



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:44 PM UTC

PDB ID : 3TTV / pdb_00003ttv
Title : Structure of the F413E variant of E. coli KatE
Authors : Loewen, P.C.; Jha, V.
Deposited on : 2011-09-15
Resolution : 1.45 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

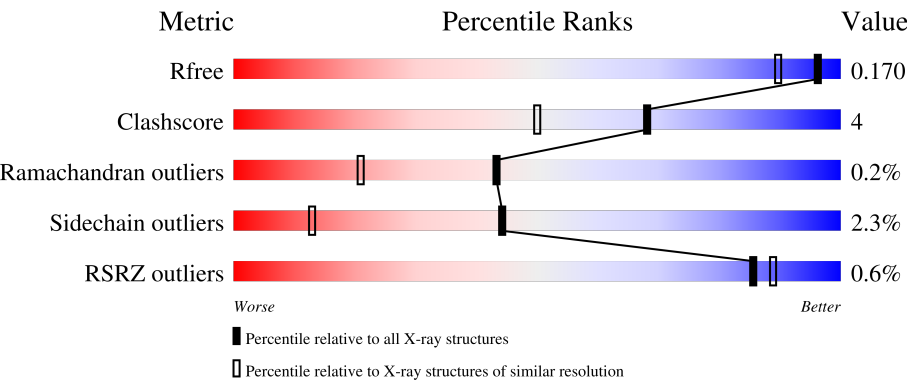
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.45 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	1756 (1.46-1.46)
Clashscore	190562	1795 (1.46-1.46)
Ramachandran outliers	187476	1776 (1.46-1.46)
Sidechain outliers	187428	1776 (1.46-1.46)
RSRZ outliers	180081	1756 (1.46-1.46)

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	81%14% . .
1	B	753	% 81%13% . . .
1	C	753	% 82%13% . .
1	D	753	% 82%12% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26511 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.

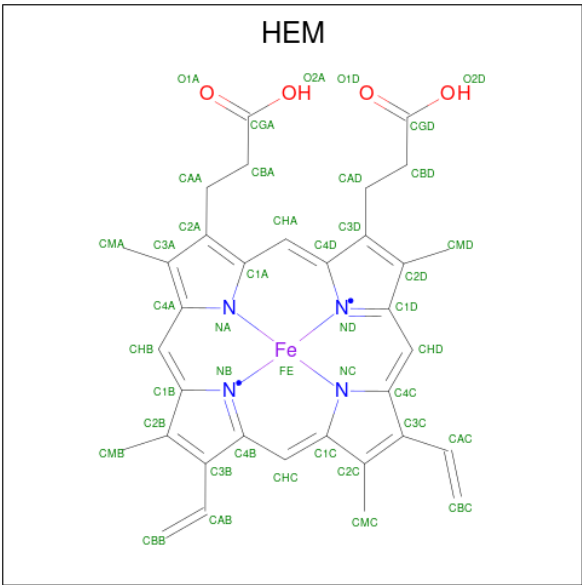
- Molecule 1 is a protein called Catalase HP11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	3	0
			5755	3652	1006	1085	12			
1	B	726	Total	C	N	O	S	0	3	0
			5758	3654	1006	1086	12			
1	C	726	Total	C	N	O	S	0	2	0
			5750	3649	1006	1083	12			
1	D	726	Total	C	N	O	S	0	2	0
			5750	3649	1006	1083	12			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	ALA	THR	engineered mutation	UNP P21179
A	413	TYR	PHE	engineered mutation	UNP P21179
B	115	ALA	THR	engineered mutation	UNP P21179
B	413	TYR	PHE	engineered mutation	UNP P21179
C	115	ALA	THR	engineered mutation	UNP P21179
C	413	TYR	PHE	engineered mutation	UNP P21179
D	115	ALA	THR	engineered mutation	UNP P21179
D	413	TYR	PHE	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

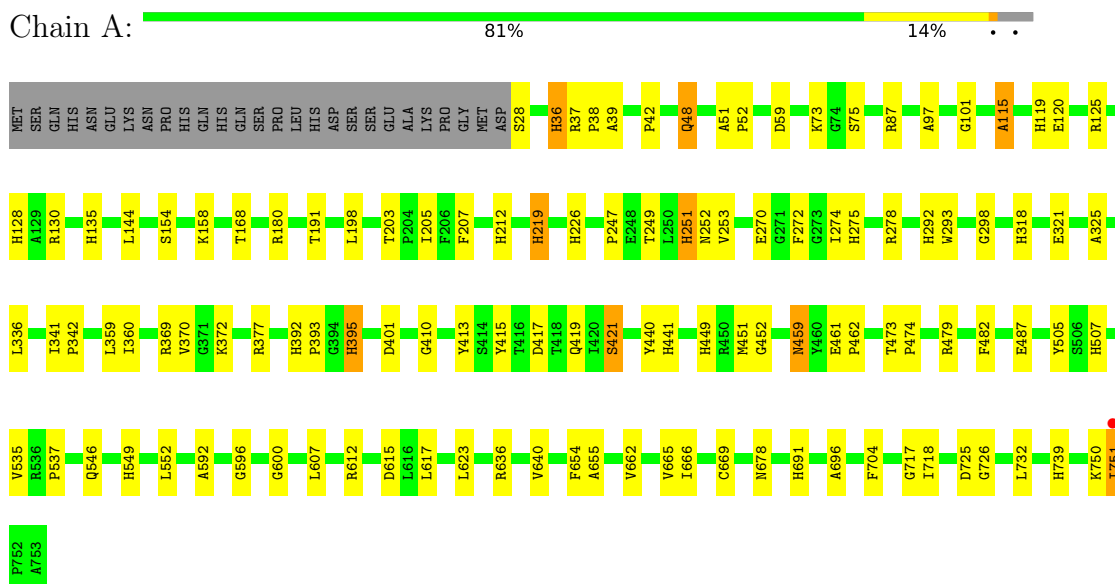
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	864	Total	O	0	0
			864	864		
3	B	775	Total	O	0	0
			775	775		
3	C	797	Total	O	0	0
			797	797		
3	D	890	Total	O	0	0
			890	890		

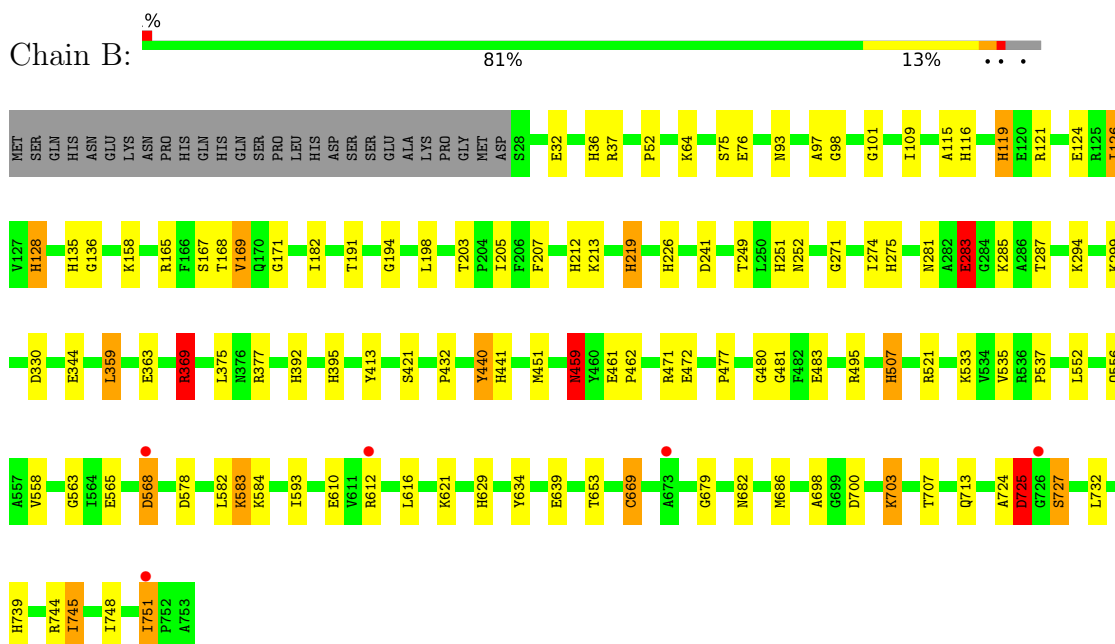
3 Residue-property plots

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.

