



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:18 AM UTC

PDB ID : 1GGH / pdb_00001ggh
Title : CRYSTAL STRUCTURE OF CATALASE HP11 FROM ESCHERICHIA COLI, HIS128ALA VARIANT.
Authors : Melik-Adamyan, W.R.; Bravo, J.; Carpena, X.; Switala, J.; Mate, M.J.; Fita, I.; Loewen, P.C.
Deposited on : 2000-08-21
Resolution : 2.15 Å(reported)

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

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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

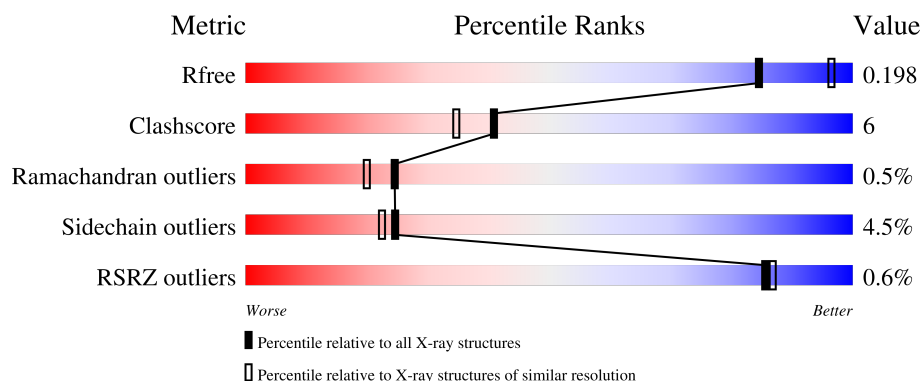
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	% 79% 15% ..
1	B	753	77% 16% ..
1	C	753	74% 19% ..
1	D	753	% 76% 18% ...

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25922 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

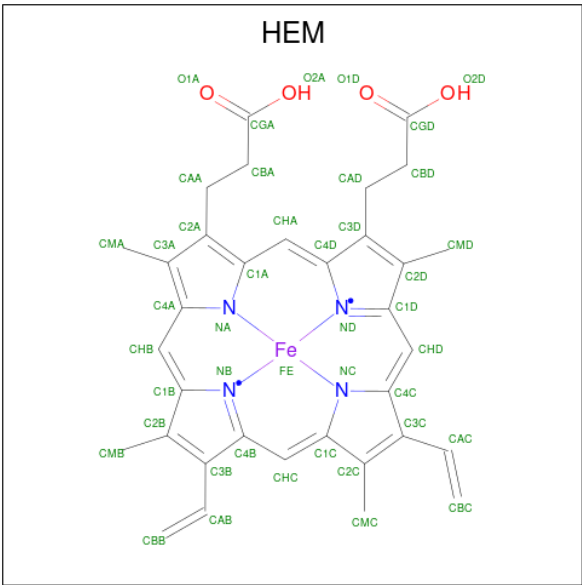
- Molecule 1 is a protein called CATALASE HPIL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5741	3644	1003	1082	12			
1	B	727	Total	C	N	O	S	0	0	0
			5741	3644	1003	1082	12			
1	C	727	Total	C	N	O	S	0	0	0
			5741	3644	1003	1082	12			
1	D	727	Total	C	N	O	S	0	0	0
			5741	3644	1003	1082	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	128	ALA	HIS	engineered mutation	UNP P21179
B	128	ALA	HIS	engineered mutation	UNP P21179
C	128	ALA	HIS	engineered mutation	UNP P21179
D	128	ALA	HIS	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

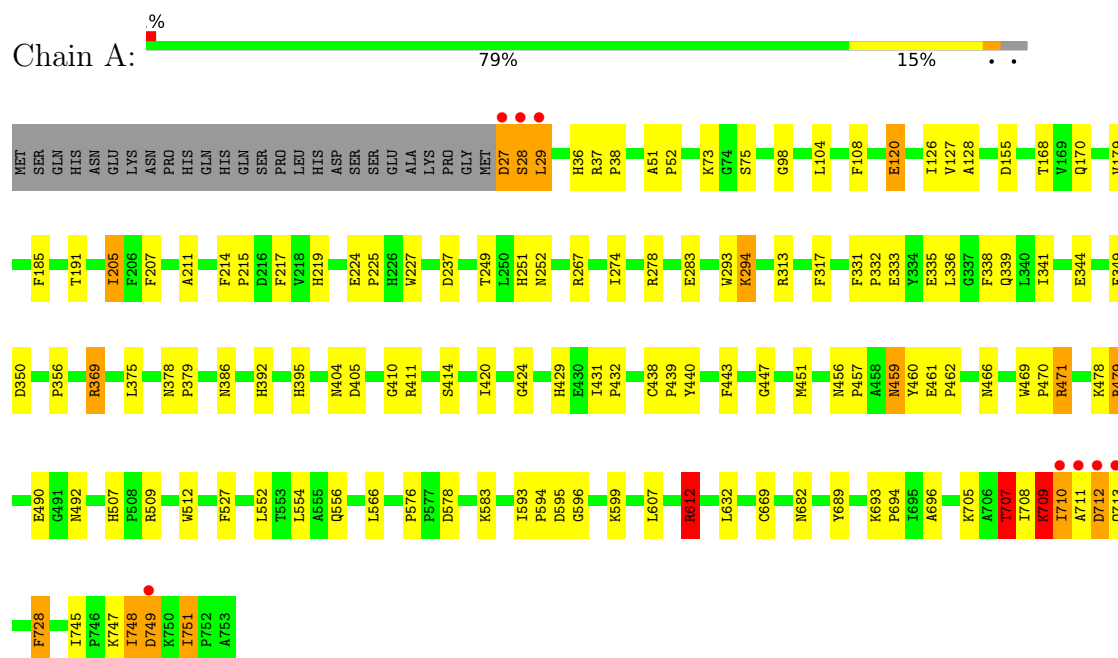
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	737	Total	O	0	0
			737	737		
3	B	661	Total	O	0	0
			661	661		
3	C	675	Total	O	0	0
			675	675		
3	D	713	Total	O	0	0
			713	713		

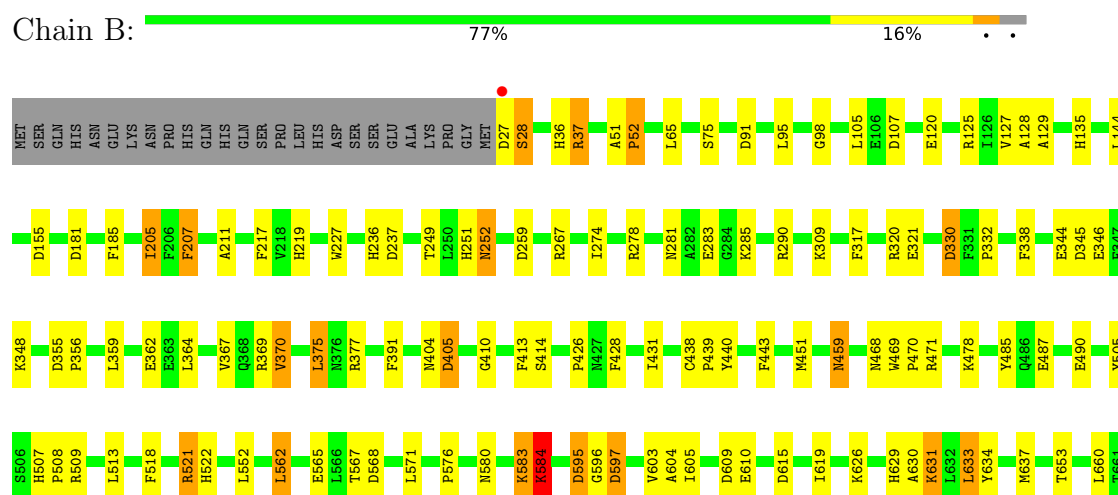
3 Residue-property plots

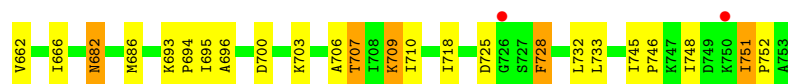
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 HP11



