



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2020 – 09:12 AM BST

PDB ID : 4ENP
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

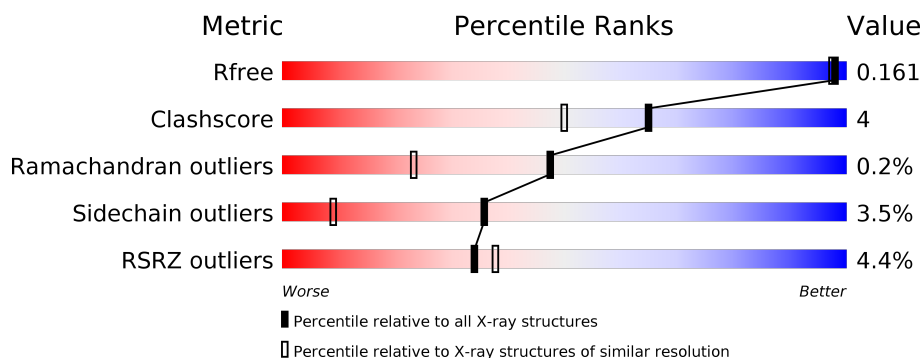
1 Overall quality at a glance

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}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (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 on 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	<div> <div>3%</div> <div> <div></div> <div>83%</div> <div>12%</div> <div>• •</div> </div> </div>
1	B	753	<div> <div>7%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>• •</div> </div> </div>
1	C	753	<div> <div>5%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>• •</div> </div> </div>
1	D	753	<div> <div>2%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>• •</div> </div> </div>

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.

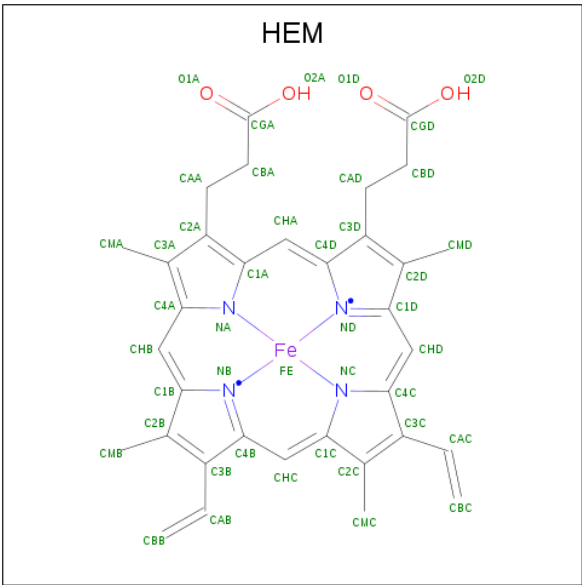
- Molecule 1 is a protein called Catalase HPIL.

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 (three-letter code: 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

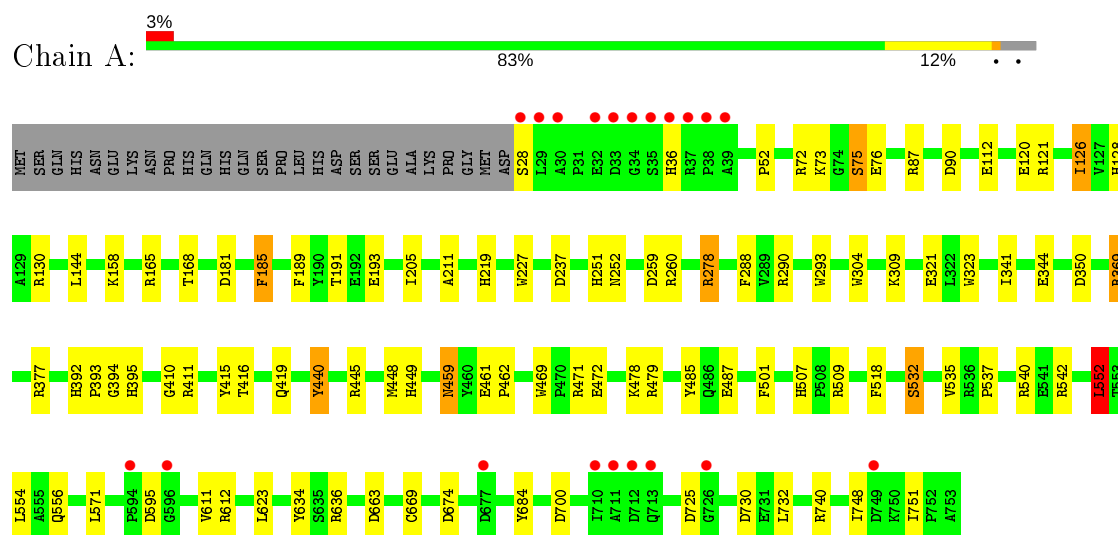
- Molecule 3 is water.

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

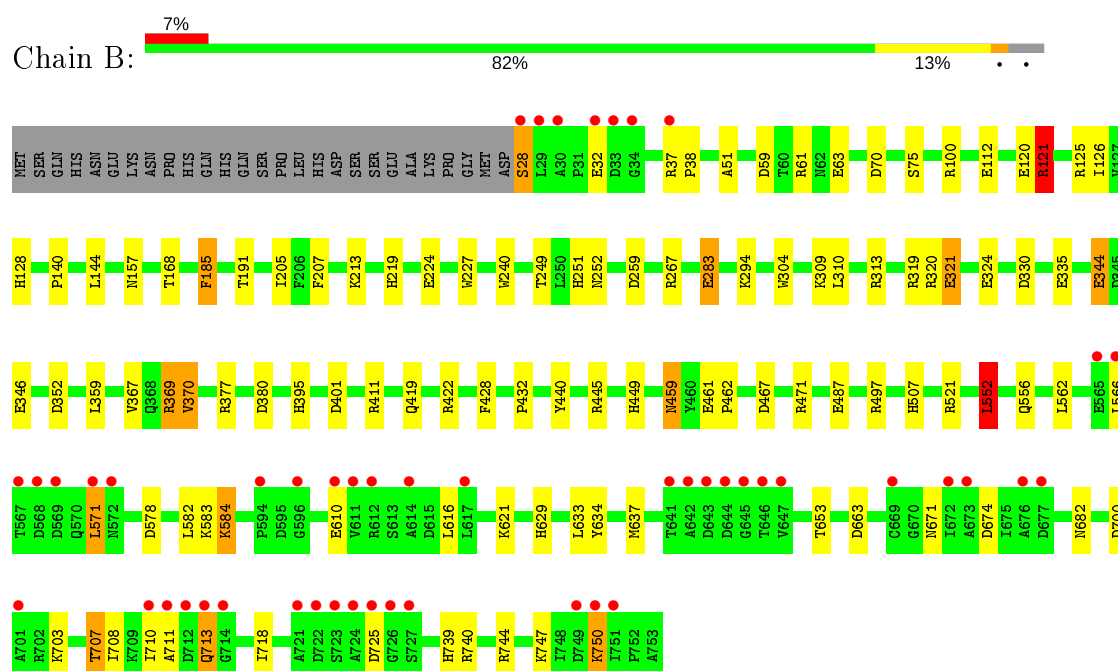
3 Residue-property plots [i](#)

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.