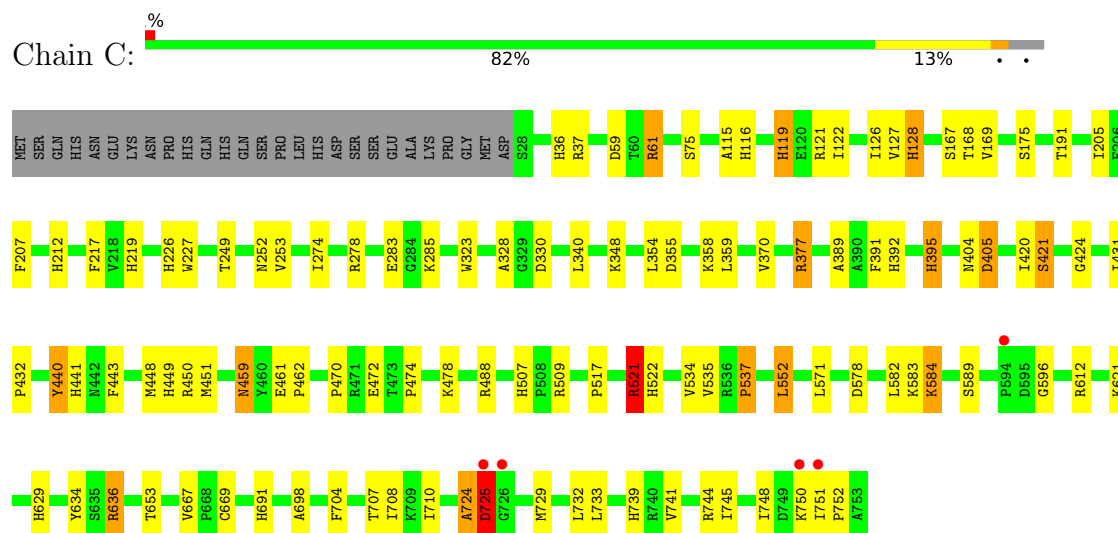
• Molecule 1: Catalase HPII



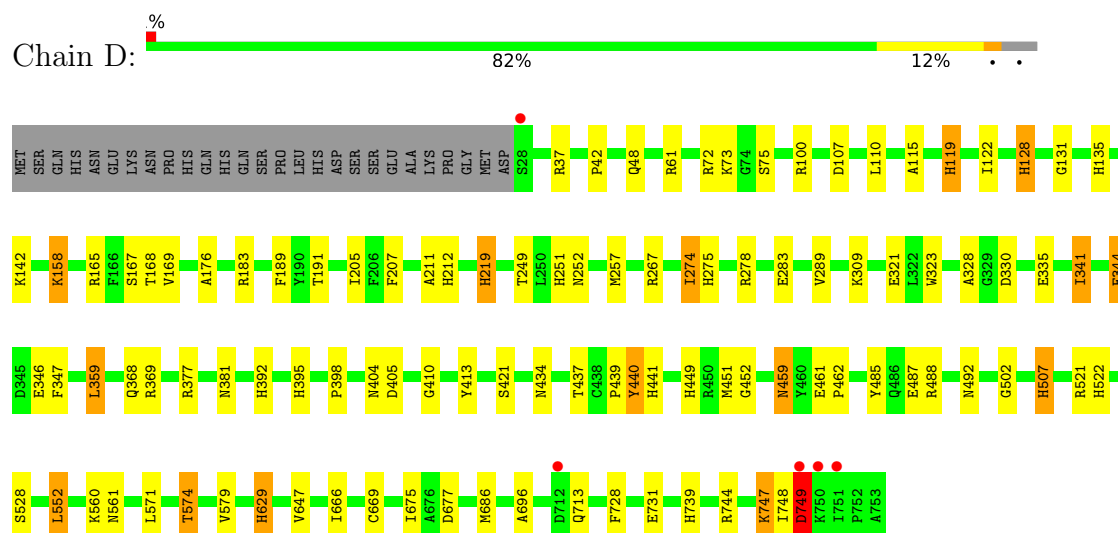
• Molecule 1: Catalase HPII



● Molecule 1: Catalase HP1I



● Molecule 1: Catalase HP1I



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.56Å 133.05Å 122.64Å 90.00° 109.29° 90.00°	Depositor
Resolution (Å)	32.16 – 1.45 32.16 – 1.45	Depositor EDS
% Data completeness (in resolution range)	96.8 (32.16-1.45) 96.8 (32.16-1.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.45Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.145 , 0.172 0.144 , 0.170	Depositor DCC
R_{free} test set	24236 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	12.4	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.1	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	0.97	EDS
Total number of atoms	26511	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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	1.71	68/5911 (1.2%)	1.44	10/8035 (0.1%)
1	B	1.65	53/5914 (0.9%)	1.39	17/8040 (0.2%)
1	C	1.66	48/5903 (0.8%)	1.40	21/8024 (0.3%)
1	D	1.73	59/5903 (1.0%)	1.42	9/8024 (0.1%)
All	All	1.69	228/23631 (1.0%)	1.41	57/32123 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	3
All	All	0	4

All (228) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	392	HIS	ND1-CE1	11.38	1.44	1.32
1	C	116	HIS	ND1-CE1	10.84	1.43	1.32
1	B	441	HIS	ND1-CE1	10.30	1.42	1.32
1	C	119	HIS	ND1-CE1	9.40	1.42	1.32
1	B	36	HIS	CE1-NE2	9.07	1.41	1.32
1	A	441	HIS	ND1-CE1	8.97	1.41	1.32
1	B	128	HIS	ND1-CE1	8.83	1.41	1.32
1	B	392	HIS	ND1-CE1	8.59	1.41	1.32
1	A	275	HIS	CE1-NE2	8.55	1.41	1.32
1	D	251	HIS	ND1-CE1	8.41	1.41	1.32
1	B	135	HIS	ND1-CE1	7.90	1.40	1.32
1	A	662	VAL	N-CA	7.88	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	452	GLY	C-O	7.83	1.31	1.24
1	C	226	HIS	ND1-CE1	7.82	1.40	1.32
1	B	219	HIS	ND1-CE1	7.72	1.40	1.32
1	D	341	ILE	N-CA	7.65	1.51	1.45
1	C	522	HIS	CE1-NE2	7.60	1.40	1.32
1	D	131	GLY	N-CA	7.57	1.53	1.45
1	A	48	GLN	N-CA	7.45	1.52	1.45
1	A	341	ILE	N-CA	7.45	1.51	1.45
1	D	749	ASP	N-CA	7.42	1.55	1.46
1	D	666	ILE	N-CA	7.31	1.54	1.46
1	D	219	HIS	CG-CD2	7.30	1.43	1.35
1	D	368	GLN	CD-OE1	7.30	1.37	1.23
1	A	36	HIS	ND1-CE1	7.29	1.39	1.32
1	A	275	HIS	ND1-CE1	7.28	1.39	1.32
1	C	212	HIS	ND1-CE1	7.24	1.39	1.32
1	D	507	HIS	ND1-CE1	7.17	1.39	1.32
1	B	219	HIS	CG-CD2	7.03	1.43	1.35
1	B	739	HIS	CG-CD2	6.99	1.43	1.35
1	C	392	HIS	ND1-CE1	6.91	1.39	1.32
1	C	59	ASP	CB-CG	6.89	1.69	1.52
1	A	219	HIS	CE1-NE2	6.86	1.39	1.32
1	B	698	ALA	N-CA	6.86	1.54	1.46
1	C	441	HIS	ND1-CE1	6.80	1.39	1.32
1	A	212	HIS	ND1-CE1	6.69	1.39	1.32
1	C	340	LEU	C-O	6.67	1.32	1.24
1	A	474	PRO	CA-C	6.65	1.55	1.51
1	B	745	ILE	CA-CB	6.65	1.57	1.54
1	C	392	HIS	CE1-NE2	6.60	1.39	1.32
1	D	257	MET	C-O	6.59	1.32	1.24
1	C	691	HIS	CE1-NE2	6.55	1.39	1.32
1	C	217	PHE	CA-CB	6.54	1.63	1.53
1	D	189	PHE	C-O	6.53	1.32	1.24
1	D	629	HIS	CD2-NE2	-6.53	1.30	1.37
1	A	549	HIS	ND1-CE1	6.50	1.39	1.32
1	C	698	ALA	N-CA	6.50	1.53	1.46
1	C	739	HIS	CG-CD2	6.48	1.43	1.35
1	D	377	ARG	CZ-NH1	6.48	1.41	1.32
1	B	495	ARG	N-CA	6.46	1.55	1.46
1	C	522	HIS	ND1-CE1	6.46	1.39	1.32
1	A	401	ASP	N-CA	6.43	1.53	1.46
1	C	358	LYS	N-CA	6.42	1.53	1.46
1	B	203	THR	N-CA	6.42	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	VAL	C-O	6.41	1.31	1.24
1	A	623	LEU	N-CA	6.40	1.54	1.46
1	D	398	PRO	CA-CB	6.40	1.62	1.53
1	D	528	SER	N-CA	6.39	1.54	1.46
1	A	292	HIS	ND1-CE1	6.39	1.39	1.32
1	B	287	THR	C-O	6.37	1.31	1.24
1	A	135	HIS	CE1-NE2	6.36	1.39	1.32
1	B	275	HIS	ND1-CE1	6.36	1.39	1.32
1	C	729	MET	N-CA	6.36	1.54	1.46
1	A	321	GLU	CD-OE1	6.34	1.37	1.25
1	B	459	ASN	CG-OD1	6.34	1.35	1.23
1	A	452	GLY	C-O	6.33	1.30	1.24
1	A	251	HIS	ND1-CE1	6.28	1.38	1.32
1	B	36	HIS	CG-CD2	6.25	1.42	1.35
1	B	480	GLY	N-CA	6.22	1.51	1.44
1	A	135	HIS	N-CA	6.20	1.53	1.45
1	C	59	ASP	CG-OD1	6.19	1.37	1.25
1	B	226	HIS	CG-CD2	6.17	1.42	1.35
1	D	135	HIS	CE1-NE2	6.17	1.38	1.32
1	D	359	LEU	C-N	6.15	1.38	1.33
1	C	61	ARG	CA-CB	6.13	1.64	1.53
1	C	167	SER	N-CA	6.12	1.53	1.46
1	B	194	GLY	N-CA	6.09	1.50	1.45
1	D	73	LYS	N-CA	6.08	1.53	1.46
1	A	739	HIS	ND1-CE1	6.07	1.38	1.32
1	D	37	ARG	CZ-NH1	6.05	1.41	1.32
1	B	375	LEU	N-CA	6.05	1.54	1.46
1	D	167	SER	N-CA	6.04	1.53	1.46
1	B	136	GLY	N-CA	6.03	1.52	1.45
1	C	667	VAL	N-CA	-6.03	1.41	1.46
1	A	359	LEU	N-CA	6.01	1.52	1.45
1	C	522	HIS	CG-CD2	6.00	1.42	1.35
1	C	377	ARG	CZ-NH1	5.98	1.41	1.32
1	C	127	VAL	C-O	5.97	1.30	1.23
1	C	733	LEU	CA-C	5.90	1.60	1.52
1	A	39	ALA	C-O	5.90	1.30	1.23
1	C	253	VAL	CA-C	5.90	1.60	1.52
1	A	691	HIS	CE1-NE2	5.90	1.38	1.32
1	C	227	TRP	N-CA	5.88	1.54	1.45
1	A	377	ARG	CZ-NH1	5.86	1.41	1.32
1	C	391	PHE	N-CA	5.85	1.53	1.46
1	B	271	GLY	CA-C	-5.83	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	119	HIS	ND1-CE1	5.82	1.38	1.32
1	A	600	GLY	N-CA	5.78	1.53	1.45
1	D	321	GLU	CD-OE1	5.76	1.36	1.25
1	D	492	ASN	C-O	5.76	1.31	1.23
1	A	392	HIS	ND1-CE1	5.74	1.38	1.32
1	D	739	HIS	CG-CD2	5.74	1.42	1.35
1	A	691	HIS	ND1-CE1	5.74	1.38	1.32
1	A	270	GLU	N-CA	5.73	1.53	1.45
1	B	472	GLU	CA-C	5.73	1.59	1.52
1	B	37	ARG	CA-C	5.73	1.59	1.52
1	B	251	HIS	CG-CD2	5.73	1.42	1.35
1	C	370	VAL	CA-CB	5.72	1.63	1.55
1	D	522	HIS	ND1-CE1	5.72	1.38	1.32
1	A	654	PHE	C-O	5.72	1.30	1.24
1	B	64	LYS	C-O	5.72	1.30	1.24
1	D	413	TYR	CA-C	5.71	1.60	1.52
1	A	704	PHE	N-CA	5.71	1.53	1.46
1	A	607	LEU	N-CA	5.70	1.53	1.45
1	B	483	GLU	C-O	5.69	1.30	1.24
1	A	293	TRP	N-CA	5.67	1.52	1.46
1	B	745	ILE	C-O	5.67	1.29	1.24
1	A	360	ILE	N-CA	5.66	1.50	1.46
1	D	289	VAL	N-CA	5.65	1.53	1.46
1	A	505	TYR	CA-CB	5.65	1.61	1.54
1	C	534	VAL	C-O	5.65	1.29	1.24
1	A	318	HIS	CE1-NE2	5.64	1.38	1.32
1	D	328	ALA	N-CA	5.63	1.53	1.46
1	B	116	HIS	ND1-CE1	5.63	1.38	1.32
1	A	473	THR	C-N	5.62	1.38	1.33
1	B	507	HIS	CE1-NE2	5.61	1.38	1.32
1	D	158	LYS	CA-CB	-5.59	1.46	1.53
1	A	42	PRO	C-O	5.57	1.30	1.23
1	B	109	ILE	C-O	5.56	1.30	1.24
1	B	481	GLY	N-CA	5.54	1.52	1.45
1	D	42	PRO	C-O	5.54	1.30	1.23
1	D	507	HIS	CE1-NE2	5.53	1.38	1.32
1	B	98	GLY	N-CA	5.52	1.51	1.45
1	C	424	GLY	N-CA	5.52	1.53	1.45
1	A	115	ALA	N-CA	5.51	1.53	1.46
1	D	122	ILE	CA-CB	5.50	1.59	1.55
1	C	421	SER	CA-C	5.49	1.59	1.52
1	C	584	LYS	C-O	5.48	1.29	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	647	VAL	N-CA	5.48	1.52	1.46
1	B	363	GLU	N-CA	5.47	1.53	1.46
1	A	180	ARG	CZ-NH1	5.47	1.40	1.32
1	A	717	GLY	N-CA	5.47	1.52	1.45
1	D	323	TRP	NE1-CE2	5.47	1.43	1.37
1	A	125	ARG	CD-NE	5.46	1.53	1.46
1	A	154	SER	N-CA	5.45	1.53	1.46
1	C	421	SER	N-CA	5.43	1.52	1.46
1	D	439	PRO	N-CA	5.41	1.53	1.47
1	A	696	ALA	N-CA	5.40	1.52	1.46
1	A	87	ARG	CZ-NH1	-5.39	1.25	1.32
1	B	359	LEU	N-CA	5.39	1.52	1.45
1	A	655	ALA	C-O	5.38	1.30	1.24
1	B	212	HIS	ND1-CE1	5.38	1.38	1.32
1	B	283	GLU	N-CA	5.37	1.53	1.46
1	B	251	HIS	ND1-CE1	5.37	1.38	1.32
1	C	377	ARG	CZ-NH2	5.36	1.40	1.33
1	A	410	GLY	C-O	5.36	1.30	1.23
1	A	482	PHE	CA-CB	5.36	1.61	1.53
1	D	441	HIS	ND1-CE1	5.35	1.38	1.32
1	A	718	ILE	C-O	5.35	1.29	1.24
1	B	568	ASP	CB-CG	5.35	1.65	1.52
1	A	52	PRO	CA-CB	5.34	1.60	1.53
1	D	561	ASN	CA-C	-5.34	1.45	1.52
1	D	72	ARG	C-O	5.34	1.30	1.23
1	B	76	GLU	CA-C	-5.32	1.45	1.52
1	D	183	ARG	CD-NE	5.32	1.53	1.46
1	D	502	GLY	C-O	5.32	1.31	1.23
1	C	323	TRP	NE1-CE2	5.32	1.43	1.37
1	C	474	PRO	CA-C	5.32	1.57	1.52
1	A	342	PRO	CA-C	-5.32	1.46	1.52
1	A	203	THR	N-CA	5.31	1.50	1.45
1	D	274	ILE	N-CA	5.31	1.52	1.46
1	A	247	PRO	C-O	5.31	1.31	1.24
1	C	36	HIS	CE1-NE2	5.30	1.37	1.32
1	A	612	ARG	C-O	5.29	1.30	1.23
1	D	507	HIS	CG-CD2	5.29	1.41	1.35
1	D	107	ASP	CA-C	5.28	1.59	1.52
1	B	563	GLY	N-CA	5.28	1.52	1.45
1	D	128	HIS	CE1-NE2	5.28	1.37	1.32
1	B	124	GLU	N-CA	5.27	1.52	1.45
1	B	471	ARG	CZ-NH2	5.27	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	579	VAL	CA-CB	5.27	1.60	1.53
1	C	395	HIS	CG-CD2	5.26	1.41	1.35
1	B	158	LYS	CA-CB	-5.25	1.46	1.53
1	A	298	GLY	N-CA	5.25	1.50	1.45
1	A	325	ALA	N-CA	5.24	1.52	1.46
1	A	739	HIS	CG-ND1	-5.24	1.32	1.38
1	D	275	HIS	CG-CD2	5.24	1.41	1.35
1	C	175	SER	N-CA	5.24	1.52	1.45
1	C	589	SER	CA-CB	5.24	1.61	1.53
1	C	744	ARG	CZ-NH1	5.23	1.40	1.32
1	D	165	ARG	CZ-NH2	5.23	1.40	1.33
1	D	212	HIS	ND1-CE1	5.22	1.37	1.32
1	C	741	VAL	N-CA	5.22	1.52	1.46
1	B	167	SER	N-CA	5.22	1.52	1.46
1	D	434	ASN	N-CA	5.21	1.52	1.46
1	A	226	HIS	ND1-CE1	5.21	1.37	1.32
1	C	621	LYS	N-CA	-5.21	1.40	1.46
1	A	36	HIS	CG-CD2	5.20	1.41	1.35
1	B	119	HIS	ND1-CE1	5.20	1.37	1.32
1	A	640	VAL	N-CA	5.20	1.51	1.46
1	D	560	LYS	N-CA	5.20	1.52	1.46
1	B	725	ASP	CA-C	5.20	1.59	1.52
1	A	419	GLN	CD-OE1	5.19	1.33	1.23
1	D	189	PHE	N-CA	5.18	1.52	1.46
1	A	615	ASP	N-CA	5.17	1.52	1.46
1	B	126	ILE	CA-C	5.17	1.59	1.52
1	A	336	LEU	N-CA	5.16	1.52	1.46
1	B	727	SER	CA-C	5.16	1.59	1.52
1	C	405	ASP	C-O	5.14	1.30	1.24
1	A	592	ALA	N-CA	5.13	1.52	1.46
1	C	389	ALA	N-CA	5.13	1.52	1.45
1	D	346	GLU	N-CA	5.13	1.52	1.46
1	D	347	PHE	CA-CB	5.11	1.60	1.53
1	A	417	ASP	CA-C	5.09	1.59	1.52
1	C	128	HIS	CG-CD2	5.09	1.41	1.35
1	B	744	ARG	CZ-NH1	5.08	1.39	1.32
1	A	395	HIS	ND1-CE1	5.08	1.37	1.32
1	D	485	TYR	CA-C	5.08	1.59	1.52
1	A	272	PHE	N-CA	5.07	1.52	1.46
1	B	171	GLY	N-CA	5.06	1.51	1.45
1	D	135	HIS	ND1-CE1	5.06	1.37	1.32
1	B	558	VAL	CA-CB	5.05	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	299	LYS	CA-C	-5.04	1.46	1.52
1	D	176	ALA	N-CA	5.04	1.52	1.45
1	C	328	ALA	N-CA	5.03	1.52	1.46
1	A	678	ASN	CA-C	5.02	1.59	1.52
1	D	437	THR	N-CA	5.02	1.52	1.46
1	D	142	LYS	N-CA	5.02	1.52	1.45