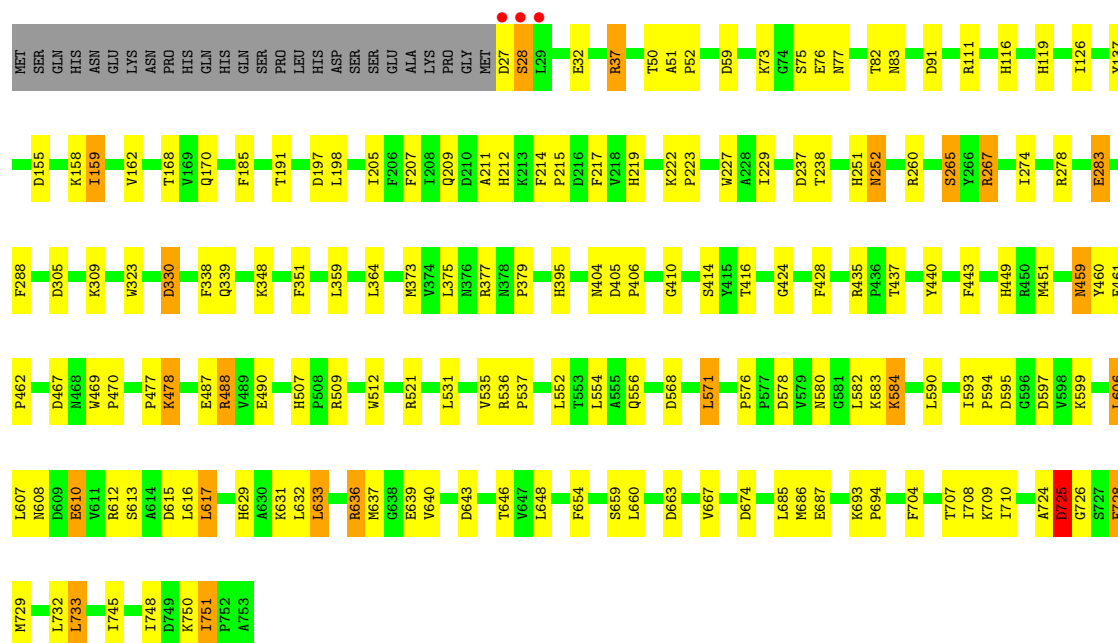
• Molecule 1: CATALASE HP11





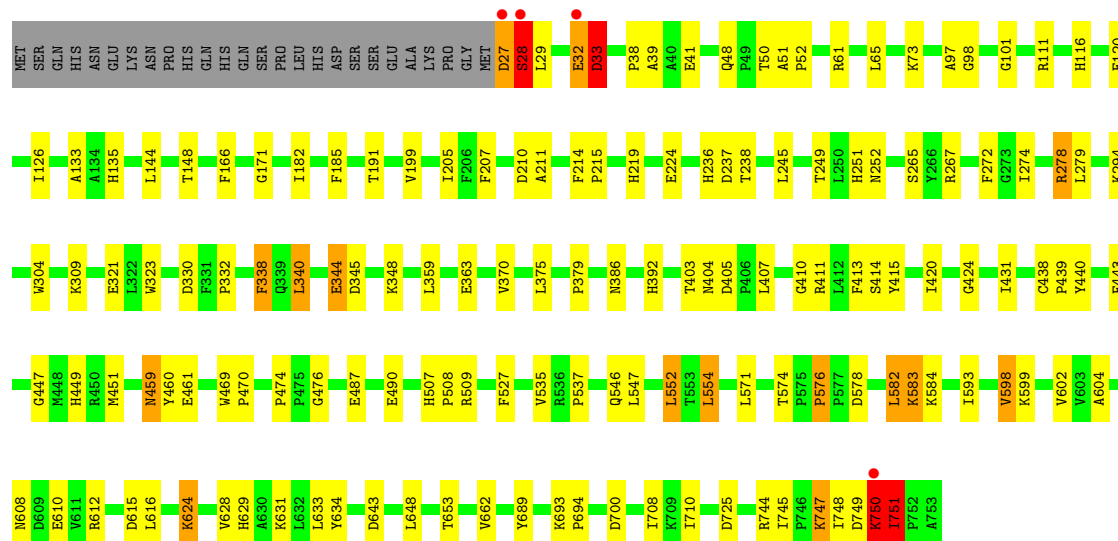
• Molecule 1: CATALASE HPII

Chain C: 74% 19%



• Molecule 1: CATALASE HPII

Chain D: 76% 18%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.04Å 132.34Å 121.20Å 90.00° 109.63° 90.00°	Depositor
Resolution (Å)	87.65 – 2.15 87.65 – 2.15	Depositor EDS
% Data completeness (in resolution range)	95.8 (87.65-2.15) 95.7 (87.65-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 2.15Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.150 , 0.206 0.145 , 0.198	Depositor DCC
R_{free} test set	7176 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	8.7	Xtriage
Anisotropy	0.244	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25922	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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	0.56	0/5896	1.45	37/8016 (0.5%)
1	B	0.57	0/5896	1.47	47/8016 (0.6%)
1	C	0.57	0/5896	1.48	46/8016 (0.6%)
1	D	0.57	0/5896	1.46	41/8016 (0.5%)
All	All	0.57	0/23584	1.47	171/32064 (0.5%)

There are no bond length outliers.

All (171) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	725	ASP	CA-C-N	14.86	150.54	121.41
1	C	725	ASP	C-N-CA	14.86	150.54	121.41
1	D	33	ASP	CA-CB-CG	14.02	126.62	112.60
1	D	449	HIS	CA-CB-CG	13.61	127.41	113.80
1	C	725	ASP	CA-C-O	12.85	138.89	120.51
1	C	488	ARG	CD-NE-CZ	11.81	140.93	124.40
1	B	595	ASP	CA-CB-CG	11.13	123.73	112.60
1	B	185	PHE	CA-CB-CG	10.79	124.59	113.80
1	A	350	ASP	CA-CB-CG	10.51	123.11	112.60
1	D	27	ASP	CA-CB-CG	10.48	123.08	112.60
1	A	748	ILE	N-CA-C	10.45	121.28	110.72
1	C	283	GLU	CB-CG-CD	10.31	130.13	112.60
1	C	330	ASP	CA-CB-CG	10.22	122.82	112.60
1	B	330	ASP	CA-CB-CG	9.84	122.44	112.60
1	A	338	PHE	CA-CB-CG	9.79	123.59	113.80
1	B	414	SER	N-CA-C	9.31	121.42	111.28
1	B	597	ASP	CA-CB-CG	9.26	121.86	112.60
1	A	414	SER	N-CA-C	9.01	121.10	111.28
1	D	414	SER	N-CA-C	8.71	120.39	111.07
1	C	338	PHE	CA-CB-CG	8.54	122.34	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	414	SER	N-CA-C	8.24	120.27	111.28
1	D	615	ASP	CA-CB-CG	7.73	120.33	112.60
1	B	320	ARG	CD-NE-CZ	7.60	135.04	124.40
1	A	27	ASP	CA-CB-CG	7.55	120.15	112.60
1	B	707	THR	N-CA-CB	7.42	121.77	110.28
1	C	663	ASP	CA-CB-CG	-7.28	105.32	112.60
1	C	28	SER	N-CA-C	-7.18	102.54	112.30
1	A	185	PHE	CA-CB-CG	7.14	120.94	113.80
1	B	521	ARG	CD-NE-CZ	7.14	134.39	124.40
1	D	61	ARG	CD-NE-CZ	7.11	134.35	124.40
1	C	428	PHE	CA-CB-CG	-7.03	106.77	113.80
1	D	236	HIS	CA-CB-CG	7.02	120.82	113.80
1	A	751	ILE	N-CA-CB	7.01	117.95	110.17
1	D	166	PHE	CA-C-O	-6.96	113.30	121.16
1	D	111	ARG	CD-NE-CZ	6.93	134.11	124.40
1	C	726	GLY	N-CA-C	-6.93	96.76	113.18
1	D	61	ARG	NE-CZ-NH2	6.92	125.43	119.20
1	B	431	ILE	N-CA-C	-6.91	102.17	108.95
1	C	168	THR	N-CA-C	-6.90	99.10	109.94
1	D	61	ARG	NE-CZ-NH1	-6.85	114.65	121.50
1	C	185	PHE	CA-CB-CG	6.80	120.61	113.80
1	D	32	GLU	N-CA-C	-6.75	99.84	109.96
1	A	707	THR	N-CA-CB	6.72	120.00	110.12
1	A	728	PHE	CA-CB-CG	6.67	120.47	113.80
1	C	217	PHE	CA-CB-CG	-6.66	107.14	113.80
1	C	158	LYS	CA-C-N	-6.65	114.95	123.19
1	C	158	LYS	C-N-CA	-6.65	114.95	123.19
1	B	28	SER	N-CA-CB	6.61	121.66	110.49
1	B	338	PHE	CA-CB-CG	6.52	120.32	113.80
1	A	479	ARG	CD-NE-CZ	6.46	133.44	124.40
1	C	667	VAL	CB-CA-C	-6.41	104.99	111.08
1	D	237	ASP	N-CA-C	6.41	118.80	111.11
1	C	615	ASP	CA-CB-CG	6.40	119.00	112.60
1	D	210	ASP	CA-CB-CG	6.32	118.92	112.60
1	C	237	ASP	N-CA-C	6.29	118.70	111.02
1	D	278	ARG	NE-CZ-NH1	-6.22	115.28	121.50
1	D	725	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	98	GLY	N-CA-C	-6.17	105.01	112.48
1	B	521	ARG	CA-CB-CG	6.16	126.42	114.10
1	D	431	ILE	N-CA-C	-6.14	102.93	108.95
1	C	725	ASP	O-C-N	-6.12	114.44	122.59
1	D	447	GLY	CA-C-O	-6.11	116.92	122.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	212	HIS	CA-CB-CG	-6.11	107.69	113.80
1	D	185	PHE	CA-CB-CG	6.10	119.90	113.80
1	D	98	GLY	N-CA-C	-6.08	104.03	112.18
1	B	706	ALA	CA-C-O	-6.04	114.15	120.55
1	B	283	GLU	N-CA-C	-6.03	104.62	111.07
1	C	437	THR	N-CA-C	-6.01	106.11	113.50
1	C	674	ASP	CA-CB-CG	5.96	118.56	112.60
1	D	546	GLN	OE1-CD-NE2	-5.92	116.68	122.60
1	A	596	GLY	N-CA-C	5.92	127.20	113.18
1	D	612	ARG	CD-NE-CZ	5.92	132.68	124.40
1	B	283	GLU	CA-CB-CG	5.90	125.90	114.10
1	D	265	SER	N-CA-CB	-5.89	102.61	111.56
1	A	339	GLN	CA-C-O	-5.88	114.42	120.54
1	A	707	THR	CB-CA-C	-5.88	101.03	110.79
1	C	170	GLN	N-CA-C	5.87	118.56	111.40
1	C	597	ASP	CA-CB-CG	5.87	118.47	112.60
1	C	351	PHE	CA-CB-CG	-5.84	107.96	113.80
1	B	281	ASN	CA-CB-CG	5.84	118.44	112.60
1	A	492	ASN	CA-C-O	-5.82	114.56	121.66
1	D	386	ASN	OD1-CG-ND2	-5.82	116.78	122.60
1	A	595	ASP	CA-CB-CG	5.81	118.41	112.60
1	C	339	GLN	N-CA-C	-5.75	99.36	108.73
1	B	217	PHE	CA-CB-CG	-5.74	108.06	113.80
1	B	405	ASP	CA-CB-CG	5.72	118.32	112.60
1	B	207	PHE	CA-CB-CG	5.72	119.52	113.80
1	C	728	PHE	CA-CB-CG	5.71	119.51	113.80
1	D	576	PRO	O-C-N	5.70	123.83	121.15
1	A	168	THR	N-CA-C	-5.69	101.01	109.94
1	B	391	PHE	CA-CB-CG	5.68	119.48	113.80
1	A	155	ASP	CA-CB-CG	5.68	118.28	112.60
1	B	596	GLY	N-CA-C	5.61	117.92	111.36
1	A	278	ARG	NE-CZ-NH1	-5.60	115.90	121.50
1	C	155	ASP	CA-CB-CG	5.58	118.19	112.60
1	C	288	PHE	CA-C-O	-5.58	114.91	121.16
1	C	595	ASP	CA-CB-CG	5.58	118.18	112.60
1	A	237	ASP	N-CA-C	5.57	117.80	111.11
1	D	643	ASP	CA-CB-CG	5.55	118.15	112.60
1	D	33	ASP	N-CA-CB	5.54	119.86	110.49
1	B	237	ASP	N-CA-C	5.51	117.73	111.11
1	B	236	HIS	CA-CB-CG	5.51	119.31	113.80
1	C	536	ARG	CA-C-O	5.50	122.86	119.29
1	B	98	GLY	N-CA-C	-5.49	105.84	112.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	709	LYS	N-CA-C	5.47	118.88	111.17
1	B	155	ASP	CA-CB-CG	5.46	118.06	112.60
1	A	108	PHE	CA-CB-CG	5.45	119.25	113.80
1	D	272	PHE	CA-CB-CG	5.45	119.25	113.80
1	A	749	ASP	CA-CB-CG	-5.44	107.16	112.60
1	C	339	GLN	N-CA-CB	5.40	119.22	110.42
1	A	424	GLY	N-CA-C	5.38	123.19	114.90
1	B	52	PRO	CA-C-N	5.35	126.04	119.99
1	B	52	PRO	C-N-CA	5.35	126.04	119.99
1	D	133	ALA	N-CA-C	5.35	117.82	109.52
1	C	640	VAL	N-CA-CB	5.35	121.43	112.44
1	B	428	PHE	CA-CB-CG	-5.35	108.45	113.80
1	A	349	PHE	CA-CB-CG	-5.34	108.46	113.80
1	B	471	ARG	N-CA-C	5.34	118.45	109.95
1	B	283	GLU	N-CA-CB	5.34	117.75	110.01
1	B	485	TYR	CA-C-O	-5.33	114.84	120.92
1	B	370	VAL	CB-CA-C	-5.31	106.39	111.06
1	A	414	SER	CA-C-O	-5.31	114.92	120.55
1	C	536	ARG	CG-CD-NE	5.30	123.65	112.00
1	D	593	ILE	CB-CA-C	-5.29	105.09	111.18
1	B	609	ASP	CA-CB-CG	5.28	117.88	112.60
1	D	182	ILE	N-CA-C	-5.28	104.30	110.05
1	C	111	ARG	CD-NE-CZ	5.28	131.79	124.40
1	A	447	GLY	CA-C-O	-5.27	118.02	122.29
1	C	330	ASP	CB-CA-C	-5.27	104.45	111.88
1	D	424	GLY	N-CA-C	5.27	122.88	115.30
1	D	304	TRP	N-CA-C	5.26	117.42	111.11
1	A	471	ARG	N-CA-C	5.25	118.30	109.95
1	A	224	GLU	CA-C-N	5.25	125.05	119.28
1	A	224	GLU	C-N-CA	5.25	125.05	119.28
1	B	290	ARG	N-CA-CB	5.24	119.48	110.68
1	B	181	ASP	CA-CB-CG	5.24	117.84	112.60
1	D	608	ASN	CA-C-O	-5.24	115.42	121.49
1	A	217	PHE	CA-CB-CG	-5.23	108.57	113.80
1	A	170	GLN	OE1-CD-NE2	-5.22	117.38	122.60
1	C	59	ASP	CA-CB-CG	-5.22	107.38	112.60
1	C	659	SER	CA-C-N	5.21	127.52	120.38
1	C	659	SER	C-N-CA	5.21	127.52	120.38
1	D	474	PRO	O-C-N	5.21	123.71	121.31
1	B	631	LYS	CB-CA-C	5.21	118.47	110.14
1	D	527	PHE	CA-CB-CG	5.20	119.00	113.80
1	D	199	VAL	N-CA-CB	-5.17	106.51	111.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	171	GLY	N-CA-C	5.17	119.15	112.54
1	D	403	THR	N-CA-CB	5.17	119.38	111.22
1	C	725	ASP	N-CA-C	5.16	121.80	110.80
1	C	424	GLY	N-CA-C	5.15	122.72	115.30
1	B	567	THR	CA-C-N	5.15	129.38	121.19
1	B	567	THR	C-N-CA	5.15	129.38	121.19
1	D	224	GLU	CB-CA-C	5.14	117.64	109.52
1	A	456	ASN	CA-CB-CG	5.12	117.72	112.60
1	A	612	ARG	CD-NE-CZ	5.11	131.55	124.40
1	C	116	HIS	CA-CB-CG	-5.09	108.71	113.80
1	B	98	GLY	CA-C-O	-5.09	117.81	122.24
1	A	225	PRO	N-CA-C	5.09	120.52	113.65
1	B	413	PHE	CA-C-N	5.08	127.09	120.28
1	B	413	PHE	C-N-CA	5.08	127.09	120.28
1	D	338	PHE	CA-CB-CG	5.08	118.88	113.80
1	B	682	ASN	CA-CB-CG	-5.07	107.53	112.60
1	A	527	PHE	CA-C-O	-5.06	115.19	120.55
1	C	82	THR	N-CA-C	-5.05	103.38	110.35
1	B	728	PHE	CA-CB-CG	5.05	118.85	113.80
1	A	120	GLU	N-CA-C	5.05	116.86	111.36
1	B	707	THR	CA-C-O	-5.05	114.17	119.97
1	C	608	ASN	CA-C-O	-5.04	115.65	121.49
1	B	317	PHE	N-CA-C	5.03	116.45	111.07
1	A	317	PHE	CA-C-O	-5.01	115.53	120.90
1	B	707	THR	CB-CA-C	-5.01	101.06	110.67

