



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:50 PM UTC

PDB ID : 3TTT / pdb_00003ttt
Title : Structure of F413Y variant of E. coli KatE
Authors : Loewen, P.C.; Jha, V.
Deposited on : 2011-09-15
Resolution : 1.58 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

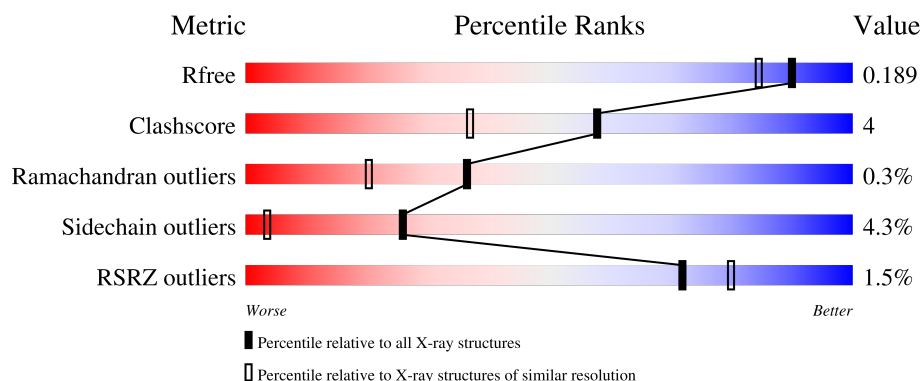
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.58 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	2% 83% 11% ..
1	B	753	% 82% 13% ..
1	C	753	% 80% 14% ..
1	D	753	% 81% 13% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26162 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.

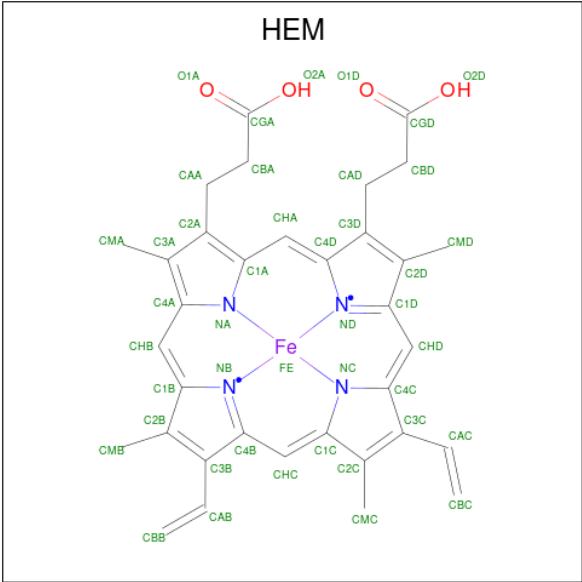
- Molecule 1 is a protein called Catalase HP11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	1	0
			5745	3647	1006	1080	12			
1	B	726	Total	C	N	O	S	0	1	0
			5746	3648	1006	1080	12			
1	C	726	Total	C	N	O	S	0	1	0
			5745	3647	1006	1080	12			
1	D	726	Total	C	N	O	S	0	1	0
			5746	3648	1006	1080	12			

There are 4 discrepancies between the modelled and reference sequences:

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

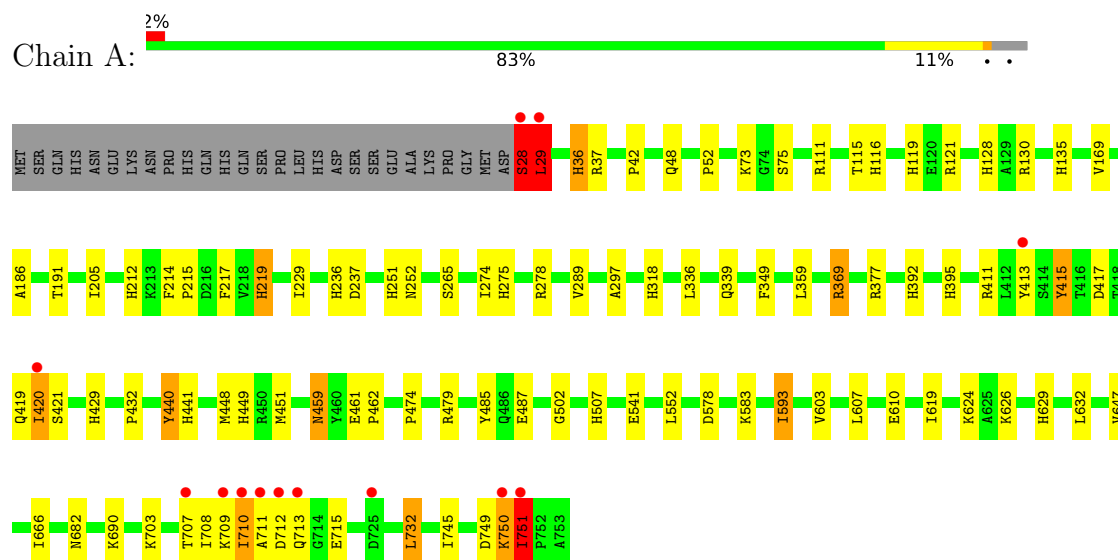
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	815	Total	O	0	0
			815	815		
3	B	673	Total	O	0	0
			673	673		
3	C	737	Total	O	0	0
			737	737		
3	D	783	Total	O	0	0
			783	783		

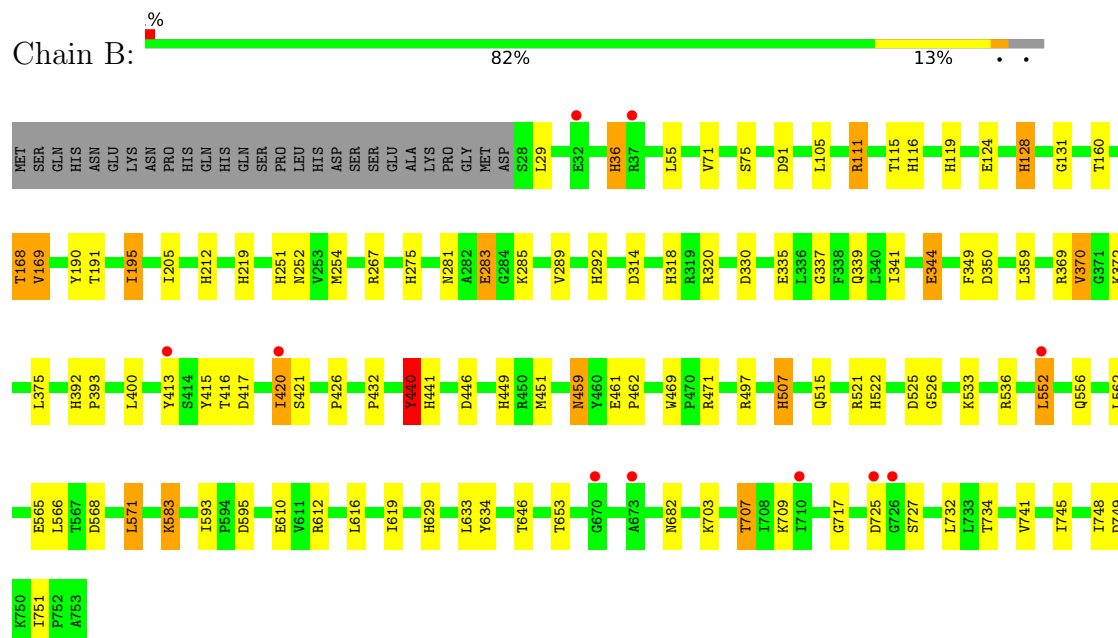
3 Residue-property plots [i](#)

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.

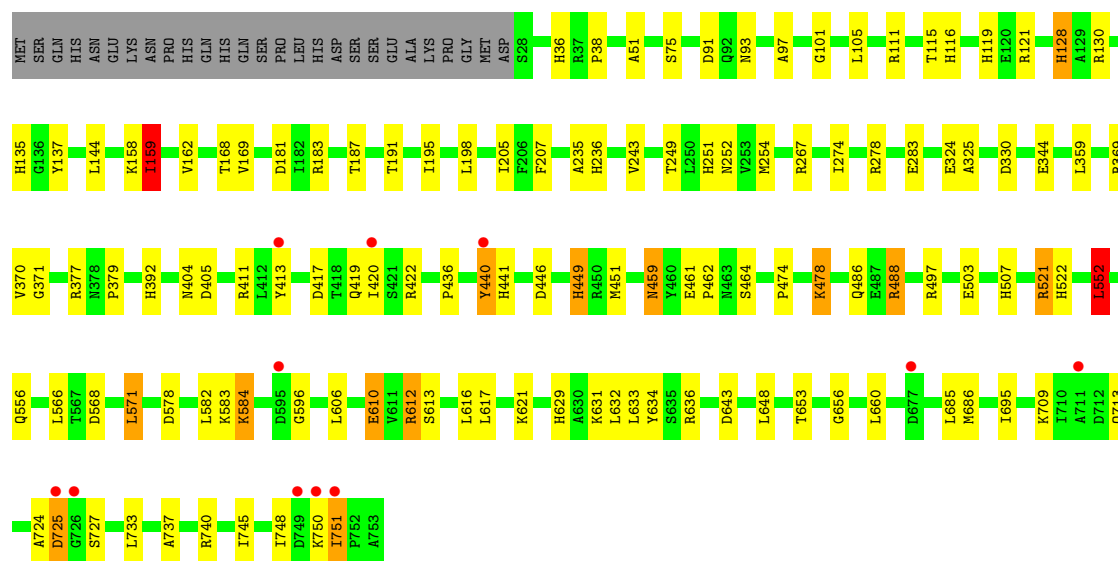
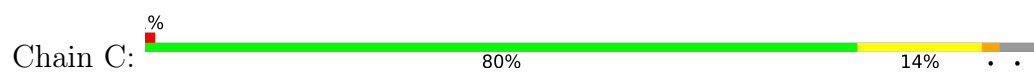
• Molecule 1: Catalase HPII



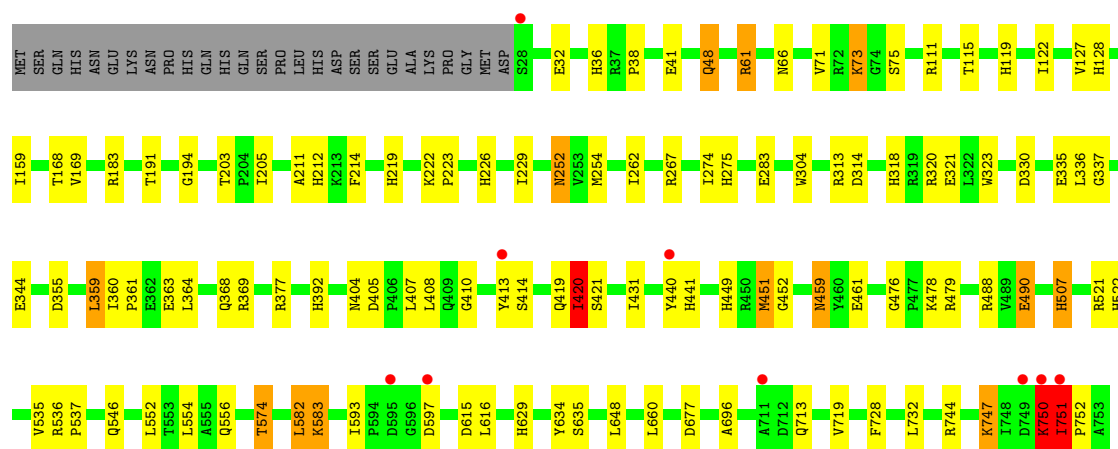
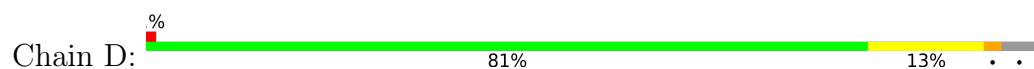
• Molecule 1: Catalase HPII



