



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:54 AM UTC

PDB ID : 4ENR / pdb_00004enr
Title : Structure of E530I variant E. coli KatE
Authors : Loewen, P.C.; Jha, V.
Deposited on : 2012-04-13
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

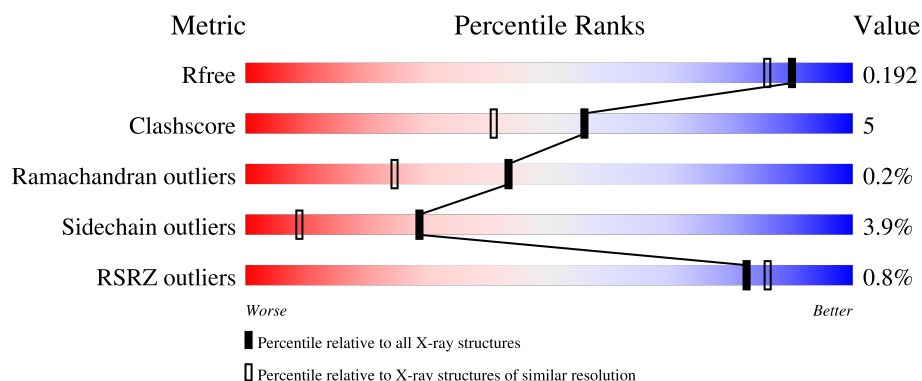
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

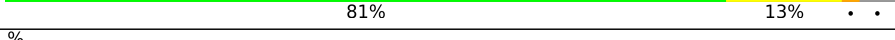
The reported resolution of this entry is 1.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	753	
1	B	753	
1	C	753	
1	D	753	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26152 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.

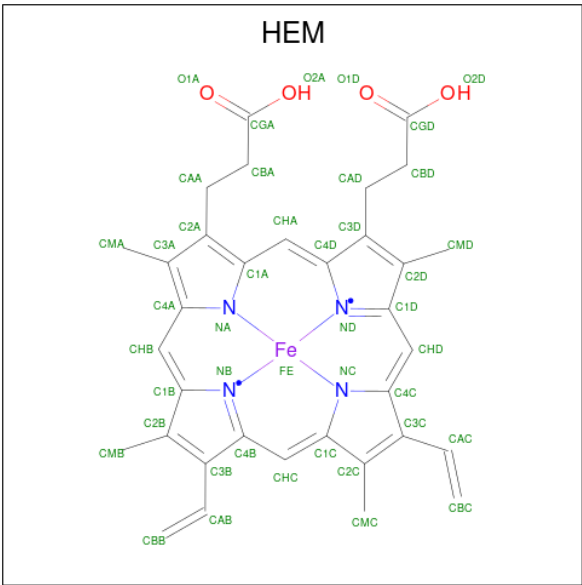
- Molecule 1 is a protein called Catalase HP11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	4	0
			5758	3658	1006	1082	12			
1	B	726	Total	C	N	O	S	0	4	0
			5761	3661	1007	1081	12			
1	C	726	Total	C	N	O	S	0	3	0
			5755	3656	1006	1081	12			
1	D	726	Total	C	N	O	S	0	4	0
			5758	3658	1006	1082	12			

There are 4 discrepancies between the modelled and reference sequences:

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

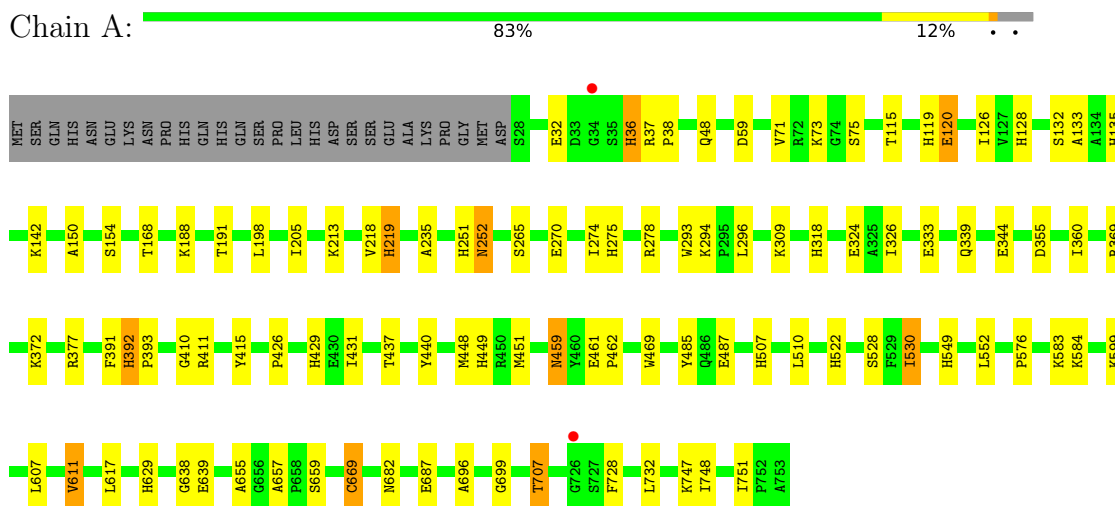
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	747	Total	O	0	0
			747	747		
3	B	690	Total	O	0	0
			690	690		
3	C	733	Total	O	0	0
			733	733		
3	D	778	Total	O	0	0
			778	778		

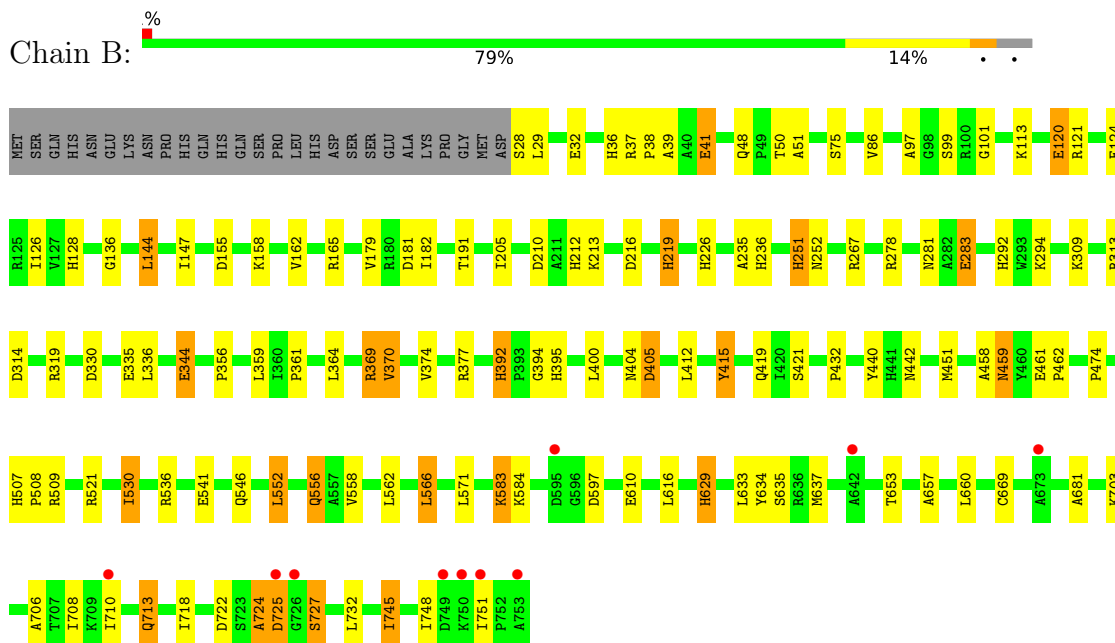
3 Residue-property plots

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

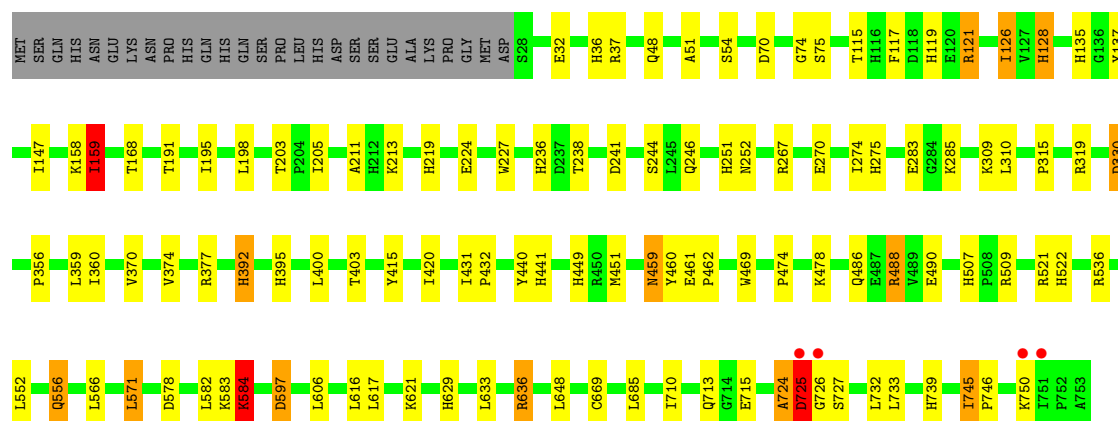
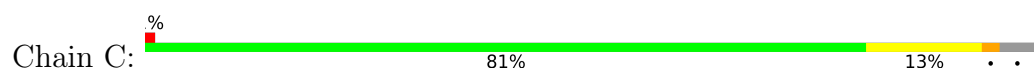
• Molecule 1: Catalase HP1I



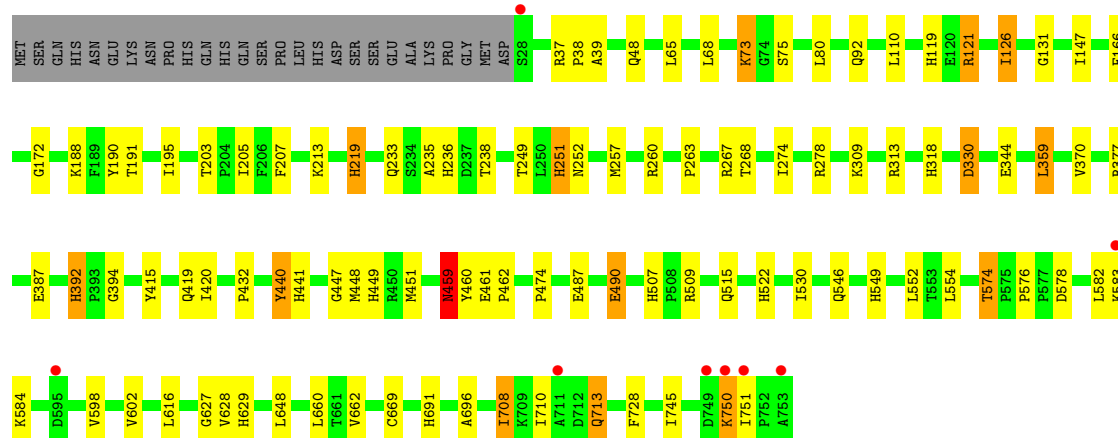
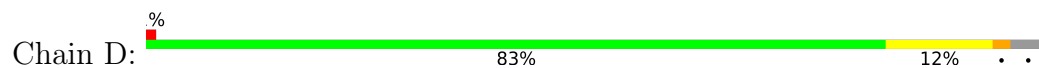
• Molecule 1: Catalase HP1I