There are no chirality outliers.

There are no planarity outliers.

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	5741	0	5576	79	0
1	B	5741	0	5576	81	0
1	C	5741	0	5575	86	0
1	D	5741	0	5576	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	43	0	30	3	0
2	B	43	0	30	1	0
2	C	43	0	30	1	0
2	D	43	0	30	3	0
3	A	737	0	0	10	0
3	B	661	0	0	10	0
3	C	675	0	0	10	0
3	D	713	0	0	7	0
All	All	25922	0	22423	296	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (296) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:MET:HE2	1:C:451:MET:HE2	1.44	0.99
1:B:451:MET:HE2	1:D:451:MET:HE2	1.49	0.91
1:A:490:GLU:HG2	1:B:490:GLU:HG2	1.57	0.87
1:D:750:LYS:HD3	1:D:751:ILE:H	1.52	0.75
1:B:468:ASN:HD22	1:D:27:ASP:N	1.86	0.73
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.72	0.72
1:B:144:LEU:HD11	1:B:370:VAL:HG13	1.72	0.70
1:D:744:ARG:HA	1:D:747:LYS:HD3	1.74	0.70
1:A:28:SER:HB2	1:D:245:LEU:HD13	1.73	0.70
1:D:267:ARG:HG3	3:D:1248:HOH:O	1.93	0.68
1:D:700:ASP:HB2	3:D:1403:HOH:O	1.93	0.68
1:C:751:ILE:HB	3:C:1414:HOH:O	1.94	0.67
1:D:552:LEU:HD11	1:D:571:LEU:HD23	1.75	0.67
1:C:477:PRO:HB2	1:C:478:LYS:HD3	1.76	0.67
1:C:724:ALA:O	1:C:725:ASP:HB2	1.94	0.67
1:B:710:ILE:HD13	1:B:718:ILE:HG13	1.74	0.67
1:A:612:ARG:HE	1:A:669:CYS:HB3	1.60	0.66
1:B:583:LYS:O	1:B:584:LYS:HB3	1.95	0.65
1:D:27:ASP:O	1:D:28:SER:HB2	1.96	0.65
1:B:345:ASP:HA	1:B:348:LYS:HD2	1.78	0.64
1:D:274:ILE:HD12	2:D:760:HEM:HMB1	1.80	0.62
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.30	0.62
1:C:330:ASP:OD2	1:C:599:LYS:HE2	2.00	0.62
1:D:32:GLU:O	1:D:33:ASP:HB3	2.00	0.62
1:C:725:ASP:HA	1:C:728:PHE:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:38:PRO:HA	1:D:48:GLN:HE21	1.65	0.61
1:C:490:GLU:HG3	1:D:490:GLU:HG3	1.83	0.61
1:B:583:LYS:H	1:B:583:LYS:CE	2.12	0.61
1:C:435:ARG:HD3	3:C:1110:HOH:O	2.02	0.60
1:B:748:ILE:O	1:B:751:ILE:HG22	2.01	0.60
1:B:274:ILE:HD12	2:B:760:HEM:HMB1	1.84	0.59
1:C:704:PHE:O	1:C:707:THR:HG22	2.01	0.59
1:A:335:GLU:OE1	1:A:369:ARG:HG2	2.01	0.59
1:A:748:ILE:O	1:A:751:ILE:HG13	2.03	0.59
1:B:478:LYS:HD2	3:B:1356:HOH:O	2.03	0.59
1:B:583:LYS:H	1:B:583:LYS:NZ	2.00	0.58
1:B:634:TYR:O	1:B:653:THR:HA	2.03	0.58
1:A:709:LYS:HE3	1:A:709:LYS:HA	1.86	0.58
1:C:274:ILE:HD12	2:C:760:HEM:HMB1	1.84	0.58
1:C:323:TRP:CZ3	1:C:379:PRO:HD2	2.39	0.58
1:C:613:SER:HB3	1:C:643:ASP:OD1	2.04	0.57
1:A:607:LEU:HD11	1:A:632:LEU:HB3	1.87	0.57
1:A:214:PHE:HB3	1:A:215:PRO:HD3	1.87	0.57
1:B:686:MET:HB3	1:B:751:ILE:HD11	1.87	0.56
1:A:126:ILE:CD1	1:D:120:GLU:HB2	2.35	0.56
1:A:745:ILE:O	1:A:748:ILE:HG12	2.05	0.56
1:D:267:ARG:HG2	1:D:332:PRO:HB3	1.87	0.56
1:D:51:ALA:HB1	1:D:52:PRO:HD2	1.88	0.55
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.41	0.55
1:D:748:ILE:O	1:D:751:ILE:HG22	2.06	0.55
1:A:708:ILE:O	1:A:710:ILE:N	2.39	0.55
1:B:27:ASP:HB3	3:B:1386:HOH:O	2.07	0.55
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.22	0.55
1:B:605:ILE:HD12	1:B:630:ALA:HB1	1.88	0.55
1:A:51:ALA:HB1	1:A:52:PRO:HD2	1.88	0.55
1:D:359:LEU:H	1:D:507:HIS:HD2	1.55	0.55
1:A:705:LYS:HE3	3:A:1424:HOH:O	2.07	0.54
1:B:631:LYS:HG3	1:B:633:LEU:HD13	1.90	0.54
1:C:260:ARG:HD3	1:C:590:LEU:HD21	1.89	0.54
1:D:750:LYS:CD	1:D:751:ILE:H	2.21	0.54
1:D:27:ASP:HB2	1:D:29:LEU:HD21	1.89	0.54
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.91	0.54
1:A:438:CYS:HB2	1:A:439:PRO:CD	2.38	0.53
1:B:710:ILE:CD1	1:B:718:ILE:HG13	2.38	0.53
1:A:599:LYS:HE3	3:A:1283:HOH:O	2.08	0.53
1:D:629:HIS:HD2	3:D:1119:HOH:O	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:617:LEU:HD12	3:C:1326:HOH:O	2.08	0.53
1:C:636:ARG:NH2	1:C:639:GLU:O	2.40	0.53
1:D:338:PHE:HB3	1:D:340:LEU:HD13	1.89	0.53
1:C:309:LYS:NZ	1:C:687:GLU:OE2	2.41	0.53
1:A:36:HIS:CD2	1:A:36:HIS:H	2.26	0.53
1:B:521:ARG:HE	1:B:745:ILE:HG21	1.72	0.53
1:A:457:PRO:HG2	1:C:37:ARG:NH2	2.23	0.53
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.24	0.53
1:C:509:ARG:HD2	1:C:576:PRO:HD2	1.90	0.53
1:A:478:LYS:HG2	3:A:1257:HOH:O	2.09	0.53
1:B:51:ALA:HB1	1:B:52:PRO:HD2	1.90	0.53
1:D:359:LEU:H	1:D:507:HIS:CD2	2.27	0.53
1:B:344:GLU:CD	1:B:344:GLU:H	2.17	0.52
1:D:32:GLU:O	1:D:33:ASP:CB	2.58	0.52
1:A:52:PRO:HG3	3:C:1004:HOH:O	2.09	0.52
2:A:760:HEM:HBC2	2:A:760:HEM:CMC	2.39	0.52
1:B:309:LYS:HG2	1:B:660:LEU:HD11	1.91	0.52
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.41	0.51
1:C:552:LEU:HD22	1:C:556:GLN:HG3	1.93	0.51
1:A:127:VAL:O	1:A:128:ALA:HB3	2.10	0.51
1:C:631:LYS:HG3	1:C:633:LEU:HD13	1.92	0.51
1:B:267:ARG:HG3	3:B:1255:HOH:O	2.10	0.51
1:B:603:VAL:HG11	1:B:666:ILE:HD12	1.93	0.51
1:C:404:ASN:O	1:C:405:ASP:C	2.54	0.51
1:A:29:LEU:HB2	1:C:467:ASP:OD1	2.11	0.51
1:C:745:ILE:O	1:C:748:ILE:HG12	2.11	0.51
1:B:745:ILE:O	1:B:748:ILE:HG12	2.10	0.51
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.41	0.51
1:A:682:ASN:HB3	1:A:707:THR:HG21	1.92	0.51
1:D:438:CYS:HB2	1:D:439:PRO:CD	2.41	0.51
1:A:751:ILE:HD12	1:A:751:ILE:O	2.11	0.50
1:C:197:ASP:OD1	1:C:395:HIS:ND1	2.41	0.50
1:D:65:LEU:HD21	1:D:135:HIS:CG	2.46	0.50
1:D:207:PHE:O	1:D:249:THR:HA	2.10	0.50
1:B:36:HIS:HD1	1:B:36:HIS:H	1.60	0.50
1:B:120:GLU:HB2	1:C:126:ILE:HD11	1.94	0.50
1:A:578:ASP:OD1	1:A:583:LYS:NZ	2.45	0.50
1:D:214:PHE:HB3	1:D:215:PRO:HD3	1.93	0.50
1:D:404:ASN:O	1:D:405:ASP:C	2.55	0.50
1:A:205:ILE:HB	1:A:356:PRO:O	2.12	0.50
1:B:359:LEU:H	1:B:507:HIS:HD2	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:LYS:HB3	1:C:223:PRO:CD	2.42	0.50
1:A:404:ASN:O	1:A:405:ASP:C	2.55	0.49
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.27	0.49
1:A:420:ILE:HG21	1:C:119:HIS:CE1	2.48	0.49
1:A:612:ARG:HH11	1:A:669:CYS:CB	2.25	0.49
1:A:251:HIS:CE1	1:A:507:HIS:HB3	2.47	0.49
1:D:578:ASP:OD2	1:D:583:LYS:HG3	2.12	0.49
1:D:547:LEU:HB3	1:D:554:LEU:HD13	1.95	0.49
1:D:574:THR:HG22	3:D:1165:HOH:O	2.12	0.49
1:C:416:THR:HA	3:C:1341:HOH:O	2.12	0.49
1:C:459:ASN:H	1:C:459:ASN:HD22	1.60	0.48
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.28	0.48
1:D:602:VAL:HG13	1:D:662:VAL:HA	1.94	0.48
1:B:700:ASP:HB2	3:B:1410:HOH:O	2.12	0.48
1:D:345:ASP:HA	1:D:348:LYS:HG3	1.95	0.48
1:A:443:PHE:CZ	1:A:470:PRO:HD2	2.48	0.48
1:B:127:VAL:O	1:B:128:ALA:HB3	2.13	0.48
1:B:207:PHE:O	1:B:249:THR:HA	2.13	0.48
1:C:251:HIS:CE1	1:C:507:HIS:HB3	2.49	0.48
1:A:179:VAL:HA	3:A:1131:HOH:O	2.14	0.47
1:B:278:ARG:HH22	1:B:487:GLU:CD	2.22	0.47
1:B:604:ALA:HB2	1:B:662:VAL:HG11	1.96	0.47
1:A:378:ASN:HB3	1:A:379:PRO:HD2	1.97	0.47
3:A:909:HOH:O	1:C:52:PRO:HG3	2.14	0.47
1:D:509:ARG:HD2	1:D:576:PRO:HD2	1.97	0.47
1:C:137:TYR:HB2	1:C:159:ILE:HD12	1.96	0.47
1:C:222:LYS:HB3	1:C:223:PRO:HD2	1.97	0.47
1:A:104:LEU:HB3	3:C:781:HOH:O	2.13	0.47
1:B:469:TRP:HA	1:B:470:PRO:C	2.39	0.47
1:A:512:TRP:CZ3	1:A:554:LEU:HD13	2.48	0.47
1:A:37:ARG:HA	1:A:38:PRO:HD3	1.83	0.47
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.50	0.47
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.97	0.47
1:D:745:ILE:O	1:D:748:ILE:HG12	2.14	0.47
1:C:51:ALA:HB1	1:C:52:PRO:HD2	1.97	0.46
1:C:583:LYS:O	1:C:584:LYS:HB3	2.14	0.46
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.45	0.46