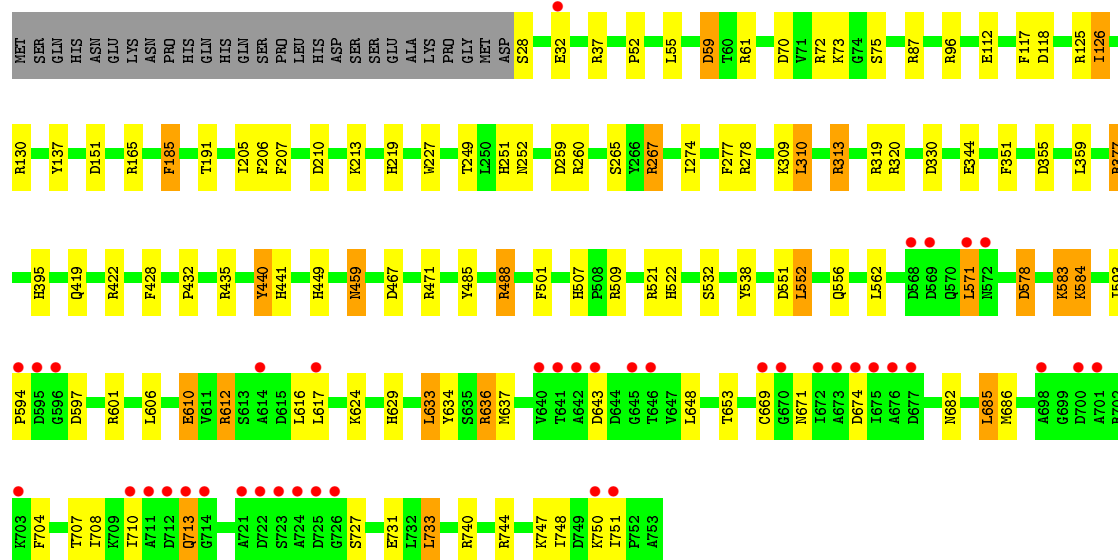
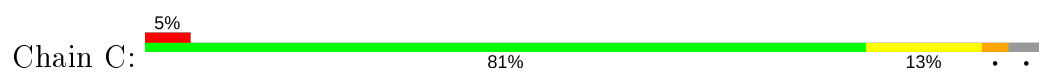
• Molecule 1: Catalase HP11



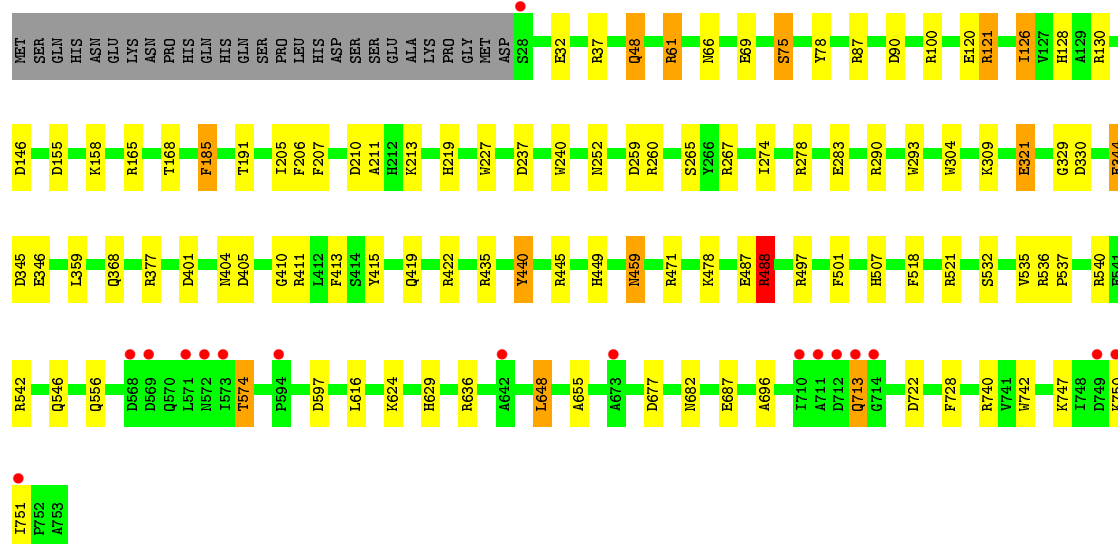
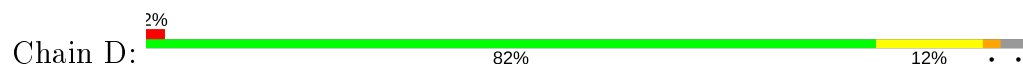
• Molecule 1: Catalase HP11



• 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 0.136 , 0.161	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)	0.34 , 45.9	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	1.34	25/6023 (0.4%)	1.37	52/8188 (0.6%)
1	B	1.27	14/5972 (0.2%)	1.25	34/8119 (0.4%)
1	C	1.30	13/5984 (0.2%)	1.36	62/8134 (0.8%)
1	D	1.35	29/5976 (0.5%)	1.35	55/8123 (0.7%)
All	All	1.31	81/23955 (0.3%)	1.33	203/32564 (0.6%)

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

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

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	377	ARG	CZ-NH1	9.10	1.44	1.33
1	C	59	ASP	CB-CG	8.98	1.70	1.51
1	C	265	SER	CB-OG	-8.40	1.31	1.42
1	A	440	TYR	CE1-CZ	8.24	1.49	1.38
1	A	344	GLU	CD-OE2	7.78	1.34	1.25
1	A	344	GLU	CD-OE1	7.55	1.33	1.25
1	C	419	GLN	CD-NE2	7.50	1.51	1.32
1	B	344	GLU	CD-OE2	7.34	1.33	1.25
1	D	419	GLN	CD-OE1	7.32	1.40	1.24
1	C	59	ASP	CG-OD1	7.29	1.42	1.25
1	B	419	GLN	CD-NE2	7.27	1.51	1.32
1	D	293	TRP	CD2-CE2	7.26	1.50	1.41
1	D	440	TYR	CE1-CZ	7.23	1.48	1.38
1	D	69	GLU	CD-OE2	-7.05	1.17	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	377	ARG	CZ-NH1	7.02	1.42	1.33
1	A	532[A]	SER	CB-OG	6.80	1.51	1.42
1	A	532[B]	SER	CB-OG	6.80	1.51	1.42
1	A	419	GLN	CD-OE1	6.76	1.38	1.24
1	D	329	GLY	C-O	6.70	1.34	1.23
1	D	532[A]	SER	CB-OG	6.52	1.50	1.42
1	D	532[B]	SER	CB-OG	6.52	1.50	1.42
1	D	321	GLU	CD-OE1	6.49	1.32	1.25
1	C	344	GLU	CD-OE1	6.46	1.32	1.25
1	A	304	TRP	CD2-CE2	6.43	1.49	1.41
1	A	321	GLU	CD-OE1	6.26	1.32	1.25
1	D	265	SER	CA-CB	6.24	1.62	1.52
1	D	265	SER	CB-OG	-6.21	1.34	1.42
1	B	37	ARG	CZ-NH2	6.10	1.41	1.33
1	A	350	ASP	CB-CG	-6.02	1.39	1.51
1	D	344	GLU	CD-OE2	6.00	1.32	1.25
1	A	472	GLU	CD-OE2	5.97	1.32	1.25
1	B	304	TRP	CD2-CE2	5.97	1.48	1.41
1	D	445	ARG	CZ-NH2	5.94	1.40	1.33
1	A	419	GLN	CD-NE2	5.92	1.47	1.32
1	D	487	GLU	CD-OE2	-5.90	1.19	1.25
1	A	288	PHE	CG-CD2	5.89	1.47	1.38
1	C	419	GLN	CD-OE1	5.80	1.36	1.24
1	D	435	ARG	NE-CZ	5.79	1.40	1.33
1	C	419	GLN	CG-CD	5.76	1.64	1.51
1	D	75	SER	CB-OG	5.74	1.49	1.42
1	A	469	TRP	CD2-CE2	5.71	1.48	1.41
1	D	419	GLN	CD-NE2	5.62	1.46	1.32
1	D	240	TRP	CD2-CE2	5.58	1.48	1.41
1	D	290	ARG	CZ-NH2	5.58	1.40	1.33
1	B	739	HIS	CG-CD2	5.55	1.45	1.35
1	D	304	TRP	CD2-CE2	5.53	1.48	1.41
1	B	370	VAL	CA-CB	5.51	1.66	1.54
1	D	419	GLN	CA-CB	5.50	1.66	1.53
1	B	63	GLU	CD-OE2	5.50	1.31	1.25
1	C	351	PHE	CG-CD2	5.50	1.47	1.38
1	B	224	GLU	CD-OE1	5.50	1.31	1.25
1	A	323	TRP	CD2-CE2	5.49	1.48	1.41
1	A	290	ARG	CZ-NH2	5.48	1.40	1.33
1	B	521	ARG	CZ-NH1	5.47	1.40	1.33
1	D	368[A]	GLN	CD-NE2	-5.45	1.19	1.32
1	D	368[B]	GLN	CD-NE2	-5.45	1.19	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	419	GLN	CG-CD	5.43	1.63	1.51
1	C	320	ARG	CZ-NH2	5.43	1.40	1.33
1	A	193	GLU	CD-OE1	5.41	1.31	1.25
1	A	419	GLN	CG-CD	5.41	1.63	1.51
1	D	682	ASN	N-CA	-5.38	1.35	1.46
1	D	413	PHE	CG-CD1	5.38	1.46	1.38
1	C	344	GLU	CD-OE2	5.34	1.31	1.25
1	A	75	SER	CA-CB	5.33	1.60	1.52
1	C	522	HIS	CG-CD2	5.28	1.44	1.35
1	B	346	GLU	CD-OE1	5.27	1.31	1.25
1	B	497	ARG	CZ-NH2	5.23	1.39	1.33
1	C	206	PHE	CG-CD1	5.20	1.46	1.38
1	A	445	ARG	CZ-NH2	5.19	1.39	1.33
1	C	278	ARG	CZ-NH2	5.14	1.39	1.33
1	D	742	TRP	CD2-CE2	5.13	1.47	1.41
1	A	540	ARG	CZ-NH1	5.12	1.39	1.33
1	A	293	TRP	CD2-CE2	5.12	1.47	1.41
1	A	377	ARG	CZ-NH2	5.11	1.39	1.33
1	A	623	LEU	C-O	5.11	1.33	1.23
1	D	240	TRP	CG-CD1	5.09	1.43	1.36
1	A	87	ARG	CZ-NH1	-5.07	1.26	1.33
1	D	206	PHE	CG-CD2	5.06	1.46	1.38
1	D	655	ALA	C-O	5.03	1.32	1.23
1	B	157	ASN	CB-CG	5.01	1.62	1.51
1	B	240	TRP	CD2-CE2	5.01	1.47	1.41

