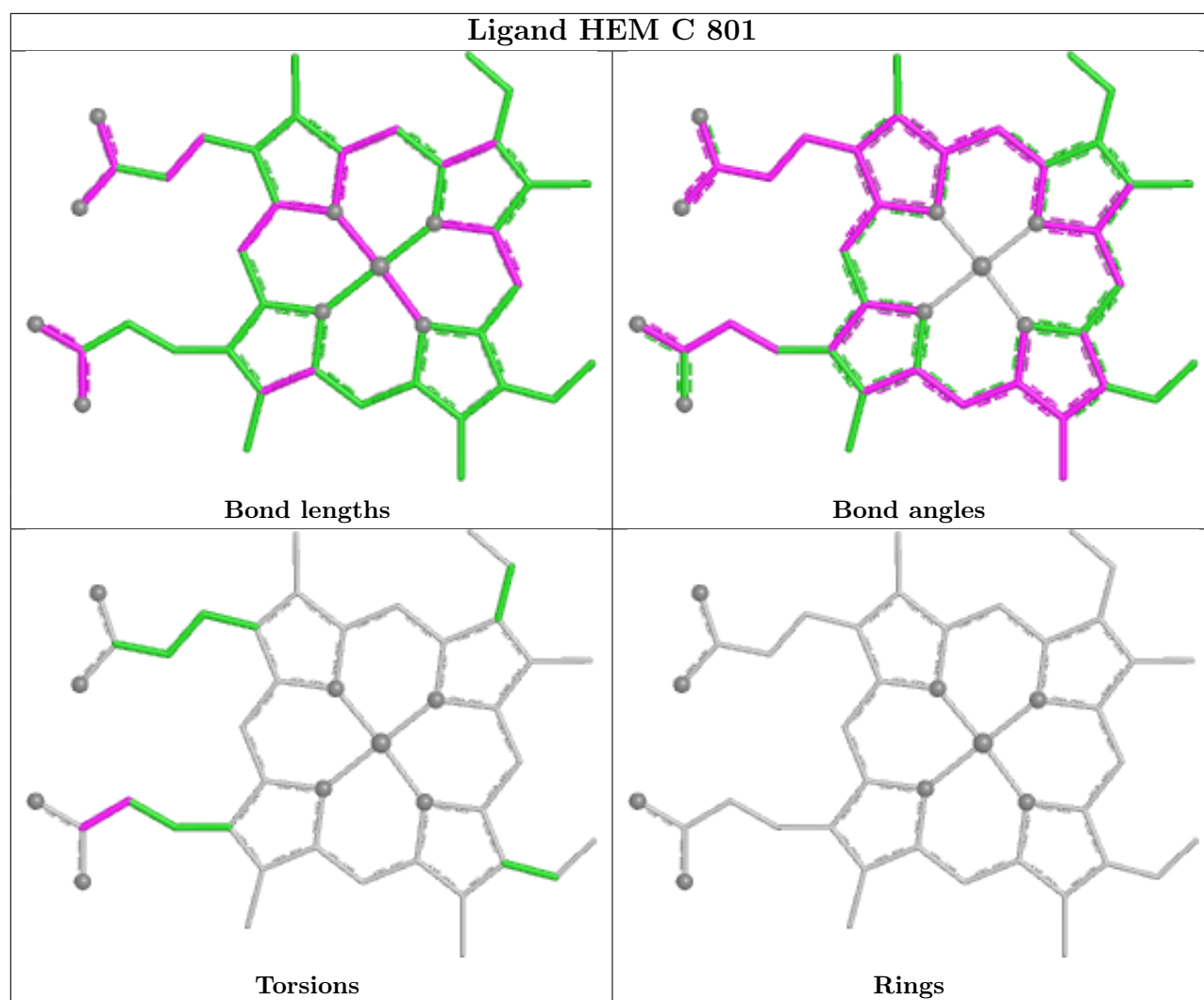
There are no ring outliers.