1:D:251:HIS:CE1	1:D:507:HIS:HB3	2.50	0.46
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.98	0.46
1:B:362:GLU:HG2	1:B:367:VAL:HG23	1.97	0.46
1:C:552:LEU:HD21	1:C:571:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.98	0.46
1:B:518:PHE:HB3	1:B:521:ARG:NH2	2.30	0.46
1:B:211:ALA:CB	1:B:410:GLY:HA3	2.46	0.46
1:B:369:ARG:HG3	3:B:768:HOH:O	2.15	0.46
1:A:438:CYS:HB2	1:A:439:PRO:HD2	1.97	0.46
1:C:686:MET:HB3	1:C:751:ILE:HD11	1.98	0.46
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.24	0.46
1:C:359:LEU:H	1:C:507:HIS:HD2	1.64	0.45
1:C:607:LEU:HD11	1:C:632:LEU:HB3	1.99	0.45
1:B:332:PRO:HD2	1:B:375:LEU:O	2.17	0.45
1:D:411:ARG:HG2	2:D:760:HEM:C2C	2.51	0.45
1:D:689:TYR:HA	1:D:744:ARG:NH1	2.31	0.45
1:D:634:TYR:O	1:D:653:THR:HA	2.17	0.45
1:A:126:ILE:HD11	1:D:120:GLU:HB2	1.97	0.45
1:B:438:CYS:HB2	1:B:439:PRO:HD2	1.97	0.45
1:D:535:VAL:O	1:D:537:PRO:HD3	2.15	0.45
1:C:443:PHE:CZ	1:C:470:PRO:HD2	2.52	0.45
1:D:323:TRP:CZ3	1:D:379:PRO:HD2	2.52	0.45
1:C:460:TYR:CE2	1:D:238:THR:HB	2.52	0.45
1:A:227:TRP:CZ3	1:D:50:THR:HG21	2.51	0.45
1:C:267:ARG:HD3	3:C:1245:HOH:O	2.16	0.45
1:D:148:THR:HB	1:D:279:LEU:HB3	1.98	0.45
1:B:745:ILE:HB	1:B:746:PRO:HD3	1.97	0.45
1:C:305:ASP:O	1:C:309:LYS:HG3	2.17	0.44
1:A:274:ILE:HD12	2:A:760:HEM:HMB1	1.98	0.44
1:A:712:ASP:HB3	3:A:1436:HOH:O	2.17	0.44
1:B:364:LEU:HD11	1:B:580:ASN:HB2	1.98	0.44
1:C:748:ILE:O	1:C:751:ILE:HG22	2.17	0.44
1:A:267:ARG:HG2	1:A:332:PRO:HB3	1.99	0.44
1:A:708:ILE:O	1:A:709:LYS:C	2.59	0.44
1:B:120:GLU:HB2	1:C:126:ILE:CD1	2.48	0.44
1:B:695:ILE:HB	1:B:718:ILE:CD1	2.48	0.44
1:D:599:LYS:HD3	3:D:1288:HOH:O	2.17	0.44
1:D:708:ILE:HG13	1:D:710:ILE:HG12	1.99	0.44
1:C:709:LYS:HD3	1:C:709:LYS:N	2.32	0.44
1:A:38:PRO:HG2	1:A:51:ALA:HB2	2.00	0.44
1:A:689:TYR:OH	1:A:710:ILE:HG21	2.17	0.44
1:B:693:LYS:HA	1:B:694:PRO:HD3	1.86	0.44
1:C:535:VAL:O	1:C:537:PRO:HD3	2.17	0.44
1:D:624:LYS:HD3	1:D:624:LYS:C	2.43	0.44
1:B:513:LEU:HD12	3:B:1392:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:748:ILE:HA	1:C:751:ILE:HG22	2.00	0.44
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.53	0.44
1:D:469:TRP:HA	1:D:470:PRO:C	2.43	0.44
1:D:39:ALA:H	1:D:48:GLN:NE2	2.15	0.44
1:D:598:VAL:HG13	1:D:628:VAL:CG2	2.48	0.44
1:A:461:GLU:OE1	1:C:91:ASP:OD1	2.36	0.44
1:B:205:ILE:HB	1:B:356:PRO:O	2.18	0.44
1:C:278:ARG:HH12	1:C:487:GLU:CD	2.26	0.44
1:B:105:LEU:HD11	1:D:413:PHE:HB2	2.00	0.43
1:B:521:ARG:NH2	3:B:1092:HOH:O	2.51	0.43
1:A:37:ARG:HD3	3:A:1321:HOH:O	2.18	0.43
1:A:459:ASN:HD22	1:A:460:TYR:HD2	1.66	0.43
1:A:556:GLN:HG3	1:A:566:LEU:HD12	1.99	0.43
1:A:207:PHE:O	1:A:249:THR:HA	2.18	0.43
1:B:91:ASP:OD1	1:D:461:GLU:OE1	2.36	0.43
1:B:259:ASP:OD1	1:B:522:HIS:ND1	2.42	0.43
1:B:267:ARG:HG2	1:B:332:PRO:HB3	2.00	0.43
1:D:144:LEU:HD11	1:D:370:VAL:HG13	2.00	0.43
1:C:606:LEU:HG	1:C:654:PHE:CE2	2.54	0.43
1:D:27:ASP:HB2	1:D:29:LEU:CD2	2.48	0.43
1:A:120:GLU:HB2	1:D:126:ILE:CD1	2.48	0.43
1:B:443:PHE:CZ	1:B:470:PRO:HD2	2.53	0.43
1:C:646:THR:O	1:C:648:LEU:HD13	2.19	0.43
1:D:97:ALA:O	1:D:101:GLY:HA3	2.19	0.43
1:B:631:LYS:HG3	1:B:633:LEU:CD1	2.48	0.43
1:A:593:ILE:HA	1:A:594:PRO:HD2	1.87	0.43
1:C:28:SER:HA	3:C:1435:HOH:O	2.18	0.43
1:A:429:HIS:CG	1:C:83:ASN:HB3	2.54	0.43
1:B:144:LEU:CD1	1:B:370:VAL:HG13	2.43	0.43
1:B:562:LEU:HA	1:C:637:MET:HB2	2.01	0.43
1:B:751:ILE:HD13	1:B:752:PRO:HD2	2.01	0.43
1:C:207:PHE:CD2	1:C:252:ASN:HB3	2.54	0.43
1:A:713:GLN:HG2	3:A:1319:HOH:O	2.20	0.42
1:B:583:LYS:H	1:B:583:LYS:HE2	1.83	0.42
1:D:407:LEU:HD11	2:D:760:HEM:HMC2	2.02	0.42
1:D:693:LYS:HA	1:D:694:PRO:HD3	1.93	0.42
1:A:457:PRO:HG2	1:C:37:ARG:HH21	1.84	0.42
1:B:65:LEU:HD21	1:B:135:HIS:CG	2.54	0.42
1:B:637:MET:HE3	3:B:1284:HOH:O	2.19	0.42
1:A:469:TRP:CE3	1:A:471:ARG:HG3	2.54	0.42
1:C:252:ASN:HD22	1:C:252:ASN:HA	1.63	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:GLU:HB2	1:A:462:PRO:HA	2.02	0.42
1:B:95:LEU:HB3	1:B:107:ASP:HB2	2.00	0.42
1:B:626:LYS:HG3	1:B:733:LEU:HD13	2.00	0.42
1:C:364:LEU:HD11	1:C:580:ASN:HB2	2.02	0.42
1:D:583:LYS:HB2	1:D:583:LYS:NZ	2.35	0.42
1:B:227:TRP:CZ3	1:C:50:THR:HG21	2.54	0.42
1:C:265:SER:OG	1:C:267:ARG:HB2	2.19	0.42
1:A:27:ASP:O	1:A:29:LEU:HG	2.20	0.42
1:A:509:ARG:HD2	1:A:576:PRO:HD2	2.01	0.42
1:A:612:ARG:HG3	3:A:1487:HOH:O	2.19	0.42
1:C:729:MET:O	1:C:733:LEU:HB2	2.19	0.42
1:D:321:GLU:HG3	3:D:1316:HOH:O	2.20	0.42
1:A:294:LYS:NZ	3:A:1135:HOH:O	2.53	0.41
1:A:461:GLU:HA	1:A:462:PRO:C	2.44	0.41
1:C:76:GLU:O	1:C:77:ASN:HB2	2.18	0.41
1:B:505:TYR:HA	1:B:508:PRO:HG2	2.02	0.41
1:D:344:GLU:CD	1:D:344:GLU:H	2.28	0.41
1:A:27:ASP:O	1:A:28:SER:C	2.64	0.41
1:A:293:TRP:CZ3	1:A:336:LEU:HB2	2.56	0.41
1:B:509:ARG:HD2	1:B:576:PRO:HD2	2.02	0.41
1:D:583:LYS:O	1:D:584:LYS:HB3	2.19	0.41
1:A:431:ILE:HG13	1:C:449:HIS:CE1	2.55	0.41
1:B:125:ARG:HB2	1:B:129:ALA:HA	2.02	0.41
1:C:209:GLN:O	1:C:406:PRO:HG2	2.20	0.41
1:B:426:PRO:HB2	1:D:116:HIS:CD2	2.55	0.41
1:C:162:VAL:HG21	1:C:373:MET:SD	2.60	0.41
1:C:227:TRP:CE2	1:C:229:ILE:HB	2.56	0.41
1:D:547:LEU:HD22	1:D:554:LEU:HD11	2.02	0.41
1:A:479:ARG:HD3	3:C:1163:HOH:O	2.21	0.41
1:B:615:ASP:O	1:B:619:ILE:HG13	2.20	0.41
1:C:578:ASP:HB2	1:C:582:LEU:O	2.21	0.41
1:D:438:CYS:HB2	1:D:439:PRO:HD2	2.01	0.41
1:D:507:HIS:N	1:D:508:PRO:HD2	2.35	0.41
1:A:429:HIS:CD2	1:C:83:ASN:HB3	2.55	0.41
1:B:37:ARG:HD2	3:B:1358:HOH:O	2.21	0.41
1:B:696:ALA:HB1	1:B:728:PHE:CZ	2.55	0.41
1:B:252:ASN:HD22	1:B:252:ASN:HA	1.63	0.41
1:B:459:ASN:HD22	1:B:459:ASN:H	1.68	0.41
1:C:469:TRP:HA	1:C:470:PRO:C	2.45	0.41
1:D:476:GLY:HA3	3:D:872:HOH:O	2.20	0.41
1:A:313:ARG:NH1	1:D:309:LYS:HD2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:PHE:O	1:A:333:GLU:HG3	2.20	0.41
1:B:345:ASP:O	1:B:346:GLU:C	2.64	0.41
1:B:355:ASP:HA	1:B:356:PRO:HD2	1.97	0.41
1:C:686:MET:HG2	1:C:751:ILE:HD11	2.02	0.41
1:D:211:ALA:HB3	1:D:410:GLY:HA3	2.02	0.41
1:D:507:HIS:N	1:D:508:PRO:CD	2.83	0.41
1:D:604:ALA:HB2	1:D:662:VAL:HG11	2.03	0.41
1:C:507:HIS:HE1	3:C:923:HOH:O	2.03	0.41
1:B:404:ASN:O	1:B:405:ASP:C	2.64	0.40
1:C:512:TRP:CZ3	1:C:554:LEU:HD13	2.56	0.40
1:C:593:ILE:HA	1:C:594:PRO:HD2	1.90	0.40
1:A:411:ARG:HG2	2:A:760:HEM:C2C	2.56	0.40
1:C:238:THR:HB	1:D:460:TYR:CE2	2.57	0.40
1:C:610:GLU:O	1:C:610:GLU:HG3	2.20	0.40
1:A:386:ASN:OD1	1:A:386:ASN:C	2.63	0.40
1:A:392:HIS:HB3	1:A:395:HIS:CG	2.57	0.40
1:B:629:HIS:HD2	3:B:1034:HOH:O	2.03	0.40
1:C:214:PHE:HB3	1:C:215:PRO:HD3	2.02	0.40
1:C:693:LYS:HA	1:C:694:PRO:HD3	1.97	0.40
1:D:392:HIS:CE1	1:D:415:TYR:HB2	2.57	0.40
1:A:466:ASN:HA	1:C:37:ARG:HH22	1.86	0.40
1:A:748:ILE:HG13	1:A:749:ASP:N	2.35	0.40
1:A:693:LYS:HA	1:A:694:PRO:HD3	1.86	0.40
1:C:461:GLU:HA	1:C:462:PRO:C	2.47	0.40
1:D:363:GLU:HB2	1:D:582:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	725/753 (96%)	701 (97%)	20 (3%)	4 (1%)	21 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	725/753 (96%)	700 (97%)	21 (3%)	4 (1%)	21	15
1	C	725/753 (96%)	701 (97%)	22 (3%)	2 (0%)	36	34
1	D	725/753 (96%)	693 (96%)	28 (4%)	4 (1%)	21	15
All	All	2900/3012 (96%)	2795 (96%)	91 (3%)	14 (0%)	24	20