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	521	ARG	CG-CD-NE	8.55	130.81	112.00
1	D	344	GLU	CA-CB-CG	8.24	130.58	114.10
1	A	341	ILE	CA-C-O	7.82	124.01	119.94
1	A	636	ARG	NE-CZ-NH2	7.20	125.67	119.20
1	C	377	ARG	CA-CB-CG	-6.78	100.53	114.10
1	D	748	ILE	N-CA-C	6.74	121.86	112.50
1	C	552	LEU	N-CA-C	6.71	118.60	111.28
1	C	348	LYS	CA-CB-CG	-6.65	100.81	114.10
1	B	745	ILE	CA-C-N	-6.40	113.55	119.82
1	B	745	ILE	C-N-CA	-6.40	113.55	119.82
1	B	182	ILE	N-CA-C	-6.39	103.08	110.05
1	C	725	ASP	N-CA-C	6.12	123.84	110.80
1	D	377	ARG	CG-CD-NE	-6.11	98.55	112.00
1	C	431	ILE	N-CA-C	-5.99	103.45	109.02
1	C	37	ARG	NE-CZ-NH2	-5.98	113.82	119.20
1	B	556	GLN	N-CA-C	5.95	117.77	111.28
1	A	130	ARG	NE-CZ-NH2	-5.93	113.87	119.20
1	C	745	ILE	O-C-N	5.82	124.14	120.42
1	A	421	SER	N-CA-C	-5.74	104.94	111.14
1	A	751	ILE	N-CA-CB	5.73	116.36	110.23
1	C	596	GLY	N-CA-C	5.69	118.47	111.93
1	A	154	SER	CA-C-O	-5.67	112.90	119.14
1	B	369	ARG	NE-CZ-NH1	-5.53	115.97	121.50
1	A	665	VAL	O-C-N	5.53	129.17	123.20
1	C	278	ARG	NE-CZ-NH1	-5.49	116.01	121.50
1	D	675	ILE	CA-C-O	5.47	124.14	119.38
1	B	377	ARG	NE-CZ-NH1	-5.45	116.05	121.50
1	D	100	ARG	CB-CA-C	-5.37	102.79	111.28
1	B	165	ARG	NE-CZ-NH1	-5.36	116.14	121.50
1	C	355	ASP	CA-C-O	5.36	122.77	119.29
1	A	158	LYS	CA-C-O	5.35	126.10	120.54
1	D	309	LYS	CB-CG-CD	-5.34	99.02	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	198	LEU	CB-CG-CD1	5.33	126.68	110.70
1	C	61	ARG	NE-CZ-NH1	-5.31	116.19	121.50
1	B	568	ASP	N-CA-CB	-5.30	101.54	110.49
1	A	120	GLU	N-CA-C	5.27	117.03	111.28
1	C	509	ARG	NE-CZ-NH2	5.27	123.94	119.20
1	D	381	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	B	241	ASP	N-CA-C	-5.22	105.48	111.07
1	C	450	ARG	CD-NE-CZ	-5.22	117.09	124.40
1	C	472	GLU	CA-C-O	-5.20	116.04	121.55
1	B	392	HIS	CB-CA-C	5.19	116.40	109.65
1	B	194	GLY	CA-C-O	5.18	126.16	122.37
1	C	354	LEU	CD1-CG-CD2	5.14	122.10	110.80
1	B	169	VAL	CB-CA-C	-5.13	106.48	111.05
1	C	126	ILE	CB-CA-C	-5.13	105.22	112.14
1	B	679	GLY	N-CA-C	-5.12	106.59	112.73
1	B	93	ASN	CA-CB-CG	-5.07	107.53	112.60
1	A	596	GLY	N-CA-C	5.04	118.64	112.14
1	C	37	ARG	CB-CG-CD	-5.04	99.71	111.30
1	C	61	ARG	CA-C-O	5.03	126.77	121.33
1	D	110	LEU	N-CA-C	-5.03	105.71	111.14
1	C	122	ILE	N-CA-CB	5.02	115.29	111.83
1	C	285	LYS	CD-CE-NZ	-5.01	95.85	111.90
1	B	477	PRO	N-CD-CG	-5.01	95.68	103.20
1	D	61	ARG	NE-CZ-NH2	5.01	123.71	119.20
1	B	377	ARG	CG-CD-NE	-5.01	100.98	112.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	121	ARG	Sidechain
1	C	121	ARG	Sidechain
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	5755	0	5587	38	2
1	B	5758	0	5589	55	2
1	C	5750	0	5583	40	0
1	D	5750	0	5583	44	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
2	C	43	0	30	1	0
2	D	43	0	30	1	0
3	A	864	0	0	10	1
3	B	775	0	0	15	0
3	C	797	0	0	10	0
3	D	890	0	0	16	1
All	All	26511	0	22462	163	3