• Molecule 1: Catalase HP1I



• 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	93.58Å 132.78Å 122.81Å 90.00° 109.35° 90.00°	Depositor
Resolution (Å)	33.20 – 1.60 33.20 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.2 (33.20-1.60) 96.2 (33.20-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 1.60Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.158 , 0.193 0.156 , 0.192	Depositor DCC
R_{free} test set	18012 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	12.2	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26152	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: OCS, 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	1.60	46/5917 (0.8%)	1.33	12/8043 (0.1%)
1	B	1.55	40/5920 (0.7%)	1.32	29/8046 (0.4%)
1	C	1.54	40/5911 (0.7%)	1.32	21/8035 (0.3%)
1	D	1.62	41/5917 (0.7%)	1.33	9/8043 (0.1%)
All	All	1.58	167/23665 (0.7%)	1.32	71/32167 (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	C	0	2

All (167) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	392	HIS	ND1-CE1	9.88	1.42	1.32
1	B	474	PRO	CA-C	9.50	1.57	1.51
1	B	128	HIS	ND1-CE1	8.98	1.41	1.32
1	A	275	HIS	ND1-CE1	8.44	1.41	1.32
1	D	251	HIS	ND1-CE1	8.31	1.40	1.32
1	D	318	HIS	CD2-NE2	8.13	1.46	1.37
1	C	745	ILE	CA-CB	7.61	1.57	1.54
1	A	275	HIS	CE1-NE2	7.56	1.40	1.32
1	B	226	HIS	ND1-CE1	7.47	1.40	1.32
1	A	629	HIS	ND1-CE1	7.46	1.40	1.32
1	D	251	HIS	CG-CD2	7.39	1.44	1.35
1	C	159	ILE	CB-CG1	-7.39	1.38	1.53
1	D	147	ILE	N-CA	7.30	1.53	1.46
1	C	392	HIS	ND1-CE1	7.25	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	236	HIS	CG-CD2	7.25	1.43	1.35
1	B	292	HIS	ND1-CE1	7.24	1.39	1.32
1	B	236	HIS	ND1-CE1	7.08	1.39	1.32
1	A	355	ASP	C-N	7.07	1.39	1.33
1	A	115	THR	N-CA	7.03	1.54	1.46
1	C	522	HIS	CG-CD2	6.99	1.43	1.35
1	D	119	HIS	ND1-CE1	6.96	1.39	1.32
1	D	219	HIS	CG-CD2	6.90	1.43	1.35
1	B	136	GLY	N-CA	6.88	1.53	1.45
1	B	226	HIS	CG-CD2	6.87	1.43	1.35
1	A	392	HIS	ND1-CE1	6.81	1.39	1.32
1	B	219	HIS	CG-CD2	6.80	1.43	1.35
1	D	459	ASN	N-CA	6.75	1.54	1.46
1	A	132	SER	N-CA	6.72	1.54	1.46
1	D	691	HIS	CE1-NE2	6.66	1.39	1.32
1	B	251	HIS	ND1-CE1	6.65	1.39	1.32
1	A	142	LYS	C-O	6.62	1.31	1.23
1	D	387	GLU	N-CA	-6.62	1.38	1.46
1	B	314	ASP	N-CA	6.51	1.52	1.46
1	C	51	ALA	CA-C	6.43	1.59	1.52
1	A	360	ILE	N-CA	6.34	1.51	1.46
1	D	474	PRO	CA-C	6.34	1.55	1.51
1	A	377	ARG	CZ-NH1	6.33	1.41	1.32
1	B	210	ASP	C-O	-6.31	1.16	1.24
1	A	293	TRP	N-CA	6.29	1.53	1.46
1	D	392	HIS	ND1-CE1	6.28	1.38	1.32
1	A	324	GLU	N-CA	6.21	1.54	1.46
1	D	419	GLN	CD-NE2	6.16	1.46	1.33
1	C	441	HIS	CG-CD2	6.15	1.42	1.35
1	B	629	HIS	CE1-NE2	6.15	1.38	1.32
1	C	203	THR	CA-C	6.11	1.58	1.52
1	A	391	PHE	N-CA	6.11	1.53	1.45
1	D	522	HIS	CE1-NE2	6.11	1.38	1.32
1	D	522	HIS	ND1-CE1	6.09	1.38	1.32
1	A	429	HIS	CG-ND1	-6.09	1.31	1.38
1	C	121	ARG	CD-NE	6.08	1.54	1.46
1	B	162	VAL	N-CA	6.06	1.52	1.46
1	C	395	HIS	CG-CD2	6.05	1.42	1.35
1	A	318	HIS	CE1-NE2	6.01	1.38	1.32
1	C	119	HIS	ND1-CE1	6.01	1.38	1.32
1	C	395	HIS	CB-CG	-5.99	1.41	1.50
1	B	179	VAL	N-CA	5.99	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	181	ASP	N-CA	5.98	1.53	1.46
1	A	638	GLY	N-CA	5.91	1.51	1.45
1	D	370	VAL	CA-CB	5.90	1.64	1.54
1	A	119	HIS	ND1-CE1	5.90	1.38	1.32
1	D	121	ARG	CZ-NH2	5.89	1.41	1.33
1	A	135	HIS	CG-CD2	5.88	1.42	1.35
1	D	691	HIS	CG-CD2	5.88	1.42	1.35
1	B	415	TYR	CA-C	5.88	1.60	1.52
1	A	485	TYR	C-O	5.87	1.30	1.23
1	B	278	ARG	N-CA	5.85	1.53	1.46
1	A	133	ALA	N-CA	5.84	1.53	1.45
1	D	447	GLY	N-CA	5.84	1.51	1.45
1	B	236	HIS	CG-CD2	5.81	1.42	1.35
1	A	275	HIS	CG-CD2	5.79	1.42	1.35
1	D	203	THR	N-CA	5.79	1.50	1.45
1	B	727	SER	CA-C	5.77	1.60	1.52
1	A	659	SER	N-CA	-5.73	1.38	1.46
1	B	158	LYS	C-O	5.73	1.30	1.24
1	A	510	LEU	C-O	5.72	1.30	1.24
1	C	474	PRO	CA-C	5.69	1.57	1.52
1	D	80	LEU	N-CA	5.65	1.52	1.46
1	C	244	SER	C-O	5.64	1.31	1.24
1	D	233	GLN	C-O	5.62	1.30	1.23
1	A	326	ILE	N-CA	5.61	1.53	1.46
1	C	36	HIS	CE1-NE2	5.60	1.38	1.32
1	B	442	ASN	C-O	-5.59	1.18	1.24
1	C	135	HIS	CG-ND1	-5.59	1.32	1.38
1	A	522	HIS	CG-CD2	5.59	1.42	1.35
1	A	270	GLU	N-CA	5.57	1.53	1.45
1	B	458	ALA	C-O	5.53	1.30	1.23
1	A	135	HIS	CE1-NE2	5.53	1.38	1.32
1	C	395	HIS	ND1-CE1	5.53	1.38	1.32
1	B	124	GLU	N-CA	5.52	1.52	1.45
1	A	611	VAL	CA-CB	5.51	1.59	1.54
1	B	412	LEU	N-CA	5.51	1.53	1.46
1	D	263	PRO	N-CA	5.50	1.53	1.47
1	C	469	TRP	CD2-CE2	5.50	1.50	1.41
1	D	549	HIS	CG-CD2	5.50	1.41	1.35
1	B	50	THR	N-CA	5.49	1.53	1.45
1	C	115	THR	N-CA	5.49	1.52	1.46
1	A	657	ALA	C-O	-5.49	1.18	1.24
1	A	549	HIS	CG-CD2	5.46	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	41	GLU	C-O	5.46	1.29	1.24
1	A	426	PRO	CA-C	5.46	1.58	1.52
1	C	211	ALA	N-CA	5.44	1.53	1.46
1	B	374	VAL	N-CA	5.42	1.52	1.46
1	C	246	GLN	C-O	-5.42	1.18	1.24
1	B	405	ASP	C-N	5.40	1.39	1.34
1	B	37	ARG	CA-C	5.39	1.58	1.52
1	C	275	HIS	CG-CD2	5.38	1.41	1.35
1	A	36	HIS	CE1-NE2	5.37	1.38	1.32
1	A	339	GLN	N-CA	5.36	1.52	1.46
1	D	359	LEU	N-CA	5.35	1.52	1.45
1	C	135	HIS	CG-CD2	5.35	1.41	1.35
1	B	558	VAL	N-CA	5.35	1.52	1.46
1	D	377	ARG	CZ-NH2	5.34	1.40	1.33
1	A	188	LYS	C-O	5.33	1.30	1.24
1	D	377	ARG	CZ-NH1	5.32	1.40	1.32
1	C	739	HIS	CG-CD2	5.32	1.41	1.35
1	A	522	HIS	ND1-CE1	5.32	1.37	1.32
1	D	268	THR	N-CA	5.32	1.52	1.46
1	D	166	PHE	C-O	-5.32	1.17	1.23
1	A	218	VAL	CA-CB	-5.30	1.47	1.54
1	D	691	HIS	CG-ND1	-5.30	1.32	1.38
1	A	599	LYS	C-O	5.29	1.30	1.23
1	A	469	TRP	CD2-CE2	5.29	1.50	1.41
1	C	319	ARG	CZ-NH1	5.25	1.40	1.32
1	D	627	GLY	N-CA	5.24	1.52	1.45
1	C	403	THR	C-O	5.24	1.31	1.23
1	C	400	LEU	N-CA	5.23	1.52	1.45
1	C	147	ILE	N-CA	5.23	1.51	1.46
1	D	236	HIS	CE1-NE2	5.23	1.37	1.32
1	D	188	LYS	CA-CB	5.22	1.60	1.53
1	C	236	HIS	CG-ND1	-5.21	1.32	1.38
1	C	441	HIS	CA-C	-5.20	1.46	1.52
1	D	172	GLY	N-CA	5.20	1.51	1.45
1	D	260	ARG	CZ-NH2	5.19	1.40	1.33
1	A	293	TRP	CA-C	-5.19	1.46	1.52
1	D	236	HIS	CG-ND1	-5.18	1.32	1.38
1	C	224	GLU	CA-C	-5.17	1.47	1.53
1	C	374	VAL	C-O	-5.17	1.18	1.24
1	A	150	ALA	N-CA	5.17	1.52	1.46
1	A	411	ARG	CD-NE	5.16	1.53	1.46
1	B	400	LEU	N-CA	5.16	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	212	HIS	ND1-CE1	5.16	1.37	1.32
1	C	74	GLY	C-O	5.16	1.28	1.23
1	D	65	LEU	C-O	-5.15	1.18	1.24
1	D	515	GLN	CA-C	5.15	1.60	1.53
1	B	216	ASP	N-CA	5.14	1.52	1.46
1	C	370	VAL	CA-CB	5.14	1.61	1.54
1	C	356	PRO	CA-C	5.13	1.59	1.52
1	D	68	LEU	CA-C	-5.12	1.45	1.52
1	B	356	PRO	C-O	-5.09	1.17	1.24
1	C	54	SER	N-CA	5.09	1.52	1.46
1	A	36	HIS	CG-CD2	5.05	1.41	1.35
1	C	128	HIS	CG-ND1	-5.05	1.32	1.38
1	A	528	SER	N-CA	5.05	1.52	1.46
1	D	318	HIS	ND1-CE1	5.04	1.37	1.32
1	B	541	GLU	C-O	5.04	1.30	1.24
1	B	681	ALA	C-O	5.04	1.30	1.24
1	A	219	HIS	ND1-CE1	5.03	1.37	1.32
1	C	536	ARG	N-CA	5.03	1.52	1.46
1	B	86	VAL	CA-C	-5.03	1.47	1.52
1	D	131	GLY	N-CA	5.02	1.50	1.45
1	A	154	SER	C-O	-5.01	1.17	1.24
1	B	99	SER	C-O	-5.01	1.17	1.24
1	C	126[A]	ILE	N-CA	5.01	1.52	1.46
1	C	126[B]	ILE	N-CA	5.01	1.52	1.46
1	B	113	LYS	CA-C	5.01	1.59	1.52
1	A	410	GLY	C-O	5.01	1.29	1.24
1	D	441	HIS	ND1-CE1	5.00	1.37	1.32