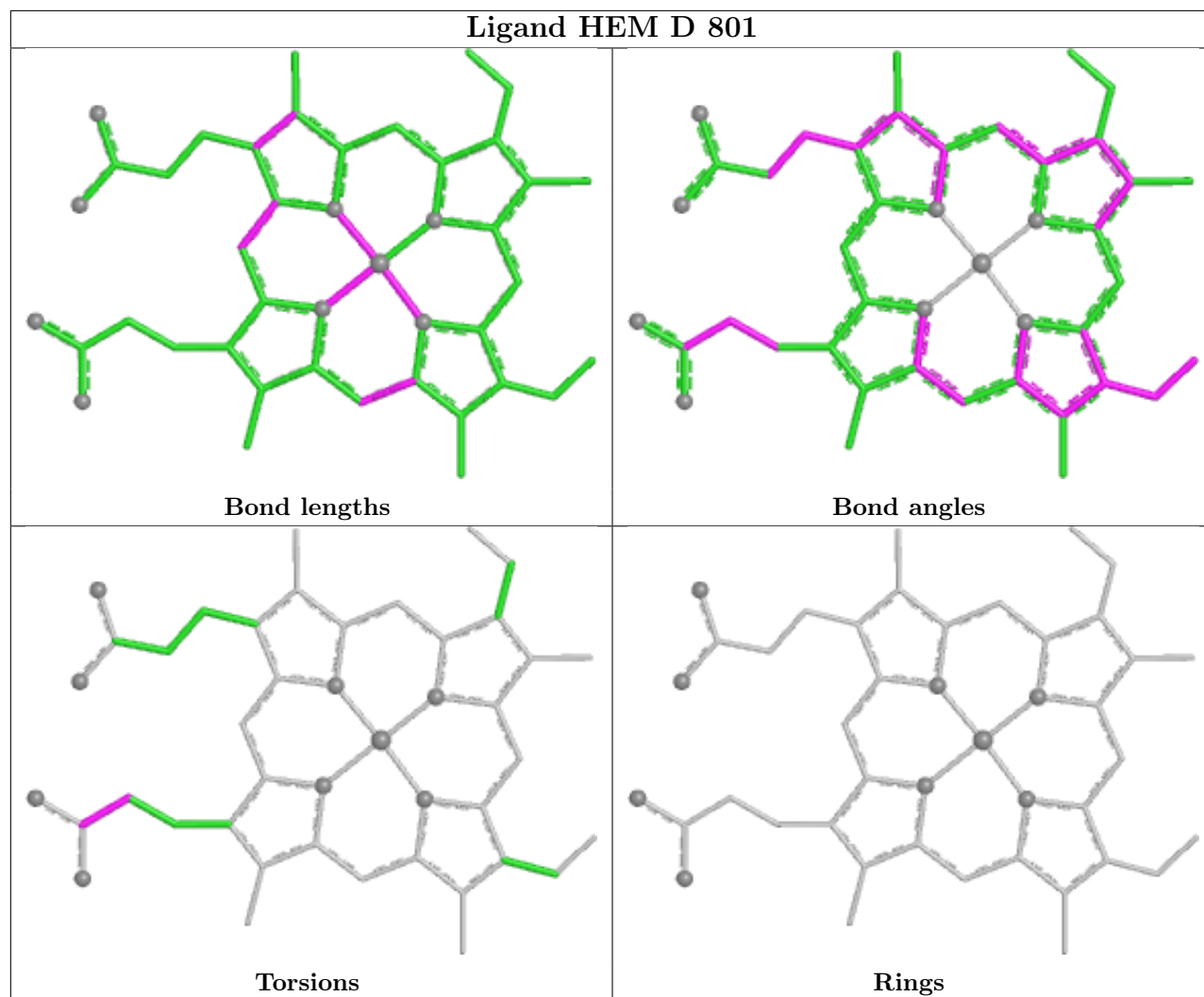
3 monomers are involved in 8 short contacts:

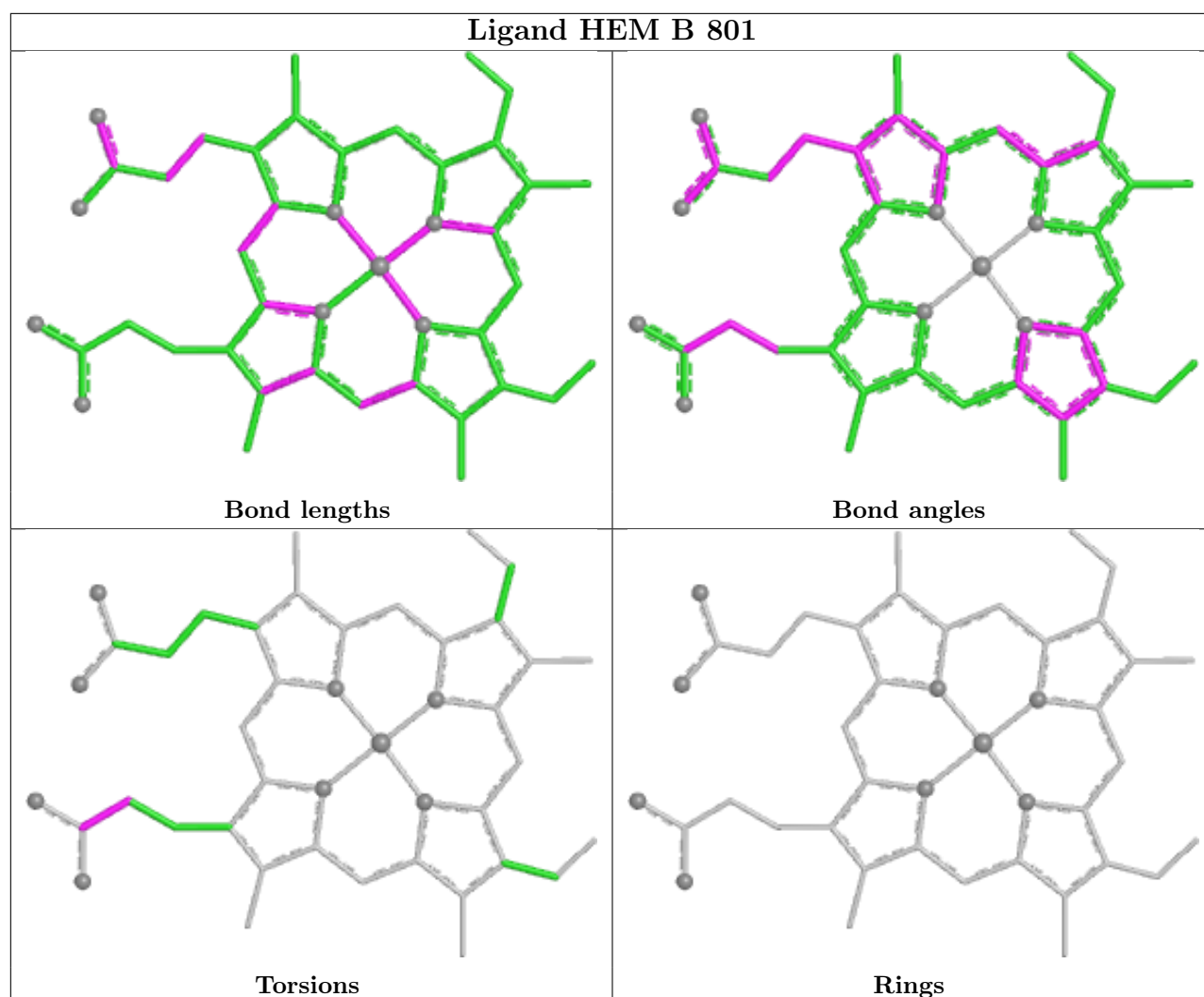
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	801	HEM	2	0
2	D	801	HEM	3	0
2	B	801	HEM	3	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	726/753 (96%)	-0.56	5 (0%) 84 87	5, 12, 29, 57	18 (2%)
1	B	726/753 (96%)	-0.34	16 (2%) 62 66	5, 13, 43, 72	11 (1%)
1	C	726/753 (96%)	-0.36	22 (3%) 52 56	4, 14, 41, 74	13 (1%)
1	D	726/753 (96%)	-0.51	6 (0%) 82 86	5, 13, 31, 69	11 (1%)
All	All	2904/3012 (96%)	-0.44	49 (1%) 69 72	4, 13, 38, 74	53 (1%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	28	SER	3.8