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 (163) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:521:ARG:HD3	3:B:3047:HOH:O	1.27	1.33
1:B:533:LYS:HE3	3:C:2623:HOH:O	1.28	1.26
1:D:449[B]:HIS:NE2	3:D:2501:HOH:O	1.65	1.24
1:B:451:MET:HE2	1:D:451:MET:HE2	1.24	1.18
1:A:546:GLN:HG3	3:A:3434:HOH:O	1.45	1.16
1:A:479:ARG:NH2	3:A:2607:HOH:O	1.89	1.05
1:B:294:LYS:HD2	3:B:3483:HOH:O	1.55	1.03
1:A:369:ARG:HD3	3:A:2403:HOH:O	1.61	1.00
1:D:341:ILE:HG13	3:D:3022:HOH:O	1.60	1.00
1:A:451:MET:HE2	1:C:451:MET:HE2	1.47	0.95
1:B:521:ARG:NH2	1:B:745:ILE:HD13	1.88	0.89
1:A:546:GLN:CG	3:A:3434:HOH:O	2.12	0.84
1:C:283:GLU:OE1	3:C:2292:HOH:O	1.95	0.84
1:D:521:ARG:HD3	3:D:3213:HOH:O	1.78	0.83
1:B:521:ARG:HH22	1:B:745:ILE:HD13	1.45	0.80
1:C:636:ARG:NH1	3:C:2717:HOH:O	2.17	0.77
1:A:546:GLN:CD	3:A:3434:HOH:O	2.33	0.70
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.73	0.70
1:D:731:GLU:OE2	3:D:3028:HOH:O	2.09	0.69
1:D:574:THR:HG22	3:D:1614:HOH:O	1.93	0.67
1:D:449[B]:HIS:CE1	3:D:2501:HOH:O	2.27	0.67
1:D:283:GLU:OE1	3:D:2496:HOH:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.78	0.66
1:D:341:ILE:CG1	3:D:3022:HOH:O	2.27	0.66
1:B:294:LYS:CE	3:B:3483:HOH:O	2.42	0.66
1:B:583:LYS:H	1:B:583:LYS:NZ	1.96	0.64
1:C:751:ILE:HG13	1:C:752:PRO:HD2	1.80	0.62
1:A:36:HIS:CD2	1:A:36:HIS:H	2.17	0.62
1:D:488:ARG:NE	3:D:2698:HOH:O	1.63	0.62
1:D:158:LYS:HB3	3:D:3454:HOH:O	2.00	0.61
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.84	0.60
1:B:521:ARG:HH22	1:B:745:ILE:CD1	2.15	0.60
1:B:583:LYS:O	1:B:584:LYS:HB3	2.03	0.59
1:C:521:ARG:O	1:C:521:ARG:HD2	2.01	0.59
1:B:119:HIS:CE1	1:C:421:SER:HB2	2.38	0.59
1:B:629:HIS:HD2	3:B:1057:HOH:O	1.86	0.58
1:B:748:ILE:O	1:B:751:ILE:HG22	2.02	0.58
1:D:629:HIS:HD2	3:D:1554:HOH:O	1.87	0.58
1:A:751:ILE:O	1:A:751:ILE:HD12	2.05	0.57
1:C:629:HIS:HD2	3:C:1129:HOH:O	1.87	0.57
1:B:359:LEU:H	1:B:507:HIS:HD2	1.51	0.57
3:A:3442:HOH:O	1:D:686:MET:HE1	2.05	0.57
1:B:294:LYS:NZ	3:B:2778:HOH:O	2.37	0.56
1:D:359:LEU:H	1:D:507:HIS:HD2	1.52	0.56
1:D:574:THR:HG23	3:D:3354:HOH:O	2.06	0.56
1:B:521:ARG:NH2	1:B:745:ILE:HG21	2.20	0.56
1:A:119:HIS:CE1	1:D:421:SER:HB2	2.42	0.55
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.88	0.55
1:B:32:GLU:HG2	3:B:2850:HOH:O	2.06	0.54
1:B:621:LYS:HG2	3:B:2721:HOH:O	2.07	0.54
1:A:421:SER:HB2	1:D:119:HIS:CE1	2.43	0.54
1:B:669:OCS:OD1	1:B:700:ASP:HB2	2.07	0.54
1:A:28:SER:N	3:A:3144:HOH:O	2.41	0.53
1:C:535:VAL:O	1:C:537:PRO:HD3	2.08	0.53
1:B:578:ASP:HB2	1:B:582:LEU:O	2.09	0.53
1:C:583:LYS:O	1:C:584:LYS:HB3	2.09	0.53
1:A:395:HIS:HE1	3:A:3225:HOH:O	1.91	0.52
1:D:341:ILE:CD1	3:D:3022:HOH:O	2.55	0.52
1:B:552:LEU:HB2	3:B:3202:HOH:O	2.10	0.52
1:B:686:MET:HB3	1:B:751:ILE:HD11	1.92	0.52
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.91	0.51
1:B:724:ALA:O	1:B:725:ASP:O	2.28	0.51
1:B:294:LYS:HE3	3:B:3483:HOH:O	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:LEU:H	1:C:507:HIS:HD2	1.60	0.50
1:C:395:HIS:HE1	3:C:3337:HOH:O	1.93	0.50
1:D:488:ARG:NH2	3:D:2698:HOH:O	2.43	0.50
1:B:634:TYR:O	1:B:653:THR:HA	2.11	0.50
1:A:369:ARG:HG3	1:A:369:ARG:HH21	1.77	0.50
1:B:610:GLU:HG2	3:B:3191:HOH:O	2.12	0.49
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.28	0.48
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.43	0.48
1:B:359:LEU:H	1:B:507:HIS:CD2	2.30	0.48
1:C:115:ALA:O	1:C:119:HIS:HD2	1.96	0.48
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.29	0.47
1:A:372:LYS:NZ	3:A:2965:HOH:O	2.47	0.47
1:D:461:GLU:HA	1:D:462:PRO:C	2.39	0.47
1:D:713:GLN:O	1:D:713:GLN:HG2	2.15	0.47
1:A:535:VAL:O	1:A:537:PRO:HD3	2.14	0.47
1:B:421:SER:HB2	1:C:119:HIS:CE1	2.50	0.47
1:C:274:ILE:HD12	2:C:760:HEM:HMB1	1.97	0.47
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.30	0.47
1:A:207:PHE:O	1:A:249:THR:HA	2.15	0.46
1:B:535:VAL:O	1:B:537:PRO:HD3	2.15	0.46
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.24	0.46
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.31	0.46
1:A:552:LEU:HD12	3:A:2786:HOH:O	2.16	0.46
1:B:461:GLU:HA	1:B:462:PRO:C	2.39	0.46
1:A:115:ALA:O	1:A:119:HIS:HD2	1.99	0.46
1:B:281:ASN:OD1	1:B:283:GLU:HG3	2.16	0.46
1:D:274:ILE:HD12	2:D:760:HEM:HMB1	1.98	0.46
1:A:97:ALA:O	1:A:101:GLY:HA3	2.16	0.46
1:A:750:LYS:NZ	1:D:677:ASP:HB3	2.31	0.46
1:B:440:TYR:CD2	1:B:440:TYR:C	2.94	0.46
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.51	0.46
1:C:552:LEU:HD11	1:C:571:LEU:HD23	1.97	0.45
1:D:749:ASP:OD1	1:D:749:ASP:N	2.44	0.45
1:C:61:ARG:HG3	3:C:2648:HOH:O	2.15	0.45
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.25	0.45
1:C:128:HIS:CE1	1:C:169:VAL:HG22	2.51	0.45
1:D:552:LEU:HD11	1:D:571:LEU:HA	1.98	0.45
1:C:359:LEU:H	1:C:507:HIS:CD2	2.36	0.45
1:C:724:ALA:O	1:C:725:ASP:HB2	2.18	0.44
1:B:369:ARG:HG3	3:B:778:HOH:O	2.17	0.44
1:B:395:HIS:HE1	3:B:3281:HOH:O	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335:GLU:OE1	1:D:369:ARG:HG2	2.17	0.44
1:C:448:MET:O	1:C:449[B]:HIS:HB2	2.18	0.44
1:A:144:LEU:HD11	1:A:370:VAL:HG13	1.98	0.44
1:A:274:ILE:HD12	2:A:760:HEM:HMB1	2.00	0.44
1:C:634:TYR:O	1:C:653:THR:HA	2.18	0.44
1:A:36:HIS:H	1:A:36:HIS:HD2	1.64	0.44
1:B:359:LEU:HD12	1:B:359:LEU:C	2.42	0.44
1:A:449[B]:HIS:CG	1:C:449[B]:HIS:CG	2.40	0.44
1:B:745:ILE:O	1:B:748:ILE:HG12	2.18	0.43
1:C:128:HIS:HA	1:C:168:THR:O	2.17	0.43
1:B:294:LYS:CD	3:B:3483:HOH:O	2.27	0.43
1:D:359:LEU:H	1:D:507:HIS:CD2	2.35	0.43
1:D:128:HIS:HA	1:D:168:THR:O	2.18	0.43
1:D:404:ASN:O	1:D:405:ASP:C	2.61	0.43
1:D:459:ASN:HD22	1:D:459:ASN:H	1.67	0.43
1:B:583:LYS:H	1:B:583:LYS:HZ2	1.65	0.43
3:B:1038:HOH:O	1:D:449[B]:HIS:HD2	2.01	0.43
1:D:696:ALA:HB1	1:D:728:PHE:CZ	2.54	0.43
1:B:128:HIS:HA	1:B:168:THR:O	2.19	0.43
1:C:461:GLU:HA	1:C:462:PRO:C	2.43	0.42
1:A:119:HIS:CE1	1:C:420:ILE:HG21	2.54	0.42
1:B:274:ILE:HD12	2:B:760:HEM:HMB1	1.99	0.42
1:D:207:PHE:O	1:D:249:THR:HA	2.19	0.42
1:C:552:LEU:HB2	3:C:3296:HOH:O	2.19	0.42
1:A:461:GLU:HA	1:A:462:PRO:C	2.43	0.42
1:C:404:ASN:O	1:C:405:ASP:C	2.61	0.42
1:D:115:ALA:O	1:D:119:HIS:HD2	2.02	0.42
1:A:128:HIS:HA	1:A:168:THR:O	2.20	0.42
1:A:666:ILE:HD11	1:A:732:LEU:CD2	2.50	0.42
1:B:533:LYS:CE	3:C:2623:HOH:O	2.14	0.42
1:C:440:TYR:CD2	1:C:440:TYR:C	2.98	0.42
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.55	0.42
1:B:725:ASP:OD2	1:B:727:SER:N	2.53	0.42
1:D:395:HIS:HE1	3:D:3312:HOH:O	2.03	0.42
1:A:725:ASP:HB2	1:A:726:GLY:H	1.66	0.41
1:C:704:PHE:O	1:C:707:THR:HG22	2.19	0.41
1:A:38:PRO:HG2	1:A:51:ALA:HB2	2.01	0.41
1:A:38:PRO:HA	1:A:48:GLN:OE1	2.21	0.41
1:C:612:ARG:HG3	3:C:3087:HOH:O	2.19	0.41
1:B:703:LYS:N	1:B:703:LYS:HD3	2.36	0.41
1:C:521:ARG:HD3	1:C:521:ARG:HA	1.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:HIS:CE1	1:A:507:HIS:HB3	2.55	0.41
1:B:97:ALA:O	1:B:101:GLY:HA3	2.20	0.41
1:B:724:ALA:O	1:B:725:ASP:C	2.63	0.41
1:D:267:ARG:HH21	1:D:267:ARG:HD2	1.75	0.41
1:D:440:TYR:CD2	1:D:440:TYR:C	2.98	0.41
1:B:52:PRO:HG3	3:D:1451:HOH:O	2.21	0.41
1:C:748:ILE:O	1:C:751:ILE:HG22	2.20	0.41
1:B:128:HIS:CE1	1:B:169:VAL:HG22	2.56	0.41
1:D:744:ARG:HA	1:D:747:LYS:HD3	2.02	0.41
1:C:440:TYR:OH	3:C:1028:HOH:O	2.22	0.40
1:A:37:ARG:HA	1:A:38:PRO:HD3	1.96	0.40
1:B:126:ILE:HG12	3:B:928:HOH:O	2.21	0.40
1:B:207:PHE:O	1:B:249:THR:HA	2.21	0.40
1:C:207:PHE:O	1:C:249:THR:HA	2.21	0.40
1:A:393:PRO:HD2	1:A:415:TYR:CD2	2.56	0.40
1:A:413:TYR:CE2	1:B:413:TYR:HE2	2.39	0.40
1:B:115:ALA:O	1:B:119:HIS:HD2	2.04	0.40
1:C:578:ASP:HB3	1:C:582:LEU:O	2.21	0.40