• Molecule 1: Catalase HPII



• Molecule 1: Catalase HPII



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 133.33Å 122.16Å 90.00° 109.58° 90.00°	Depositor
Resolution (Å)	29.23 – 1.58 29.23 – 1.58	Depositor EDS
% Data completeness (in resolution range)	98.8 (29.23-1.58) 98.7 (29.23-1.58)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 1.58Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.157 , 0.189 0.157 , 0.189	Depositor DCC
R_{free} test set	18949 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	11.8	Xtriage
Anisotropy	0.077	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26162	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 4.08% 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	1.61	41/5906 (0.7%)	1.34	15/8030 (0.2%)
1	B	1.51	43/5906 (0.7%)	1.31	16/8030 (0.2%)
1	C	1.49	28/5906 (0.5%)	1.30	18/8030 (0.2%)
1	D	1.58	41/5906 (0.7%)	1.33	21/8030 (0.3%)
All	All	1.55	153/23624 (0.6%)	1.32	70/32120 (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	A	0	2
1	C	0	3
All	All	0	5

All (153) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	745	ILE	CA-CB	10.24	1.59	1.54
1	A	441	HIS	ND1-CE1	8.70	1.41	1.32
1	B	441	HIS	ND1-CE1	8.49	1.41	1.32
1	D	275	HIS	ND1-CE1	8.18	1.40	1.32
1	D	522	HIS	ND1-CE1	8.02	1.40	1.32
1	B	392	HIS	ND1-CE1	7.52	1.40	1.32
1	A	29	LEU	N-CA	-7.47	1.36	1.45
1	A	48	GLN	N-CA	7.43	1.53	1.45
1	C	392	HIS	ND1-CE1	7.18	1.39	1.32
1	B	341	ILE	CA-C	-7.11	1.47	1.52
1	C	441	HIS	ND1-CE1	7.03	1.39	1.32
1	B	522	HIS	ND1-CE1	6.99	1.39	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	128	HIS	ND1-CE1	6.98	1.39	1.32
1	D	377	ARG	CZ-NH1	6.83	1.42	1.32
1	D	414	SER	C-O	6.82	1.32	1.24
1	B	314	ASP	N-CA	6.76	1.53	1.46
1	B	168	THR	C-O	6.74	1.31	1.23
1	A	417	ASP	CA-C	6.72	1.61	1.52
1	A	229	ILE	C-O	-6.71	1.19	1.24
1	A	359	LEU	N-CA	6.69	1.53	1.45
1	D	304	TRP	N-CA	6.68	1.54	1.46
1	D	203	THR	N-CA	6.64	1.51	1.45
1	C	497	ARG	CZ-NH2	6.64	1.42	1.33
1	B	131	GLY	N-CA	6.60	1.52	1.45
1	B	128	HIS	ND1-CE1	6.56	1.39	1.32
1	C	324	GLU	N-CA	6.54	1.54	1.46
1	D	419	GLN	CA-CB	6.53	1.64	1.53
1	A	42	PRO	C-O	6.52	1.30	1.23
1	D	359	LEU	N-CA	6.44	1.53	1.45
1	D	318	HIS	ND1-CE1	6.43	1.39	1.32
1	A	219	HIS	CD2-NE2	6.43	1.45	1.37
1	A	339	GLN	N-CA	6.42	1.54	1.46
1	B	471	ARG	CZ-NH2	6.39	1.41	1.33
1	D	194	GLY	N-CA	6.38	1.50	1.45
1	D	536	ARG	N-CA	6.36	1.53	1.46
1	C	159	ILE	CB-CG1	-6.36	1.40	1.53
1	A	186	ALA	N-CA	6.35	1.53	1.46
1	D	392	HIS	ND1-CE1	6.33	1.38	1.32
1	D	212	HIS	ND1-CE1	6.28	1.38	1.32
1	D	226	HIS	ND1-CE1	6.23	1.38	1.32
1	B	318	HIS	ND1-CE1	6.21	1.38	1.32
1	A	275	HIS	ND1-CE1	6.19	1.38	1.32
1	A	135	HIS	CG-CD2	6.17	1.42	1.35
1	D	719	VAL	C-O	-6.17	1.17	1.24
1	A	629	HIS	ND1-CE1	6.14	1.38	1.32
1	C	371	GLY	N-CA	6.11	1.52	1.45
1	A	219	HIS	ND1-CE1	6.09	1.38	1.32
1	B	497	ARG	CZ-NH2	6.02	1.41	1.33
1	C	116	HIS	ND1-CE1	5.99	1.38	1.32
1	A	395	HIS	ND1-CE1	5.95	1.38	1.32
1	C	36	HIS	CE1-NE2	5.92	1.38	1.32
1	B	124	GLU	N-CA	5.92	1.53	1.45
1	C	235	ALA	N-CA	5.91	1.54	1.46
1	D	212	HIS	CG-ND1	-5.90	1.31	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	HIS	ND1-CE1	5.82	1.38	1.32
1	A	429	HIS	ND1-CE1	5.82	1.38	1.32
1	D	593	ILE	N-CA	5.81	1.50	1.46
1	A	336	LEU	N-CA	5.76	1.53	1.46
1	D	122	ILE	CA-C	5.76	1.58	1.52
1	D	36	HIS	ND1-CE1	5.75	1.38	1.32
1	A	502	GLY	N-CA	5.74	1.53	1.45
1	B	515	GLN	C-O	5.72	1.31	1.23
1	A	217	PHE	N-CA	-5.71	1.39	1.46
1	C	236	HIS	ND1-CE1	5.68	1.38	1.32
1	A	419	GLN	CA-CB	5.66	1.62	1.53
1	A	377	ARG	CZ-NH1	5.66	1.40	1.32
1	D	128	HIS	CD2-NE2	5.65	1.44	1.37
1	D	169	VAL	N-CA	5.64	1.53	1.46
1	A	212	HIS	ND1-CE1	5.64	1.38	1.32
1	A	52	PRO	C-O	5.63	1.30	1.23
1	C	464	SER	N-CA	5.63	1.53	1.46
1	B	522	HIS	CG-CD2	5.62	1.42	1.35
1	B	400	LEU	N-CA	5.62	1.52	1.45
1	A	135	HIS	CE1-NE2	5.60	1.38	1.32
1	D	507	HIS	ND1-CE1	5.58	1.38	1.32
1	B	169	VAL	N-CA	5.57	1.53	1.46
1	A	289	VAL	CA-C	5.56	1.59	1.52
1	B	275	HIS	ND1-CE1	5.56	1.38	1.32
1	C	632	LEU	C-O	5.55	1.30	1.24
1	A	629	HIS	CG-CD2	5.54	1.42	1.35
1	C	522	HIS	CG-CD2	5.54	1.42	1.35
1	B	212	HIS	ND1-CE1	5.54	1.38	1.32
1	C	135	HIS	ND1-CE1	5.54	1.38	1.32
1	C	325	ALA	N-CA	5.53	1.53	1.46
1	B	36	HIS	CG-CD2	5.50	1.42	1.35
1	A	624	LYS	C-O	5.50	1.30	1.24
1	A	411	ARG	CA-C	-5.49	1.45	1.52
1	A	318	HIS	ND1-CE1	5.48	1.38	1.32
1	B	36	HIS	CE1-NE2	5.46	1.38	1.32
1	A	36	HIS	ND1-CE1	5.44	1.38	1.32
1	A	275	HIS	CE1-NE2	5.44	1.38	1.32
1	B	320	ARG	CZ-NH2	5.43	1.40	1.33
1	B	441	HIS	CG-CD2	5.43	1.41	1.35
1	A	474	PRO	CA-CB	5.40	1.58	1.53
1	B	416	THR	N-CA	5.40	1.53	1.46
1	C	251	HIS	C-O	5.39	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	411	ARG	CA-C	-5.39	1.45	1.52
1	C	740	ARG	CZ-NH2	5.38	1.40	1.33
1	D	314	ASP	N-CA	5.38	1.51	1.46
1	C	135	HIS	CG-ND1	-5.35	1.32	1.38
1	D	408	LEU	N-CA	5.35	1.52	1.46
1	D	593	ILE	CA-CB	5.34	1.59	1.53
1	A	593	ILE	N-CA	5.32	1.50	1.46
1	B	375	LEU	N-CA	5.32	1.53	1.46
1	D	183	ARG	CD-NE	5.32	1.53	1.46
1	C	130	ARG	N-CA	5.31	1.52	1.46
1	D	214	PHE	C-O	-5.30	1.19	1.24
1	B	55	LEU	CA-C	5.30	1.60	1.52
1	B	526	GLY	N-CA	5.28	1.53	1.45
1	B	507	HIS	ND1-CE1	5.28	1.37	1.32
1	D	337	GLY	CA-C	-5.28	1.46	1.51
1	B	292	HIS	CG-CD2	5.27	1.41	1.35
1	B	440	TYR	CE1-CZ	5.26	1.50	1.38
1	B	522	HIS	CE1-NE2	5.24	1.37	1.32
1	D	431	ILE	N-CA	5.24	1.53	1.47
1	A	116	HIS	CE1-NE2	5.22	1.37	1.32
1	D	507	HIS	CE1-NE2	5.22	1.37	1.32
1	C	128	HIS	ND1-CE1	5.21	1.37	1.32
1	C	181	ASP	CA-CB	5.19	1.62	1.53
1	D	360	ILE	CA-C	5.18	1.57	1.53
1	B	190	TYR	C-O	5.18	1.29	1.23
1	D	355	ASP	CA-C	5.18	1.58	1.52
1	D	262	ILE	N-CA	5.17	1.52	1.46
1	B	71	VAL	N-CA	-5.16	1.40	1.46
1	D	452	GLY	N-CA	5.16	1.52	1.45
1	C	183	ARG	CD-NE	5.15	1.53	1.46
1	B	734	THR	CA-C	5.15	1.59	1.52
1	A	415	TYR	CA-C	-5.15	1.46	1.52
1	D	441	HIS	ND1-CE1	5.14	1.37	1.32
1	B	219	HIS	ND1-CE1	5.12	1.37	1.32
1	B	292	HIS	ND1-CE1	5.12	1.37	1.32
1	B	337	GLY	N-CA	5.12	1.50	1.45
1	C	187	THR	N-CA	5.11	1.52	1.46
1	B	131	GLY	C-O	5.10	1.28	1.23
1	D	336	LEU	N-CA	5.10	1.52	1.46
1	A	647	VAL	CA-C	5.09	1.58	1.52
1	B	400	LEU	C-O	5.09	1.30	1.23
1	B	469	TRP	N-CA	5.09	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	320	ARG	CZ-NH1	5.09	1.39	1.32
1	B	116	HIS	ND1-CE1	5.07	1.37	1.32
1	C	419	GLN	CA-CB	5.07	1.61	1.53
1	D	479	ARG	CA-CB	5.07	1.61	1.53
1	C	162	VAL	N-CA	5.07	1.51	1.46
1	B	426	PRO	N-CA	-5.06	1.41	1.47
1	A	732	LEU	C-O	5.06	1.29	1.24
1	C	243	VAL	N-CA	5.06	1.52	1.46
1	D	452	GLY	C-O	5.05	1.29	1.24
1	D	323	TRP	C-O	-5.05	1.18	1.24
1	B	160	THR	C-O	-5.04	1.19	1.24
1	A	749	ASP	N-CA	5.03	1.52	1.46
1	C	446	ASP	N-CA	5.03	1.52	1.46
1	A	485	TYR	N-CA	5.01	1.52	1.46
1	B	420	ILE	CA-CB	5.00	1.59	1.54