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	SER
1	A	709	LYS
1	B	28	SER
1	C	725	ASP
1	D	28	SER
1	D	750	LYS
1	D	751	ILE
1	B	725	ASP
1	C	75	SER
1	D	33	ASP
1	A	75	SER
1	A	711	ALA
1	B	584	LYS
1	B	75	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	611/635 (96%)	590 (97%)	21 (3%)	32	33
1	B	611/635 (96%)	587 (96%)	24 (4%)	28	28
1	C	611/635 (96%)	573 (94%)	38 (6%)	16	12
1	D	611/635 (96%)	583 (95%)	28 (5%)	24	22
All	All	2444/2540 (96%)	2333 (96%)	111 (4%)	24	22

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	73	LYS
1	A	191	THR
1	A	205	ILE
1	A	252	ASN
1	A	283	GLU
1	A	294	LYS
1	A	341	ILE
1	A	344	GLU
1	A	369	ARG
1	A	375	LEU
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	612	ARG
1	A	707	THR
1	A	709	LYS
1	A	710	ILE
1	A	712	ASP
1	A	747	LYS
1	B	37	ARG
1	B	205	ILE
1	B	252	ASN
1	B	285	LYS
1	B	321	GLU
1	B	375	LEU
1	B	377	ARG
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	584	LYS
1	B	595	ASP
1	B	597	ASP
1	B	610	GLU
1	B	633	LEU
1	B	703	LYS

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Mol	Chain	Res	Type
1	B	709	LYS
1	B	732	LEU
1	B	751	ILE
1	C	27	ASP
1	C	32	GLU
1	C	37	ARG
1	C	73	LYS
1	C	159	ILE
1	C	191	THR
1	C	198	LEU
1	C	205	ILE
1	C	252	ASN
1	C	265	SER
1	C	267	ARG
1	C	283	GLU
1	C	348	LYS
1	C	375	LEU
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	531	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	616	LEU
1	C	617	LEU
1	C	633	LEU
1	C	636	ARG
1	C	660	LEU
1	C	685	LEU
1	C	725	ASP
1	C	732	LEU
1	C	733	LEU
1	C	750	LYS
1	C	751	ILE
1	D	28	SER

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Mol	Chain	Res	Type
1	D	41	GLU
1	D	73	LYS
1	D	191	THR
1	D	205	ILE
1	D	252	ASN
1	D	294	LYS
1	D	340	LEU
1	D	344	GLU
1	D	375	LEU
1	D	420	ILE
1	D	440	TYR
1	D	459	ASN
1	D	552	LEU
1	D	554	LEU
1	D	582	LEU
1	D	583	LYS
1	D	598	VAL
1	D	610	GLU
1	D	616	LEU
1	D	624	LYS
1	D	631	LYS
1	D	633	LEU
1	D	648	LEU
1	D	747	LYS
1	D	749	ASP
1	D	750	LYS
1	D	751	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	84	GLN
1	A	252	ASN
1	A	368	GLN
1	A	459	ASN
1	A	515	GLN
1	A	713	GLN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	546	GLN