All (3) 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]	1.97	0.23
3:A:2805:HOH:O	3:D:2468:HOH:O[1_455]	1.97	0.23
1:A:59:ASP:OD1	1:B:369:ARG:NH1[2_545]	2.19	0.01

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	726/753 (96%)	709 (98%)	16 (2%)	1 (0%)	48 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	726/753 (96%)	706 (97%)	17 (2%)	3 (0%)	30	11
1	C	725/753 (96%)	705 (97%)	18 (2%)	2 (0%)	36	16
1	D	725/753 (96%)	708 (98%)	16 (2%)	1 (0%)	48	22
All	All	2902/3012 (96%)	2828 (98%)	67 (2%)	7 (0%)	43	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	725	ASP
1	C	75	SER
1	A	75	SER
1	B	75	SER
1	C	725	ASP
1	B	612	ARG
1	D	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	612/634 (96%)	604 (99%)	8 (1%)	61	31
1	B	612/634 (96%)	591 (97%)	21 (3%)	32	5
1	C	611/634 (96%)	595 (97%)	16 (3%)	40	10
1	D	611/634 (96%)	600 (98%)	11 (2%)	51	19
All	All	2446/2536 (96%)	2390 (98%)	56 (2%)	44	13

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	LYS
1	A	191	THR
1	A	198	LEU
1	A	205	ILE

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Mol	Chain	Res	Type
1	A	252	ASN
1	A	440	TYR
1	A	459	ASN
1	A	617	LEU
1	B	191	THR
1	B	205	ILE
1	B	213	LYS
1	B	252	ASN
1	B	283	GLU
1	B	285	LYS
1	B	344	GLU
1	B	369	ARG
1	B	432	PRO
1	B	440	TYR
1	B	459	ASN
1	B	565	GLU
1	B	568	ASP
1	B	583	LYS
1	B	593	ILE
1	B	616	LEU
1	B	639	GLU
1	B	703	LYS
1	B	713	GLN
1	B	732	LEU
1	B	751	ILE
1	C	191	THR
1	C	205	ILE
1	C	252	ASN
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	517	PRO
1	C	521	ARG
1	C	537	PRO
1	C	636	ARG
1	C	725	ASP
1	C	732	LEU
1	C	750	LYS
1	D	48	GLN

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Mol	Chain	Res	Type
1	D	191	THR
1	D	205	ILE
1	D	252	ASN
1	D	344	GLU
1	D	440	TYR
1	D	459	ASN
1	D	552	LEU
1	D	574	THR
1	D	747	LYS
1	D	749	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	119	HIS
1	A	139	GLN
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	A	546	GLN
1	B	77	ASN
1	B	157	ASN
1	B	252	ASN
1	B	419	GLN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	B	713	GLN
1	C	77	ASN
1	C	119	HIS
1	C	252	ASN
1	C	419	GLN
1	C	459	ASN
1	C	507	HIS
1	C	546	GLN
1	C	629	HIS
1	C	671	ASN
1	C	682	ASN
1	D	48	GLN
1	D	157	ASN
1	D	252	ASN

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Mol	Chain	Res	Type
1	D	459	ASN
1	D	507	HIS
1	D	546	GLN
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	D	669	1	6,8,9	2.87	2 (33%)	7,11,13	1.72	2 (28%)
1	OCS	C	669	1	6,8,9	1.86	2 (33%)	7,11,13	1.94	2 (28%)
1	OCS	B	669	1	6,8,9	2.02	1 (16%)	7,11,13	3.22	3 (42%)
1	OCS	A	669	1	6,8,9	2.53	2 (33%)	7,11,13	1.77	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	D	669	1	-	1/4/7/9	-
1	OCS	C	669	1	-	1/4/7/9	-
1	OCS	B	669	1	-	3/4/7/9	-
1	OCS	A	669	1	-	3/4/7/9	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	669	OCS	CB-CA	6.09	1.58	1.53
1	B	669	OCS	OD2-SG	4.53	1.64	1.47
1	A	669	OCS	OD2-SG	4.27	1.63	1.47
1	A	669	OCS	CB-CA	3.86	1.56	1.53
1	C	669	OCS	CB-CA	3.16	1.55	1.53
1	D	669	OCS	OD2-SG	2.98	1.58	1.47
1	C	669	OCS	OD2-SG	2.83	1.57	1.47

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	669	OCS	OD1-SG-CB	5.95	115.65	106.76
1	B	669	OCS	OD3-SG-CB	-4.50	100.04	106.76
1	B	669	OCS	OD2-SG-CB	-3.44	99.32	105.97
1	C	669	OCS	OD1-SG-CB	-3.38	101.72	106.76
1	D	669	OCS	OD3-SG-CB	-3.18	102.01	106.76
1	C	669	OCS	CA-CB-SG	3.15	118.29	113.61
1	A	669	OCS	CA-CB-SG	2.90	117.92	113.61
1	D	669	OCS	OD2-SG-OD3	2.28	117.09	111.40
1	A	669	OCS	OD2-SG-OD1	2.15	116.79	111.40

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	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	A	760	1	50,50,50	2.00	17 (34%)	67,82,82	2.03	22 (32%)
2	HEM	C	760	1	50,50,50	1.81	13 (26%)	67,82,82	1.93	18 (26%)
2	HEM	B	760	1	50,50,50	1.55	10 (20%)	67,82,82	1.67	14 (20%)
2	HEM	D	760	1	50,50,50	1.62	14 (28%)	67,82,82	2.07	20 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	760	1	-	3/14/54/54	-
2	HEM	C	760	1	-	3/14/54/54	-
2	HEM	B	760	1	-	3/14/54/54	-
2	HEM	D	760	1	-	3/14/54/54	-

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HEM	FE-NB	4.84	2.09	1.94
2	A	760	HEM	C1C-NC	4.20	1.47	1.39
2	A	760	HEM	C3D-C2D	4.08	1.45	1.36
2	B	760	HEM	FE-NB	4.04	2.07	1.94
2	A	760	HEM	C4A-NA	4.00	1.47	1.39
2	D	760	HEM	FE-NB	3.89	2.06	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	760	HEM	CHA-C4D	3.58	1.45	1.38
2	A	760	HEM	FE-ND	3.31	2.05	1.94
2	C	760	HEM	FE-ND	3.29	2.05	1.94
2	C	760	HEM	FE-NB	3.24	2.04	1.94
2	A	760	HEM	C1A-NA	3.17	1.45	1.39
2	C	760	HEM	C3C-C2C	3.13	1.43	1.37
2	C	760	HEM	CHB-C4A	3.01	1.46	1.39
2	A	760	HEM	CHA-C4D	3.01	1.44	1.38
2	C	760	HEM	CHB-C1B	2.96	1.44	1.38
2	C	760	HEM	CHC-C1C	2.94	1.44	1.38
2	D	760	HEM	C1C-NC	2.93	1.45	1.39
2	C	760	HEM	C1C-NC	2.92	1.45	1.39
2	B	760	HEM	FE-NC	2.76	2.04	1.95
2	B	760	HEM	O1A-CGA	2.73	1.31	1.22
2	D	760	HEM	C3C-C2C	2.72	1.42	1.37
2	A	760	HEM	CHB-C1B	2.71	1.43	1.38
2	B	760	HEM	C4A-C3A	2.68	1.49	1.43
2	B	760	HEM	CHB-C1B	2.64	1.43	1.38
2	D	760	HEM	FE-NC	2.61	2.03	1.95
2	D	760	HEM	C1B-C2B	2.58	1.49	1.44
2	D	760	HEM	CHD-C1D	2.58	1.45	1.39
2	A	760	HEM	CHD-C1D	2.56	1.45	1.39
2	A	760	HEM	C2A-C3A	2.53	1.45	1.38
2	C	760	HEM	C4D-C3D	2.47	1.49	1.45
2	C	760	HEM	CHC-C4B	2.42	1.44	1.39
2	A	760	HEM	CMC-C2C	2.42	1.55	1.50
2	B	760	HEM	CHD-C1D	2.41	1.44	1.39
2	D	760	HEM	C3D-C2D	2.40	1.42	1.36
2	A	760	HEM	C1B-C2B	2.38	1.49	1.44
2	C	760	HEM	C3C-C4C	2.37	1.50	1.46
2	B	760	HEM	CHB-C4A	2.36	1.44	1.39
2	D	760	HEM	CBA-CAA	2.36	1.60	1.51
2	D	760	HEM	FE-NA	2.36	2.02	1.95
2	A	760	HEM	CMB-C2B	-2.30	1.46	1.50
2	D	760	HEM	CHA-C4D	2.29	1.43	1.38
2	D	760	HEM	O2A-CGA	-2.28	1.23	1.30
2	B	760	HEM	FE-ND	2.24	2.01	1.94
2	B	760	HEM	CHA-C4D	2.24	1.43	1.38
2	B	760	HEM	C4A-NA	2.18	1.43	1.39
2	D	760	HEM	FE-ND	2.17	2.01	1.94
2	C	760	HEM	CHD-C1D	2.15	1.44	1.39
2	A	760	HEM	C3C-C2C	2.14	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HEM	FE-NA	2.14	2.02	1.95
2	D	760	HEM	CMA-C3A	-2.14	1.46	1.50
2	C	760	HEM	FE-NC	2.11	2.02	1.95
2	D	760	HEM	CHB-C1B	2.10	1.42	1.38
2	A	760	HEM	C4C-NC	-2.08	1.35	1.39
2	A	760	HEM	FE-NC	2.02	2.01	1.95