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	420	ILE	N-CA-C	13.00	124.01	110.36
1	C	420	ILE	N-CA-C	12.29	123.27	110.36
1	C	159	ILE	CB-CG1-CD1	-10.45	91.85	113.80
1	B	420	ILE	N-CA-C	8.23	118.79	110.23
1	B	370	VAL	N-CA-CB	-7.95	102.87	112.33
1	C	725	ASP	N-CA-C	7.65	127.09	110.80
1	D	229	ILE	N-CA-C	-7.59	102.96	109.19
1	D	420	ILE	N-CA-C	7.39	118.12	110.36
1	A	751	ILE	N-CA-CB	7.09	117.82	110.23
1	D	61	ARG	NE-CZ-NH2	6.97	125.47	119.20
1	D	615	ASP	N-CA-C	-6.91	103.68	111.14
1	B	349	PHE	CA-C-N	-6.60	112.11	122.73
1	B	349	PHE	C-N-CA	-6.60	112.11	122.73
1	B	619	ILE	N-CA-C	-6.58	104.35	110.53
1	D	368	GLN	CA-CB-CG	-6.31	101.48	114.10
1	B	536	ARG	CA-C-N	-6.29	112.52	119.19
1	B	536	ARG	C-N-CA	-6.29	112.52	119.19
1	C	449[A]	HIS	CB-CA-C	6.26	120.62	111.73
1	C	449[B]	HIS	CB-CA-C	6.26	120.62	111.73
1	B	727	SER	N-CA-C	6.23	118.15	111.36
1	C	158	LYS	CA-C-N	-6.17	115.14	123.10
1	C	158	LYS	C-N-CA	-6.17	115.14	123.10
1	C	159	ILE	CA-CB-CG2	6.14	120.94	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	130	ARG	NE-CZ-NH2	-6.12	113.69	119.20
1	D	168	THR	CA-C-N	-6.08	116.94	123.08
1	D	168	THR	C-N-CA	-6.08	116.94	123.08
1	B	370	VAL	CG1-CB-CG2	6.04	124.09	110.80
1	D	377	ARG	CA-CB-CG	-6.02	102.05	114.10
1	A	28	SER	CA-C-N	-6.01	112.01	122.64
1	A	28	SER	C-N-CA	-6.01	112.01	122.64
1	D	71	VAL	CB-CA-C	-5.98	104.36	110.93
1	D	431	ILE	N-CA-C	-5.98	103.09	108.95
1	C	552	LEU	N-CA-C	5.94	117.75	111.28
1	B	446	ASP	CB-CA-C	-5.92	108.08	115.89
1	D	732	LEU	N-CA-C	-5.87	104.97	111.36
1	A	419	GLN	N-CA-C	-5.86	104.85	112.23
1	B	593	ILE	N-CA-C	5.83	113.33	107.55
1	C	422	ARG	NE-CZ-NH1	-5.81	115.69	121.50
1	D	419	GLN	N-CA-C	-5.78	105.12	111.82
1	A	421	SER	N-CA-CB	5.75	119.16	110.30
1	C	278	ARG	NE-CZ-NH1	-5.73	115.77	121.50
1	A	237	ASP	N-CA-C	5.73	117.20	111.07
1	C	379	PRO	CB-CA-C	-5.65	102.70	111.40
1	A	229	ILE	N-CA-C	-5.64	104.57	109.19
1	D	169	VAL	CB-CA-C	-5.63	106.09	111.44
1	B	525	ASP	CA-C-O	-5.62	114.59	120.55
1	A	297	ALA	N-CA-C	-5.59	106.41	113.18
1	A	415	TYR	N-CA-C	5.57	117.43	111.36
1	B	195	ILE	CA-CB-CG1	-5.56	100.95	110.40
1	A	349	PHE	CA-C-N	-5.55	113.01	122.56
1	A	349	PHE	C-N-CA	-5.55	113.01	122.56
1	C	631	LYS	CB-CA-C	5.45	118.86	110.14
1	B	421	SER	N-CA-CB	5.43	118.67	110.30
1	C	695	ILE	N-CA-C	-5.41	100.27	108.17
1	D	419	GLN	CB-CA-C	5.35	120.95	110.67
1	C	417	ASP	N-CA-CB	-5.32	102.29	110.01
1	D	407	LEU	N-CA-C	-5.32	104.38	112.04
1	D	335	GLU	CB-CG-CD	-5.31	103.57	112.60
1	B	111	ARG	CA-CB-CG	-5.30	103.50	114.10
1	A	619	ILE	N-CA-C	-5.29	105.55	110.53
1	A	265	SER	N-CA-CB	-5.26	103.41	111.56
1	D	38	PRO	CB-CA-C	-5.17	104.21	110.98
1	C	656	GLY	N-CA-C	5.17	118.93	112.73
1	D	377	ARG	NH1-CZ-NH2	5.14	125.98	119.30
1	C	474	PRO	O-C-N	5.12	123.67	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	421	SER	N-CA-CB	5.12	118.19	110.30
1	B	320	ARG	NE-CZ-NH1	-5.10	116.40	121.50
1	D	451	MET	CA-C-N	-5.08	115.05	120.43
1	D	451	MET	C-N-CA	-5.08	115.05	120.43
1	C	93	ASN	N-CA-C	5.04	117.04	109.23