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	ARG	NE-CZ-NH2	-18.45	111.08	120.30
1	C	37	ARG	NE-CZ-NH2	-16.93	111.83	120.30
1	D	278	ARG	NE-CZ-NH1	-13.06	113.77	120.30
1	A	740	ARG	NE-CZ-NH2	-11.90	114.35	120.30
1	C	59	ASP	CB-CG-OD1	11.59	128.73	118.30
1	D	278	ARG	NE-CZ-NH2	11.28	125.94	120.30
1	C	278	ARG	NE-CZ-NH1	-10.97	114.82	120.30
1	D	87	ARG	NE-CZ-NH2	-10.91	114.84	120.30
1	A	552[A]	LEU	CB-CG-CD1	10.84	129.42	111.00
1	A	552[B]	LEU	CB-CG-CD1	10.84	129.42	111.00
1	D	61	ARG	NE-CZ-NH2	9.98	125.29	120.30
1	C	125	ARG	NE-CZ-NH1	9.93	125.27	120.30
1	C	125	ARG	NE-CZ-NH2	-9.89	115.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	59	ASP	CB-CG-OD2	-9.51	109.74	118.30
1	C	37	ARG	NE-CZ-NH1	9.47	125.04	120.30
1	C	578[A]	ASP	CB-CG-OD1	9.28	126.65	118.30
1	C	578[B]	ASP	CB-CG-OD1	9.28	126.65	118.30
1	D	377	ARG	NE-CZ-NH2	-9.24	115.68	120.30
1	A	636	ARG	NE-CZ-NH2	9.20	124.90	120.30
1	D	401	ASP	CB-CG-OD2	9.11	126.50	118.30
1	D	422	ARG	NE-CZ-NH2	-8.94	115.83	120.30
1	C	440	TYR	CB-CG-CD2	-8.87	115.68	121.00
1	D	488[A]	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	D	488[B]	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	B	70	ASP	CB-CG-OD1	8.76	126.19	118.30
1	A	290	ARG	NE-CZ-NH2	-8.68	115.96	120.30
1	A	130	ARG	NE-CZ-NH1	8.63	124.61	120.30
1	B	377	ARG	NE-CZ-NH1	-8.59	116.01	120.30
1	C	165	ARG	NE-CZ-NH2	-8.51	116.04	120.30
1	C	740	ARG	NE-CZ-NH2	-8.47	116.07	120.30
1	D	636	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	C	130	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	C	471	ARG	NE-CZ-NH2	-8.12	116.24	120.30
1	C	96	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	D	542	ARG	NE-CZ-NH1	8.06	124.33	120.30
1	A	260	ARG	NE-CZ-NH1	8.05	124.32	120.30
1	A	471	ARG	NE-CZ-NH1	-7.99	116.31	120.30
1	A	445	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	C	509	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	C	185	PHE	CB-CG-CD2	-7.92	115.25	120.80
1	A	130	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	542	ARG	NE-CZ-NH1	7.79	124.19	120.30
1	C	87	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	B	401	ASP	CB-CG-OD2	7.69	125.22	118.30
1	A	509	ARG	NE-CZ-NH1	7.66	124.13	120.30
1	D	210	ASP	CB-CG-OD2	7.51	125.06	118.30
1	C	278	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	A	278	ARG	NE-CZ-NH2	7.50	124.05	120.30
1	B	100	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	C	267	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	A	350	ASP	CB-CG-OD2	-7.32	111.71	118.30
1	B	467	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	B	445	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	C	422	ARG	NE-CZ-NH1	-7.19	116.70	120.30
1	C	126[A]	ILE	CB-CG1-CD1	-7.11	93.98	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	126[B]	ILE	CB-CG1-CD1	-7.11	93.98	113.90
1	A	87	ARG	NE-CZ-NH1	-7.09	116.75	120.30
1	C	636	ARG	NE-CZ-NH1	7.09	123.84	120.30
1	A	684	TYR	CB-CG-CD1	6.96	125.17	121.00
1	D	207	PHE	CB-CG-CD1	-6.94	115.94	120.80
1	C	319	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	B	125	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	A	501	PHE	CB-CG-CD1	6.88	125.62	120.80
1	D	687	GLU	OE1-CD-OE2	-6.88	115.05	123.30
1	B	744	ARG	NE-CZ-NH2	6.86	123.73	120.30
1	C	419	GLN	CB-CA-C	6.86	124.12	110.40
1	D	185	PHE	CB-CG-CD2	-6.86	116.00	120.80
1	C	440	TYR	CB-CG-CD1	6.84	125.10	121.00
1	A	377	ARG	NH1-CZ-NH2	6.81	126.89	119.40
1	D	419	GLN	CB-CA-C	6.79	123.98	110.40
1	B	740	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	A	740	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	C	685	LEU	CB-CG-CD1	6.71	122.41	111.00
1	A	445	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	C	551	ASP	CB-CG-OD2	-6.69	112.28	118.30
1	D	146	ASP	CB-CG-OD2	6.64	124.28	118.30
1	A	663	ASP	CB-CG-OD1	6.61	124.25	118.30
1	C	55	LEU	CB-CG-CD2	6.61	122.23	111.00
1	A	72	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	C	70	ASP	CB-CG-OD1	-6.59	112.37	118.30
1	B	422	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	B	663	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	B	121	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	C	633	LEU	CB-CG-CD1	6.54	122.12	111.00
1	D	121	ARG	NE-CZ-NH2	-6.49	117.05	120.30
1	D	740	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	D	435	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	D	61	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	B	125	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	259	ASP	CB-CG-OD1	-6.38	112.56	118.30
1	A	185	PHE	CB-CG-CD2	-6.32	116.38	120.80
1	B	185	PHE	CB-CG-CD2	-6.31	116.38	120.80
1	D	260	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	730	ASP	CB-CG-OD1	6.27	123.94	118.30
1	B	37	ARG	NE-CZ-NH2	6.27	123.43	120.30
1	D	78	TYR	CB-CG-CD2	-6.25	117.25	121.00
1	A	611	VAL	CG1-CB-CG2	-6.24	100.91	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	213	LYS	CD-CE-NZ	-6.24	97.34	111.70
1	B	100	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	C	733	LEU	CB-CG-CD2	6.23	121.59	111.00
1	D	536	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	D	501	PHE	CB-CG-CD2	-6.19	116.47	120.80
1	A	700	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	C	70	ASP	CB-CG-OD2	6.08	123.77	118.30
1	C	313	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	C	538	TYR	CB-CG-CD1	-6.07	117.36	121.00
1	A	501	PHE	CB-CG-CD2	-6.04	116.57	120.80
1	D	90	ASP	CB-CG-OD2	6.01	123.71	118.30
1	C	37	ARG	CB-CG-CD	-6.00	95.99	111.60
1	C	351	PHE	CB-CG-CD1	5.98	124.98	120.80
1	C	72	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	C	259	ASP	CB-CG-OD1	-5.94	112.96	118.30
1	D	126[A]	ILE	CB-CG1-CD1	-5.94	97.28	113.90
1	D	126[B]	ILE	CB-CG1-CD1	-5.94	97.28	113.90
1	C	636	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	C	501	PHE	CB-CG-CD2	-5.92	116.66	120.80
1	B	259	ASP	CB-CG-OD2	5.92	123.63	118.30
1	C	467	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	D	344	GLU	CG-CD-OE1	-5.91	106.47	118.30
1	B	377	ARG	CG-CD-NE	-5.91	99.40	111.80
1	D	121	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	D	346	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	A	259	ASP	CB-CG-OD2	5.89	123.60	118.30
1	D	345	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	A	674	ASP	CB-CG-OD2	5.86	123.58	118.30
1	A	411	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	A	485	TYR	CZ-CE2-CD2	-5.86	114.53	119.80
1	D	648	LEU	CB-CG-CD2	5.84	120.93	111.00
1	A	112	GLU	OE1-CD-OE2	5.83	130.29	123.30
1	B	112	GLU	OE1-CD-OE2	5.82	130.28	123.30
1	C	521	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	A	90	ASP	CB-CG-OD2	5.80	123.52	118.30
1	C	310	LEU	CB-CG-CD1	5.75	120.78	111.00
1	C	118	ASP	CB-CG-OD1	-5.74	113.14	118.30
1	D	722	ASP	CB-CG-OD1	5.72	123.44	118.30
1	C	377	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	C	260	ARG	NE-CZ-NH1	5.69	123.15	120.30
1	D	521	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	A	595	ASP	CB-CG-OD2	5.64	123.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	377	ARG	CG-CD-NE	-5.63	99.98	111.80
1	B	324	GLU	OE1-CD-OE2	5.61	130.03	123.30
1	D	344	GLU	CA-CB-CG	5.55	125.61	113.40
1	A	369[A]	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	369[B]	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	D	540	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	552	LEU	CA-CB-CG	5.51	127.96	115.30
1	B	380	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	144	LEU	CB-CG-CD1	-5.50	101.65	111.00
1	D	165	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	B	352	ASP	CB-CG-OD2	5.48	123.24	118.30
1	B	313	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	D	155	ASP	CB-CG-OD1	-5.44	113.41	118.30
1	B	313	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	B	320	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	C	435	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	B	37	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	C	428	PHE	CB-CG-CD2	-5.41	117.01	120.80
1	C	87	ARG	NH1-CZ-NH2	5.41	125.35	119.40
1	B	344	GLU	CG-CD-OE1	-5.38	107.55	118.30
1	C	259	ASP	CB-CG-OD2	5.37	123.14	118.30
1	C	485	TYR	CD1-CE1-CZ	-5.37	114.97	119.80
1	C	112	GLU	OE1-CD-OE2	5.35	129.72	123.30
1	D	100	ARG	NE-CZ-NH2	5.33	122.97	120.30
1	D	497	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	518	PHE	CB-CG-CD1	-5.31	117.08	120.80
1	C	37	ARG	CG-CD-NE	-5.30	100.66	111.80
1	C	355	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	277	PHE	CG-CD1-CE1	-5.28	114.99	120.80
1	B	310	LEU	CB-CG-CD1	5.27	119.97	111.00
1	B	419	GLN	CB-CA-C	5.26	120.92	110.40
1	D	415	TYR	CB-CG-CD2	5.25	124.15	121.00
1	D	518	PHE	CG-CD2-CE2	-5.25	115.03	120.80
1	A	321	GLU	CG-CD-OE2	-5.25	107.80	118.30
1	A	634	TYR	CB-CG-CD2	-5.25	117.85	121.00
1	A	189	PHE	CB-CG-CD2	-5.25	117.13	120.80
1	C	485	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	D	259	ASP	CB-CG-OD2	5.24	123.01	118.30
1	D	401	ASP	CB-CG-OD1	-5.23	113.59	118.30
1	A	518	PHE	CG-CD2-CE2	-5.23	115.05	120.80
1	C	137	TYR	CB-CG-CD1	-5.22	117.87	121.00
1	D	146	ASP	CB-CG-OD1	-5.22	113.60	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	130	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	D	440	TYR	CZ-CE2-CD2	-5.21	115.11	119.80
1	A	419	GLN	CB-CA-C	5.19	120.77	110.40
1	A	684	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	B	319	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	D	471	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	D	37	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	165	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	A	126[A]	ILE	CB-CG1-CD1	-5.10	99.61	113.90
1	A	126[B]	ILE	CB-CG1-CD1	-5.10	99.61	113.90
1	A	674	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	C	151	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	485	TYR	CB-CG-CD1	-5.09	117.95	121.00
1	A	181	ASP	CB-CG-OD2	5.08	122.87	118.30
1	C	601	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	B	377	ARG	NH1-CZ-NH2	5.06	124.96	119.40
1	D	377	ARG	NH1-CZ-NH2	5.05	124.96	119.40
1	B	471	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	A	554	LEU	CB-CG-CD2	-5.04	102.42	111.00
1	C	210	ASP	CB-CG-OD2	5.04	122.84	118.30
1	D	411	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	D	78	TYR	CZ-CE2-CD2	-5.02	115.28	119.80