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Mol	Chain	Res	Type
1	B	629	HIS
1	C	139	GLN
1	C	252	ASN
1	C	368	GLN
1	C	449	HIS
1	C	459	ASN
1	C	507	HIS
1	C	515	GLN
1	C	572	ASN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	252	ASN
1	D	459	ASN
1	D	507	HIS
1	D	546	GLN
1	D	629	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	A	760	1	50,50,50	1.34	8 (16%)	67,82,82	1.10	6 (8%)
2	HEM	B	760	1	50,50,50	1.37	10 (20%)	67,82,82	0.95	4 (5%)
2	HEM	D	760	1	50,50,50	1.28	8 (16%)	67,82,82	0.97	3 (4%)
2	HEM	C	760	1	50,50,50	1.33	8 (16%)	67,82,82	0.95	3 (4%)

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	-	2/14/54/54	-
2	HEM	B	760	1	-	2/14/54/54	-
2	HEM	D	760	1	-	2/14/54/54	-
2	HEM	C	760	1	-	2/14/54/54	-

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HEM	CAC-C3C	3.02	1.55	1.47
2	D	760	HEM	CAB-C3B	2.92	1.55	1.47
2	C	760	HEM	FE-NB	2.83	2.03	1.94
2	C	760	HEM	CAB-C3B	2.79	1.54	1.47
2	D	760	HEM	CAC-C3C	2.76	1.54	1.47
2	B	760	HEM	FE-NA	2.75	2.04	1.95
2	D	760	HEM	FE-ND	2.74	2.03	1.94
2	B	760	HEM	CAB-C3B	2.73	1.54	1.47
2	C	760	HEM	CAC-C3C	2.69	1.54	1.47
2	A	760	HEM	FE-NB	2.68	2.03	1.94
2	A	760	HEM	CAB-C3B	2.67	1.54	1.47
2	D	760	HEM	FE-NC	2.58	2.03	1.95
2	A	760	HEM	FE-NC	2.47	2.03	1.95
2	B	760	HEM	CAC-C3C	2.47	1.54	1.47
2	D	760	HEM	FE-NA	2.45	2.03	1.95
2	B	760	HEM	FE-NB	2.42	2.02	1.94
2	C	760	HEM	FE-ND	2.39	2.02	1.94
2	C	760	HEM	FE-NC	2.38	2.03	1.95
2	B	760	HEM	FE-ND	2.34	2.02	1.94
2	B	760	HEM	CMC-C2C	2.34	1.55	1.50
2	B	760	HEM	CMA-C3A	2.32	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	760	HEM	FE-NC	2.31	2.02	1.95
2	A	760	HEM	FE-ND	2.31	2.02	1.94
2	D	760	HEM	FE-NB	2.28	2.01	1.94
2	A	760	HEM	CMD-C2D	2.26	1.55	1.50
2	C	760	HEM	CMB-C2B	2.17	1.55	1.50
2	B	760	HEM	C2A-C3A	-2.16	1.33	1.38
2	C	760	HEM	CMC-C2C	2.11	1.55	1.50
2	A	760	HEM	CMB-C2B	2.09	1.55	1.50
2	B	760	HEM	CMD-C2D	2.08	1.55	1.50
2	A	760	HEM	CMC-C2C	2.07	1.55	1.50
2	D	760	HEM	CMD-C2D	2.02	1.54	1.50
2	C	760	HEM	CMD-C2D	2.01	1.54	1.50
2	D	760	HEM	C2A-C3A	-2.01	1.33	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	760	HEM	O2A-CGA-O1A	4.08	133.84	123.33
2	A	760	HEM	CHD-C4C-NC	3.15	127.89	124.45
2	A	760	HEM	CHC-C1C-NC	3.14	127.87	124.45
2	A	760	HEM	O2A-CGA-O1A	3.09	131.28	123.33
2	D	760	HEM	O1A-CGA-CBA	-2.92	113.82	123.09
2	D	760	HEM	CAD-CBD-CGD	2.67	120.74	113.67
2	C	760	HEM	O1A-CGA-CBA	-2.61	114.82	123.09
2	A	760	HEM	CBC-CAC-C3C	-2.50	115.03	127.53
2	C	760	HEM	O2A-CGA-O1A	2.40	129.51	123.33
2	B	760	HEM	O1A-CGA-CBA	-2.30	115.79	123.09
2	A	760	HEM	C4C-CHD-C1D	-2.15	121.45	126.02
2	A	760	HEM	O1A-CGA-CBA	-2.09	116.48	123.09
2	B	760	HEM	O2A-CGA-O1A	2.07	128.66	123.33
2	B	760	HEM	CMD-C2D-C1D	-2.06	121.82	125.03
2	B	760	HEM	CHD-C1D-ND	2.05	126.63	124.42
2	C	760	HEM	CAD-CBD-CGD	2.03	119.06	113.67

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

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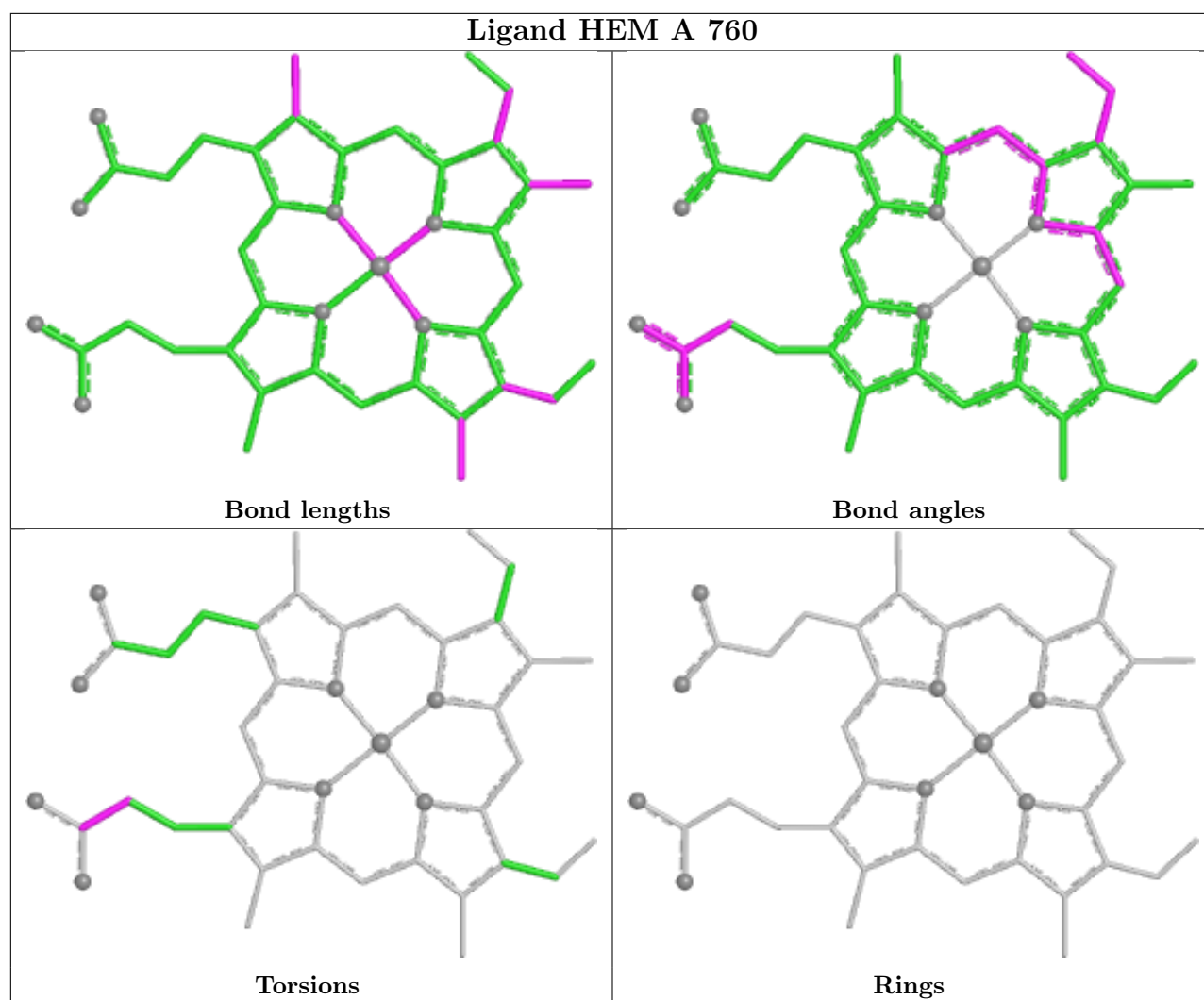
Mol	Chain	Res	Type	Atoms
2	D	760	HEM	CAA-CBA-CGA-O2A
2	C	760	HEM	CAA-CBA-CGA-O2A
2	B	760	HEM	CAA-CBA-CGA-O1A
2	B	760	HEM	CAA-CBA-CGA-O2A