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	ARG	Sidechain
1	A	708	ILE	Peptide
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	5745	0	5576	44	0
1	B	5746	0	5581	57	0
1	C	5745	0	5577	61	0
1	D	5746	0	5581	63	0
2	A	43	0	30	1	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	1	0
3	A	815	0	0	6	2
3	B	673	0	0	14	1
3	C	737	0	0	18	0
3	D	783	0	0	17	1
All	All	26162	0	22435	204	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (204) 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:D:449[B]:HIS:CE1	3:D:2501:HOH:O	1.80	1.29
1:B:521:ARG:HD3	3:B:3047:HOH:O	1.41	1.14
1:A:451:MET:HE2	1:C:451:MET:HE2	1.25	1.10
1:D:546:GLN:HG3	3:D:2742:HOH:O	1.53	1.05
1:C:267:ARG:HG3	3:C:2916:HOH:O	1.59	1.02
1:D:267:ARG:HG3	3:D:1920:HOH:O	1.56	1.02
1:B:451:MET:HE2	1:D:451:MET:HE2	1.41	1.00
1:A:413:TYR:HE2	1:B:413:TYR:CE2	1.80	0.98
1:A:413:TYR:CE2	1:B:413:TYR:HE2	1.83	0.96
1:B:267:ARG:HG3	3:B:1921:HOH:O	1.64	0.94
3:B:2705:HOH:O	1:D:73:LYS:HE3	1.68	0.93
1:C:413:TYR:CE2	1:D:413:TYR:HE2	1.87	0.92
1:C:612:ARG:HG3	1:C:612:ARG:HH11	1.34	0.92
1:A:413:TYR:CE2	1:B:413:TYR:CE2	2.59	0.90
1:A:29:LEU:HB2	3:C:2405:HOH:O	1.71	0.89
1:C:413:TYR:CE2	1:D:413:TYR:CE2	2.63	0.86
1:C:636:ARG:NH1	3:C:2717:HOH:O	2.07	0.85
1:A:111:ARG:O	1:A:115:THR:HG23	1.80	0.81
1:B:583:LYS:H	1:B:583:LYS:NZ	1.76	0.81
1:C:621:LYS:HE3	3:C:3116:HOH:O	1.80	0.81
1:A:541:GLU:OE2	3:A:2550:HOH:O	2.01	0.78
1:D:490:GLU:OE1	3:D:2308:HOH:O	2.02	0.77
1:C:612:ARG:HH11	1:C:612:ARG:CG	1.97	0.76
1:B:583:LYS:H	1:B:583:LYS:HZ2	1.30	0.74
1:D:574:THR:HG22	3:D:1614:HOH:O	1.86	0.74
1:C:413:TYR:HE2	1:D:413:TYR:CE2	2.04	0.73
1:B:533:LYS:HE2	3:B:3100:HOH:O	1.90	0.71
1:A:449[A]:HIS:CD2	1:C:449[A]:HIS:CD2	2.79	0.71
1:A:710:ILE:HG12	1:A:715:GLU:OE1	1.91	0.71
1:D:111:ARG:O	1:D:115:THR:HG23	1.91	0.70
1:A:28:SER:OG	1:A:28:SER:O	2.09	0.70
1:C:486:GLN:OE1	3:C:2892:HOH:O	2.09	0.69
1:B:449[B]:HIS:CD2	1:D:449[B]:HIS:CD2	2.81	0.68
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.77	0.67
1:D:750:LYS:HD2	1:D:751:ILE:H	1.61	0.66
2:B:760:HEM:HMC2	2:B:760:HEM:HBC2	1.77	0.66
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.78	0.66
1:A:479:ARG:NH2	3:A:2607:HOH:O	2.27	0.65
1:D:449[B]:HIS:NE2	3:D:2501:HOH:O	2.09	0.65
1:A:369:ARG:NH2	3:A:2403:HOH:O	2.03	0.65
1:C:552:LEU:HD11	1:C:571:LEU:HD12	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:GLU:OE1	3:C:2887:HOH:O	2.15	0.64
1:B:521:ARG:NH2	1:B:745:ILE:HD13	2.13	0.64
1:D:546:GLN:CD	3:D:2742:HOH:O	2.42	0.63
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.80	0.62
1:C:748:ILE:O	1:C:751:ILE:HG22	2.00	0.62
1:B:111:ARG:O	1:B:115:THR:HG23	2.00	0.62
1:C:413:TYR:HE2	1:D:413:TYR:CD2	2.18	0.62
1:A:29:LEU:HD12	1:A:29:LEU:H	1.65	0.61
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.83	0.61
1:C:610:GLU:O	1:C:610:GLU:HG3	2.00	0.61
1:D:583:LYS:NZ	1:D:583:LYS:HB2	2.16	0.61
1:A:36:HIS:CD2	1:A:36:HIS:H	2.18	0.60
1:B:350:ASP:HB2	3:B:1940:HOH:O	2.00	0.59
1:D:750:LYS:CD	1:D:751:ILE:H	2.16	0.59
1:D:750:LYS:HD2	1:D:751:ILE:N	2.18	0.58
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.85	0.58
1:C:521:ARG:HG2	3:C:2920:HOH:O	2.04	0.58
1:A:750:LYS:HE2	1:D:677:ASP:HB3	1.86	0.57
1:D:597:ASP:OD2	3:D:2709:HOH:O	2.17	0.57
1:C:111:ARG:O	1:C:115:THR:HG23	2.05	0.56
1:B:281:ASN:OD1	1:B:283:GLU:HG3	2.05	0.56
1:B:552:LEU:HD22	1:B:556:GLN:HG3	1.87	0.56
1:B:629:HIS:HD2	3:B:1045:HOH:O	1.88	0.56
1:D:61:ARG:HH11	1:D:66:ASN:HA	1.70	0.56
1:A:603:VAL:HG11	1:A:666:ILE:HD12	1.88	0.56
1:B:521:ARG:HH21	1:B:745:ILE:HD13	1.71	0.55
1:D:363:GLU:HB2	1:D:582:LEU:HD21	1.88	0.55
1:C:115:THR:O	1:C:119:HIS:HD2	1.89	0.54
1:D:478:LYS:HD2	3:D:2968:HOH:O	2.06	0.54
1:C:274:ILE:HD12	2:C:760:HEM:HMB1	1.89	0.54
1:C:629:HIS:HD2	3:C:1129:HOH:O	1.91	0.53
1:A:451:MET:CE	1:C:451:MET:HE2	2.18	0.53
1:D:546:GLN:CG	3:D:2742:HOH:O	2.26	0.53
1:D:629:HIS:HD2	3:D:1554:HOH:O	1.91	0.53
1:B:420:ILE:HG21	1:D:119:HIS:CE1	2.42	0.53
1:C:503:GLU:OE1	3:C:1142:HOH:O	2.18	0.53
1:D:750:LYS:O	1:D:751:ILE:O	2.26	0.52
1:B:449[A]:HIS:CG	1:D:449[A]:HIS:CG	2.42	0.52
1:C:359:LEU:H	1:C:507:HIS:HD2	1.57	0.52
1:C:612:ARG:CG	1:C:612:ARG:NH1	2.65	0.52
1:C:488:ARG:HD2	3:C:2379:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:283:GLU:N	1:C:283:GLU:OE1	2.43	0.51
1:C:556:GLN:HG2	1:C:566:LEU:HD12	1.93	0.51
1:B:359:LEU:H	1:B:507:HIS:HD2	1.59	0.51
1:A:29:LEU:CB	3:C:2405:HOH:O	2.45	0.51
1:C:596:GLY:HA3	1:C:737:ALA:O	2.10	0.51
2:C:760:HEM:HBC2	2:C:760:HEM:HMC2	1.94	0.50
1:A:448:MET:O	1:A:449[B]:HIS:HB2	2.12	0.50
1:C:578:ASP:HB2	1:C:582:LEU:O	2.12	0.50
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.94	0.49
1:D:521:ARG:HD2	3:D:2912:HOH:O	2.11	0.49
1:C:478:LYS:HG3	3:C:3207:HOH:O	2.12	0.49
1:C:610:GLU:OE1	1:C:643:ASP:HA	2.12	0.49
1:A:751:ILE:O	1:A:751:ILE:HD12	2.12	0.49
1:C:745:ILE:HD13	3:C:2920:HOH:O	2.11	0.49
1:B:521:ARG:NH2	1:B:745:ILE:HG21	2.28	0.49
1:C:195:ILE:HD11	1:C:436:PRO:HA	1.94	0.49
1:D:583:LYS:HB2	1:D:583:LYS:HZ3	1.77	0.49
1:D:321:GLU:HG3	3:D:2151:HOH:O	2.11	0.48
1:A:578:ASP:OD1	1:A:583:LYS:NZ	2.43	0.48
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.43	0.48
1:D:61:ARG:NH1	1:D:66:ASN:HA	2.28	0.48
1:D:283:GLU:OE2	3:D:2496:HOH:O	2.20	0.48
1:B:344:GLU:H	1:B:344:GLU:CD	2.22	0.48
1:B:571:LEU:HD22	3:B:2758:HOH:O	2.14	0.48
1:A:449[B]:HIS:CG	1:C:449[B]:HIS:CG	2.54	0.47
1:C:584:LYS:NZ	3:C:1767:HOH:O	2.46	0.47
1:C:634:TYR:O	1:C:653:THR:HA	2.14	0.47
1:A:682:ASN:HB3	1:A:707:THR:HG21	1.97	0.47
1:C:612:ARG:NH1	1:C:612:ARG:HB2	2.29	0.47
3:B:2705:HOH:O	1:D:73:LYS:CD	2.63	0.47
1:C:552:LEU:HD13	1:C:556:GLN:HG3	1.97	0.47
1:A:115:THR:O	1:A:119:HIS:HD2	1.97	0.46
1:C:713:GLN:HG2	3:C:2154:HOH:O	2.15	0.46
1:B:36:HIS:H	1:B:36:HIS:HD1	1.63	0.46
1:C:686:MET:HB3	1:C:751:ILE:HD11	1.96	0.46
1:A:461:GLU:OE1	1:C:91:ASP:OD1	2.33	0.46
1:A:603:VAL:HG11	1:A:666:ILE:CD1	2.45	0.46
1:A:128:HIS:CE1	1:A:169:VAL:HG22	2.50	0.46
1:C:621:LYS:HG2	3:C:3116:HOH:O	2.16	0.46
1:B:634:TYR:O	1:B:653:THR:HA	2.16	0.46
1:C:128:HIS:HA	1:C:168:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:THR:HA	3:B:1822:HOH:O	2.16	0.46
1:C:583:LYS:HB2	1:C:583:LYS:HE2	1.60	0.46
1:B:91:ASP:OD1	1:D:461:GLU:OE1	2.34	0.45
1:D:115:THR:O	1:D:119:HIS:HD2	2.00	0.45
1:B:115:THR:O	1:B:119:HIS:HD2	2.00	0.45
1:B:566:LEU:HD23	3:B:812:HOH:O	2.16	0.45
1:A:607:LEU:HD11	1:A:632:LEU:HB3	1.99	0.45
1:A:459:ASN:HD22	1:A:459:ASN:H	1.65	0.44
1:B:566:LEU:N	1:B:566:LEU:HD22	2.32	0.44
1:A:461:GLU:HA	1:A:462:PRO:C	2.42	0.44
1:B:128:HIS:HA	1:B:168:THR:O	2.18	0.44
1:B:372:LYS:NZ	3:B:2242:HOH:O	2.41	0.44
1:D:404:ASN:O	1:D:405:ASP:C	2.59	0.44
1:D:222:LYS:HB3	1:D:223:PRO:CD	2.48	0.44
1:B:29:LEU:N	3:B:2571:HOH:O	2.24	0.44
1:D:252:ASN:HD22	1:D:252:ASN:HA	1.63	0.44
1:D:313:ARG:HG3	1:D:660:LEU:HD12	1.99	0.44
1:C:128:HIS:CE1	1:C:169:VAL:HG22	2.53	0.43
1:C:727:SER:HA	3:C:2714:HOH:O	2.17	0.43
1:D:751:ILE:HA	1:D:752:PRO:HD3	1.75	0.43
1:D:359:LEU:H	1:D:507:HIS:HD2	1.67	0.43
1:B:359:LEU:H	1:B:507:HIS:CD2	2.35	0.43
1:C:105:LEU:HA	1:C:105:LEU:HD12	1.76	0.43
1:A:274:ILE:HD12	2:A:760:HEM:HMB1	1.99	0.43
1:B:461:GLU:HA	1:B:462:PRO:C	2.43	0.43
1:C:404:ASN:O	1:C:405:ASP:C	2.60	0.43
1:A:440:TYR:HD1	3:A:1918:HOH:O	2.01	0.43
1:B:267:ARG:HD2	3:B:1023:HOH:O	2.18	0.43
1:A:610:GLU:CG	3:A:2551:HOH:O	2.67	0.43
1:D:556:GLN:NE2	3:D:2773:HOH:O	2.51	0.43
1:C:38:PRO:HG2	1:C:51:ALA:HB2	2.01	0.42
1:D:744:ARG:HA	1:D:747:LYS:HD3	2.01	0.42
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.27	0.42
1:B:119:HIS:CE1	1:D:420:ILE:HG21	2.54	0.42
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.55	0.42
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.35	0.42
1:D:254:MET:HB3	1:D:254:MET:HE3	1.77	0.42
1:C:461:GLU:HA	1:C:462:PRO:C	2.44	0.42
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.50	0.42
1:B:459:ASN:H	1:B:459:ASN:HD22	1.67	0.42
1:A:214:PHE:HB3	1:A:215:PRO:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:LYS:HA	1:A:703:LYS:HD2	1.96	0.41
1:C:254:MET:HE3	1:C:254:MET:HB3	1.72	0.41
1:B:128:HIS:CE1	1:B:169:VAL:HG22	2.55	0.41
1:B:583:LYS:H	1:B:583:LYS:HZ3	1.60	0.41
1:B:289:VAL:HA	1:B:339:GLN:O	2.20	0.41
1:B:335:GLU:OE1	1:B:369:ARG:HG2	2.20	0.41
1:B:717:GLY:HA3	1:B:741:VAL:HG11	2.02	0.41
2:B:760:HEM:CMB	2:B:760:HEM:HBB2	2.50	0.41
1:C:97:ALA:O	1:C:101:GLY:HA3	2.20	0.41
1:C:207:PHE:O	1:C:249:THR:HA	2.20	0.41
1:A:251:HIS:CE1	1:A:507:HIS:HB3	2.55	0.41
1:B:105:LEU:HD11	1:D:413:TYR:HB2	2.02	0.41
1:D:488:ARG:NE	3:D:2698:HOH:O	2.01	0.41
1:A:392:HIS:CE1	1:A:415:TYR:H	2.39	0.41
1:A:610:GLU:HG2	3:A:2551:HOH:O	2.21	0.41
1:D:274:ILE:HD12	2:D:760:HEM:HMB1	2.01	0.41
1:A:115:THR:HG22	1:D:413:TYR:OH	2.21	0.41
1:D:48:GLN:HE21	1:D:48:GLN:HB3	1.65	0.41
1:D:459:ASN:HD22	1:D:459:ASN:H	1.68	0.41
1:A:626:LYS:HA	1:A:626:LYS:HD3	1.88	0.41
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.56	0.41
1:B:417:ASP:O	1:B:420:ILE:HB	2.21	0.41
1:C:144:LEU:HD11	1:C:370:VAL:HG13	2.02	0.41
1:C:440:TYR:CD2	1:C:440:TYR:C	2.98	0.41
1:C:459:ASN:H	1:C:459:ASN:HD22	1.68	0.41
1:C:556:GLN:HG2	1:C:566:LEU:CD1	2.51	0.41
1:D:696:ALA:HB1	1:D:728:PHE:CZ	2.56	0.41
3:B:2705:HOH:O	1:D:73:LYS:CE	2.44	0.41
1:D:361:PRO:HD2	1:D:364:LEU:HD12	2.02	0.41
1:D:634:TYR:CG	1:D:635:SER:N	2.88	0.41
1:A:413:TYR:CD2	1:B:413:TYR:HE2	2.34	0.40
1:B:533:LYS:CD	3:C:2623:HOH:O	2.69	0.40
1:D:222:LYS:HB3	1:D:223:PRO:HD2	2.02	0.40
1:D:476:GLY:HA3	3:D:1112:HOH:O	2.20	0.40
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.36	0.40
1:B:372:LYS:HB3	1:B:372:LYS:HE3	1.78	0.40
1:B:440:TYR:CD2	1:B:440:TYR:C	2.99	0.40
1:B:745:ILE:O	1:B:748:ILE:HG12	2.21	0.40
1:D:535:VAL:O	1:D:537:PRO:HD3	2.20	0.40
1:B:254:MET:HE3	1:B:254:MET:HB3	1.91	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2402:HOH:O	3:D:2299:HOH:O[1_455]	2.14	0.06
3:A:2627:HOH:O	3:B:2418:HOH:O[2_545]	2.14	0.06