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	46	0
1	B	5789	0	5618	62	0
1	C	5796	0	5631	59	0
1	D	5789	0	5632	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	43	0	30	0	0
2	B	43	0	30	2	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	14	0
3	C	808	0	0	24	0
3	D	886	0	0	18	0
All	All	26715	0	22672	187	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 (187) 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: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:369:ARG:CZ	1:B:369:ARG:HB3	1.96	0.87
1:B:487:GLU:CD	3:B:1647:HOH:O	2.17	0.83
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
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:597:ASP:OD2	3:C:1412:HOH:O	2.07	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:583:LYS:C	3:C:1673:HOH:O	2.32	0.66
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:CG	1:A:369[A]:ARG:HH21	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:B:610:GLU:O	1:B:610:GLU:HG3	1.99	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: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: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:583:LYS:O	1:C:584:LYS:HB3	2.05	0.57
1:C:73:LYS:HD2	3:C:1519:HOH:O	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:C:449[B]:HIS:ND1	3:C:1704:HOH:O	0.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:278:ARG:HH12	1:A:487[A]:GLU:CD	2.10	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
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: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:478:LYS:NZ	3:D:1001:HOH:O	2.35	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:B:126[B]:ILE:HD12	1:C:117:PHE:CZ	2.48	0.48
1:D:158:LYS:HB3	3:D:1761:HOH:O	2.13	0.48
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:B:700:ASP:O	1:B:703:LYS:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:211:ALA:CB	1:A:410:GLY:HA3	2.47	0.45
1:A:76:GLU:OE1	3:A:1708:HOH:O	2.21	0.45
1:B:120:GLU:HB2	1:C:126[A]:ILE:HD11	1.97	0.45
1:D:574:THR:HG23	3:D:1303:HOH:O	2.17	0.45
1:D:309:LYS:CE	3:D:1732:HOH:O	2.61	0.45
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.46	0.45
1:C:449[B]:HIS:CE1	3:C:1704:HOH:O	1.65	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:D:48:GLN:HB3	1:D:48:GLN:HE21	1.68	0.44
1:A:73[A]:LYS:HD3	1:C:441:HIS:CD2	2.52	0.44
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:C:578[B]:ASP:CG	1:C:583:LYS:HG3	2.39	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:448:MET:O	1:A:449[A]:HIS:HB2	2.19	0.43
1:A:251:HIS:CE1	1:A:507:HIS:HB3	2.53	0.43
1:D:404:ASN:O	1:D:405:ASP:C	2.56	0.43
1:B:449[B]:HIS:CD2	1:D:449[B]:HIS:CD2	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:459:ASN:HD22	1:D:459:ASN:H	1.68	0.42
1:D:61:ARG:HH11	1:D:66:ASN:HA	1.83	0.42
1:A:52:PRO:HG3	3:C:1138:HOH:O	2.19	0.42
1:A:461:GLU:HA	1:A:462:PRO:C	2.40	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:H	1:B:713:GLN:NE2	2.18	0.42
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: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
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:B:461:GLU:HA	1:B:462:PRO:C	2.40	0.41
1:C:593:ILE:HA	1:C:594:PRO:HD3	1.94	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:HG3	1:C:713:GLN:H	1.69	0.40
1:A:121:ARG:CZ	1:D:126[B]:ILE:HG12	2.52	0.40
1:B:359:LEU:HD12	1:B:359:LEU:C	2.41	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%)	41	18
1	B	735/753 (98%)	712 (97%)	21 (3%)	2 (0%)	41	18
1	C	736/753 (98%)	718 (98%)	17 (2%)	1 (0%)	51	25
1	D	735/753 (98%)	717 (98%)	17 (2%)	1 (0%)	51	25
All	All	2947/3012 (98%)	2870 (97%)	71 (2%)	6 (0%)	47	23