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	745	ILE	CA-C-N	-9.14	110.33	119.56
1	D	745	ILE	C-N-CA	-9.14	110.33	119.56
1	C	159	ILE	CB-CG1-CD1	-9.06	94.76	113.80
1	C	330	ASP	CB-CA-C	-7.67	101.06	111.88
1	D	330	ASP	CB-CA-C	-6.94	102.09	111.88
1	B	745	ILE	CA-C-N	-6.70	112.79	119.56
1	B	745	ILE	C-N-CA	-6.70	112.79	119.56
1	B	530	ILE	N-CA-C	6.59	116.73	110.53
1	D	213	LYS	CA-CB-CG	-6.34	101.42	114.10
1	B	41	GLU	CA-C-N	-6.26	113.31	119.76
1	B	41	GLU	C-N-CA	-6.26	113.31	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	536	ARG	CA-C-N	-6.03	113.47	119.56
1	B	536	ARG	C-N-CA	-6.03	113.47	119.56
1	B	48	GLN	O-C-N	5.97	125.53	121.71
1	A	431	ILE	N-CA-C	-5.97	103.10	108.95
1	A	377	ARG	CG-CD-NE	-5.93	98.95	112.00
1	C	48	GLN	CA-C-N	-5.93	113.86	119.85
1	C	48	GLN	C-N-CA	-5.93	113.86	119.85
1	B	369	ARG	NE-CZ-NH1	-5.89	115.61	121.50
1	B	419	GLN	CB-CA-C	5.86	121.92	110.67
1	C	315	PRO	N-CA-C	-5.83	106.86	114.03
1	C	270	GLU	N-CA-C	5.81	118.20	110.53
1	C	195	ILE	CB-CA-C	-5.80	103.61	111.15
1	A	120	GLU	N-CA-C	5.79	117.59	111.28
1	B	182	ILE	N-CA-C	-5.75	103.72	110.21
1	B	421	SER	N-CA-C	-5.74	105.94	113.12
1	B	724	ALA	N-CA-C	5.71	119.95	113.15
1	C	509	ARG	NE-CZ-NH2	5.71	124.34	119.20
1	C	158	LYS	CA-C-N	-5.62	115.84	123.10
1	C	158	LYS	C-N-CA	-5.62	115.84	123.10
1	C	556	GLN	N-CA-C	5.57	117.35	111.28
1	C	115	THR	CA-C-N	-5.53	113.26	120.44
1	C	115	THR	C-N-CA	-5.53	113.26	120.44
1	D	574	THR	CB-CA-C	5.53	117.38	109.26
1	B	722	ASP	N-CA-C	5.52	117.30	111.28
1	C	420	ILE	N-CA-C	5.49	116.88	110.62
1	C	597	ASP	N-CA-C	-5.43	99.42	108.32
1	A	265	SER	N-CA-CB	-5.42	102.61	111.66
1	A	71	VAL	CB-CA-C	-5.41	104.50	111.20
1	B	509	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	B	657	ALA	CA-C-N	5.35	126.53	119.84
1	B	657	ALA	C-N-CA	5.35	126.53	119.84
1	B	283	GLU	CB-CG-CD	5.34	121.68	112.60
1	B	377	ARG	CA-CB-CG	-5.34	103.42	114.10
1	C	241	ASP	N-CA-C	-5.32	105.38	111.07
1	A	576	PRO	CA-C-N	5.26	125.20	119.78
1	A	576	PRO	C-N-CA	5.26	125.20	119.78
1	A	638	GLY	N-CA-C	-5.26	104.98	111.45
1	B	556	GLN	N-CA-C	5.26	117.01	111.28
1	A	748	ILE	N-CA-C	5.25	118.48	111.44
1	B	144	LEU	N-CA-C	5.22	118.67	112.72
1	B	147	ILE	CB-CA-C	5.20	115.64	111.06
1	A	437	THR	N-CA-C	-5.20	106.99	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	420	ILE	CB-CA-C	-5.19	105.13	112.14
1	D	110	LEU	N-CA-C	-5.15	105.56	111.07
1	A	530	ILE	N-CA-C	5.14	115.36	110.53
1	B	336	LEU	CA-C-N	5.12	125.13	121.65
1	B	336	LEU	C-N-CA	5.12	125.13	121.65
1	B	597	ASP	N-CA-C	-5.10	100.14	108.76
1	C	726	GLY	N-CA-C	-5.10	101.10	113.18
1	C	360	ILE	CA-C-N	-5.10	114.51	119.76
1	C	360	ILE	C-N-CA	-5.10	114.51	119.76
1	C	431	ILE	N-CA-C	-5.10	104.28	109.02
1	D	377	ARG	NH1-CZ-NH2	5.08	125.91	119.30
1	C	745	ILE	N-CA-CB	5.08	113.92	110.52
1	A	655	ALA	N-CA-C	5.04	117.67	111.82
1	D	377	ARG	CA-CB-CG	-5.04	104.03	114.10
1	B	165	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	B	120	GLU	N-CA-C	5.00	117.62	111.82
1	B	405	ASP	CA-C-N	-5.00	114.64	120.04
1	B	405	ASP	C-N-CA	-5.00	114.64	120.04

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	724	ALA	Peptide
1	C	725	ASP	Peptide

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	5758	0	5606	43	1
1	B	5761	0	5615	76	1
1	C	5755	0	5601	55	0
1	D	5758	0	5606	62	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
2	C	43	0	30	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	43	0	30	3	0
3	A	747	0	0	6	0
3	B	690	0	0	16	0
3	C	733	0	0	13	0
3	D	778	0	0	16	0
All	All	26152	0	22548	215	1

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 5.