1	C	676	ALA	3.2
1	B	642	ALA	3.1
1	A	751	ILE	3.0
1	B	676	ALA	2.9
1	C	711	ALA	2.9
1	C	675	ILE	2.9
1	C	750	LYS	2.8
1	C	714	GLY	2.6
1	B	726	GLY	2.6
1	B	673	ALA	2.5
1	C	724	ALA	2.5
1	B	749	ASP	2.5
1	B	611	VAL	2.5
1	C	751	ILE	2.5
1	C	614	ALA	2.5
1	C	701	ALA	2.5
1	C	669	CYS	2.4
1	D	724	ALA	2.4
1	B	677	ASP	2.4
1	B	724	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	751	ILE	2.4
1	B	750	LYS	2.4
1	A	713	GLN	2.3
1	C	595	ASP	2.3
1	C	699	GLY	2.3
1	C	726	GLY	2.3
1	D	749	ASP	2.3
1	D	711	ALA	2.3
1	B	617	LEU	2.3
1	B	725	ASP	2.2
1	C	643	ASP	2.2
1	B	612	ARG	2.2
1	C	672	ILE	2.2
1	D	750	LYS	2.2
1	B	710	ILE	2.2
1	C	721	ALA	2.2
1	C	677	ASP	2.2
1	A	710	ILE	2.1
1	B	751	ILE	2.1
1	C	634	TYR	2.1
1	A	726	GLY	2.1
1	A	725	ASP	2.1
1	B	634	TYR	2.1
1	C	635	SER	2.1
1	C	670	GLY	2.1
1	C	700	ASP	2.0
1	C	673	ALA	2.0
1	B	635	SER	2.0

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

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

6.3 Carbohydrates [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,

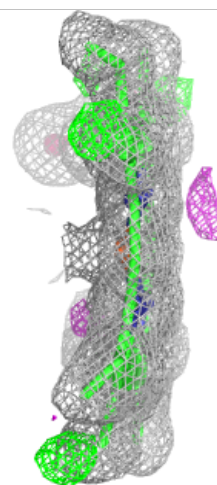
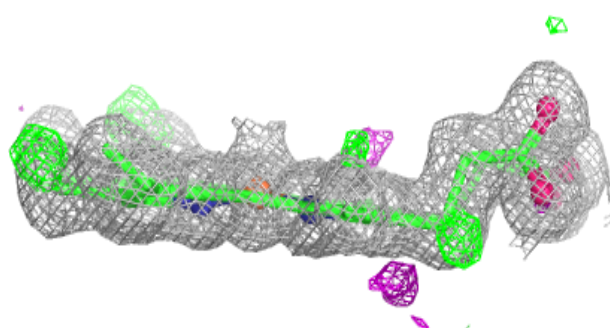
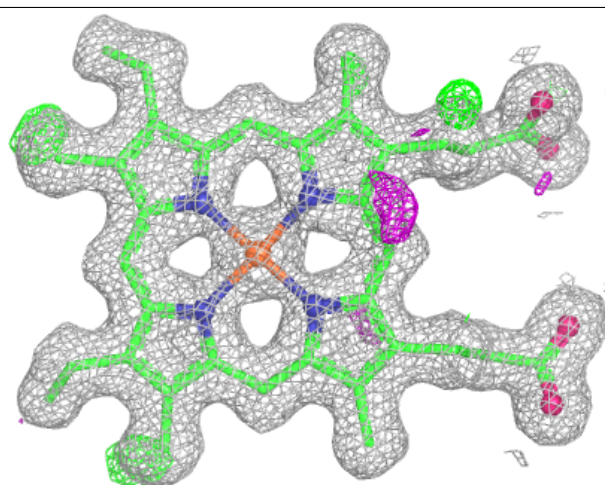
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	A	801	43/43	0.99	0.04	6,8,9,15	0