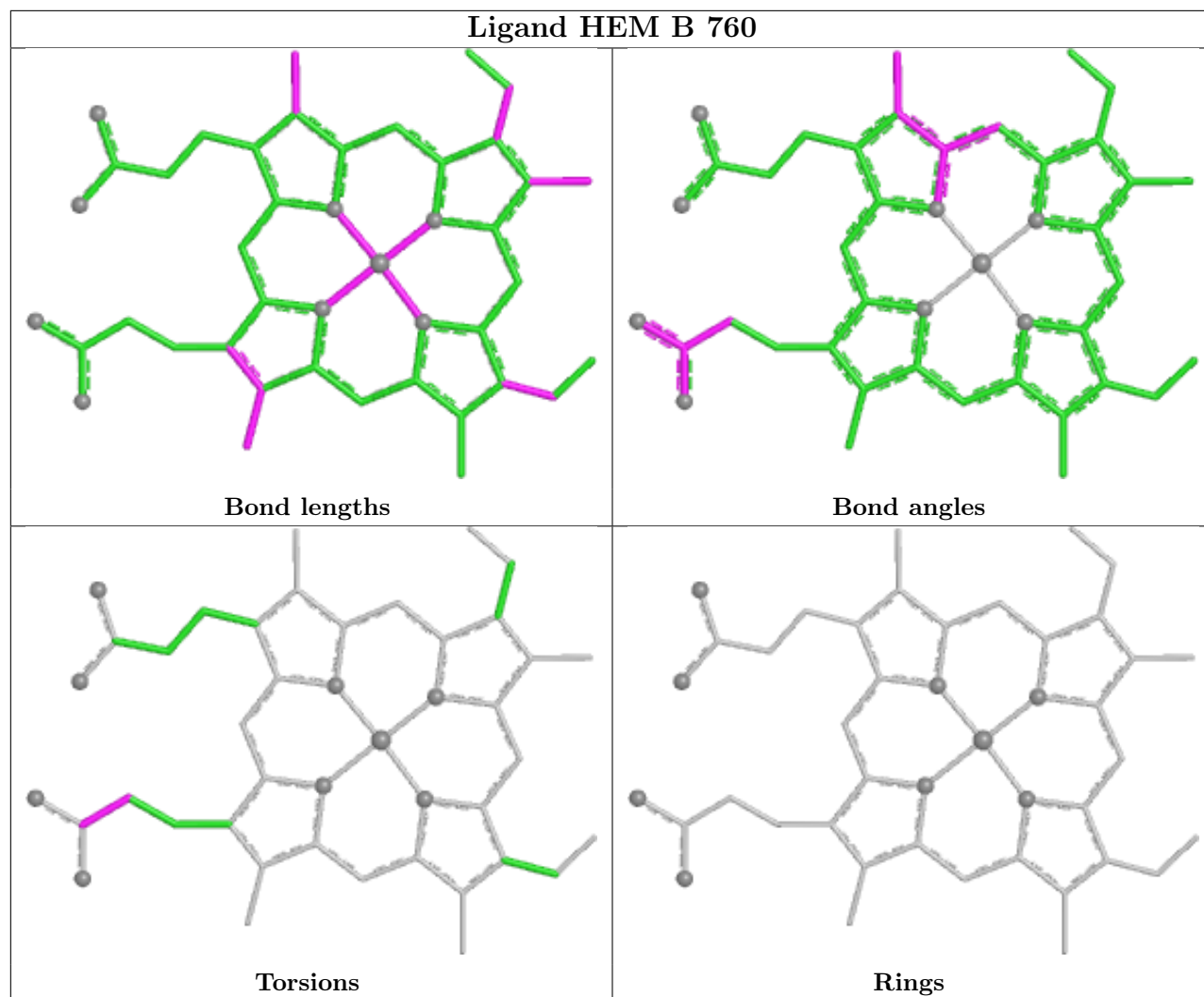
There are no ring outliers.

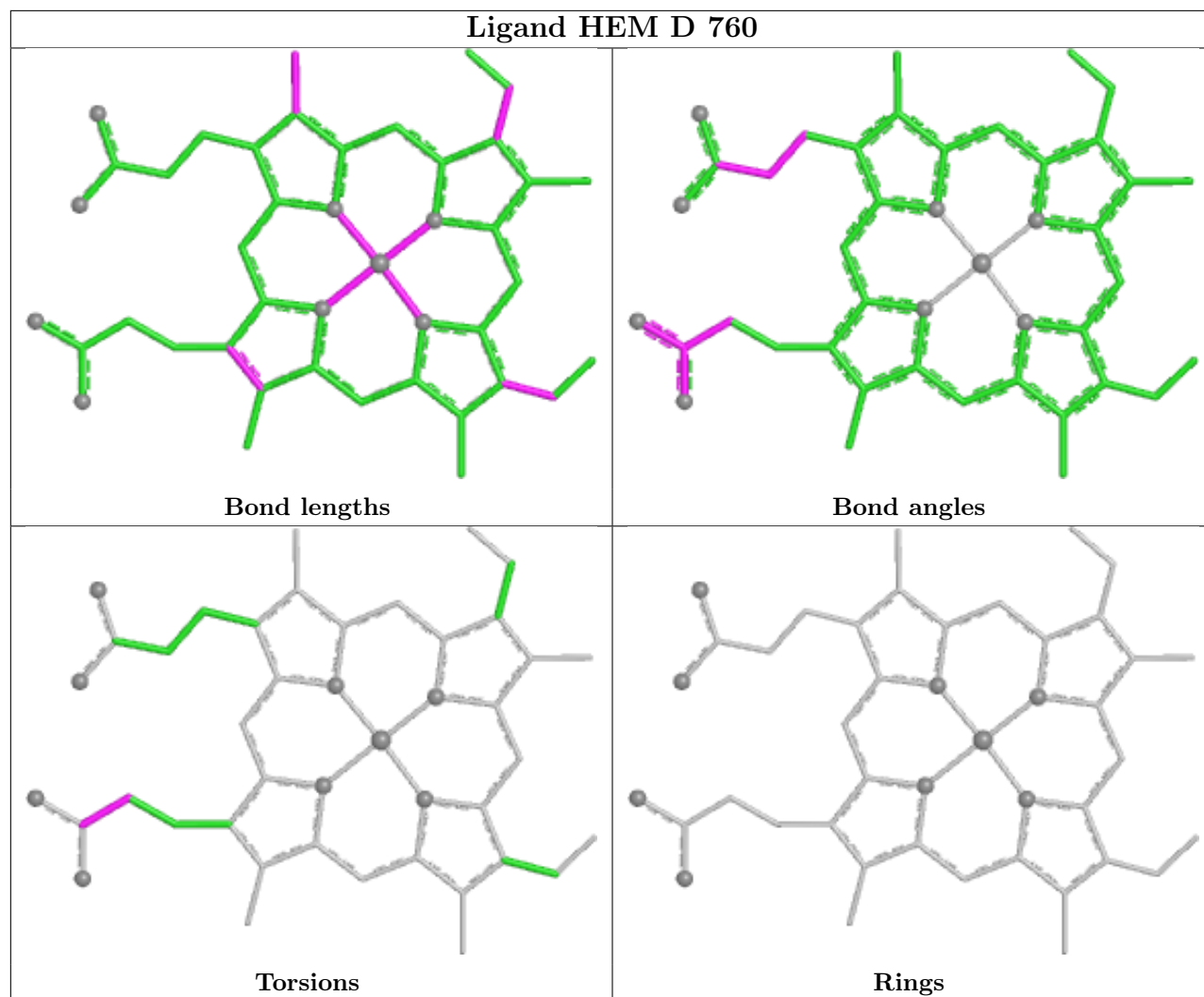
4 monomers are involved in 8 short contacts:

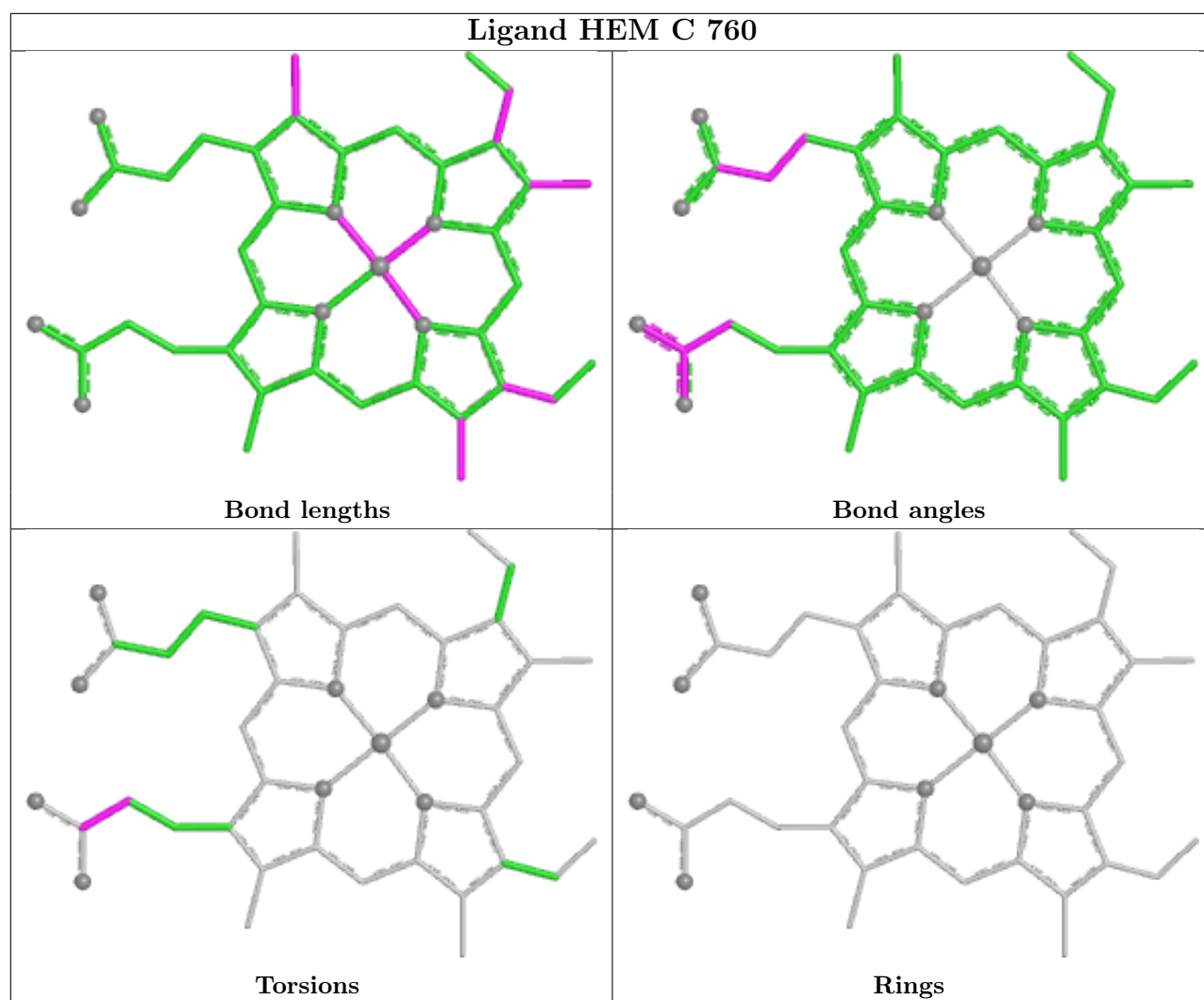
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	760	HEM	3	0
2	B	760	HEM	1	0
2	D	760	HEM	3	0
2	C	760	HEM	1	0

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

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	727/753 (96%)	-0.64	8 (1%) 78 80	3, 8, 26, 50	1 (0%)
1	B	727/753 (96%)	-0.62	3 (0%) 88 90	3, 9, 28, 47	1 (0%)
1	C	727/753 (96%)	-0.63	3 (0%) 88 90	3, 9, 28, 46	1 (0%)
1	D	727/753 (96%)	-0.65	4 (0%) 85 87	3, 8, 27, 47	1 (0%)
All	All	2908/3012 (96%)	-0.63	18 (0%) 85 87	3, 8, 27, 50	4 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	27	ASP	6.5
1	A	28	SER	5.4
1	A	710	ILE	4.5
1	A	711	ALA	3.7
1	C	27	ASP	3.7
1	B	27	ASP	3.7
1	D	27	ASP	3.7
1	A	712	ASP	3.5
1	A	29	LEU	2.7
1	A	713	GLN	2.6
1	B	750	LYS	2.4
1	C	28	SER	2.3
1	D	28	SER	2.3
1	B	726	GLY	2.3
1	A	749	ASP	2.2
1	C	29	LEU	2.1
1	D	750	LYS	2.1
1	D	32	GLU	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](#)