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	760	HEM	C3D-C4D-ND	6.57	117.38	110.17
2	C	760	HEM	C3B-C2B-C1B	-6.02	101.89	106.41
2	A	760	HEM	C2D-C1D-ND	5.53	116.30	109.90
2	A	760	HEM	C1D-C2D-C3D	-5.28	101.42	106.98
2	C	760	HEM	C2D-C1D-ND	4.86	115.52	109.90
2	D	760	HEM	C3B-C2B-C1B	-4.42	103.09	106.41
2	A	760	HEM	C3D-C4D-ND	4.38	114.97	110.17
2	A	760	HEM	CBD-CAD-C3D	-4.29	100.67	112.53
2	A	760	HEM	CAA-CBA-CGA	-4.06	102.89	113.67
2	B	760	HEM	CAA-CBA-CGA	-4.04	102.95	113.67
2	A	760	HEM	C3B-C2B-C1B	-4.01	103.40	106.41
2	C	760	HEM	C3B-C4B-NB	3.95	112.30	109.47
2	B	760	HEM	CHC-C4B-NB	-3.91	120.22	124.42
2	D	760	HEM	C4D-ND-C1D	-3.90	100.59	105.21
2	D	760	HEM	CAA-CBA-CGA	-3.88	103.36	113.67
2	D	760	HEM	CHA-C4D-ND	-3.84	119.62	124.37
2	D	760	HEM	CBD-CAD-C3D	-3.84	101.92	112.53
2	C	760	HEM	C2A-C1A-NA	3.71	114.27	110.15
2	C	760	HEM	CBD-CAD-C3D	-3.67	102.38	112.53
2	B	760	HEM	C3B-C2B-C1B	-3.56	103.74	106.41
2	D	760	HEM	C4C-C3C-C2C	-3.56	103.73	106.81
2	A	760	HEM	O2D-CGD-CBD	3.44	124.88	114.00
2	D	760	HEM	C4D-C3D-C2D	-3.38	101.97	106.89
2	C	760	HEM	CHD-C1D-C2D	-3.38	119.70	125.03
2	C	760	HEM	CAA-CBA-CGA	-3.34	104.82	113.67
2	D	760	HEM	CHB-C1B-NB	3.33	128.48	124.37
2	D	760	HEM	C2D-C1D-ND	3.23	113.64	109.90
2	C	760	HEM	C2B-C1B-NB	3.22	113.54	109.84
2	B	760	HEM	CBD-CAD-C3D	-3.17	103.75	112.53
2	A	760	HEM	O2D-CGD-O1D	-3.16	115.20	123.33
2	A	760	HEM	C4C-C3C-C2C	-3.16	104.08	106.81
2	D	760	HEM	CHD-C1D-C2D	-3.06	120.20	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	760	HEM	CHA-C4D-ND	3.06	128.15	124.37
2	A	760	HEM	C4B-C3B-C2B	3.04	110.08	107.28
2	A	760	HEM	CHB-C1B-NB	3.01	128.09	124.37
2	A	760	HEM	CHD-C4C-NC	-3.01	121.18	124.45
2	B	760	HEM	CHA-C4D-C3D	-3.00	119.70	125.23
2	A	760	HEM	C4D-ND-C1D	-2.85	101.83	105.21
2	D	760	HEM	O1A-CGA-CBA	-2.85	114.05	123.09
2	C	760	HEM	C1D-C2D-C3D	-2.84	103.99	106.98
2	A	760	HEM	CMD-C2D-C1D	2.80	129.40	125.03
2	B	760	HEM	CHD-C4C-NC	2.74	127.44	124.45
2	B	760	HEM	O2D-CGD-CBD	2.74	122.66	114.00
2	C	760	HEM	CHB-C1B-C2B	-2.73	119.20	126.95
2	D	760	HEM	C4B-C3B-C2B	2.66	109.73	107.28
2	B	760	HEM	CHD-C4C-C3C	-2.63	120.77	125.21
2	D	760	HEM	O2D-CGD-CBD	2.63	122.31	114.00
2	C	760	HEM	C4A-CHB-C1B	-2.57	120.21	126.25
2	A	760	HEM	CHD-C1D-C2D	-2.55	121.00	125.03
2	B	760	HEM	C2B-C1B-NB	2.52	112.74	109.84
2	C	760	HEM	CMB-C2B-C3B	2.46	134.39	128.43
2	D	760	HEM	CAD-C3D-C2D	2.43	132.41	127.87
2	C	760	HEM	C3D-C4D-ND	2.37	112.77	110.17
2	C	760	HEM	C4A-NA-C1A	-2.36	101.98	105.82
2	B	760	HEM	CHB-C1B-C2B	-2.34	120.30	126.95
2	C	760	HEM	O1A-CGA-CBA	-2.29	115.84	123.09
2	C	760	HEM	CHB-C1B-NB	2.28	127.19	124.37
2	D	760	HEM	O2D-CGD-O1D	-2.28	117.48	123.33
2	D	760	HEM	CHB-C1B-C2B	-2.26	120.51	126.95
2	C	760	HEM	C4D-ND-C1D	-2.24	102.55	105.21
2	D	760	HEM	CBB-CAB-C3B	-2.24	116.34	127.53
2	B	760	HEM	CMA-C3A-C2A	2.21	130.32	125.62
2	D	760	HEM	CMB-C2B-C3B	2.21	133.76	128.43
2	A	760	HEM	C4C-NC-C1C	-2.20	102.24	105.82
2	D	760	HEM	O2A-CGA-CBA	2.19	120.93	114.00
2	A	760	HEM	C1B-NB-C4B	2.17	107.77	105.21
2	B	760	HEM	C2A-C1A-NA	2.11	112.49	110.15
2	A	760	HEM	CMB-C2B-C3B	2.10	133.51	128.43
2	A	760	HEM	CHB-C1B-C2B	-2.08	121.04	126.95
2	B	760	HEM	CHB-C1B-NB	2.08	126.94	124.37
2	A	760	HEM	CAD-CBD-CGD	-2.07	108.16	113.67
2	A	760	HEM	C3B-C4B-NB	-2.05	108.00	109.47
2	A	760	HEM	C4A-CHB-C1B	-2.04	121.46	126.25
2	C	760	HEM	CHA-C4D-ND	-2.03	121.85	124.37

There are no chirality outliers.

All (12) torsion outliers are listed below:

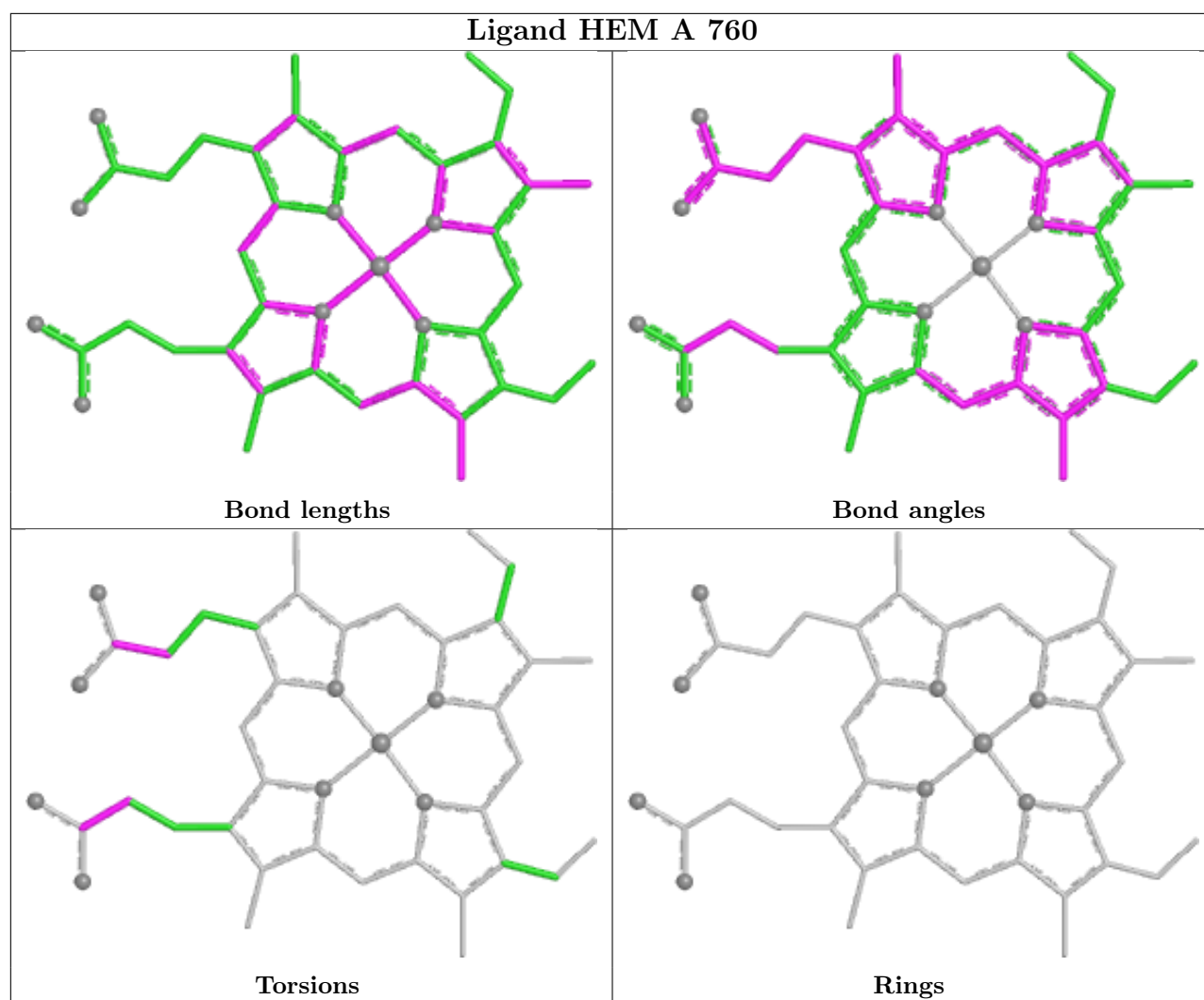
Mol	Chain	Res	Type	Atoms
2	A	760	HEM	CAA-CBA-CGA-O1A
2	D	760	HEM	CAA-CBA-CGA-O1A
2	B	760	HEM	CAA-CBA-CGA-O1A
2	B	760	HEM	CAA-CBA-CGA-O2A
2	C	760	HEM	CAA-CBA-CGA-O1A
2	C	760	HEM	CAA-CBA-CGA-O2A
2	D	760	HEM	CAA-CBA-CGA-O2A
2	A	760	HEM	CAA-CBA-CGA-O2A
2	B	760	HEM	CAD-CBD-CGD-O2D
2	A	760	HEM	CAD-CBD-CGD-O2D
2	C	760	HEM	CAD-CBD-CGD-O2D
2	D	760	HEM	CAD-CBD-CGD-O1D