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
1	D	75	SER
1	B	75	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	627/635 (99%)	616 (98%)	11 (2%)	59	30
1	B	621/635 (98%)	596 (96%)	25 (4%)	31	6
1	C	622/635 (98%)	591 (95%)	31 (5%)	24	4
1	D	621/635 (98%)	598 (96%)	23 (4%)	34	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2491/2540 (98%)	2401 (96%)	90 (4%)	36 8

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	185	PHE
1	A	191	THR
1	A	205	ILE
1	A	227	TRP
1	A	237	ASP
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	140	PRO
1	B	185	PHE
1	B	191	THR
1	B	205	ILE
1	B	213	LYS
1	B	227	TRP
1	B	252	ASN
1	B	283	GLU
1	B	321	GLU
1	B	344	GLU
1	B	369	ARG
1	B	432	PRO
1	B	440	TYR
1	B	459	ASN
1	B	552	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

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Mol	Chain	Res	Type
1	C	61	ARG
1	C	185	PHE
1	C	191	THR
1	C	205	ILE
1	C	213	LYS
1	C	227	TRP
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	633	LEU
1	C	636	ARG
1	C	648	LEU
1	C	685	LEU
1	C	713	GLN
1	C	733	LEU
1	C	750	LYS
1	D	32	GLU
1	D	48	GLN
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	227	TRP
1	D	237	ASP
1	D	252	ASN
1	D	344	GLU
1	D	440	TYR
1	D	459	ASN
1	D	488[A]	ARG

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Mol	Chain	Res	Type
1	D	488[B]	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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	A	556	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	507	HIS
1	C	572	ASN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	252	ASN
1	D	459	ASN
1	D	507	HIS
1	D	556	GLN
1	D	629	HIS
1	D	671	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	D	801	1	27,50,50	1.29	4 (14%)	17,82,82	2.49	8 (47%)
2	HEM	A	801	1	27,50,50	1.26	1 (3%)	17,82,82	2.21	5 (29%)
2	HEM	C	801	1	27,50,50	1.31	3 (11%)	17,82,82	2.91	7 (41%)
2	HEM	B	801	1	27,50,50	1.47	3 (11%)	17,82,82	2.31	6 (35%)

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	D	801	1	-	0/6/54/54	-
2	HEM	A	801	1	-	0/6/54/54	-
2	HEM	C	801	1	-	0/6/54/54	-
2	HEM	B	801	1	-	0/6/54/54	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C1A-NA	4.26	1.44	1.36
2	B	801	HEM	CAA-C2A	-3.16	1.47	1.52
2	C	801	HEM	C1A-NA	3.14	1.42	1.36
2	A	801	HEM	C4B-NB	3.10	1.42	1.36
2	B	801	HEM	C4A-NA	3.00	1.42	1.36
2	D	801	HEM	CAA-C2A	-2.76	1.48	1.52
2	D	801	HEM	C1A-NA	2.74	1.41	1.36
2	C	801	HEM	CAA-C2A	-2.46	1.48	1.52
2	D	801	HEM	CMD-C2D	-2.25	1.47	1.51
2	C	801	HEM	CMA-C3A	-2.15	1.47	1.51
2	D	801	HEM	C1C-C2C	2.08	1.47	1.42

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	HEM	C1D-C2D-C3D	-6.48	102.49	107.00
2	C	801	HEM	CBD-CAD-C3D	-6.20	101.06	112.48
2	D	801	HEM	CBD-CAD-C3D	-5.81	101.77	112.48
2	B	801	HEM	CBD-CAD-C3D	-5.47	102.41	112.48
2	A	801	HEM	CBD-CAD-C3D	-4.73	103.76	112.48
2	D	801	HEM	CAA-CBA-CGA	-4.24	105.55	112.67
2	A	801	HEM	CAA-CBA-CGA	-4.01	105.94	112.67
2	C	801	HEM	CAA-CBA-CGA	-3.94	106.07	112.67
2	B	801	HEM	CMB-C2B-C3B	3.69	131.59	124.68
2	B	801	HEM	CAA-CBA-CGA	-3.64	106.57	112.67
2	D	801	HEM	CMA-C3A-C4A	-3.63	122.88	128.46
2	C	801	HEM	CMC-C2C-C3C	3.46	131.14	124.68
2	C	801	HEM	C4A-C3A-C2A	-3.44	104.60	107.00
2	C	801	HEM	CMD-C2D-C3D	3.34	131.24	124.94
2	D	801	HEM	CMB-C2B-C3B	3.24	130.73	124.68
2	A	801	HEM	C4A-C3A-C2A	-3.14	104.81	107.00
2	D	801	HEM	CMC-C2C-C3C	3.02	130.34	124.68
2	A	801	HEM	C4C-C3C-C2C	-2.98	104.82	106.90
2	C	801	HEM	CMB-C2B-C3B	2.84	130.00	124.68
2	A	801	HEM	C1D-C2D-C3D	-2.62	105.17	107.00
2	B	801	HEM	CMD-C2D-C1D	-2.60	124.47	128.46
2	B	801	HEM	C1D-C2D-C3D	2.28	108.58	107.00
2	B	801	HEM	CMA-C3A-C4A	-2.25	125.00	128.46
2	D	801	HEM	CMD-C2D-C1D	-2.10	125.24	128.46
2	D	801	HEM	C4A-C3A-C2A	2.02	108.40	107.00
2	D	801	HEM	CMA-C3A-C2A	2.01	128.72	124.94

There are no chirality outliers.

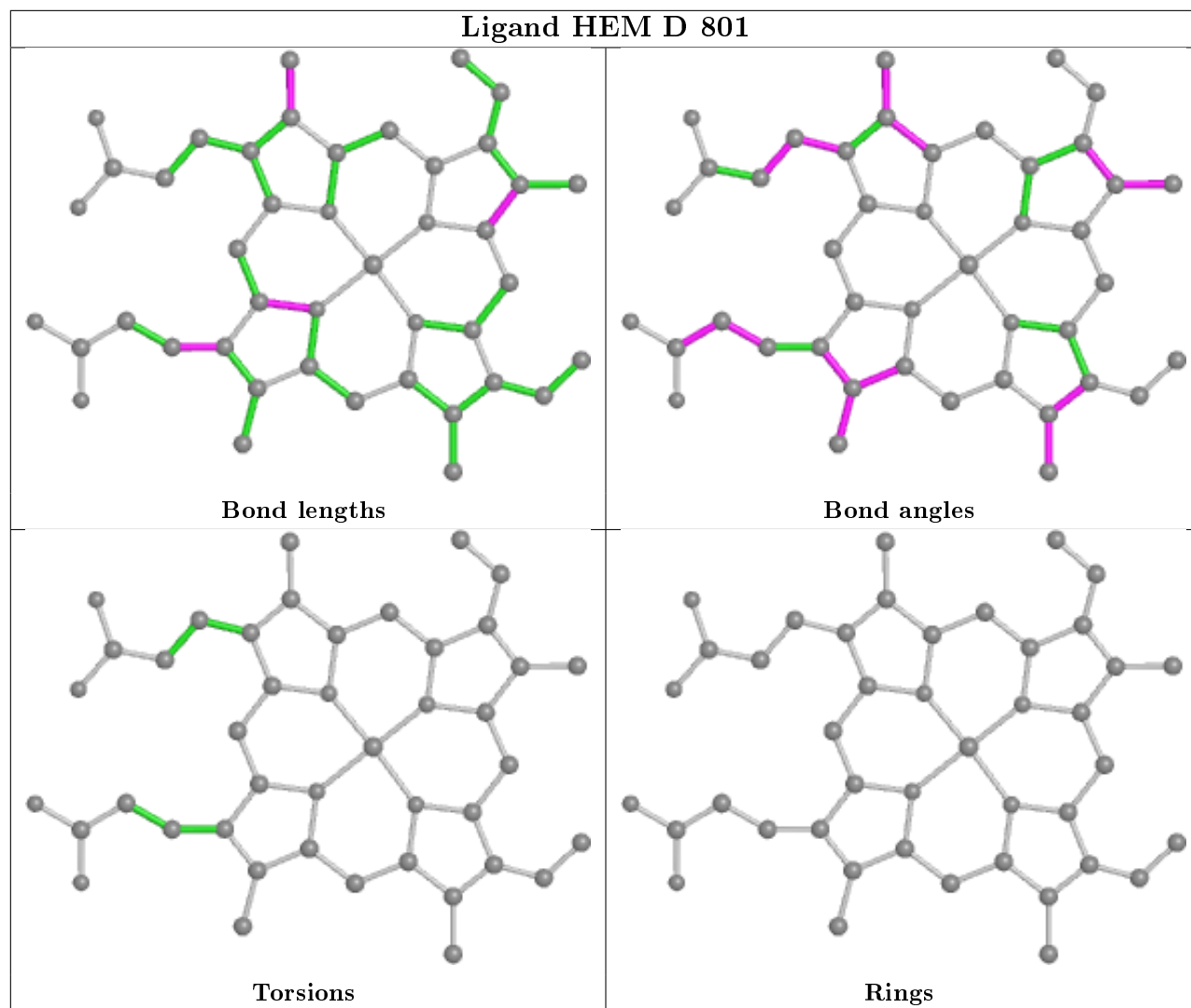
There are no torsion outliers.