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	725/753 (96%)	707 (98%)	16 (2%)	2 (0%)	36	20
1	B	725/753 (96%)	703 (97%)	20 (3%)	2 (0%)	36	20
1	C	725/753 (96%)	710 (98%)	14 (2%)	1 (0%)	48	28
1	D	725/753 (96%)	707 (98%)	15 (2%)	3 (0%)	30	12
All	All	2900/3012 (96%)	2827 (98%)	65 (2%)	8 (0%)	36	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	711	ALA
1	B	725	ASP
1	D	751	ILE
1	B	75	SER
1	D	75	SER
1	D	750	LYS
1	A	75	SER
1	C	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	612/636 (96%)	591 (97%)	21 (3%)	32	6
1	B	612/636 (96%)	584 (95%)	28 (5%)	24	3
1	C	612/636 (96%)	582 (95%)	30 (5%)	22	2
1	D	612/636 (96%)	586 (96%)	26 (4%)	26	4
All	All	2448/2544 (96%)	2343 (96%)	105 (4%)	26	3

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	29	LEU
1	A	37	ARG
1	A	73	LYS
1	A	191	THR
1	A	205	ILE
1	A	252	ASN
1	A	369	ARG
1	A	420	ILE
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	593	ILE
1	A	709	LYS
1	A	710	ILE
1	A	712	ASP
1	A	713	GLN
1	A	732	LEU
1	A	750	LYS
1	A	751	ILE
1	B	191	THR
1	B	195	ILE
1	B	205	ILE
1	B	252	ASN
1	B	283	GLU
1	B	285	LYS
1	B	344	GLU
1	B	370	VAL
1	B	432	PRO

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Mol	Chain	Res	Type
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	565	GLU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	595	ASP
1	B	610	GLU
1	B	612	ARG
1	B	616	LEU
1	B	633	LEU
1	B	703	LYS
1	B	707	THR
1	B	709	LYS
1	B	732	LEU
1	B	749	ASP
1	B	751	ILE
1	C	159	ILE
1	C	191	THR
1	C	198	LEU
1	C	205	ILE
1	C	252	ASN
1	C	369	ARG
1	C	377	ARG
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG
1	C	521	ARG
1	C	552	LEU
1	C	568	ASP
1	C	571	LEU
1	C	584	LYS
1	C	606	LEU
1	C	610	GLU
1	C	612	ARG
1	C	613	SER
1	C	616	LEU
1	C	617	LEU
1	C	633	LEU

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Mol	Chain	Res	Type
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU
1	C	709	LYS
1	C	733	LEU
1	C	750	LYS
1	C	751	ILE
1	D	32	GLU
1	D	41	GLU
1	D	48	GLN
1	D	73	LYS
1	D	127	VAL
1	D	159	ILE
1	D	191	THR
1	D	205	ILE
1	D	252	ASN
1	D	344	GLU
1	D	369	ARG
1	D	420	ILE
1	D	440	TYR
1	D	459	ASN
1	D	490	GLU
1	D	552	LEU
1	D	554	LEU
1	D	574	THR
1	D	582	LEU
1	D	583	LYS
1	D	616	LEU
1	D	648	LEU
1	D	713	GLN
1	D	747	LYS
1	D	750	LYS
1	D	751	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	66	ASN
1	A	252	ASN
1	A	419	GLN
1	A	459	ASN

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Mol	Chain	Res	Type
1	A	546	GLN
1	A	713	GLN
1	B	157	ASN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	C	84	GLN
1	C	252	ASN
1	C	368	GLN
1	C	459	ASN
1	C	486	GLN
1	C	507	HIS
1	C	546	GLN
1	C	572	ASN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	77	ASN
1	D	119	HIS
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 oligosaccharides 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	760	1	50,50,50	1.69	13 (26%)	67,82,82	2.30	23 (34%)
2	HEM	C	760	1	50,50,50	2.00	20 (40%)	67,82,82	2.64	24 (35%)
2	HEM	A	760	1	50,50,50	1.93	16 (32%)	67,82,82	2.62	25 (37%)
2	HEM	B	760	1	50,50,50	2.01	19 (38%)	67,82,82	2.34	24 (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	760	1	-	2/14/54/54	-
2	HEM	C	760	1	-	2/14/54/54	-
2	HEM	A	760	1	-	2/14/54/54	-
2	HEM	B	760	1	-	2/14/54/54	-

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HEM	C1B-NB	-5.13	1.31	1.40
2	B	760	HEM	C1B-NB	-4.65	1.32	1.40
2	B	760	HEM	FE-NB	4.33	2.08	1.94
2	A	760	HEM	CHA-C4D	4.21	1.46	1.38
2	C	760	HEM	C1B-NB	-4.12	1.33	1.40
2	B	760	HEM	CHA-C4D	4.10	1.46	1.38
2	A	760	HEM	CHB-C1B	3.63	1.45	1.38
2	D	760	HEM	FE-NB	3.59	2.06	1.94
2	A	760	HEM	CHD-C1D	3.59	1.47	1.39
2	A	760	HEM	C1C-NC	3.44	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	760	HEM	C1C-NC	3.42	1.46	1.39
2	C	760	HEM	CHB-C1B	3.41	1.45	1.38
2	C	760	HEM	C4D-ND	-3.23	1.34	1.40
2	C	760	HEM	C3C-C2C	3.21	1.43	1.37
2	B	760	HEM	CHB-C1B	3.18	1.44	1.38
2	D	760	HEM	C3D-C2D	3.12	1.43	1.36
2	C	760	HEM	C1B-C2B	3.11	1.50	1.44
2	D	760	HEM	O1D-CGD	3.10	1.32	1.22
2	C	760	HEM	CHC-C4B	3.08	1.46	1.39
2	C	760	HEM	FE-NB	3.07	2.04	1.94
2	B	760	HEM	CHC-C4B	3.03	1.46	1.39
2	D	760	HEM	CHB-C1B	2.99	1.44	1.38
2	A	760	HEM	FE-NB	2.96	2.04	1.94
2	C	760	HEM	O1D-CGD	2.91	1.31	1.22
2	C	760	HEM	FE-ND	2.90	2.03	1.94
2	A	760	HEM	CMB-C2B	-2.89	1.44	1.50
2	B	760	HEM	FE-ND	2.88	2.03	1.94
2	A	760	HEM	C3D-C2D	2.86	1.42	1.36
2	B	760	HEM	C4A-C3A	2.85	1.49	1.43
2	B	760	HEM	FE-NC	2.84	2.04	1.95
2	A	760	HEM	C3B-C2B	2.82	1.42	1.37
2	B	760	HEM	CHD-C1D	2.76	1.45	1.39
2	C	760	HEM	CHB-C4A	2.73	1.45	1.39
2	D	760	HEM	FE-ND	2.71	2.03	1.94
2	D	760	HEM	CHD-C1D	2.66	1.45	1.39
2	C	760	HEM	C1D-ND	-2.66	1.33	1.38
2	B	760	HEM	O1D-CGD	2.62	1.30	1.22
2	C	760	HEM	C4A-C3A	2.57	1.49	1.43
2	B	760	HEM	FE-NA	2.56	2.03	1.95
2	A	760	HEM	C2A-C3A	2.53	1.45	1.38
2	B	760	HEM	C3D-C2D	2.52	1.42	1.36
2	C	760	HEM	C3D-C2D	2.50	1.42	1.36
2	A	760	HEM	FE-ND	2.49	2.02	1.94
2	C	760	HEM	C3B-C4B	-2.49	1.40	1.44
2	C	760	HEM	CHC-C1C	2.46	1.43	1.38
2	C	760	HEM	CHA-C4D	2.46	1.43	1.38
2	B	760	HEM	O2D-CGD	-2.45	1.22	1.30
2	A	760	HEM	CHD-C4C	2.42	1.43	1.38
2	B	760	HEM	O1A-CGA	2.40	1.29	1.22
2	C	760	HEM	C3C-C4C	2.38	1.50	1.46
2	D	760	HEM	FE-NC	2.33	2.02	1.95
2	B	760	HEM	CHB-C4A	2.27	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	760	HEM	C1C-NC	2.26	1.43	1.39
2	A	760	HEM	C1D-ND	-2.25	1.34	1.38
2	C	760	HEM	C2A-C3A	2.25	1.44	1.38
2	A	760	HEM	O1D-CGD	2.23	1.29	1.22
2	B	760	HEM	C1C-NC	2.23	1.43	1.39
2	D	760	HEM	C3C-C4C	2.13	1.49	1.46
2	A	760	HEM	CBA-CAA	2.12	1.59	1.51
2	C	760	HEM	C4D-C3D	2.11	1.48	1.45
2	B	760	HEM	C3B-C2B	2.11	1.41	1.37
2	A	760	HEM	CBD-CAD	2.09	1.59	1.51
2	D	760	HEM	C1B-NB	-2.09	1.36	1.40
2	B	760	HEM	CHD-C4C	2.08	1.42	1.38
2	B	760	HEM	C1B-C2B	2.08	1.48	1.44
2	D	760	HEM	CBD-CAD	2.06	1.59	1.51
2	D	760	HEM	O2D-CGD	-2.05	1.24	1.30
2	D	760	HEM	C4D-ND	-2.02	1.36	1.40