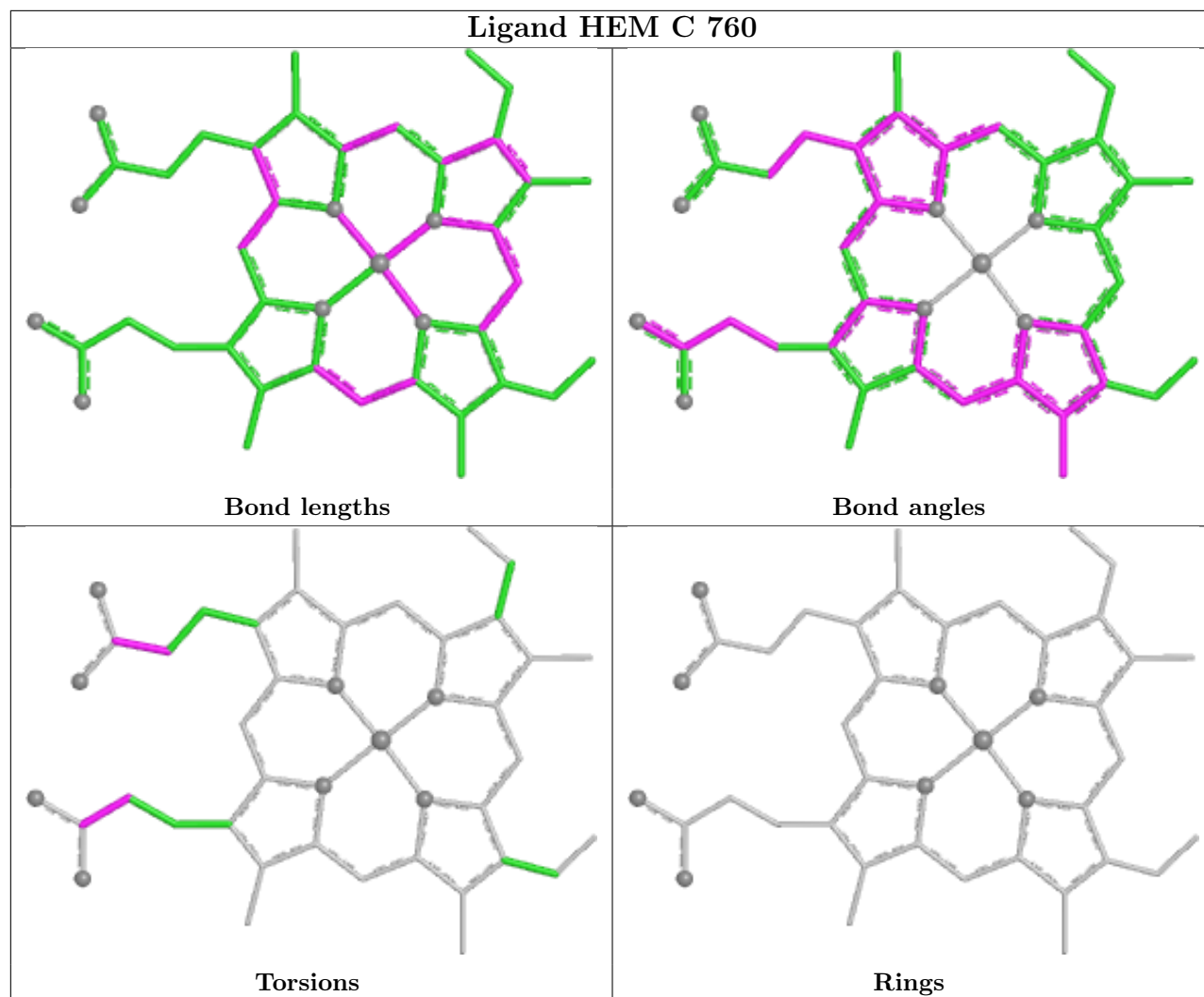
There are no ring outliers.

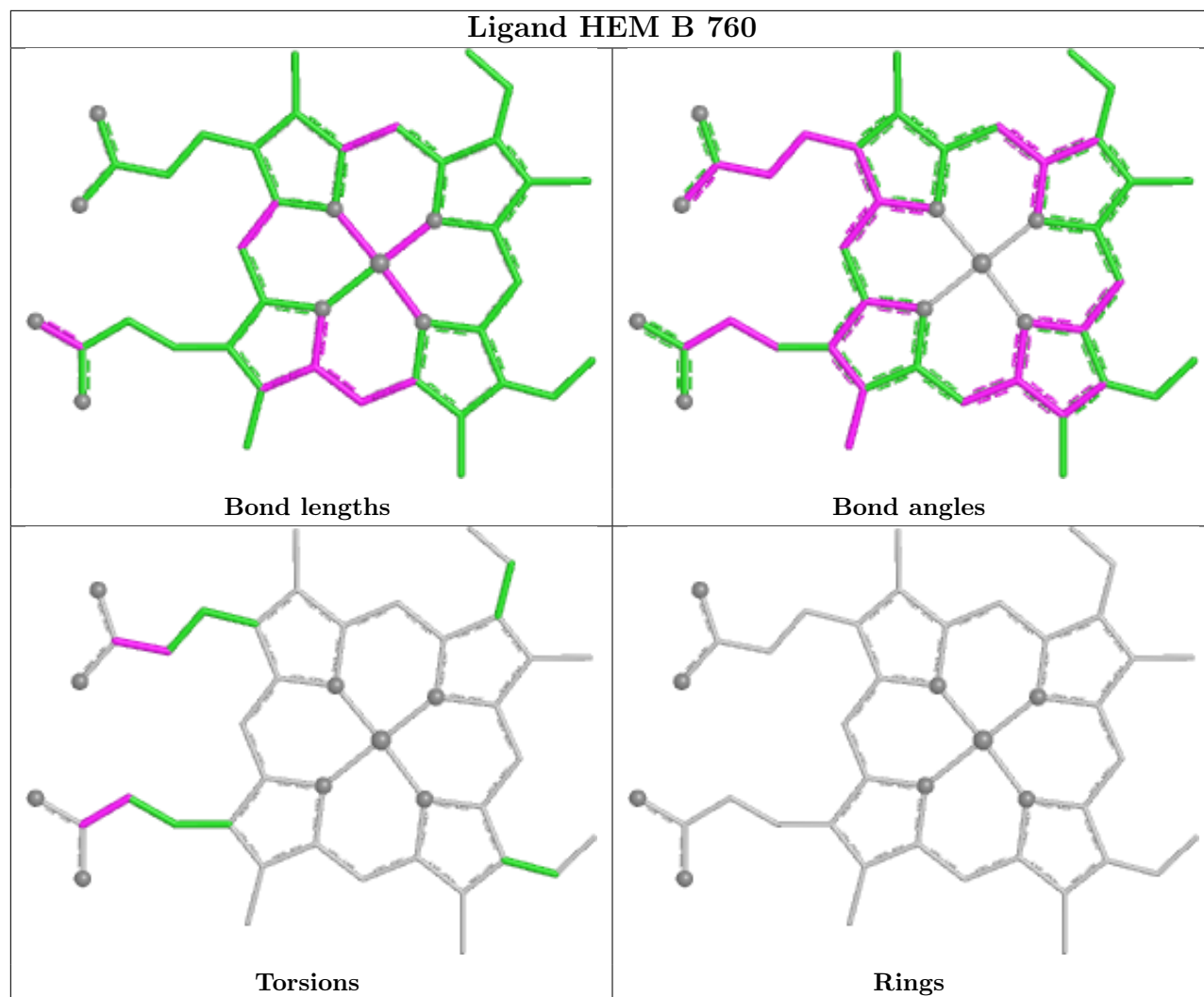
4 monomers are involved in 4 short contacts:

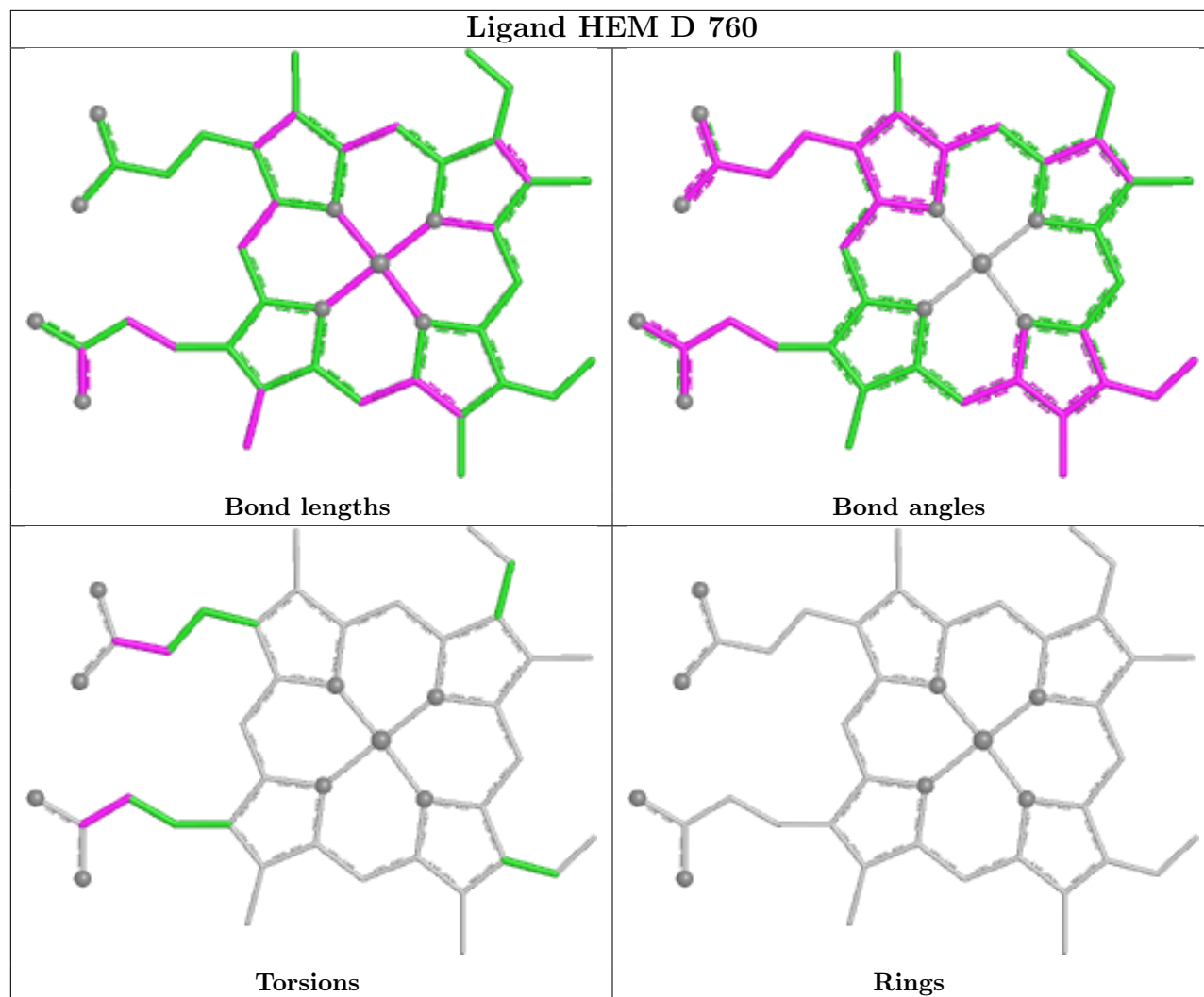
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	760	HEM	1	0
2	C	760	HEM	1	0
2	B	760	HEM	1	0
2	D	760	HEM	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	725/753 (96%)	-0.68	1 (0%) 92 93	6, 11, 25, 52	4 (0%)
1	B	725/753 (96%)	-0.49	5 (0%) 84 87	6, 13, 34, 56	4 (0%)
1	C	725/753 (96%)	-0.53	5 (0%) 84 87	6, 13, 33, 53	3 (0%)
1	D	725/753 (96%)	-0.64	5 (0%) 84 87	6, 11, 27, 56	3 (0%)
All	All	2900/3012 (96%)	-0.58	16 (0%) 85 89	6, 12, 31, 56	14 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	751	ILE	3.4
1	D	751	ILE	3.1
1	A	751	ILE	3.0
1	D	749	ASP	2.7
1	B	726	GLY	2.5
1	C	725	ASP	2.5
1	D	28	SER	2.3
1	D	750	LYS	2.2
1	C	594	PRO	2.2
1	B	612	ARG	2.2
1	B	568	ASP	2.1
1	B	751	ILE	2.1
1	C	726	GLY	2.1
1	C	750	LYS	2.0
1	B	673	ALA	2.0
1	D	712	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	0.94	0.09	27,28,33,38	0
1	OCS	C	669	9/10	0.94	0.08	27,30,36,39	0
1	OCS	D	669	9/10	0.95	0.10	19,21,27,29	0
1	OCS	A	669	9/10	0.96	0.08	16,19,26,29	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