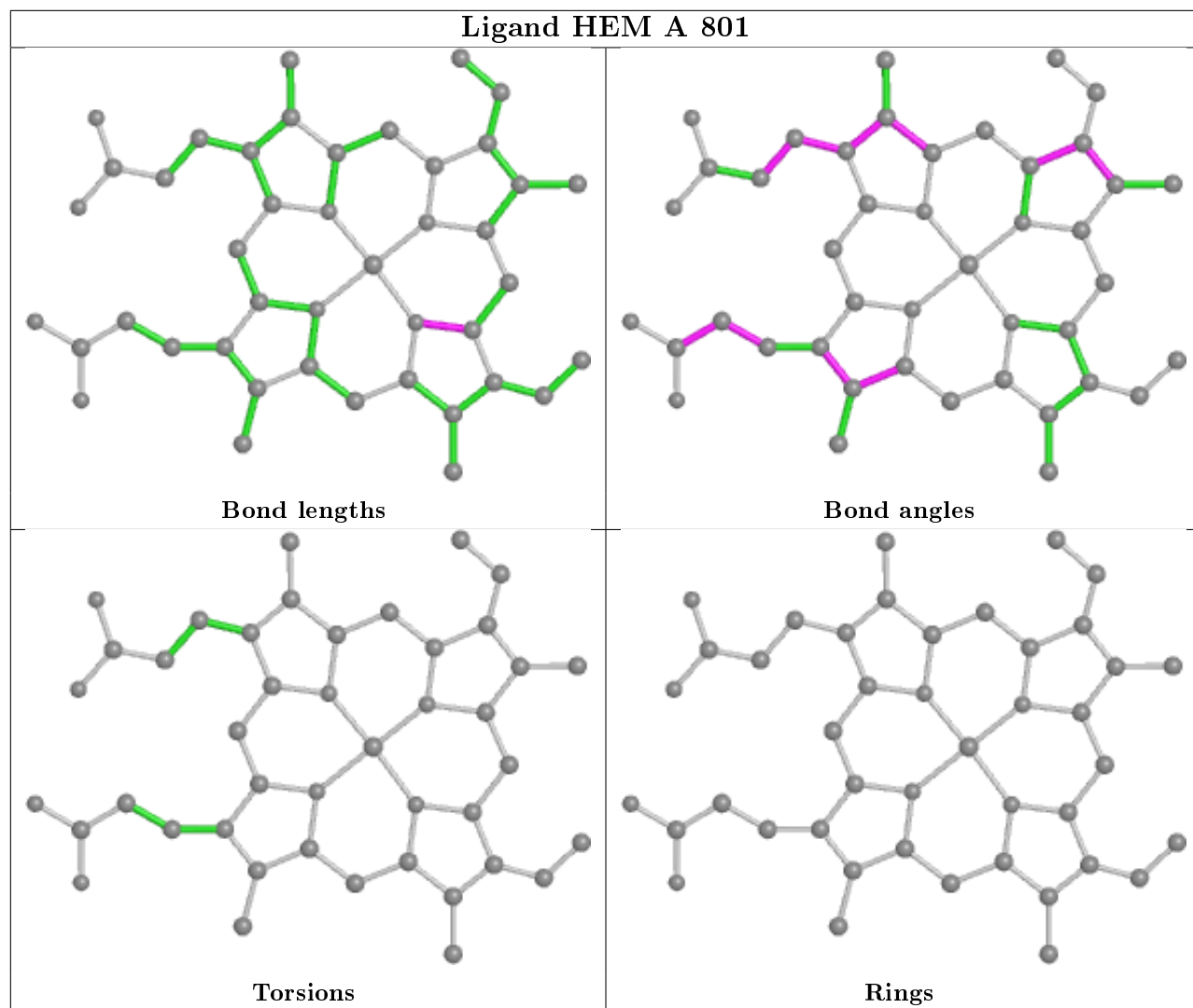
There are no ring outliers.

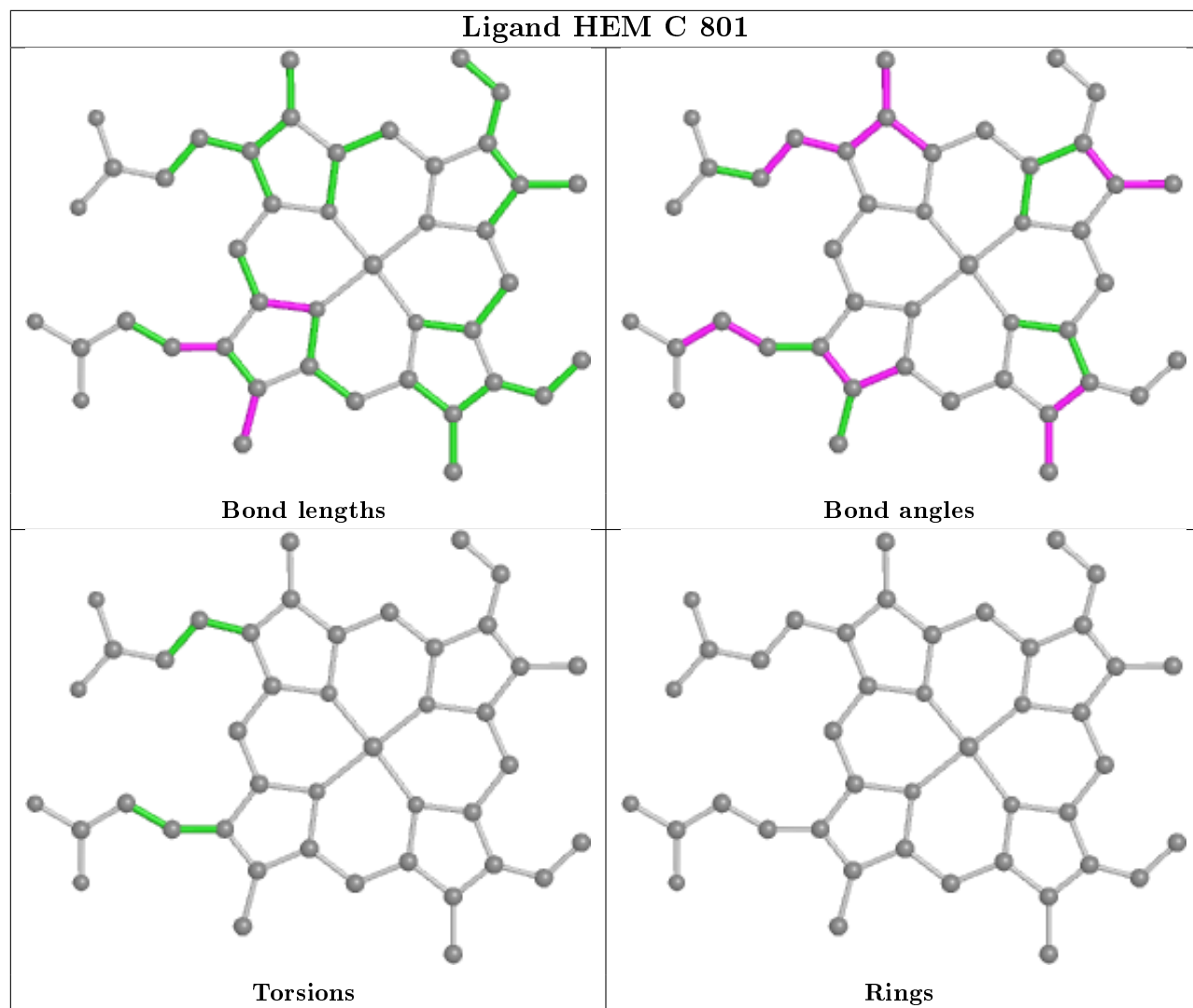
3 monomers are involved in 7 short contacts:

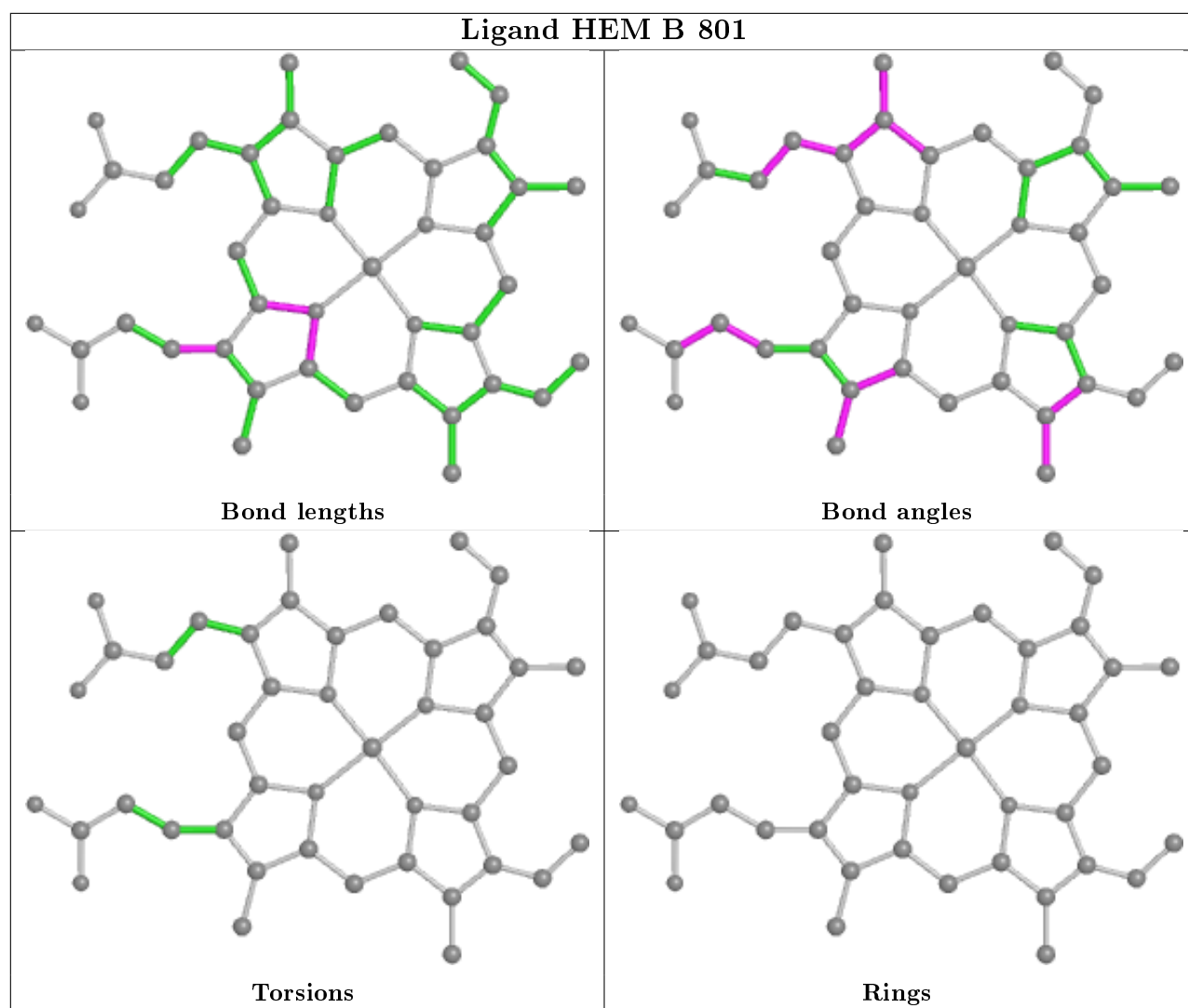
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	HEM	3	0
2	C	801	HEM	2	0
2	B	801	HEM	2	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	-0.33	20 (2%)	53	57	7, 13, 29, 57	1 (0%)
1	B	726/753 (96%)	-0.10	49 (6%)	17	19	7, 14, 43, 72	0
1	C	726/753 (96%)	-0.16	41 (5%)	24	26	7, 14, 41, 74	1 (0%)
1	D	726/753 (96%)	-0.29	17 (2%)	60	65	7, 13, 31, 69	0
All	All	2904/3012 (96%)	-0.22	127 (4%)	34	38	7, 13, 38, 74	2 (0%)

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	GLY	6.1
1	B	32	GLU	5.0
1	B	673	ALA	4.6
1	C	714	GLY	4.5
1	C	675	ILE	4.5
1	B	28	SER	4.4
1	B	672	ILE	4.3
1	C	701	ALA	4.2
1	A	28	SER	4.2
1	D	750	LYS	4.1
1	C	594	PRO	4.1
1	B	711	ALA	4.1
1	C	669	CYS	4.1
1	D	713	GLN	4.0
1	C	726	GLY	4.0
1	A	32	GLU	4.0
1	C	711	ALA	4.0
1	A	726	GLY	3.9
1	C	751	ILE	3.9
1	B	725	ASP	3.8
1	A	710	ILE	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	28	SER	3.8
1	C	673	ALA	3.7
1	B	677	ASP	3.7
1	B	713	GLN	3.6
1	C	643	ASP	3.6
1	B	645	GLY	3.5
1	B	568	ASP	3.5
1	C	698	ALA	3.4
1	B	641	THR	3.4
1	C	712	ASP	3.3
1	B	712	ASP	3.3
1	B	612	ARG	3.3
1	C	568	ASP	3.3
1	D	710	ILE	3.3
1	B	572	ASN	3.3
1	B	750	LYS	3.2
1	D	711	ALA	3.2
1	C	725	ASP	3.1
1	C	672	ILE	3.1
1	B	610	GLU	3.1
1	A	36	HIS	3.0
1	C	703	LYS	3.0
1	D	714	GLY	3.0
1	B	646	THR	3.0
1	B	594	PRO	3.0
1	D	751	ILE	3.0
1	B	566	LEU	3.0
1	B	642	ALA	3.0
1	B	647	VAL	3.0
1	B	724	ALA	3.0
1	C	676	ALA	3.0
1	C	724	ALA	3.0
1	D	712	ASP	3.0
1	C	723	SER	2.9
1	A	29	LEU	2.9
1	A	37	ARG	2.9
1	D	572	ASN	2.9
1	B	723	SER	2.9
1	B	722	ASP	2.9
1	D	673	ALA	2.9
1	B	30	ALA	2.8
1	C	710	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	594	PRO	2.8
1	B	749	ASP	2.8
1	B	644	ASP	2.8
1	B	710	ILE	2.7
1	C	645	GLY	2.7
1	C	713	GLN	2.7
1	B	33	ASP	2.7
1	A	35	SER	2.7
1	B	569	ASP	2.7
1	B	727	SER	2.7
1	C	750	LYS	2.6
1	C	569	ASP	2.6
1	C	617	LEU	2.6
1	C	674	ASP	2.6
1	C	722	ASP	2.6
1	B	714	GLY	2.6
1	D	569	ASP	2.6
1	B	29	LEU	2.6
1	A	713	GLN	2.6
1	D	568	ASP	2.5
1	B	614	ALA	2.5
1	C	646	THR	2.5
1	B	643	ASP	2.4
1	A	33	ASP	2.4
1	C	677	ASP	2.4
1	C	572	ASN	2.4
1	A	594	PRO	2.4
1	B	596	GLY	2.4
1	C	596	GLY	2.4
1	C	670	GLY	2.4
1	C	640	VAL	2.4
1	C	641	THR	2.4
1	A	30	ALA	2.4
1	D	571	LEU	2.4
1	B	701	ALA	2.3
1	B	37	ARG	2.3
1	B	611	VAL	2.3
1	A	712	ASP	2.3
1	B	617	LEU	2.2
1	B	565	GLU	2.2
1	C	721	ALA	2.2
1	B	567	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	642	ALA	2.2
1	B	34	GLY	2.2
1	C	595	ASP	2.2
1	A	711	ALA	2.2
1	C	642	ALA	2.2
1	B	751	ILE	2.2
1	B	669	CYS	2.1
1	A	596	GLY	2.1
1	C	571	LEU	2.1
1	C	32	GLU	2.1
1	B	571	LEU	2.1
1	A	39	ALA	2.1
1	C	700	ASP	2.1
1	B	721	ALA	2.1
1	D	573	ILE	2.1
1	A	38	PRO	2.1
1	A	34	GLY	2.1
1	A	749	ASP	2.1
1	D	749	ASP	2.1
1	B	676	ALA	2.0
1	A	677	ASP	2.0
1	C	614	ALA	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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	D	801	43/43	0.99	0.06	7,8,10,15	0