All (215) 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:392:HIS:ND1	1:A:415:TYR:CB	1.71	1.53
1:B:392:HIS:ND1	1:B:415:TYR:CB	1.69	1.51
1:D:392:HIS:ND1	1:D:415:TYR:CB	1.72	1.48
1:C:392:HIS:ND1	1:C:415:TYR:CB	1.73	1.48
3:B:1494:HOH:O	1:D:73:LYS:HD3	1.18	1.30
1:D:449[B]:HIS:NE2	3:D:1517:HOH:O	1.66	1.27
1:C:392:HIS:CE1	1:C:415:TYR:HB2	1.70	1.24
1:D:392:HIS:CE1	1:D:415:TYR:HB2	1.73	1.22
1:B:521:ARG:HD3	3:B:1560:HOH:O	1.41	1.20
1:B:392:HIS:CE1	1:B:415:TYR:HB2	1.76	1.19
1:A:392:HIS:CE1	1:A:415:TYR:HB2	1.80	1.17
1:D:392:HIS:ND1	1:D:415:TYR:HB2	0.83	1.16
1:C:392:HIS:ND1	1:C:415:TYR:HB2	0.83	1.15
1:B:392:HIS:ND1	1:B:415:TYR:HB2	0.78	1.10
1:A:392:HIS:ND1	1:A:415:TYR:HB2	0.77	1.09
1:B:451:MET:HE2	1:D:451:MET:HE2	1.40	1.04
1:D:267:ARG:HG3	3:D:1372:HOH:O	1.61	1.00
1:A:451:MET:HE2	1:C:451:MET:HE2	1.46	0.95
1:B:309[A]:LYS:HE2	1:C:309:LYS:HE3	1.48	0.92
1:A:392:HIS:CG	1:A:415:TYR:HB2	2.05	0.91
1:D:546:GLN:HG3	3:D:1570:HOH:O	1.73	0.89
1:B:267:ARG:HG3	3:B:1372:HOH:O	1.74	0.86
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.58	0.86
1:C:267:ARG:HG3	3:C:1558:HOH:O	1.78	0.82
1:B:552:LEU:O	1:B:552:LEU:HD23	1.80	0.81
1:B:309[A]:LYS:CE	1:C:309:LYS:HE3	2.11	0.81
1:B:309[A]:LYS:HG2	1:B:660:LEU:HD11	1.65	0.79
1:C:552:LEU:HD11	1:C:556:GLN:NE2	2.01	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:578:ASP:HB2	1:C:582:LEU:O	1.86	0.75
1:A:392:HIS:ND1	1:A:415:TYR:CG	2.53	0.75
1:B:724:ALA:O	1:B:725:ASP:O	2.05	0.73
1:B:309[A]:LYS:NZ	1:B:313:ARG:HE	1.87	0.73
3:A:1641:HOH:O	1:D:126[B]:ILE:HD11	1.89	0.73
1:B:392:HIS:ND1	1:B:415:TYR:HB3	2.02	0.69
1:B:521:ARG:NH2	1:B:745:ILE:HD13	2.06	0.69
1:B:708:ILE:HD12	1:B:710:ILE:HD11	1.75	0.69
1:C:583:LYS:O	1:C:584:LYS:HB3	1.93	0.69
3:B:1585:HOH:O	1:C:126[B]:ILE:HD11	1.92	0.68
1:B:281:ASN:OD1	1:B:283:GLU:HG2	1.93	0.68
1:B:126[B]:ILE:HD11	3:C:1628:HOH:O	1.93	0.68
2:B:801:HEM:HMC2	2:B:801:HEM:HBC2	1.73	0.68
1:D:392:HIS:ND1	1:D:415:TYR:CG	2.61	0.68
1:C:392:HIS:ND1	1:C:415:TYR:CG	2.58	0.68
1:B:126[A]:ILE:HD12	1:C:121:ARG:CZ	2.24	0.67
1:D:449[B]:HIS:CE1	3:D:1517:HOH:O	2.26	0.67
1:C:486:GLN:OE1	3:C:1555:HOH:O	2.13	0.66
1:D:309:LYS:CE	3:D:1676:HOH:O	2.44	0.66
1:B:144:LEU:HD11	1:B:370:VAL:HG13	1.76	0.66
1:B:710:ILE:CD1	1:B:718:ILE:HG13	2.25	0.65
1:C:597:ASP:OD2	3:C:1423:HOH:O	2.14	0.65
1:A:36:HIS:CD2	1:A:36:HIS:H	2.16	0.64
1:C:552:LEU:CD1	1:C:556:GLN:HE21	2.10	0.64
1:D:629:HIS:HD2	3:D:1262:HOH:O	1.81	0.63
1:B:521:ARG:NH2	1:B:745:ILE:CD1	2.61	0.63
1:B:521:ARG:HH21	1:B:745:ILE:HD13	1.60	0.63
1:B:369:ARG:HG2	3:B:1303:HOH:O	1.97	0.63
1:B:552:LEU:HD23	1:B:552:LEU:C	2.24	0.62
1:A:120:GLU:HB2	1:D:126[A]:ILE:HD11	1.82	0.62
1:B:556:GLN:HG2	1:B:566:LEU:CD2	2.29	0.62
1:D:440:TYR:HD1	3:D:1660:HOH:O	1.83	0.61
1:B:120:GLU:HB2	1:C:126[A]:ILE:HD11	1.83	0.61
1:C:629:HIS:HD2	3:C:1209:HOH:O	1.84	0.60
1:D:546:GLN:CD	3:D:1570:HOH:O	2.43	0.60
1:B:552:LEU:C	1:B:552:LEU:CD2	2.75	0.60
1:D:38:PRO:HA	1:D:48:GLN:HE21	1.67	0.58
1:C:552:LEU:CD1	1:C:556:GLN:NE2	2.66	0.58
1:B:294:LYS:NZ	3:B:1513:HOH:O	2.33	0.57
1:D:392:HIS:ND1	1:D:415:TYR:HB3	2.04	0.57
1:D:546:GLN:CG	3:D:1570:HOH:O	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.13	0.57
1:B:583:LYS:O	1:B:584:LYS:HB3	2.07	0.55
1:D:359:LEU:H	1:D:507:HIS:HD2	1.54	0.55
1:A:639:GLU:HG3	3:A:1485:HOH:O	2.06	0.54
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.90	0.54
1:A:126[B]:ILE:CD1	3:D:1009:HOH:O	2.55	0.54
3:A:1335:HOH:O	1:C:449[B]:HIS:HE1	1.89	0.54
1:C:490:GLU:HG3	1:D:490:GLU:HG3	1.88	0.54
1:D:190:TYR:CD1	1:D:195:ILE:HD11	2.43	0.54
1:A:126[A]:ILE:HD12	1:D:121:ARG:CZ	2.38	0.54
1:C:724:ALA:O	1:C:725:ASP:HB2	2.07	0.54
1:C:732:LEU:C	1:C:732:LEU:HD13	2.32	0.54
1:D:708:ILE:HG13	1:D:710:ILE:HG12	1.88	0.54
1:C:621:LYS:HG2	3:C:1608:HOH:O	2.07	0.54
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.91	0.54
1:B:392:HIS:ND1	1:B:415:TYR:CG	2.65	0.53
1:B:546:GLN:NE2	3:B:1467:HOH:O	2.41	0.53
1:B:38:PRO:HG2	1:B:51:ALA:HB2	1.91	0.53
1:B:309[A]:LYS:HG3	3:B:1588:HOH:O	2.08	0.53
1:B:521:ARG:HH22	1:B:745:ILE:HD12	1.74	0.53
1:D:598:VAL:HG22	1:D:628:VAL:HG22	1.90	0.53
1:A:120:GLU:HB2	1:D:126[A]:ILE:CD1	2.39	0.52
1:C:727:SER:HA	3:C:1526:HOH:O	2.08	0.52
1:B:461:GLU:HA	1:B:462:PRO:C	2.33	0.52
1:B:395:HIS:HE1	3:B:1589:HOH:O	1.92	0.52
1:C:552:LEU:HD13	1:C:556:GLN:HE21	1.74	0.52
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.92	0.52
1:A:449[B]:HIS:HE1	3:A:1335:HOH:O	1.92	0.52
1:B:144:LEU:HD11	1:B:370:VAL:CG1	2.40	0.51
1:B:552:LEU:HD23	1:B:556:GLN:HG3	1.91	0.51
1:D:448:MET:O	1:D:449[A]:HIS:HB2	2.10	0.51
1:D:309:LYS:HE3	3:D:1676:HOH:O	2.07	0.51
1:D:190:TYR:HA	1:D:195:ILE:HD13	1.93	0.50
1:D:190:TYR:HD1	1:D:195:ILE:HD11	1.76	0.50
1:A:344:GLU:HB3	3:A:1569:HOH:O	2.11	0.50
1:B:725:ASP:OD2	1:B:727:SER:HB3	2.11	0.50
1:C:636:ARG:NH1	3:C:1527:HOH:O	2.35	0.50
1:C:126[A]:ILE:CG2	2:C:801:HEM:HMD1	2.41	0.50
1:B:126[B]:ILE:HG21	1:C:117:PHE:CE2	2.46	0.50
1:C:274:ILE:HD12	2:C:801:HEM:HMB1	1.94	0.50
1:A:126[B]:ILE:HD11	3:D:1009:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:LEU:H	1:B:507:HIS:HD2	1.59	0.49
1:D:309:LYS:HE2	3:D:1676:HOH:O	2.08	0.49
1:A:459:ASN:HD22	1:A:459:ASN:H	1.60	0.49
1:A:682:ASN:HB3	1:A:707:THR:HG21	1.95	0.49
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.42	0.49
1:A:126[A]:ILE:CG2	2:A:801:HEM:HMD1	2.43	0.49
1:B:521:ARG:HH22	1:B:745:ILE:CD1	2.26	0.49
1:C:745:ILE:HD13	3:C:1560:HOH:O	2.13	0.49
1:B:121:ARG:HG2	1:C:126[A]:ILE:HD12	1.94	0.49
1:C:70:ASP:OD1	3:C:1495:HOH:O	2.20	0.49
2:C:801:HEM:CMC	2:C:801:HEM:HBC2	2.43	0.49
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.28	0.49
3:B:1494:HOH:O	1:D:73:LYS:CD	2.02	0.49
1:C:392:HIS:CE1	1:C:415:TYR:CB	2.63	0.48
1:D:274:ILE:HD12	2:D:801:HEM:HMB1	1.95	0.48
1:C:392:HIS:ND1	1:C:415:TYR:HB3	2.05	0.48
1:D:126[A]:ILE:HG22	2:D:801:HEM:HMD1	1.94	0.48
1:A:38:PRO:HA	1:A:48:GLN:OE1	2.13	0.47
1:B:251:HIS:HA	1:B:508:PRO:HG3	1.97	0.47
1:A:235:ALA:HA	1:A:530:ILE:HG23	1.95	0.47
1:A:309:LYS:NZ	1:A:687:GLU:OE2	2.40	0.47
1:B:344:GLU:H	1:B:344:GLU:CD	2.22	0.47
1:D:235:ALA:HA	1:D:530:ILE:HG23	1.97	0.47
1:C:488:ARG:CD	3:C:1466:HOH:O	2.62	0.47
1:C:488:ARG:HD3	3:C:1466:HOH:O	2.14	0.47
1:D:251:HIS:CE1	1:D:507:HIS:HB3	2.50	0.47
1:A:392:HIS:CG	1:A:415:TYR:CB	2.83	0.47
1:D:750:LYS:NZ	3:D:1383:HOH:O	2.41	0.47
1:C:460:TYR:CE2	1:D:238:THR:HB	2.50	0.46
1:B:629:HIS:HD2	3:B:1158:HOH:O	1.98	0.46
1:C:128:HIS:HA	1:C:168:THR:O	2.15	0.46
1:B:267:ARG:HD2	3:B:1132:HOH:O	2.14	0.46
1:D:37:ARG:HD2	3:D:1429:HOH:O	2.16	0.45
1:B:335:GLU:OE1	1:B:369:ARG:HD2	2.17	0.45
1:C:710:ILE:HG23	1:C:715:GLU:HG2	1.98	0.45
1:A:274:ILE:HD12	2:A:801:HEM:HMB1	1.99	0.45
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.31	0.45
1:B:126[B]:ILE:HG12	3:B:1040:HOH:O	2.16	0.45
1:A:36:HIS:H	1:A:36:HIS:HD2	1.63	0.45
1:A:372:LYS:NZ	3:A:1612:HOH:O	2.50	0.45
1:A:449[A]:HIS:CD2	1:C:449[A]:HIS:CD2	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309[A]:LYS:NZ	1:B:313:ARG:NE	2.60	0.45
1:B:392:HIS:CD2	1:B:394:GLY:H	2.35	0.45
1:B:724:ALA:O	1:B:725:ASP:C	2.60	0.45
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.52	0.44
1:B:319:ARG:HD3	1:C:227:TRP:O	2.16	0.44
1:B:745:ILE:O	1:B:748:ILE:HG12	2.18	0.44
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.26	0.44
1:B:556:GLN:HG2	1:B:566:LEU:HD22	1.99	0.44
1:B:634:TYR:O	1:B:653:THR:HA	2.17	0.44
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.33	0.44
1:D:602:VAL:HG13	1:D:662:VAL:HA	2.00	0.44
1:C:583:LYS:O	1:C:584:LYS:CB	2.64	0.43
1:D:207:PHE:O	1:D:249:THR:HA	2.17	0.43
1:D:461:GLU:HA	1:D:462:PRO:C	2.43	0.43
1:A:128:HIS:HA	1:A:168:THR:O	2.17	0.43
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.34	0.43
1:D:713:GLN:O	1:D:713:GLN:HG2	2.17	0.43
1:A:213:LYS:HD2	1:D:92:GLN:OE1	2.18	0.43
1:A:251:HIS:CE1	1:A:507:HIS:HB3	2.54	0.43
1:D:313:ARG:HG3	1:D:660:LEU:HD12	2.01	0.43
1:A:607:LEU:HD22	1:A:611:VAL:HG21	2.00	0.43
1:B:637:MET:HE3	3:B:1395:HOH:O	2.17	0.43
1:C:359:LEU:H	1:C:507:HIS:HD2	1.66	0.43
1:D:126[A]:ILE:CG2	2:D:801:HEM:HMD1	2.49	0.42
1:D:257:MET:SD	1:D:530:ILE:HD12	2.58	0.42
1:B:39:ALA:HB1	1:B:41:GLU:HG2	2.00	0.42
1:C:566:LEU:HB2	1:C:571:LEU:HD13	2.01	0.42
1:B:126[B]:ILE:HG21	1:C:117:PHE:CZ	2.53	0.42
1:B:708:ILE:CD1	1:B:710:ILE:HD11	2.48	0.42
1:C:251:HIS:CE1	1:C:507:HIS:HB3	2.54	0.42
1:D:38:PRO:HA	1:D:48:GLN:NE2	2.33	0.42
1:C:461:GLU:HA	1:C:462:PRO:C	2.45	0.42
1:D:696:ALA:HB1	1:D:728:PHE:CZ	2.55	0.42
1:C:746:PRO:HB2	3:C:1579:HOH:O	2.19	0.42
1:D:459:ASN:HD22	1:D:459:ASN:H	1.68	0.42
1:A:448:MET:O	1:A:449[B]:HIS:HB2	2.19	0.42
1:A:449[B]:HIS:CG	1:C:449[B]:HIS:CG	2.34	0.42
1:A:461:GLU:HA	1:A:462:PRO:C	2.45	0.42
1:B:404:ASN:O	1:B:405:ASP:C	2.63	0.42
1:B:459:ASN:H	1:B:459:ASN:HD22	1.66	0.42
1:D:392:HIS:CD2	1:D:394:GLY:H	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:HIS:CE1	1:D:415:TYR:CB	2.67	0.41
1:B:36:HIS:HD1	1:B:36:HIS:H	1.68	0.41
1:D:39:ALA:H	1:D:48:GLN:NE2	2.19	0.41
1:B:713:GLN:H	1:B:713:GLN:HG3	1.47	0.41
1:B:235:ALA:HA	1:B:530:ILE:HG23	2.02	0.41
1:B:359:LEU:H	1:B:507:HIS:CD2	2.37	0.41
1:D:359:LEU:H	1:D:507:HIS:CD2	2.37	0.41
1:A:583:LYS:O	1:A:584:LYS:HB3	2.20	0.41
1:B:97:ALA:O	1:B:101:GLY:HA3	2.21	0.41
1:D:509:ARG:HD2	1:D:576:PRO:HD2	2.01	0.41
1:A:36:HIS:CD2	1:A:36:HIS:N	2.85	0.41
1:A:296:LEU:HD12	1:A:333:GLU:HB3	2.03	0.41
1:A:393:PRO:HD2	1:A:415:TYR:CD2	2.55	0.41
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.56	0.41
1:B:309[A]:LYS:HZ3	1:B:313:ARG:NE	2.19	0.41
1:D:578:ASP:OD1	1:D:583:LYS:HE3	2.20	0.41
1:A:669:OCS:OD3	1:A:699:GLY:HA3	2.22	0.40
1:B:29:LEU:N	3:B:1478:HOH:O	2.38	0.40
1:D:267:ARG:HD2	3:D:1237:HOH:O	2.20	0.40
1:A:252:ASN:HD22	1:A:252:ASN:HA	1.71	0.40
1:B:361:PRO:HD2	1:B:364:LEU:HD12	2.03	0.40
1:C:238:THR:HB	1:D:460:TYR:CE2	2.56	0.40
1:B:706:ALA:HB3	3:B:1438:HOH:O	2.22	0.40