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	760	HEM	C3B-C2B-C1B	-10.26	98.71	106.41
2	A	760	HEM	C3B-C2B-C1B	-8.35	100.14	106.41
2	B	760	HEM	C3B-C2B-C1B	-8.33	100.16	106.41
2	A	760	HEM	C2B-C1B-NB	7.52	118.48	109.84
2	D	760	HEM	C3B-C2B-C1B	-6.67	101.40	106.41
2	A	760	HEM	C3D-C4D-ND	6.64	117.46	110.17
2	D	760	HEM	CBD-CAD-C3D	-6.36	94.94	112.53
2	C	760	HEM	CBD-CAD-C3D	-6.16	95.51	112.53
2	C	760	HEM	C2B-C1B-NB	6.09	116.84	109.84
2	A	760	HEM	CBD-CAD-C3D	-5.72	96.72	112.53
2	C	760	HEM	C3B-C4B-NB	5.65	113.53	109.47
2	B	760	HEM	CBD-CAD-C3D	-5.48	97.38	112.53
2	C	760	HEM	C2D-C1D-ND	5.41	116.16	109.90
2	D	760	HEM	CHC-C1C-NC	-5.18	118.81	124.45
2	B	760	HEM	C2B-C1B-NB	5.04	115.63	109.84
2	D	760	HEM	C3C-C2C-C1C	-4.97	102.35	107.05
2	B	760	HEM	C3C-C2C-C1C	-4.61	102.69	107.05
2	D	760	HEM	C2B-C1B-NB	4.54	115.06	109.84
2	C	760	HEM	C3D-C4D-ND	4.38	114.97	110.17
2	B	760	HEM	C3D-C4D-ND	4.35	114.94	110.17
2	B	760	HEM	C2D-C1D-ND	4.35	114.93	109.90
2	D	760	HEM	CAC-C3C-C4C	-4.18	114.83	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	760	HEM	CHB-C1B-C2B	-4.03	115.51	126.95
2	A	760	HEM	C4D-C3D-C2D	-4.00	101.07	106.89
2	A	760	HEM	CAA-CBA-CGA	-3.93	103.23	113.67
2	C	760	HEM	CHB-C1B-C2B	-3.79	116.16	126.95
2	B	760	HEM	C4D-C3D-C2D	-3.79	101.38	106.89
2	D	760	HEM	CAA-CBA-CGA	-3.79	103.62	113.67
2	A	760	HEM	C3C-C2C-C1C	-3.72	103.52	107.05
2	C	760	HEM	CAA-CBA-CGA	-3.67	103.92	113.67
2	A	760	HEM	C2D-C1D-ND	3.66	114.14	109.90
2	A	760	HEM	CAD-C3D-C4D	3.66	131.08	124.70
2	A	760	HEM	O2D-CGD-O1D	-3.61	114.06	123.33
2	C	760	HEM	C1B-NB-C4B	-3.50	101.06	105.21
2	A	760	HEM	CMB-C2B-C1B	3.50	130.50	125.03
2	C	760	HEM	CHA-C4D-C3D	-3.44	118.88	125.23
2	B	760	HEM	CAA-CBA-CGA	-3.42	104.60	113.67
2	C	760	HEM	C3C-C2C-C1C	-3.41	103.82	107.05
2	D	760	HEM	O2D-CGD-O1D	-3.41	114.57	123.33
2	D	760	HEM	C2D-C1D-ND	3.32	113.74	109.90
2	A	760	HEM	CHD-C1D-C2D	-3.31	119.81	125.03
2	A	760	HEM	C3B-C4B-NB	3.27	111.81	109.47
2	A	760	HEM	C4D-ND-C1D	-3.17	101.45	105.21
2	C	760	HEM	C4D-C3D-C2D	-3.02	102.49	106.89
2	C	760	HEM	C1D-C2D-C3D	-3.02	103.81	106.98
2	B	760	HEM	CHB-C1B-C2B	-3.00	118.43	126.95
2	C	760	HEM	O2D-CGD-CBD	2.90	123.17	114.00
2	D	760	HEM	CMC-C2C-C1C	2.89	129.82	124.73
2	C	760	HEM	O2D-CGD-O1D	-2.86	115.97	123.33
2	A	760	HEM	CHA-C4D-ND	-2.85	120.84	124.37
2	D	760	HEM	CMD-C2D-C1D	2.83	129.46	125.03
2	A	760	HEM	CAC-C3C-C4C	-2.82	118.08	124.82
2	A	760	HEM	C4C-NC-C1C	-2.81	101.24	105.82
2	B	760	HEM	C4D-ND-C1D	-2.77	101.93	105.21
2	D	760	HEM	CMB-C2B-C3B	2.75	135.09	128.43
2	C	760	HEM	O1A-CGA-CBA	-2.75	114.38	123.09
2	B	760	HEM	C4A-C3A-C2A	-2.72	103.70	106.82
2	D	760	HEM	O2D-CGD-CBD	2.71	122.58	114.00
2	D	760	HEM	C2C-C1C-NC	2.71	114.65	109.64
2	B	760	HEM	C2C-C1C-NC	2.70	114.64	109.64
2	B	760	HEM	O2D-CGD-O1D	-2.70	116.38	123.33
2	B	760	HEM	CMC-C2C-C3C	2.65	134.85	128.43
2	B	760	HEM	CHC-C1C-NC	-2.64	121.58	124.45
2	A	760	HEM	C1B-NB-C4B	-2.62	102.10	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	760	HEM	CBC-CAC-C3C	-2.61	114.50	127.53
2	B	760	HEM	O2D-CGD-CBD	2.59	122.19	114.00
2	D	760	HEM	C4C-C3C-C2C	2.58	109.05	106.81
2	B	760	HEM	C2A-C1A-NA	2.54	112.97	110.15
2	B	760	HEM	CAD-CBD-CGD	-2.48	107.08	113.67
2	A	760	HEM	CMD-C2D-C1D	2.38	128.75	125.03
2	B	760	HEM	C4C-NC-C1C	-2.37	101.95	105.82
2	C	760	HEM	CHD-C1D-C2D	-2.37	121.28	125.03
2	C	760	HEM	C4A-CHB-C1B	-2.34	120.74	126.25
2	C	760	HEM	C4D-ND-C1D	-2.33	102.45	105.21
2	B	760	HEM	CMA-C3A-C2A	2.30	130.50	125.62
2	C	760	HEM	C4B-C3B-C2B	2.29	109.39	107.28
2	D	760	HEM	C4C-NC-C1C	-2.29	102.08	105.82
2	D	760	HEM	C2A-C1A-NA	2.29	112.69	110.15
2	A	760	HEM	O2D-CGD-CBD	2.28	121.20	114.00
2	B	760	HEM	CAD-C3D-C4D	2.27	128.65	124.70
2	D	760	HEM	CBC-CAC-C3C	-2.26	116.25	127.53
2	A	760	HEM	O2A-CGA-CBA	2.24	121.07	114.00
2	D	760	HEM	CAA-C2A-C3A	2.22	132.04	127.07
2	B	760	HEM	CMB-C2B-C3B	2.21	133.78	128.43
2	D	760	HEM	O1A-CGA-CBA	-2.20	116.13	123.09
2	D	760	HEM	C1A-C2A-C3A	-2.18	103.50	106.87
2	C	760	HEM	CBB-CAB-C3B	-2.14	116.83	127.53
2	B	760	HEM	CAC-C3C-C4C	-2.14	119.71	124.82
2	A	760	HEM	CBC-CAC-C3C	-2.13	116.89	127.53
2	C	760	HEM	CAA-C2A-C1A	2.12	129.09	124.94
2	D	760	HEM	C4D-C3D-C2D	-2.11	103.82	106.89
2	D	760	HEM	CAC-C3C-C2C	2.10	135.26	128.43
2	C	760	HEM	CAC-C3C-C4C	-2.09	119.82	124.82
2	C	760	HEM	CMB-C2B-C3B	2.04	133.36	128.43
2	A	760	HEM	C4A-CHB-C1B	-2.01	121.53	126.25
2	A	760	HEM	CHA-C4D-C3D	-2.00	121.53	125.23

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	760	HEM	CAA-CBA-CGA-O2A
2	B	760	HEM	CAA-CBA-CGA-O2A
2	B	760	HEM	CAA-CBA-CGA-O1A
2	D	760	HEM	CAA-CBA-CGA-O2A
2	A	760	HEM	CAA-CBA-CGA-O1A

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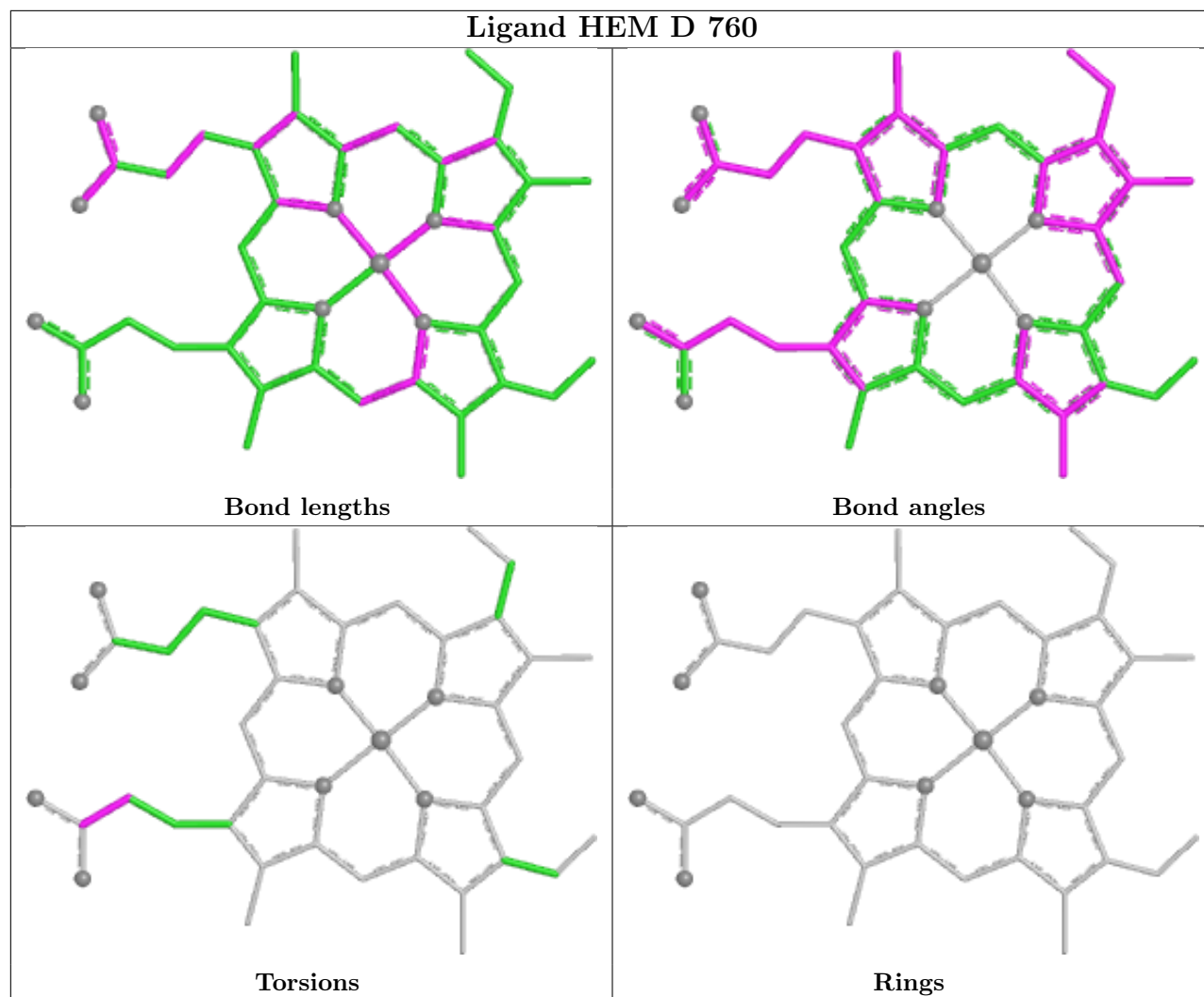
Mol	Chain	Res	Type	Atoms
2	C	760	HEM	CAA-CBA-CGA-O1A
2	C	760	HEM	CAA-CBA-CGA-O2A
2	D	760	HEM	CAA-CBA-CGA-O1A