2	HEM	B	801	43/43	0.99	0.04	7,9,11,14	0
2	HEM	C	801	43/43	0.99	0.04	7,8,11,16	0
2	HEM	D	801	43/43	0.99	0.04	7,8,10,15	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.

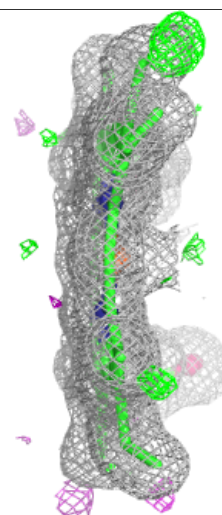
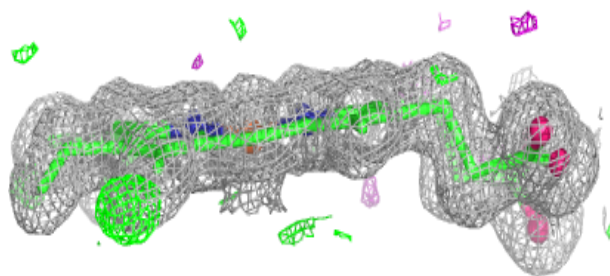
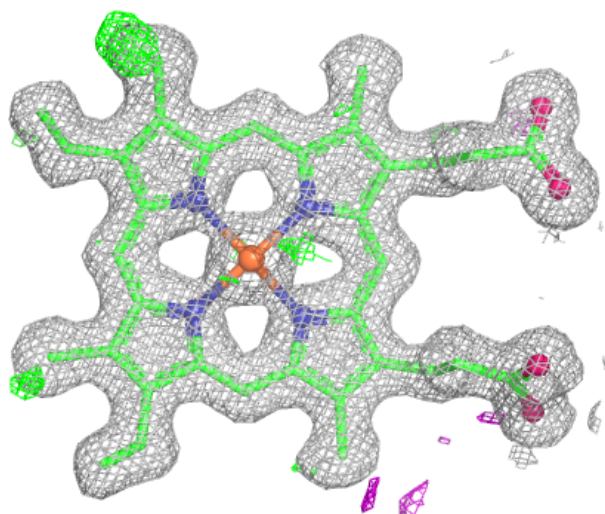
Electron density around HEM A 801:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