All (1) 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)
1:A:59:ASP:OD1	1:B:369:ARG:NH2[2_545]	1.94	0.26

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	727/753 (96%)	709 (98%)	17 (2%)	1 (0%)	48	27
1	B	727/753 (96%)	710 (98%)	15 (2%)	2 (0%)	36	20
1	C	726/753 (96%)	710 (98%)	13 (2%)	3 (0%)	30	14
1	D	727/753 (96%)	708 (97%)	18 (2%)	1 (0%)	48	27
All	All	2907/3012 (96%)	2837 (98%)	63 (2%)	7 (0%)	43	24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	ASP
1	A	75	SER
1	C	75	SER
1	C	725	ASP
1	D	75	SER
1	C	584	LYS
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	614/635 (97%)	597 (97%)	17 (3%)	38	15
1	B	614/635 (97%)	589 (96%)	25 (4%)	27	8
1	C	613/635 (96%)	582 (95%)	31 (5%)	21	5
1	D	614/635 (97%)	592 (96%)	22 (4%)	31	10
All	All	2455/2540 (97%)	2360 (96%)	95 (4%)	28	9

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	37	ARG
1	A	73	LYS
1	A	191	THR

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Mol	Chain	Res	Type
1	A	198	LEU
1	A	205	ILE
1	A	252	ASN
1	A	294	LYS
1	A	369	ARG
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	617	LEU
1	A	707	THR
1	A	732	LEU
1	A	747	LYS
1	A	751	ILE
1	B	28	SER
1	B	32	GLU
1	B	155	ASP
1	B	191	THR
1	B	205	ILE
1	B	213	LYS
1	B	252	ASN
1	B	344	GLU
1	B	370	VAL
1	B	432	PRO
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	566	LEU
1	B	571	LEU
1	B	583	LYS
1	B	610	GLU
1	B	616	LEU
1	B	633	LEU
1	B	635	SER
1	B	703	LYS
1	B	713	GLN
1	B	732	LEU
1	B	751	ILE
1	C	32	GLU
1	C	37	ARG
1	C	159	ILE
1	C	191	THR

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Mol	Chain	Res	Type
1	C	198	LEU
1	C	205	ILE
1	C	213	LYS
1	C	252	ASN
1	C	283	GLU
1	C	285	LYS
1	C	310	LEU
1	C	377	ARG
1	C	432	PRO
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG
1	C	521	ARG
1	C	571	LEU
1	C	584	LYS
1	C	606	LEU
1	C	616	LEU
1	C	617	LEU
1	C	633	LEU
1	C	636	ARG
1	C	648	LEU
1	C	685	LEU
1	C	713	GLN
1	C	725	ASP
1	C	733	LEU
1	C	750	LYS
1	D	73	LYS
1	D	126[A]	ILE
1	D	126[B]	ILE
1	D	191	THR
1	D	205	ILE
1	D	252	ASN
1	D	344	GLU
1	D	432	PRO
1	D	440	TYR
1	D	459	ASN
1	D	490	GLU
1	D	552	LEU
1	D	554	LEU
1	D	574	THR
1	D	582	LEU

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Mol	Chain	Res	Type
1	D	584	LYS
1	D	616	LEU
1	D	648	LEU
1	D	708	ILE
1	D	713	GLN
1	D	750	LYS
1	D	751	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	66	ASN
1	A	84	GLN
1	A	139	GLN
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	A	546	GLN
1	A	713	GLN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	B	713	GLN
1	C	252	ASN
1	C	459	ASN
1	C	486	GLN
1	C	507	HIS
1	C	546	GLN
1	C	556	GLN
1	C	629	HIS
1	D	48	GLN
1	D	77	ASN
1	D	252	ASN
1	D	459	ASN
1	D	507	HIS
1	D	629	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OCS	A	669	1	6,8,9	2.19	2 (33%)	7,11,13	1.51	2 (28%)
1	OCS	C	669	1	6,8,9	1.74	1 (16%)	7,11,13	1.50	1 (14%)
1	OCS	B	669	1	6,8,9	2.14	2 (33%)	7,11,13	2.77	2 (28%)
1	OCS	D	669	1	6,8,9	1.83	2 (33%)	7,11,13	2.50	2 (28%)

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	OCS	A	669	1	-	4/4/7/9	-
1	OCS	C	669	1	-	1/4/7/9	-
1	OCS	B	669	1	-	1/4/7/9	-
1	OCS	D	669	1	-	1/4/7/9	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	669	OCS	OD2-SG	4.49	1.64	1.47
1	B	669	OCS	OD2-SG	4.29	1.63	1.47
1	C	669	OCS	OD2-SG	4.00	1.62	1.47
1	D	669	OCS	OD2-SG	3.24	1.59	1.47
1	D	669	OCS	CB-CA	2.92	1.55	1.53
1	B	669	OCS	CB-CA	-2.28	1.52	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	669	OCS	CB-CA	2.21	1.55	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	669	OCS	OD3-SG-CB	-6.42	97.17	106.76
1	D	669	OCS	OD3-SG-CB	-5.53	98.50	106.76
1	C	669	OCS	CA-CB-SG	3.59	118.94	113.61
1	D	669	OCS	OD3-SG-OD1	2.58	122.23	113.82
1	A	669	OCS	OD3-SG-CB	-2.34	103.27	106.76
1	B	669	OCS	CA-CB-SG	2.33	117.07	113.61
1	A	669	OCS	CA-CB-SG	2.25	116.94	113.61

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	669	OCS	N-CA-CB-SG
1	A	669	OCS	CA-CB-SG-OD2
1	A	669	OCS	CA-CB-SG-OD3
1	B	669	OCS	N-CA-CB-SG
1	C	669	OCS	N-CA-CB-SG
1	D	669	OCS	N-CA-CB-SG
1	A	669	OCS	CA-CB-SG-OD1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	669	OCS	1	0

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	B	801	1	50,50,50	1.96	18 (36%)	67,82,82	2.37	23 (34%)
2	HEM	A	801	1	50,50,50	1.94	18 (36%)	67,82,82	2.46	26 (38%)
2	HEM	C	801	1	50,50,50	1.93	15 (30%)	67,82,82	2.66	26 (38%)
2	HEM	D	801	1	50,50,50	2.08	17 (34%)	67,82,82	2.31	28 (41%)

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	801	1	-	2/14/54/54	-
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	-

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	HEM	C3B-C2B	4.90	1.47	1.37
2	B	801	HEM	FE-NB	4.75	2.09	1.94
2	A	801	HEM	C3B-C2B	4.21	1.45	1.37
2	B	801	HEM	C1B-NB	-3.99	1.33	1.40
2	C	801	HEM	C3C-C2C	3.93	1.45	1.37
2	C	801	HEM	CHD-C1D	3.87	1.48	1.39
2	C	801	HEM	C1C-NC	3.86	1.46	1.39
2	D	801	HEM	CHB-C4A	3.83	1.48	1.39
2	D	801	HEM	CHD-C1D	3.72	1.47	1.39
2	B	801	HEM	CHB-C1B	3.67	1.45	1.38
2	D	801	HEM	CHD-C4C	3.66	1.45	1.38
2	D	801	HEM	FE-NB	3.65	2.06	1.94
2	A	801	HEM	C4A-NA	3.64	1.46	1.39
2	A	801	HEM	C3D-C2D	3.53	1.44	1.36
2	A	801	HEM	C1C-NC	3.47	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C4D-C3D	3.39	1.50	1.45
2	C	801	HEM	FE-ND	3.29	2.05	1.94
2	C	801	HEM	CHC-C4B	3.28	1.46	1.39
2	C	801	HEM	CHB-C1B	3.28	1.45	1.38
2	A	801	HEM	C1B-NB	-3.27	1.34	1.40
2	C	801	HEM	FE-NB	3.24	2.04	1.94
2	B	801	HEM	CHA-C4D	3.21	1.44	1.38
2	D	801	HEM	CHA-C4D	3.19	1.44	1.38
2	A	801	HEM	CHB-C1B	3.16	1.44	1.38
2	A	801	HEM	FE-NB	3.14	2.04	1.94
2	D	801	HEM	CHC-C4B	3.12	1.46	1.39
2	D	801	HEM	FE-ND	3.10	2.04	1.94
2	B	801	HEM	CHD-C1D	3.05	1.46	1.39
2	A	801	HEM	C2A-C3A	3.01	1.46	1.38
2	B	801	HEM	FE-ND	2.97	2.04	1.94
2	D	801	HEM	C3B-C4B	2.94	1.50	1.44
2	C	801	HEM	CHB-C4A	2.76	1.45	1.39
2	A	801	HEM	CHC-C4B	2.70	1.45	1.39
2	C	801	HEM	C4D-C3D	2.63	1.49	1.45
2	D	801	HEM	CMB-C2B	-2.58	1.45	1.50
2	B	801	HEM	C3B-C2B	2.57	1.42	1.37
2	A	801	HEM	CMC-C2C	2.54	1.56	1.50
2	B	801	HEM	CHC-C4B	2.53	1.44	1.39
2	D	801	HEM	C3D-C2D	2.52	1.42	1.36
2	D	801	HEM	CHC-C1C	2.52	1.43	1.38
2	D	801	HEM	CHB-C1B	2.51	1.43	1.38
2	B	801	HEM	C1C-NC	2.51	1.44	1.39
2	D	801	HEM	C4C-NC	2.50	1.44	1.39
2	B	801	HEM	C3C-C2C	2.50	1.42	1.37
2	B	801	HEM	C4A-C3A	2.49	1.49	1.43
2	C	801	HEM	C2A-C3A	2.47	1.45	1.38
2	A	801	HEM	CHD-C1D	2.47	1.44	1.39
2	C	801	HEM	CBD-CAD	2.45	1.60	1.51
2	A	801	HEM	C1A-NA	2.45	1.44	1.39
2	A	801	HEM	C1B-C2B	2.44	1.49	1.44
2	D	801	HEM	CBA-CAA	2.41	1.60	1.51
2	A	801	HEM	C3C-C2C	2.39	1.42	1.37
2	D	801	HEM	C3C-C4C	2.39	1.50	1.46
2	A	801	HEM	CHD-C4C	2.39	1.43	1.38
2	B	801	HEM	C1A-C2A	2.35	1.49	1.44
2	A	801	HEM	CHC-C1C	2.33	1.42	1.38
2	B	801	HEM	O2D-CGD	-2.32	1.23	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	CHD-C4C	2.21	1.42	1.38
2	C	801	HEM	FE-NC	2.20	2.02	1.95
2	C	801	HEM	C1A-NA	2.20	1.43	1.39
2	C	801	HEM	C4B-NB	-2.17	1.34	1.38
2	B	801	HEM	FE-NC	2.11	2.02	1.95
2	A	801	HEM	FE-ND	2.11	2.01	1.94
2	A	801	HEM	CMB-C2B	-2.09	1.46	1.50
2	D	801	HEM	C4A-C3A	2.08	1.48	1.43
2	C	801	HEM	CHD-C4C	2.07	1.42	1.38
2	B	801	HEM	CHB-C4A	2.07	1.44	1.39
2	B	801	HEM	O2A-CGA	-2.03	1.24	1.30