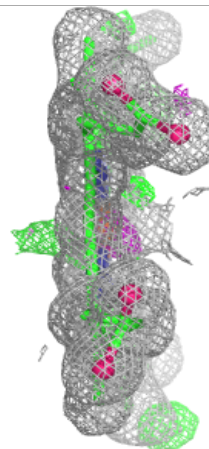
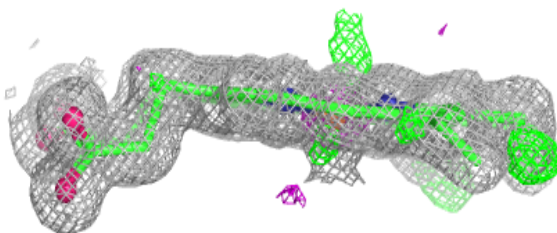
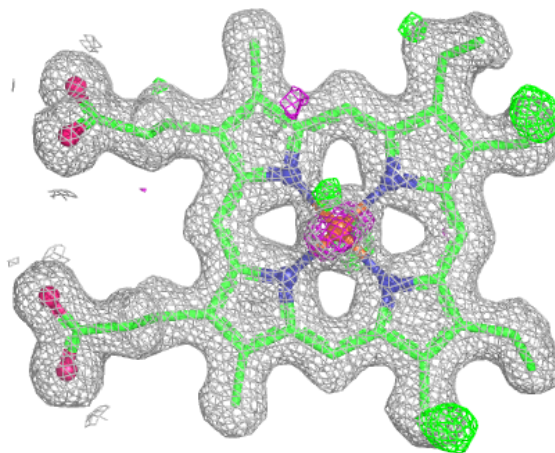
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	760	43/43	0.99	0.04	5,7,9,15	0
2	HEM	B	760	43/43	0.99	0.04	6,8,10,16	0
2	HEM	C	760	43/43	0.99	0.04	6,8,10,17	0
2	HEM	D	760	43/43	0.99	0.03	5,7,8,14	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.

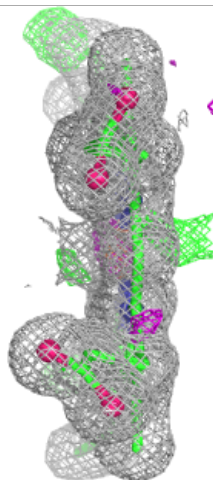
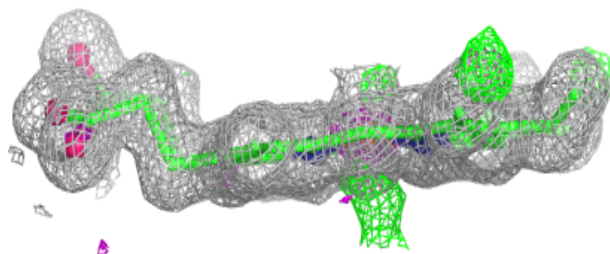
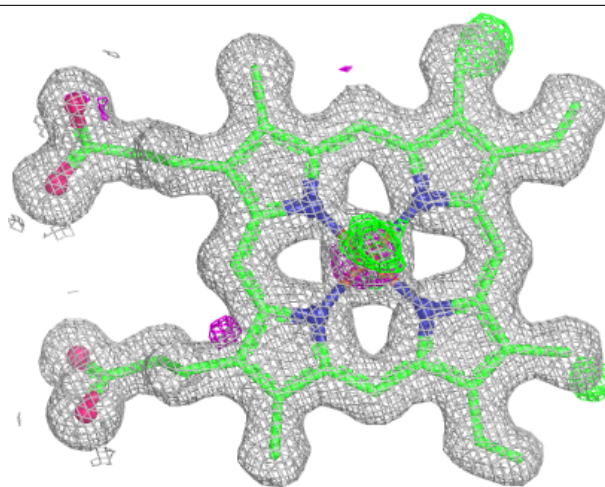
Electron density around HEM A 760:

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



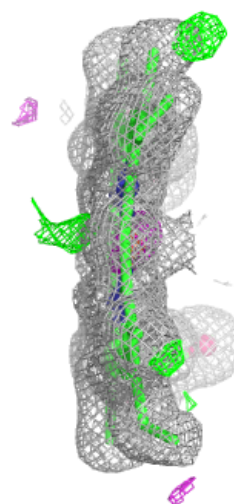
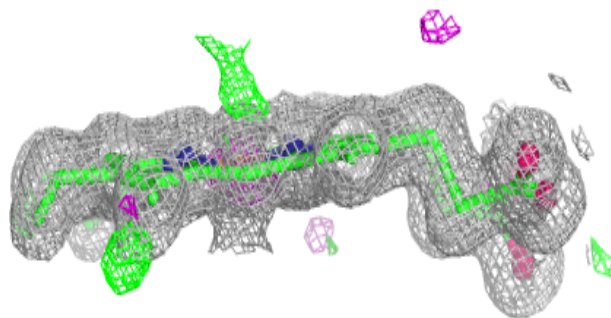
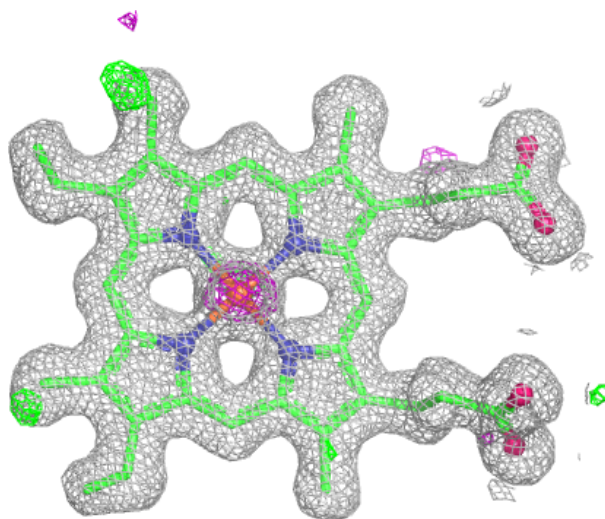
Electron density around HEM B 760:

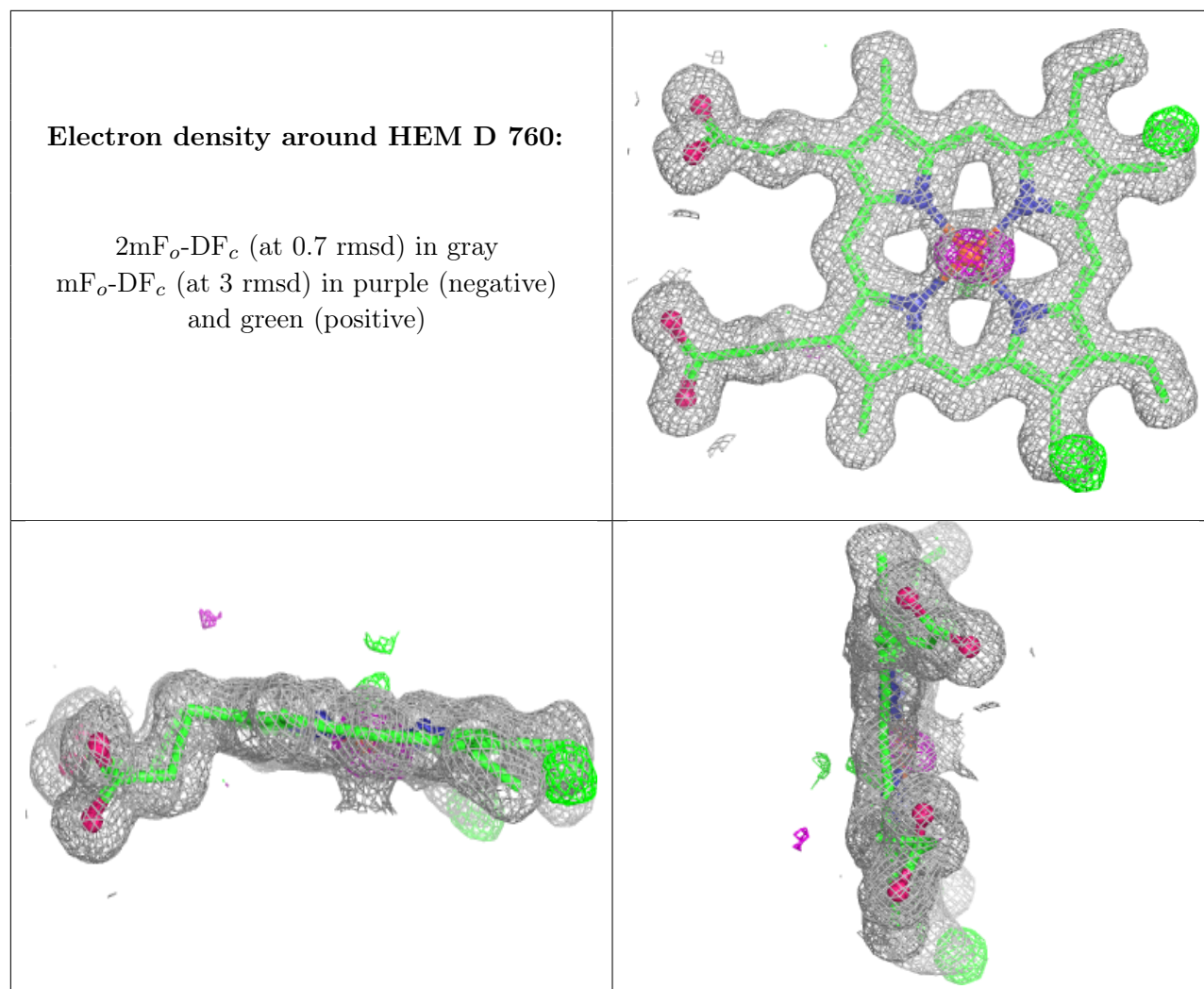
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM C 760:

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





6.5 Other polymers ⓘ

There are no such residues in this entry.