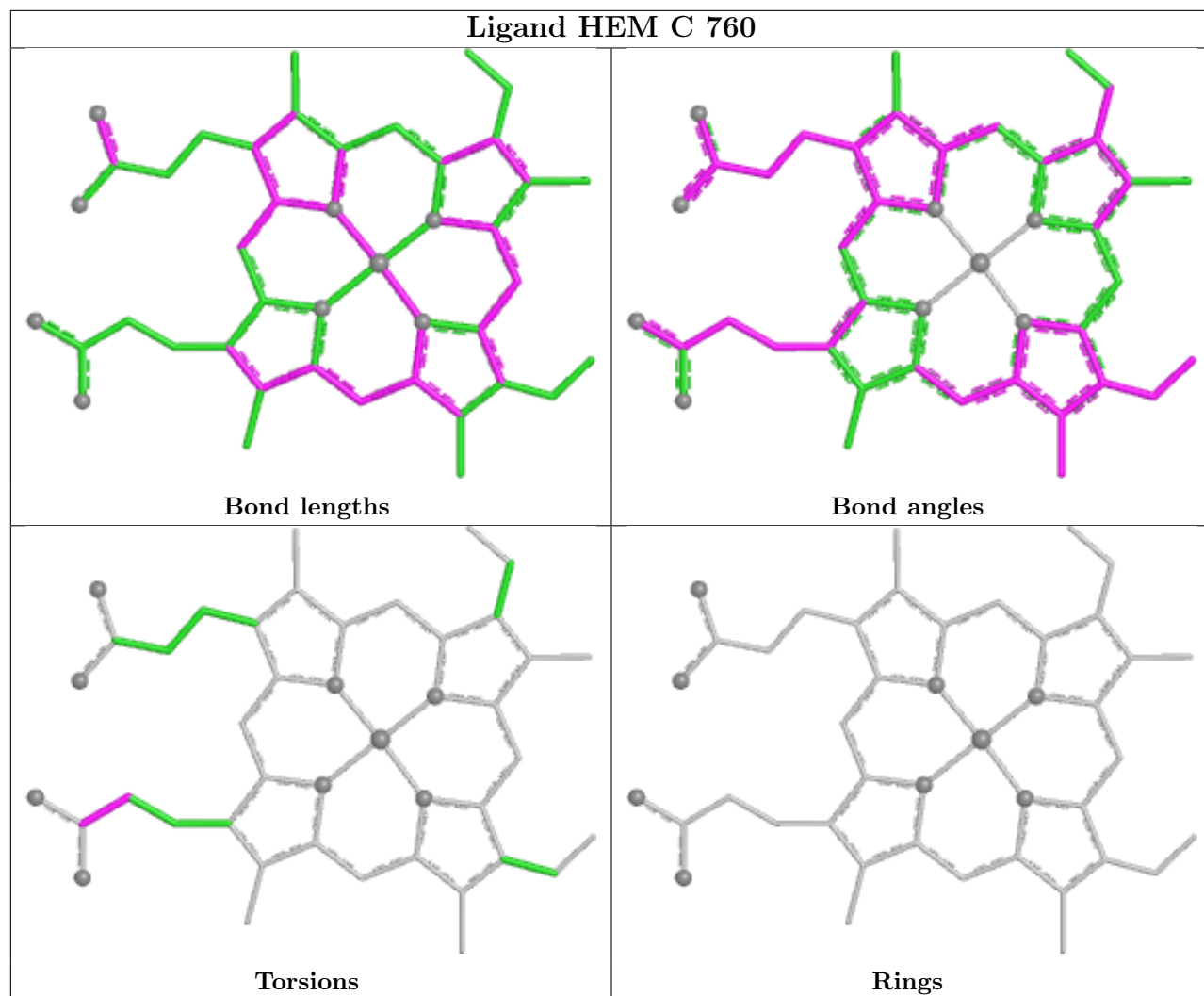
There are no ring outliers.

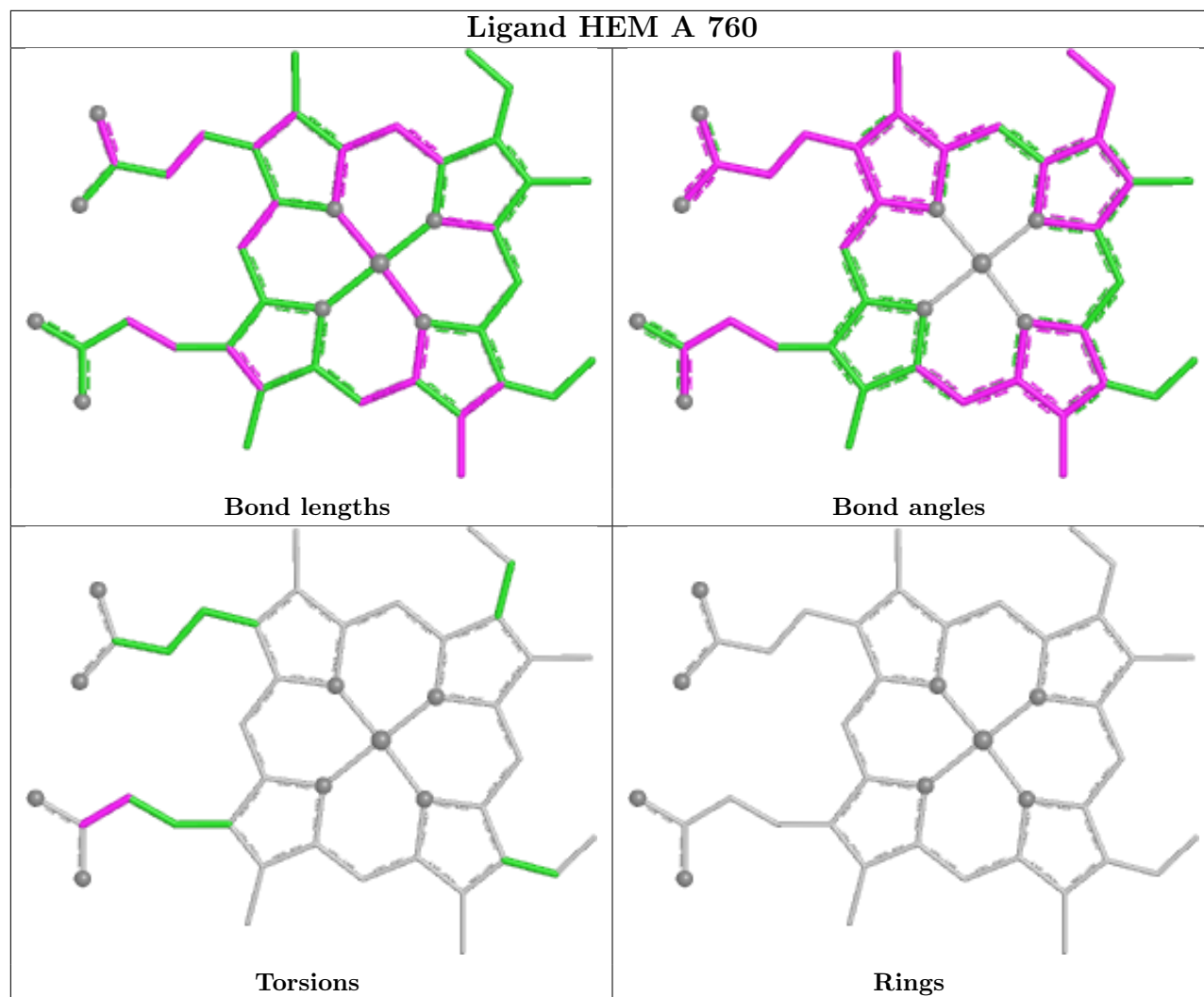
4 monomers are involved in 6 short contacts:

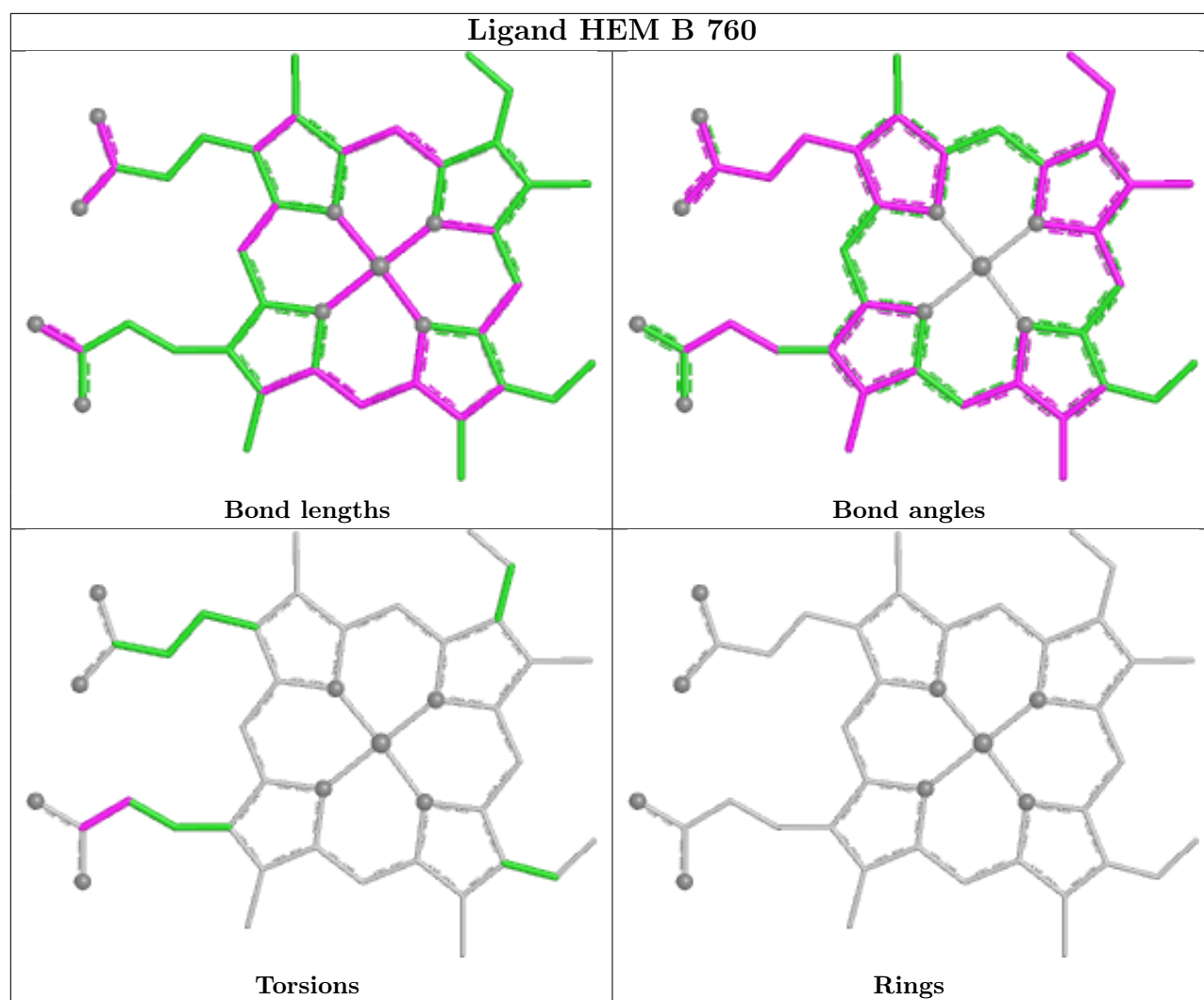
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	760	HEM	1	0
2	C	760	HEM	2	0
2	A	760	HEM	1	0
2	B	760	HEM	2	0

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%)	-0.39	13 (1%)	67 77	4, 11, 29, 84	2 (0%)
1	B	726/753 (96%)	-0.21	10 (1%)	73 81	5, 14, 39, 61	2 (0%)
1	C	726/753 (96%)	-0.26	11 (1%)	72 80	5, 14, 36, 56	2 (0%)
1	D	726/753 (96%)	-0.39	9 (1%)	76 83	4, 12, 29, 58	2 (0%)
All	All	2904/3012 (96%)	-0.31	43 (1%)	72 80	4, 13, 34, 84	8 (0%)