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	C3B-C2B-C1B	-8.51	100.02	106.41
2	C	801	HEM	C3B-C2B-C1B	-8.43	100.08	106.41
2	C	801	HEM	C2D-C1D-ND	7.20	118.23	109.90
2	B	801	HEM	C3C-C2C-C1C	-7.15	100.28	107.05
2	D	801	HEM	C3B-C2B-C1B	-6.52	101.52	106.41
2	B	801	HEM	C3B-C2B-C1B	-6.03	101.89	106.41
2	C	801	HEM	C3B-C4B-NB	5.93	113.73	109.47
2	B	801	HEM	C2D-C1D-ND	5.81	116.62	109.90
2	C	801	HEM	C2B-C1B-NB	5.65	116.33	109.84
2	B	801	HEM	C4C-C3C-C2C	5.23	111.35	106.81
2	B	801	HEM	CAA-CBA-CGA	-5.12	100.08	113.67
2	C	801	HEM	CHD-C4C-NC	-5.04	118.97	124.45
2	D	801	HEM	C2B-C1B-NB	5.03	115.62	109.84
2	A	801	HEM	C3C-C2C-C1C	-4.89	102.42	107.05
2	D	801	HEM	CAA-CBA-CGA	-4.86	100.77	113.67
2	A	801	HEM	C2B-C1B-NB	4.68	115.22	109.84
2	A	801	HEM	C3D-C4D-ND	4.53	115.14	110.17
2	A	801	HEM	CHD-C1D-C2D	-4.51	117.91	125.03
2	C	801	HEM	C4D-ND-C1D	-4.33	100.07	105.21
2	C	801	HEM	CBD-CAD-C3D	-4.28	100.69	112.53
2	A	801	HEM	CAD-C3D-C4D	4.28	132.15	124.70
2	A	801	HEM	C4C-NC-C1C	-4.09	99.14	105.82
2	A	801	HEM	CBD-CAD-C3D	-3.98	101.52	112.53
2	D	801	HEM	C2A-C1A-NA	3.94	114.52	110.15
2	B	801	HEM	CBD-CAD-C3D	-3.93	101.67	112.53
2	D	801	HEM	C4C-NC-C1C	-3.91	99.44	105.82
2	A	801	HEM	CAA-CBA-CGA	-3.82	103.54	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	HEM	CHD-C1D-ND	-3.78	120.36	124.42
2	C	801	HEM	CAA-CBA-CGA	-3.74	103.76	113.67
2	C	801	HEM	C1D-C2D-C3D	-3.69	103.09	106.98
2	D	801	HEM	C3D-C4D-ND	3.67	114.20	110.17
2	D	801	HEM	C4C-CHD-C1D	-3.62	118.32	126.02
2	D	801	HEM	C2C-C1C-NC	3.61	116.31	109.64
2	A	801	HEM	C2D-C1D-ND	3.58	114.05	109.90
2	C	801	HEM	C3D-C4D-ND	3.57	114.08	110.17
2	C	801	HEM	C3C-C2C-C1C	-3.55	103.69	107.05
2	A	801	HEM	C2C-C1C-NC	3.52	116.14	109.64
2	D	801	HEM	C3C-C2C-C1C	-3.42	103.81	107.05
2	B	801	HEM	C4D-ND-C1D	-3.39	101.19	105.21
2	C	801	HEM	CMC-C2C-C1C	3.37	130.66	124.73
2	A	801	HEM	CHB-C1B-C2B	-3.35	117.44	126.95
2	A	801	HEM	CHD-C1D-ND	3.34	128.01	124.42
2	C	801	HEM	C1B-NB-C4B	-3.28	101.33	105.21
2	D	801	HEM	CHD-C1D-C2D	-3.23	119.93	125.03
2	C	801	HEM	CBB-CAB-C3B	-3.21	111.50	127.53
2	C	801	HEM	CHB-C1B-C2B	-3.21	117.84	126.95
2	B	801	HEM	C2B-C1B-NB	3.16	113.48	109.84
2	D	801	HEM	CHC-C1C-NC	-3.16	121.01	124.45
2	B	801	HEM	C3D-C4D-ND	3.16	113.64	110.17
2	D	801	HEM	C1D-C2D-C3D	-3.16	103.66	106.98
2	B	801	HEM	C2C-C1C-NC	3.16	115.48	109.64
2	B	801	HEM	CHD-C1D-C2D	-3.13	120.08	125.03
2	B	801	HEM	CMC-C2C-C1C	3.12	130.22	124.73
2	A	801	HEM	CMC-C2C-C1C	3.07	130.14	124.73
2	A	801	HEM	CMB-C2B-C1B	3.06	129.82	125.03
2	A	801	HEM	CHC-C1C-C2C	-2.90	119.45	125.49
2	D	801	HEM	CBD-CAD-C3D	-2.89	104.55	112.53
2	D	801	HEM	CHB-C1B-C2B	-2.82	118.94	126.95
2	B	801	HEM	C1D-C2D-C3D	-2.81	104.03	106.98
2	D	801	HEM	CHD-C4C-C3C	-2.80	120.48	125.21
2	D	801	HEM	C4A-NA-C1A	-2.78	101.29	105.82
2	C	801	HEM	C2A-C1A-NA	2.71	113.16	110.15
2	D	801	HEM	C2D-C1D-ND	2.69	113.02	109.90
2	A	801	HEM	C1D-C2D-C3D	-2.68	104.16	106.98
2	B	801	HEM	C2A-C1A-NA	2.68	113.12	110.15
2	C	801	HEM	O1A-CGA-CBA	-2.67	114.62	123.09
2	A	801	HEM	CMD-C2D-C1D	2.66	129.20	125.03
2	A	801	HEM	C4D-ND-C1D	-2.64	102.08	105.21
2	A	801	HEM	C4C-CHD-C1D	-2.63	120.43	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	C3B-C4B-NB	2.61	111.34	109.47
2	C	801	HEM	CHC-C1C-C2C	-2.57	120.14	125.49
2	C	801	HEM	CHD-C1D-C2D	-2.51	121.07	125.03
2	B	801	HEM	C1A-CHA-C4D	-2.50	120.36	126.25
2	D	801	HEM	O2D-CGD-O1D	-2.48	116.96	123.33
2	D	801	HEM	C3B-C4B-NB	2.47	111.24	109.47
2	B	801	HEM	CHA-C4D-C3D	-2.47	120.68	125.23
2	B	801	HEM	CMA-C3A-C2A	2.46	130.84	125.62
2	A	801	HEM	CAD-C3D-C2D	-2.41	123.35	127.87
2	B	801	HEM	CHB-C4A-C3A	-2.39	120.49	127.43
2	D	801	HEM	CAC-C3C-C4C	-2.38	119.13	124.82
2	B	801	HEM	CAA-C2A-C1A	2.37	129.56	124.94
2	D	801	HEM	O1A-CGA-CBA	-2.34	115.66	123.09
2	D	801	HEM	CBC-CAC-C3C	-2.34	115.84	127.53
2	D	801	HEM	C4D-ND-C1D	-2.33	102.44	105.21
2	B	801	HEM	CHB-C1B-C2B	-2.32	120.37	126.95
2	D	801	HEM	CHD-C1D-ND	2.32	126.92	124.42
2	C	801	HEM	C4C-NC-C1C	-2.30	102.07	105.82
2	C	801	HEM	CMD-C2D-C3D	2.29	132.34	126.15
2	B	801	HEM	C3A-C4A-NA	2.26	113.77	110.14
2	D	801	HEM	CHC-C4B-NB	2.26	126.85	124.42
2	A	801	HEM	CHB-C1B-NB	2.26	127.16	124.37
2	A	801	HEM	CHA-C4D-C3D	-2.14	121.28	125.23
2	B	801	HEM	C4A-NA-C1A	-2.14	102.33	105.82
2	C	801	HEM	C2C-C1C-NC	2.14	113.59	109.64
2	D	801	HEM	CAD-C3D-C2D	2.13	131.86	127.87
2	A	801	HEM	CBB-CAB-C3B	-2.13	116.87	127.53
2	D	801	HEM	CAA-C2A-C1A	2.12	129.07	124.94
2	A	801	HEM	CBC-CAC-C3C	-2.07	117.16	127.53
2	D	801	HEM	CMA-C3A-C2A	2.06	130.00	125.62
2	B	801	HEM	CAC-C3C-C4C	-2.06	119.90	124.82
2	C	801	HEM	CAA-C2A-C1A	2.03	128.91	124.94
2	C	801	HEM	C1C-CHC-C4B	-2.03	121.71	126.02
2	C	801	HEM	C3A-C4A-NA	2.02	113.38	110.14

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

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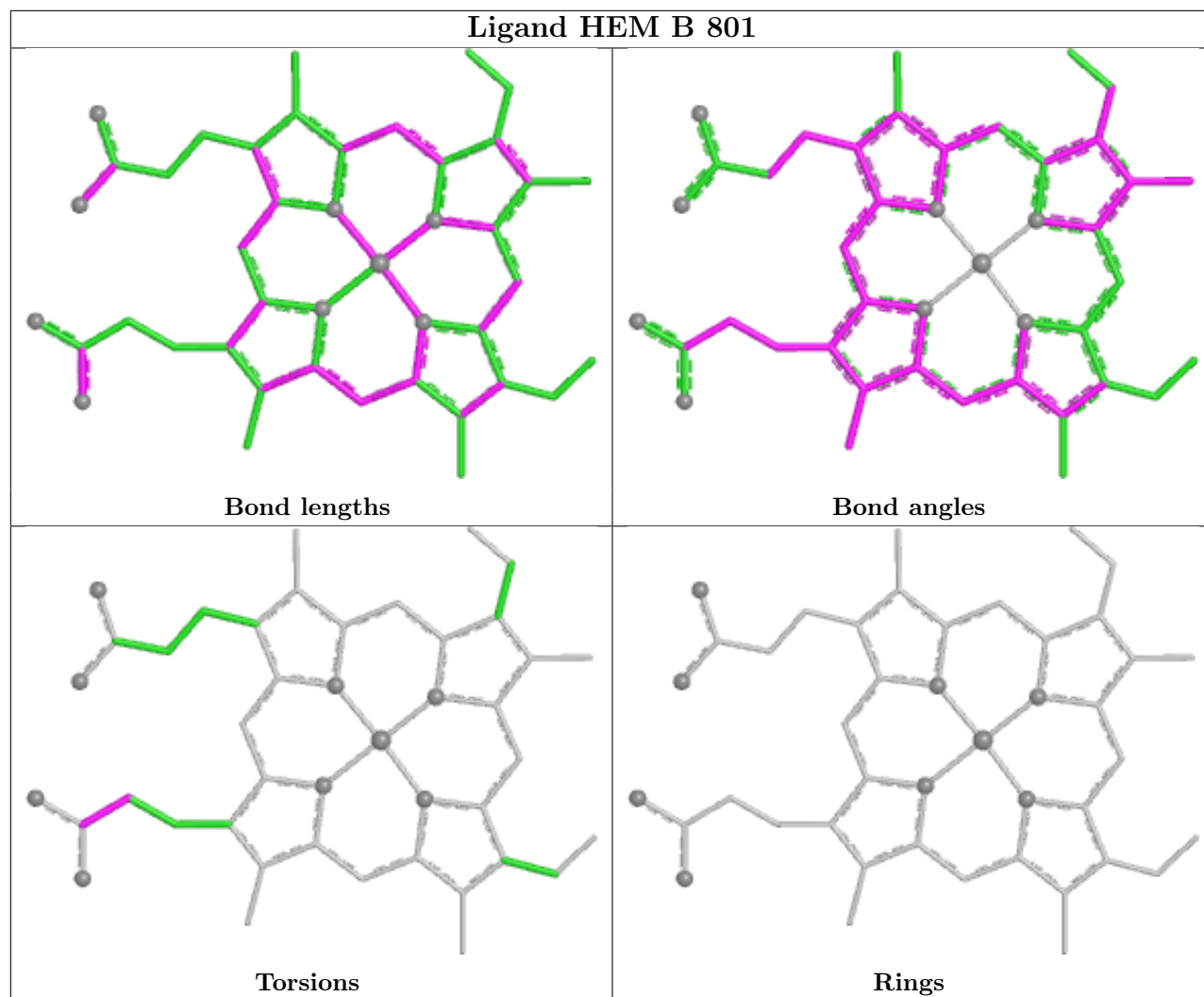
Mol	Chain	Res	Type	Atoms
2	A	801	HEM	CAA-CBA-CGA-O2A
2	C	801	HEM	CAA-CBA-CGA-O2A
2	D	801	HEM	CAA-CBA-CGA-O2A
2	D	801	HEM	CAA-CBA-CGA-O1A
2	A	801	HEM	CAA-CBA-CGA-O1A