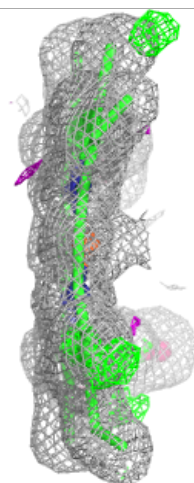
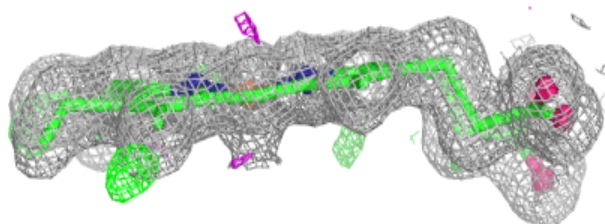
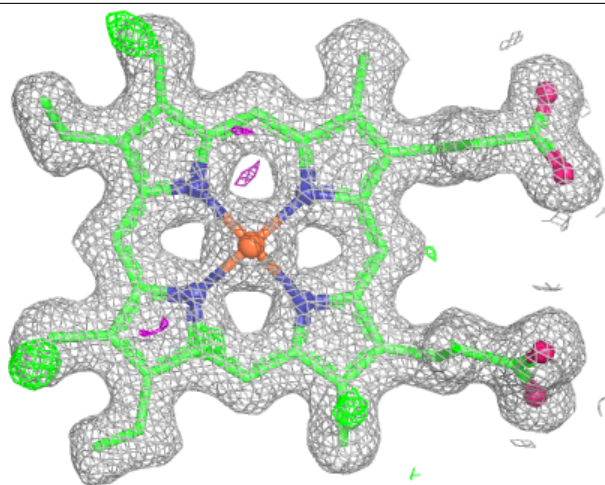
Electron density around HEM B 801:

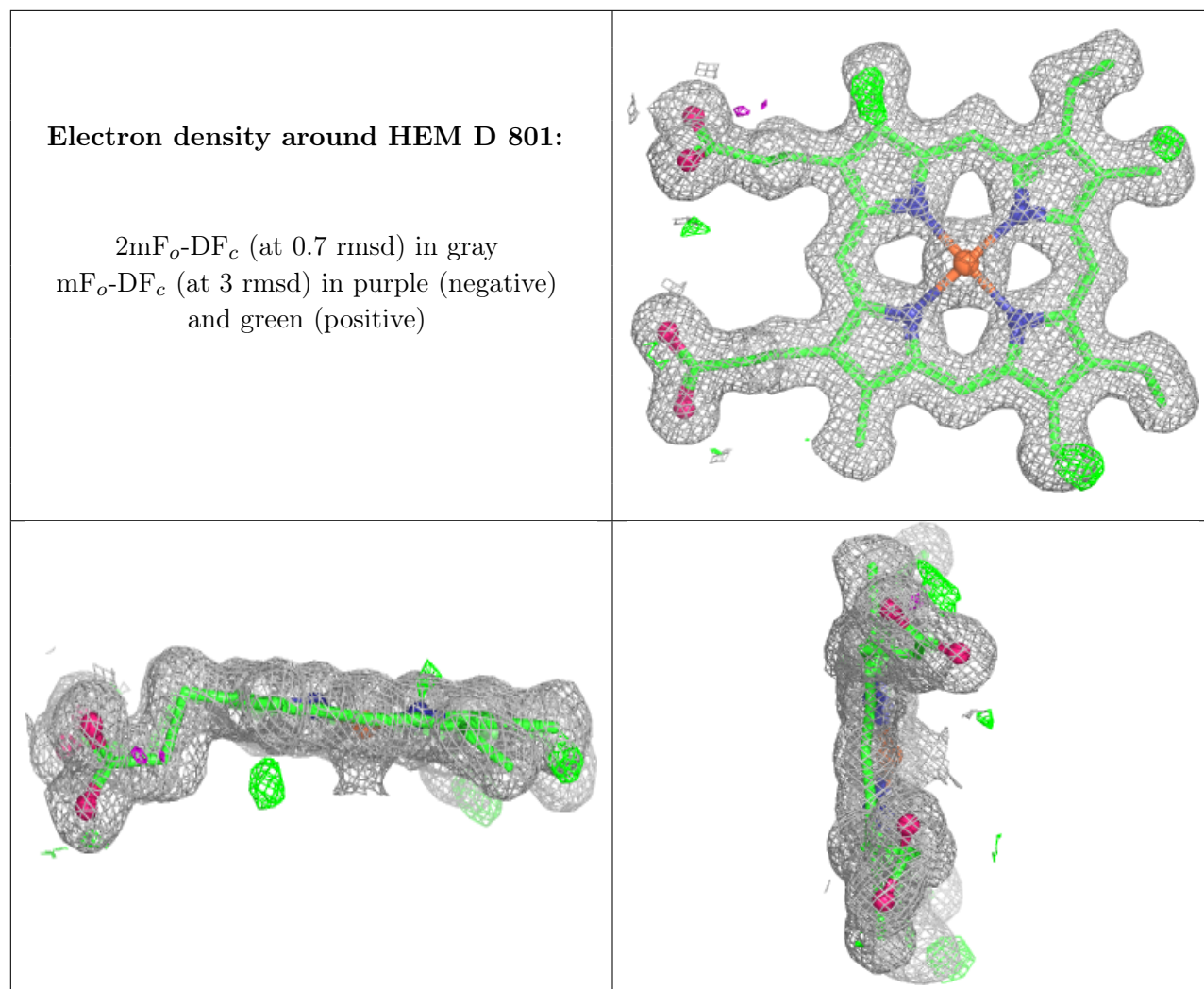
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 801:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.