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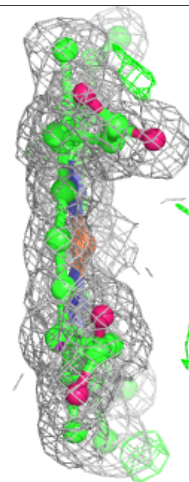
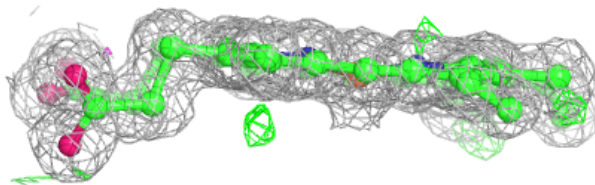
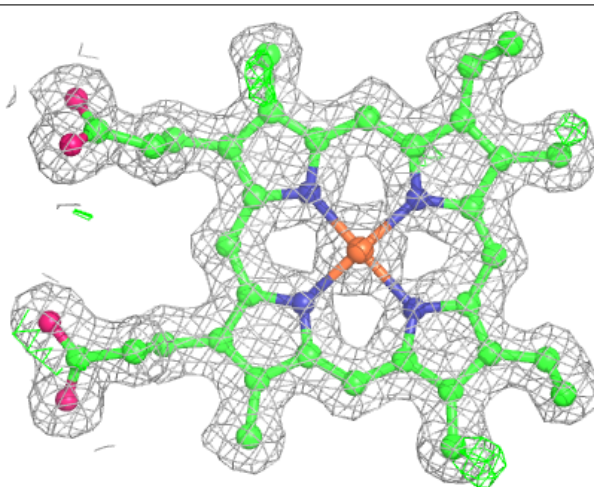
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HEM	A	801	43/43	0.99	0.10	6,8,9,15	0
2	HEM	C	801	43/43	0.99	0.08	7,8,11,16	0
2	HEM	B	801	43/43	0.99	0.06	7,9,11,14	0

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.

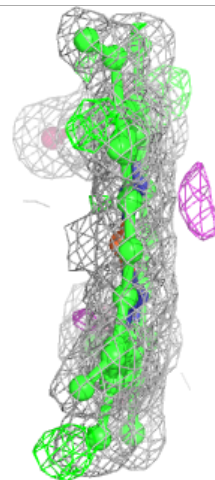
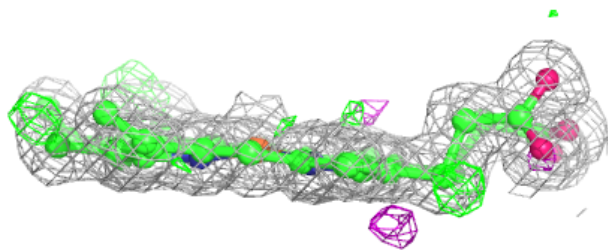
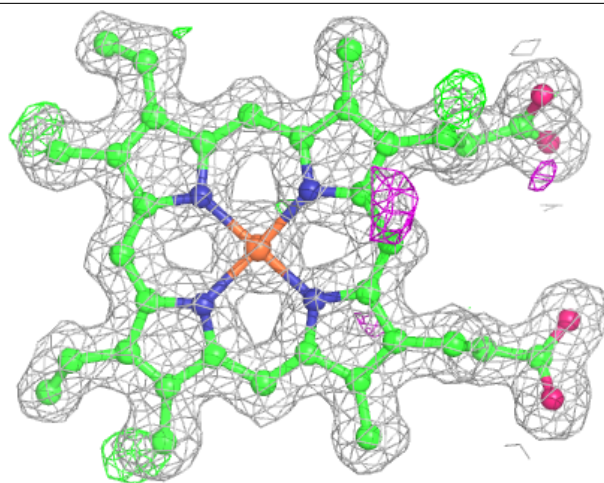
Electron density around HEM D 801:

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



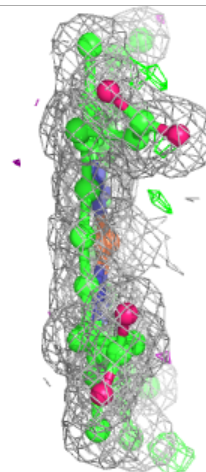
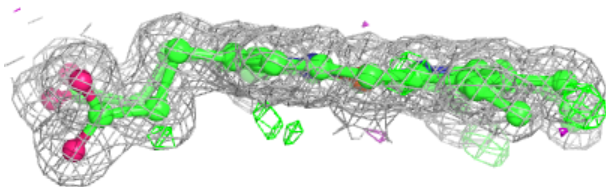
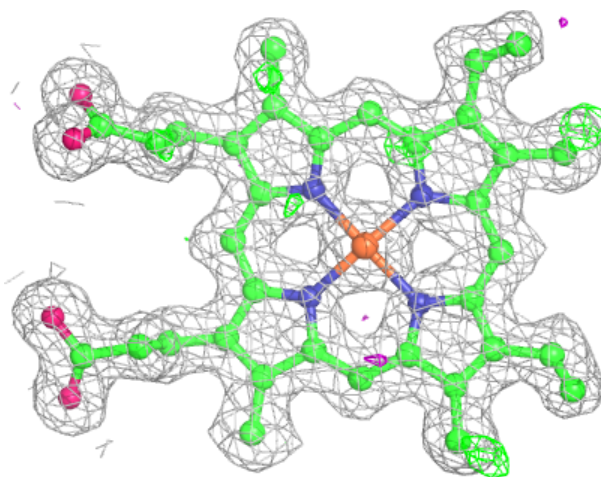
Electron density around HEM A 801:

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



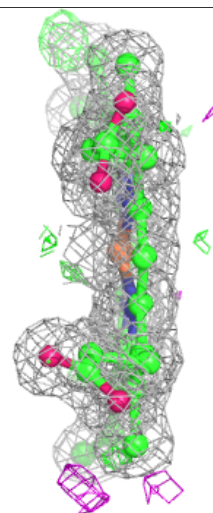
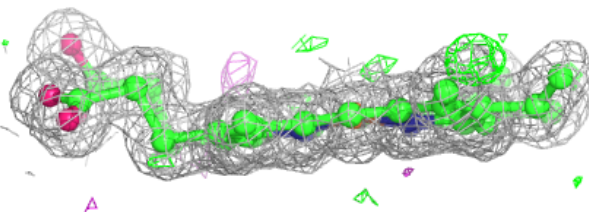
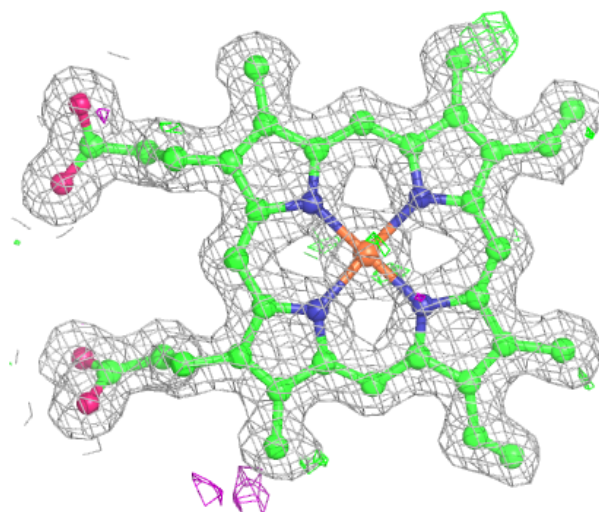
Electron density around HEM C 801:

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



Electron density around HEM B 801:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.