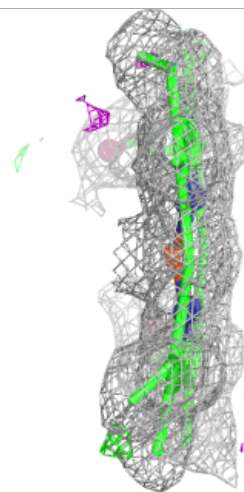
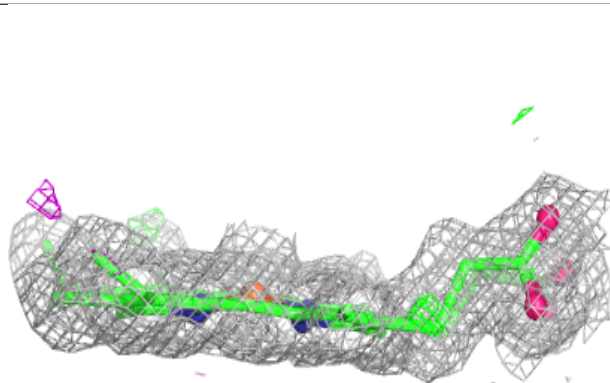
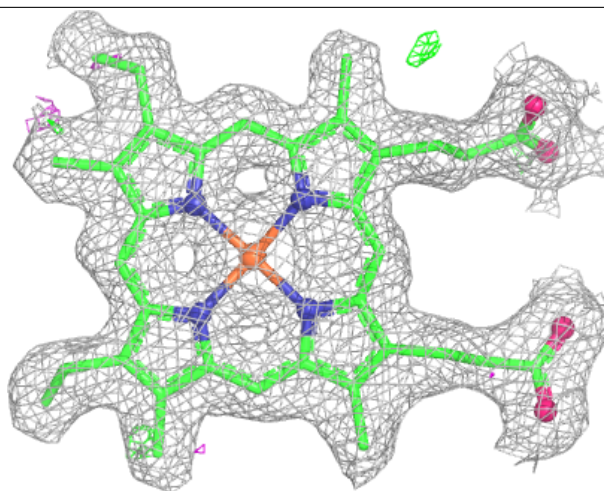
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	A	760	43/43	0.99	0.04	2,5,6,7	0
2	HEM	B	760	43/43	0.99	0.04	3,5,6,6	0
2	HEM	C	760	43/43	0.99	0.04	2,5,7,8	0
2	HEM	D	760	43/43	0.99	0.04	2,5,6,6	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.

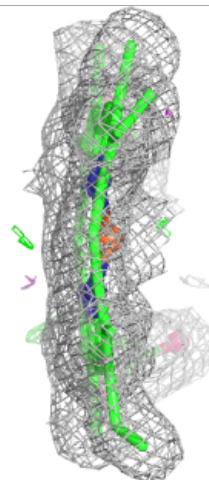
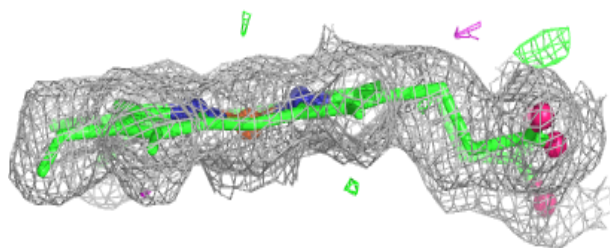
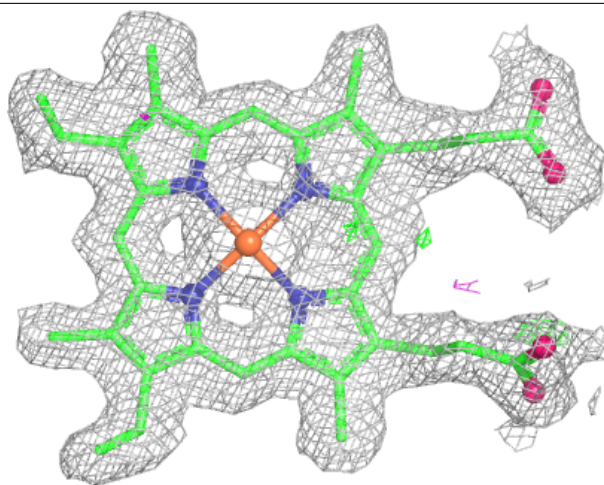
Electron density around HEM A 760:

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



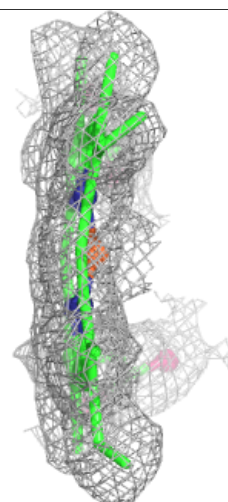
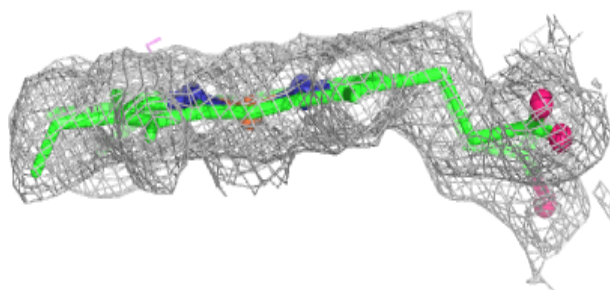
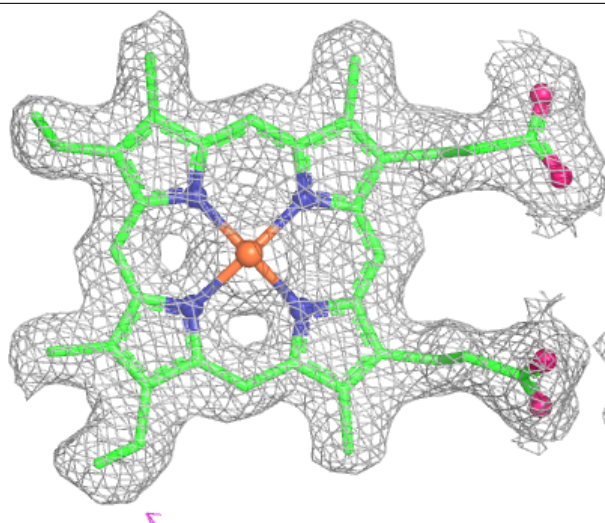
Electron density around HEM B 760:

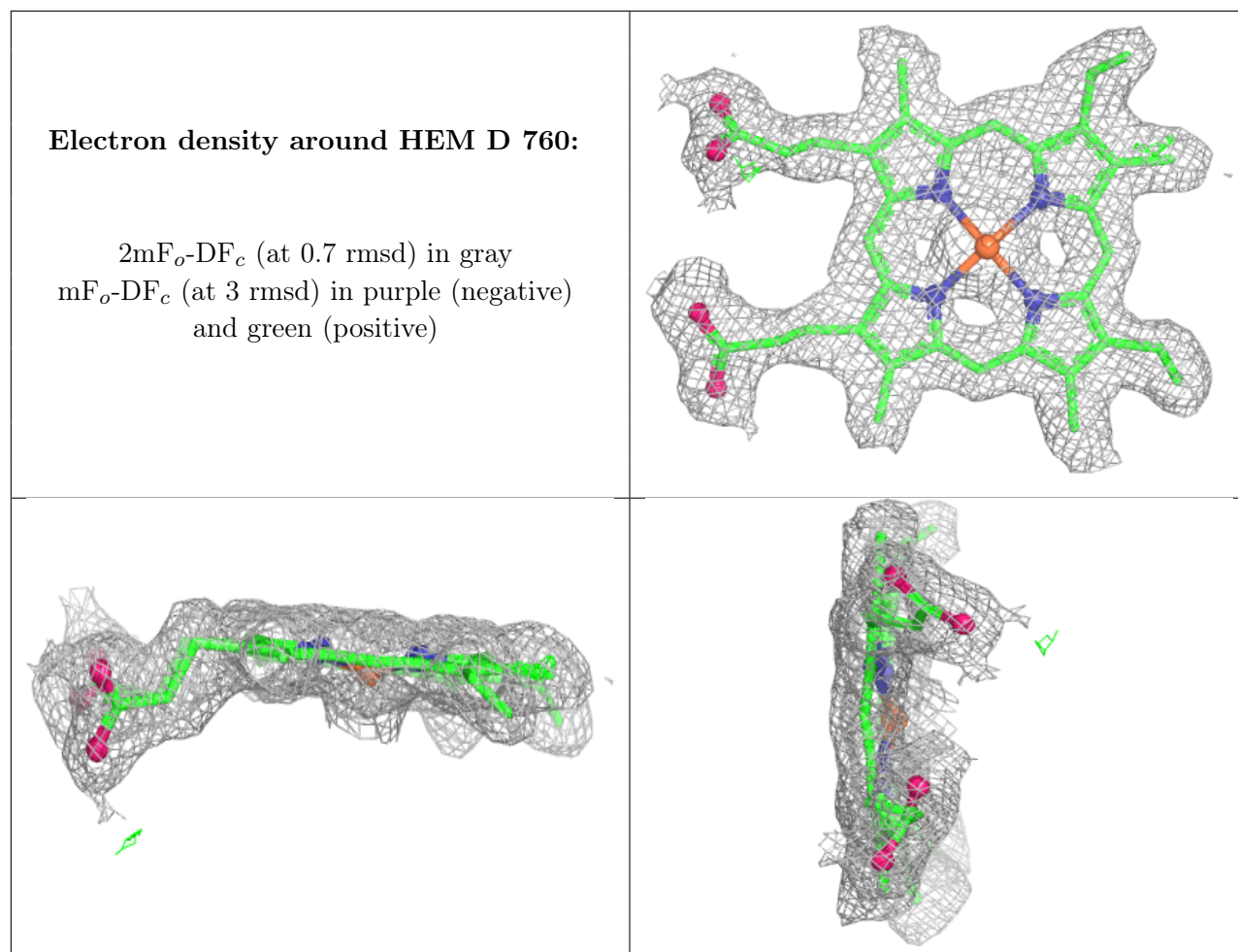
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.