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	711	ALA	8.1
1	A	710	ILE	6.0
1	A	28	SER	4.4
1	A	29	LEU	3.6
1	B	420	ILE	3.3
1	A	712	ASP	3.1
1	A	713	GLN	3.1
1	C	750	LYS	2.9
1	D	28	SER	2.9
1	A	709	LYS	2.8
1	B	726	GLY	2.8
1	C	726	GLY	2.8
1	B	725	ASP	2.7
1	D	711	ALA	2.7
1	A	751	ILE	2.7
1	A	725	ASP	2.6
1	D	750	LYS	2.6
1	C	595	ASP	2.6
1	D	751	ILE	2.5
1	C	751	ILE	2.5
1	B	413	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	673	ALA	2.4
1	C	749	ASP	2.4
1	C	413	TYR	2.4
1	D	413	TYR	2.3
1	D	595	ASP	2.3
1	A	413	TYR	2.3
1	D	440	TYR	2.2
1	D	749	ASP	2.2
1	A	707	THR	2.1
1	C	725	ASP	2.1
1	A	420	ILE	2.1
1	B	710	ILE	2.1
1	C	440	TYR	2.1
1	C	677	ASP	2.1
1	B	32	GLU	2.1
1	C	420	ILE	2.1
1	B	670	GLY	2.1
1	D	597	ASP	2.1
1	A	750	LYS	2.0
1	C	711	ALA	2.0
1	B	37	ARG	2.0
1	B	552	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	A	760	43/43	0.99	0.04	4,6,10,13	0

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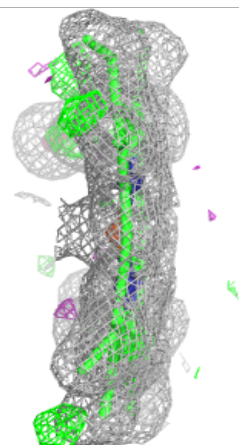
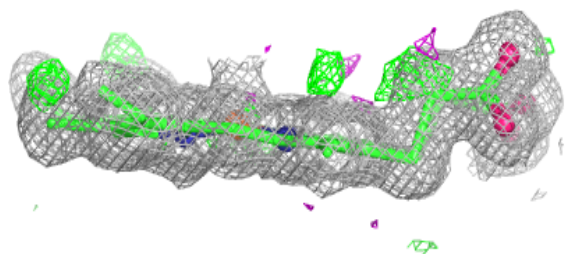
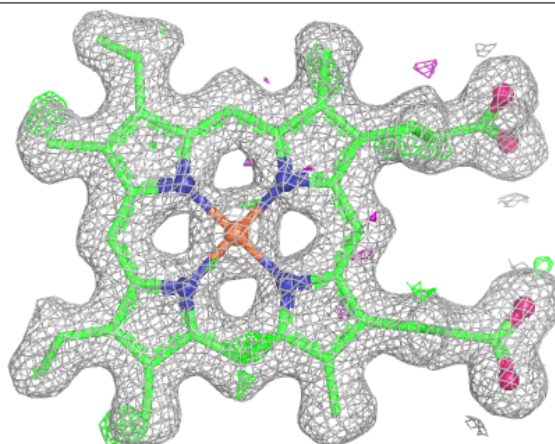
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	B	760	43/43	0.99	0.04	6,8,12,15	0
2	HEM	C	760	43/43	0.99	0.04	6,8,12,15	0
2	HEM	D	760	43/43	0.99	0.04	5,7,11,16	0

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.

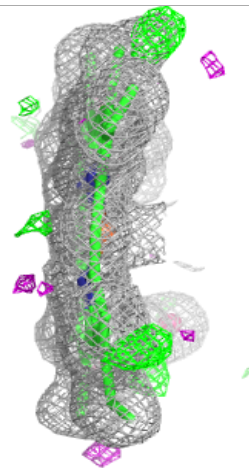
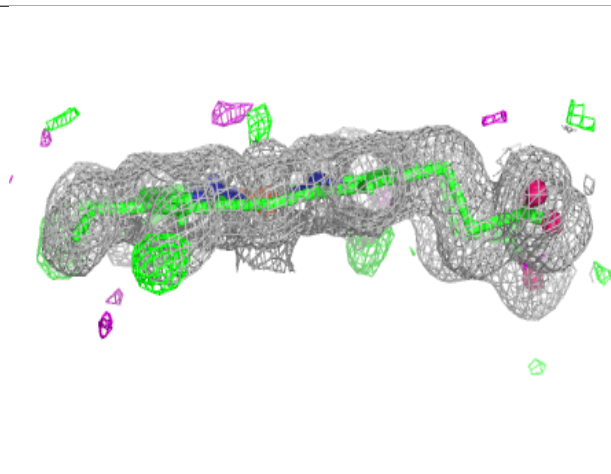
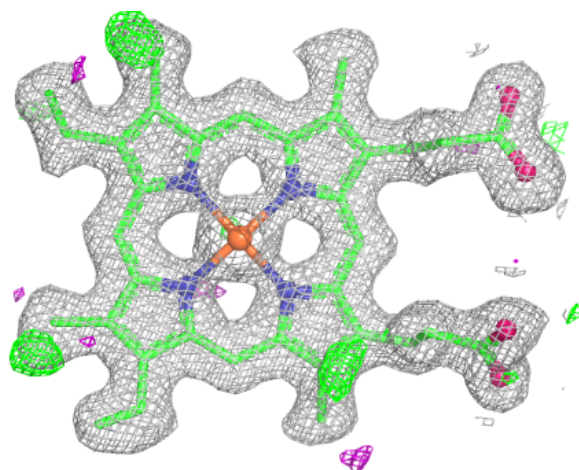
Electron density around HEM A 760:

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



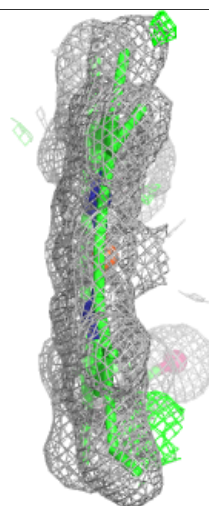
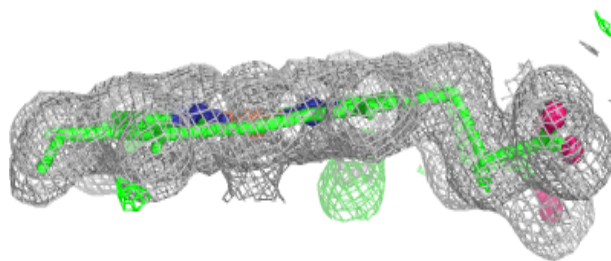
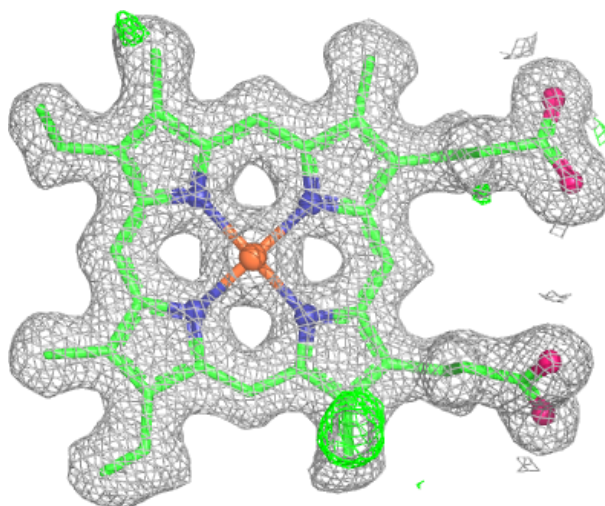
Electron density around HEM B 760:

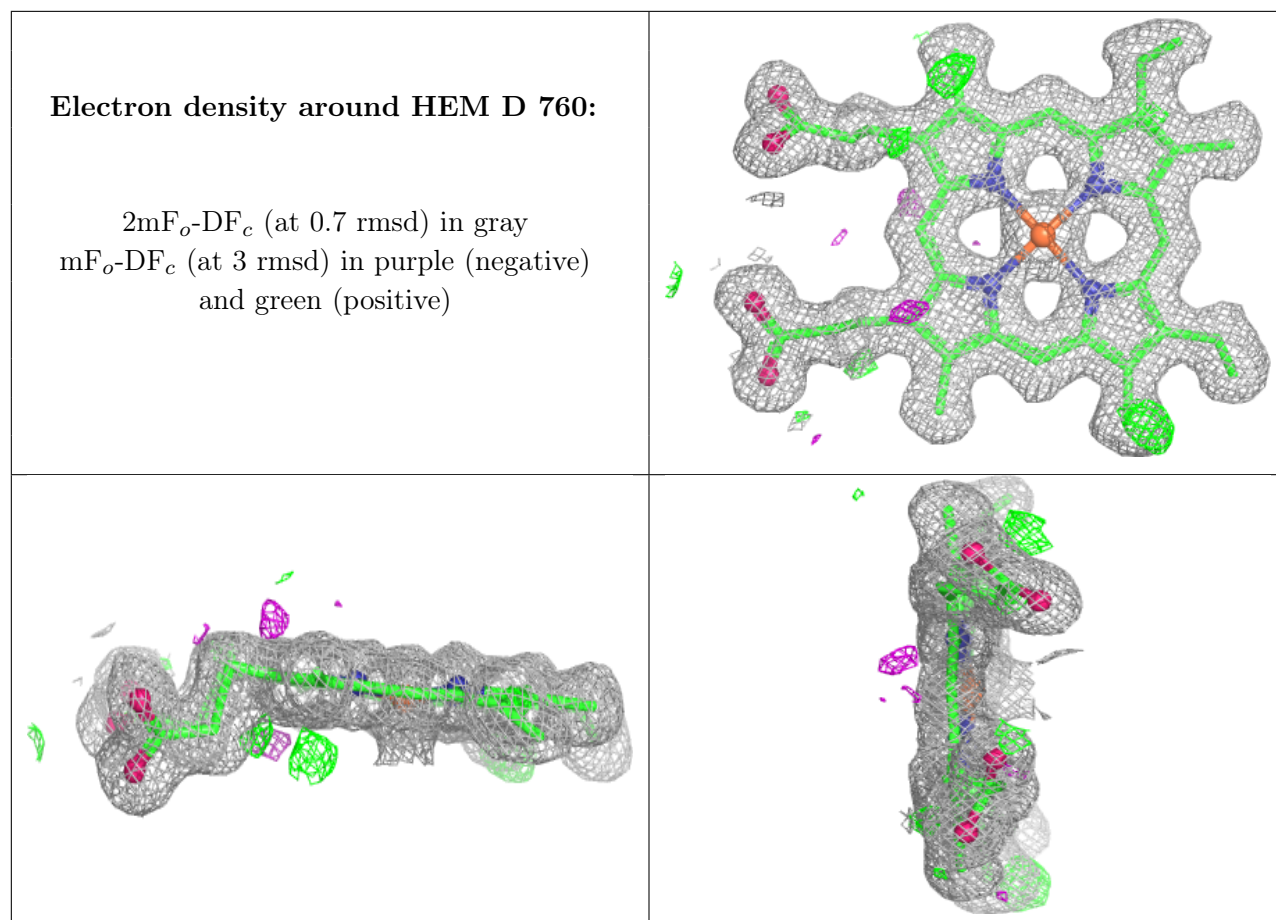
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 [i](#)

There are no such residues in this entry.