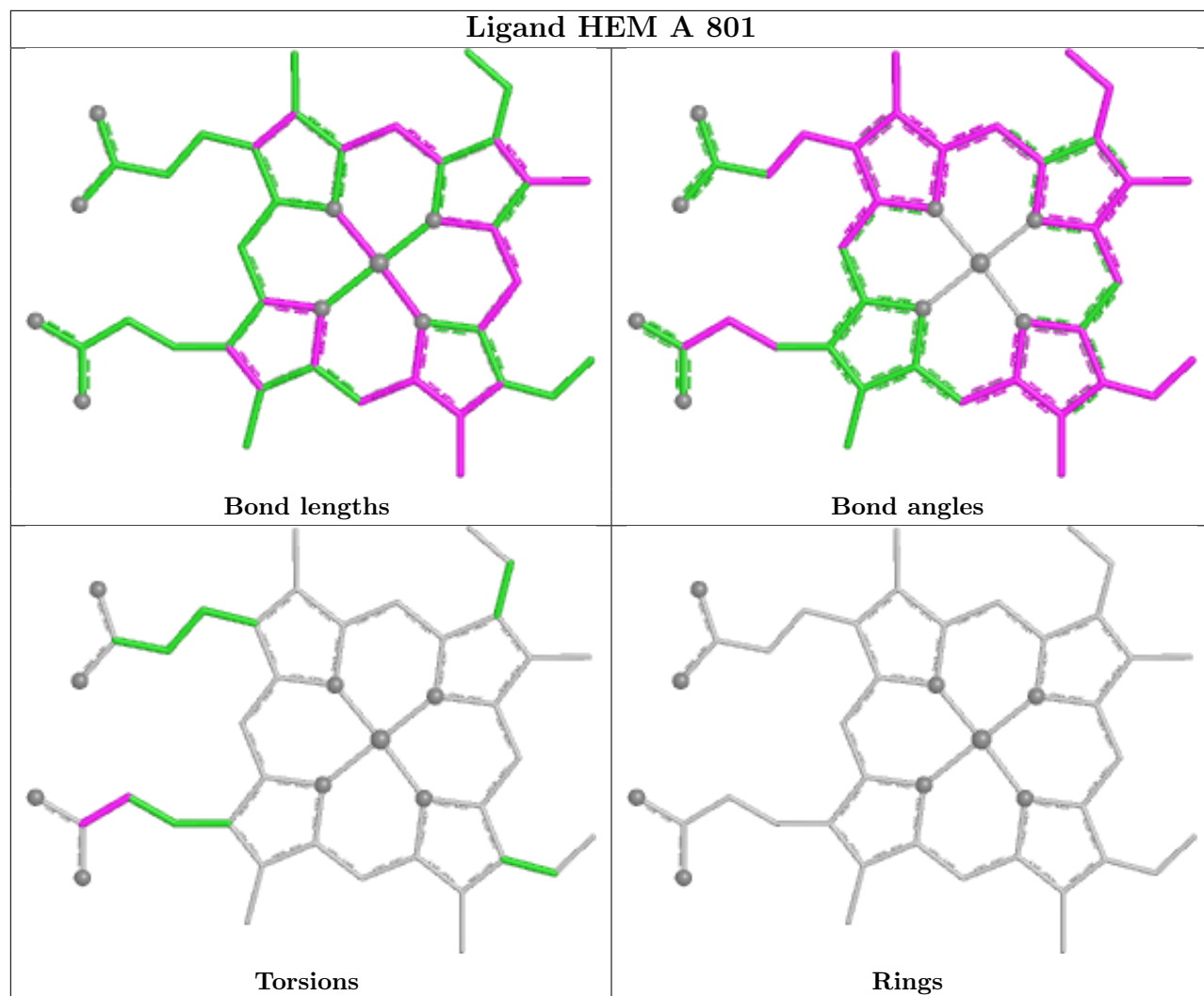
There are no ring outliers.

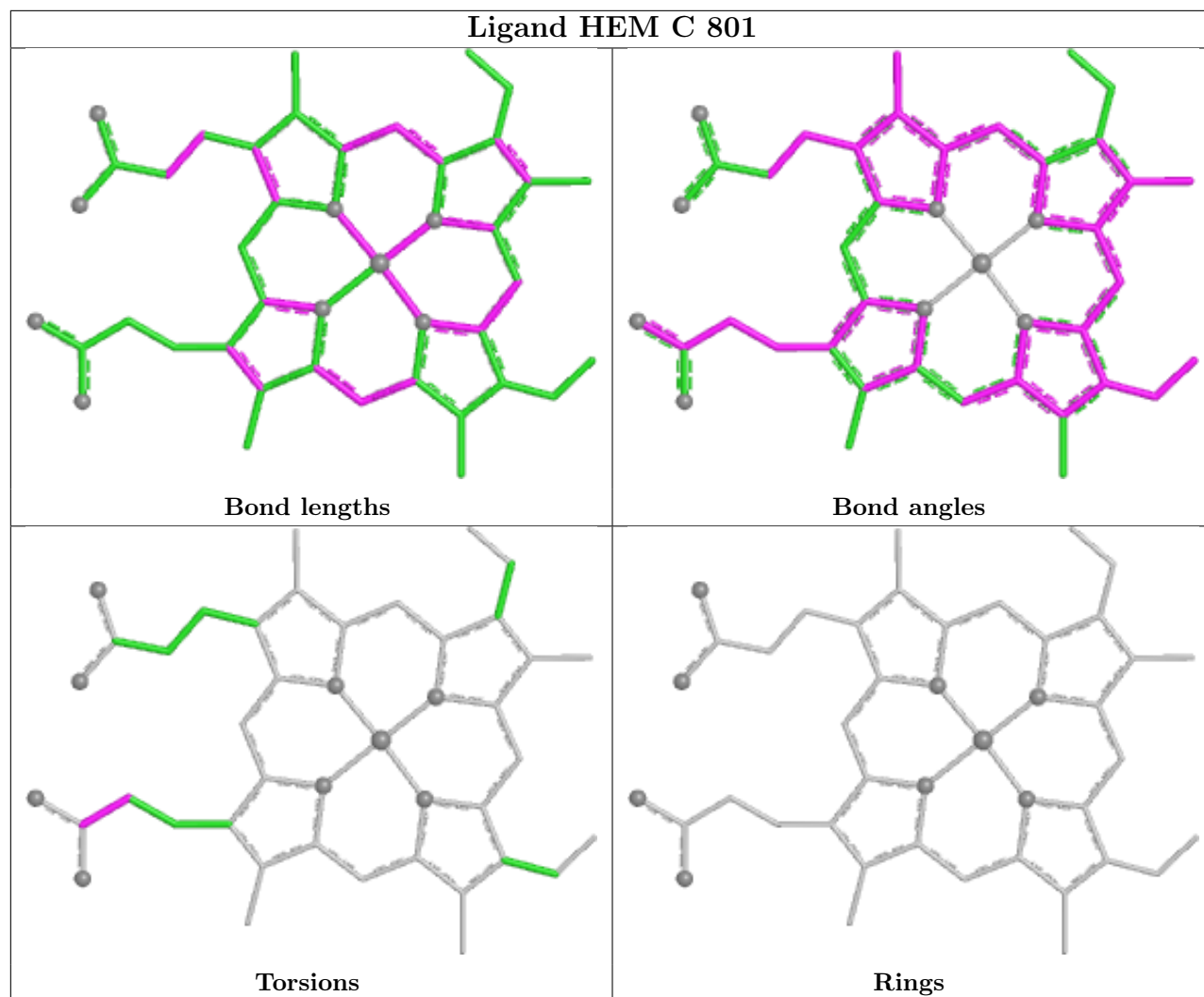
4 monomers are involved in 9 short contacts:

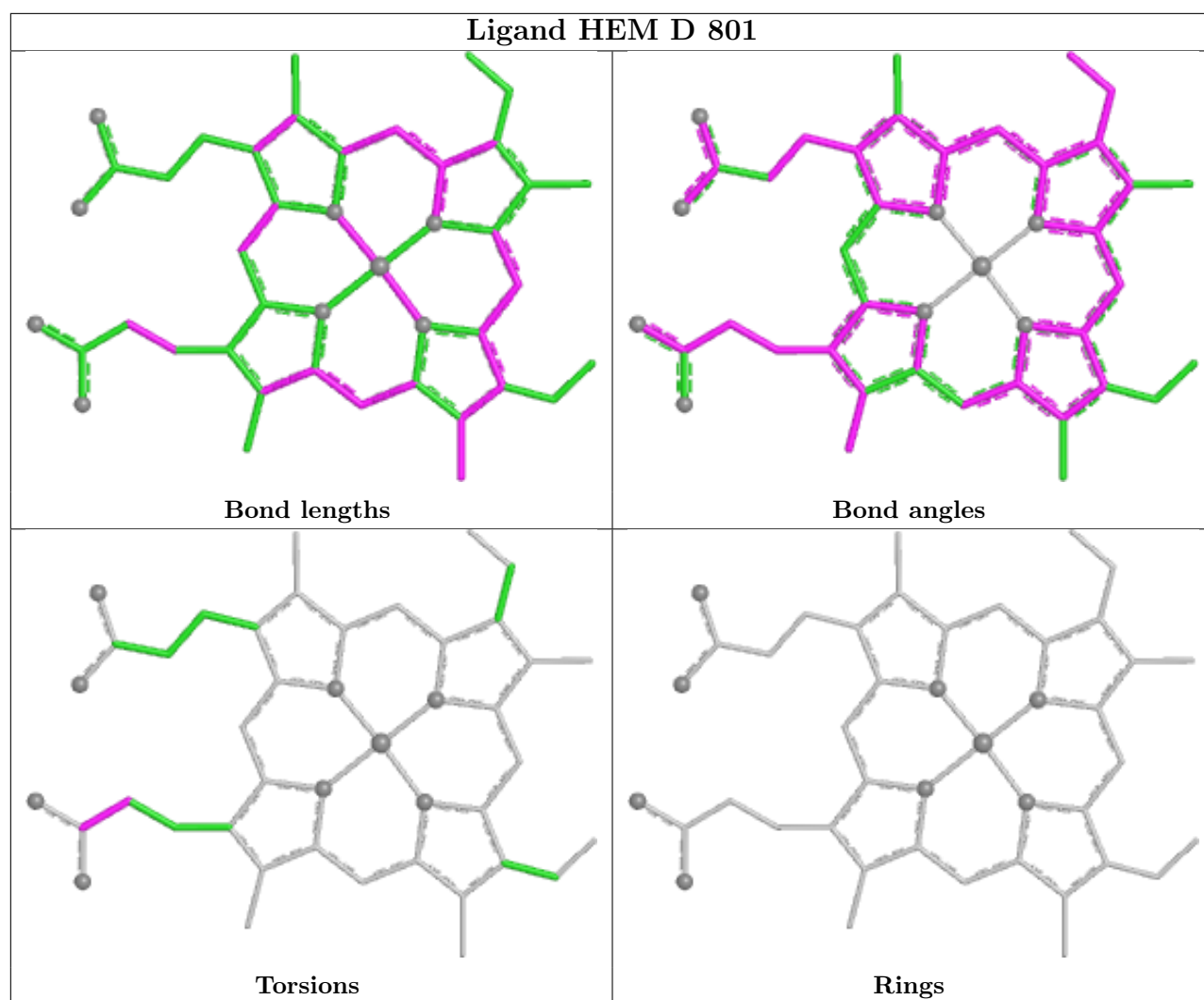
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	HEM	1	0
2	A	801	HEM	2	0
2	C	801	HEM	3	0
2	D	801	HEM	3	0

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	725/753 (96%)	-0.60	2 (0%) 90 91	4, 11, 27, 57	5 (0%)
1	B	725/753 (96%)	-0.42	10 (1%) 73 78	5, 13, 35, 68	5 (0%)
1	C	725/753 (96%)	-0.48	4 (0%) 85 88	5, 13, 36, 53	4 (0%)
1	D	725/753 (96%)	-0.56	8 (1%) 78 82	4, 11, 29, 68	5 (0%)
All	All	2900/3012 (96%)	-0.52	24 (0%) 82 86	4, 12, 33, 68	19 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	28	SER	3.4
1	D	751	ILE	3.4
1	B	749	ASP	3.2
1	B	726	GLY	3.2
1	B	725	ASP	3.2
1	B	751	ILE	3.0
1	D	749	ASP	2.9
1	C	751	ILE	2.8
1	D	750	LYS	2.7
1	B	750	LYS	2.7
1	C	725	ASP	2.6
1	C	726	GLY	2.5
1	C	750	LYS	2.5
1	B	753	ALA	2.3
1	D	583	LYS	2.2
1	B	595	ASP	2.2
1	A	726	GLY	2.2
1	B	673	ALA	2.1
1	D	711	ALA	2.1
1	B	710	ILE	2.1
1	D	753	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	34	GLY	2.1
1	B	642	ALA	2.0
1	D	595	ASP	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	OCS	B	669	9/10	0.93	0.10	25,29,34,42	0
1	OCS	C	669	9/10	0.93	0.10	26,29,36,37	0
1	OCS	A	669	9/10	0.95	0.08	17,20,28,29	0
1	OCS	D	669	9/10	0.95	0.09	17,21,24,30	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

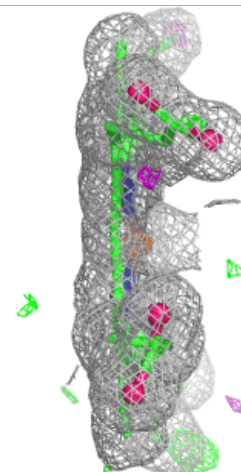
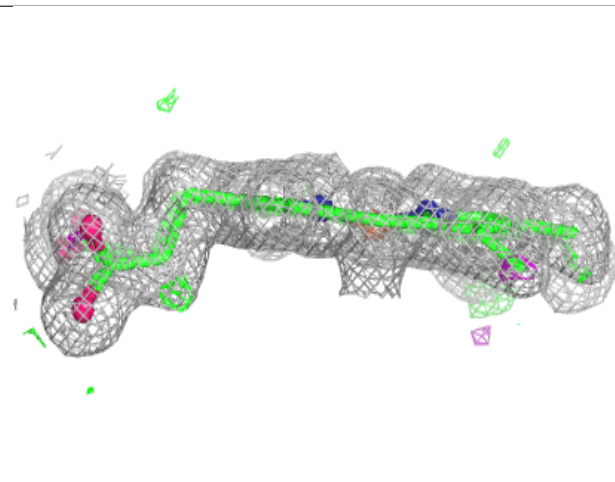
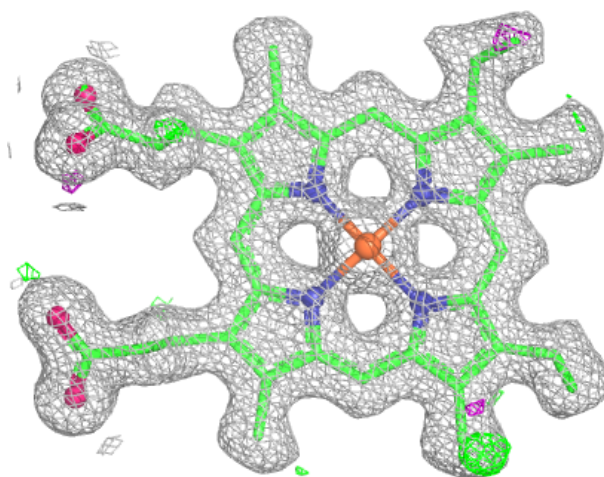
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	A	801	43/43	0.99	0.04	5,6,8,11	0
2	HEM	B	801	43/43	0.99	0.04	6,7,9,12	0
2	HEM	C	801	43/43	0.99	0.04	5,6,9,11	0
2	HEM	D	801	43/43	0.99	0.04	5,6,8,10	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.

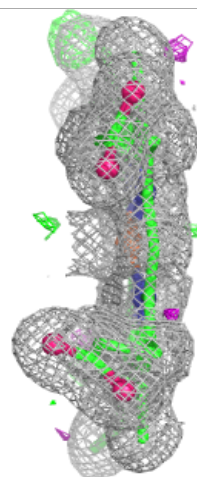
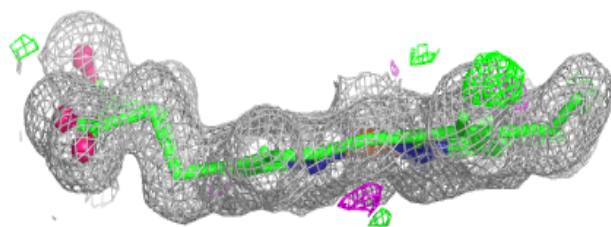
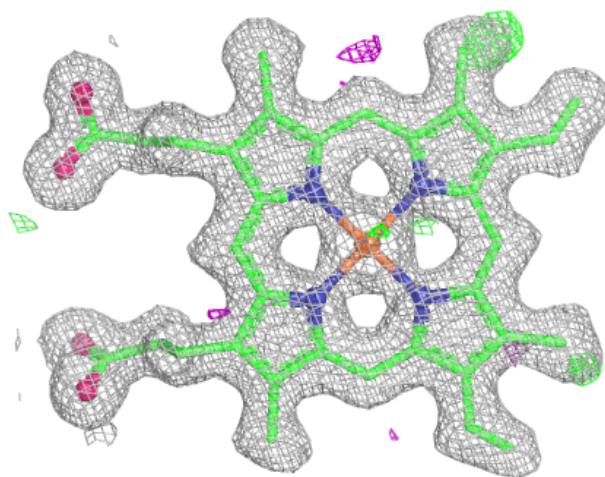
Electron density around HEM A 801:

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



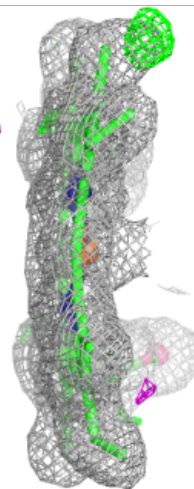
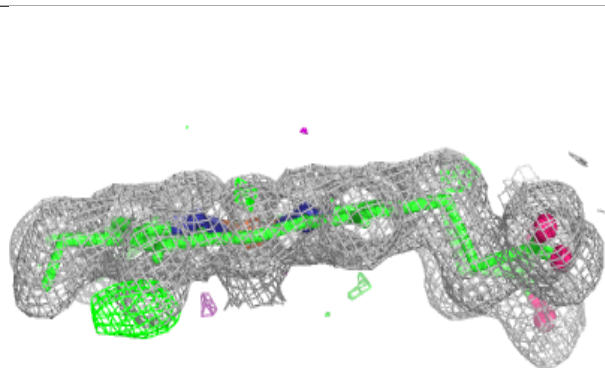
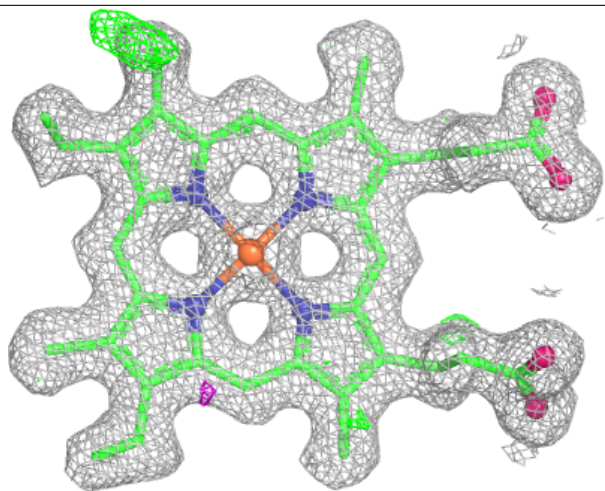
Electron density around HEM B 801:

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



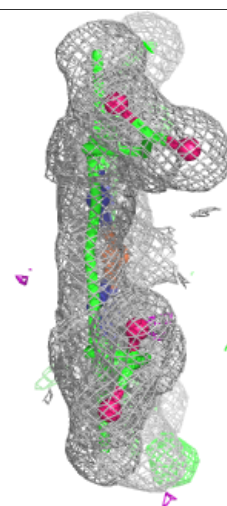
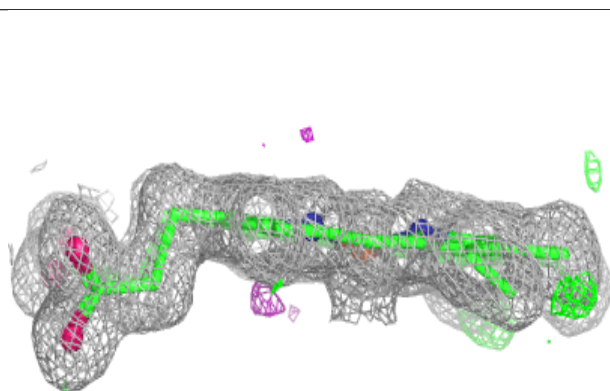
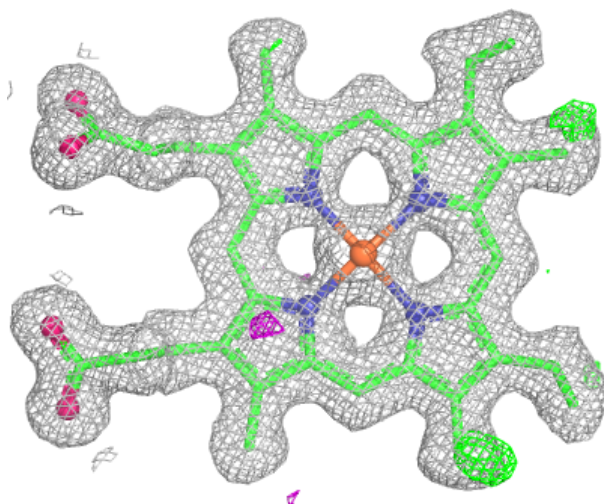
Electron density around HEM C 801:

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



Electron density around HEM D 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.