



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:43 AM UTC

PDB ID : 3TTX / pdb_00003ttx
Title : Structure of the F413K variant of E. coli KatE
Authors : Loewen, P.C.; Jha, V.
Deposited on : 2011-09-15
Resolution : 1.74 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

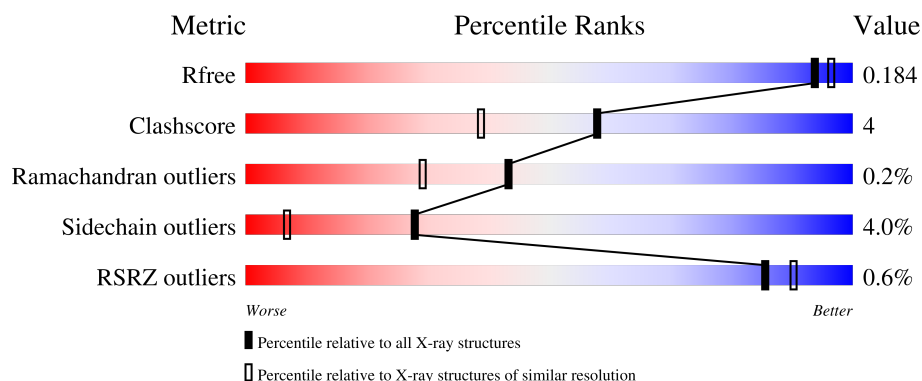
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	% 86% 9% ...
1	B	753	% 85% 9% ...
1	C	753	% 82% 13% ...
1	D	753	% 84% 11% ...

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26010 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	3644	1007	1082	12			
1	B	726	Total	C	N	O	S	0	1	0
			5746	3645	1007	1082	12			
1	C	726	Total	C	N	O	S	0	1	0
			5745	3644	1007	1082	12			
1	D	726	Total	C	N	O	S	0	1	0
			5746	3645	1007	1082	12			

There are 4 discrepancies between the modelled and reference sequences:

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

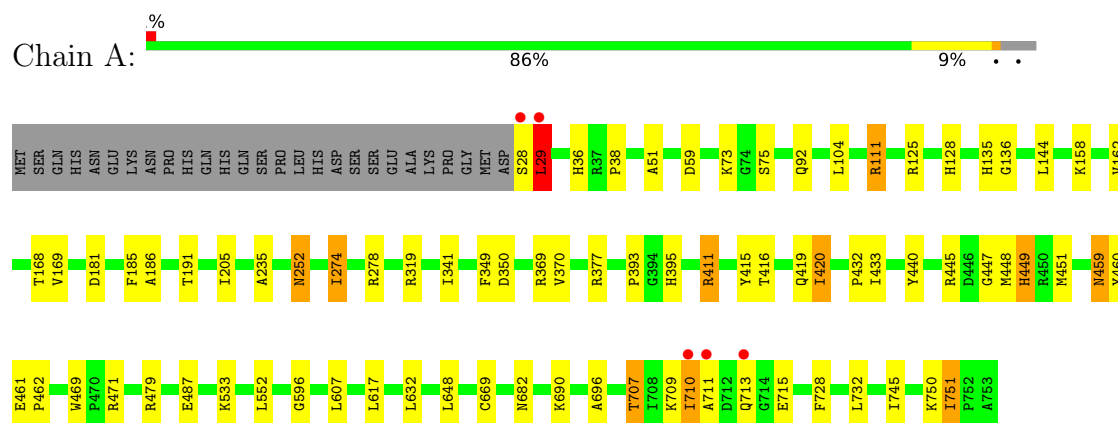
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	771	Total O 771 771	0	0
3	B	650	Total O 650 650	0	0
3	C	690	Total O 690 690	0	0
3	D	745	Total O 745 745	0	0

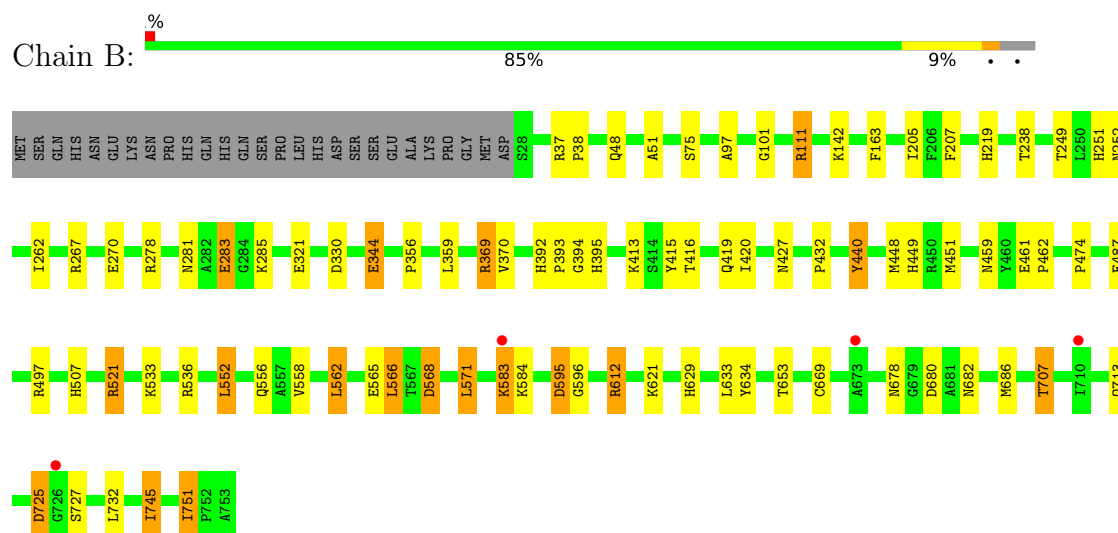
3 Residue-property plots

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.

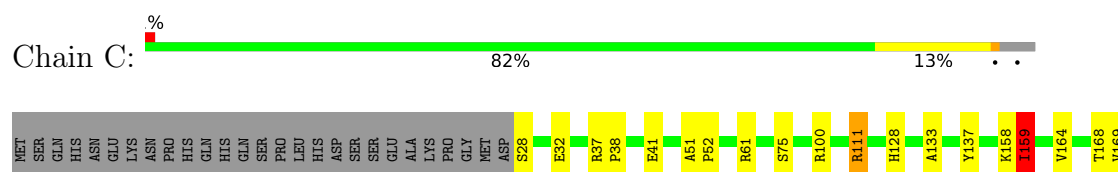
• Molecule 1: Catalase HP11

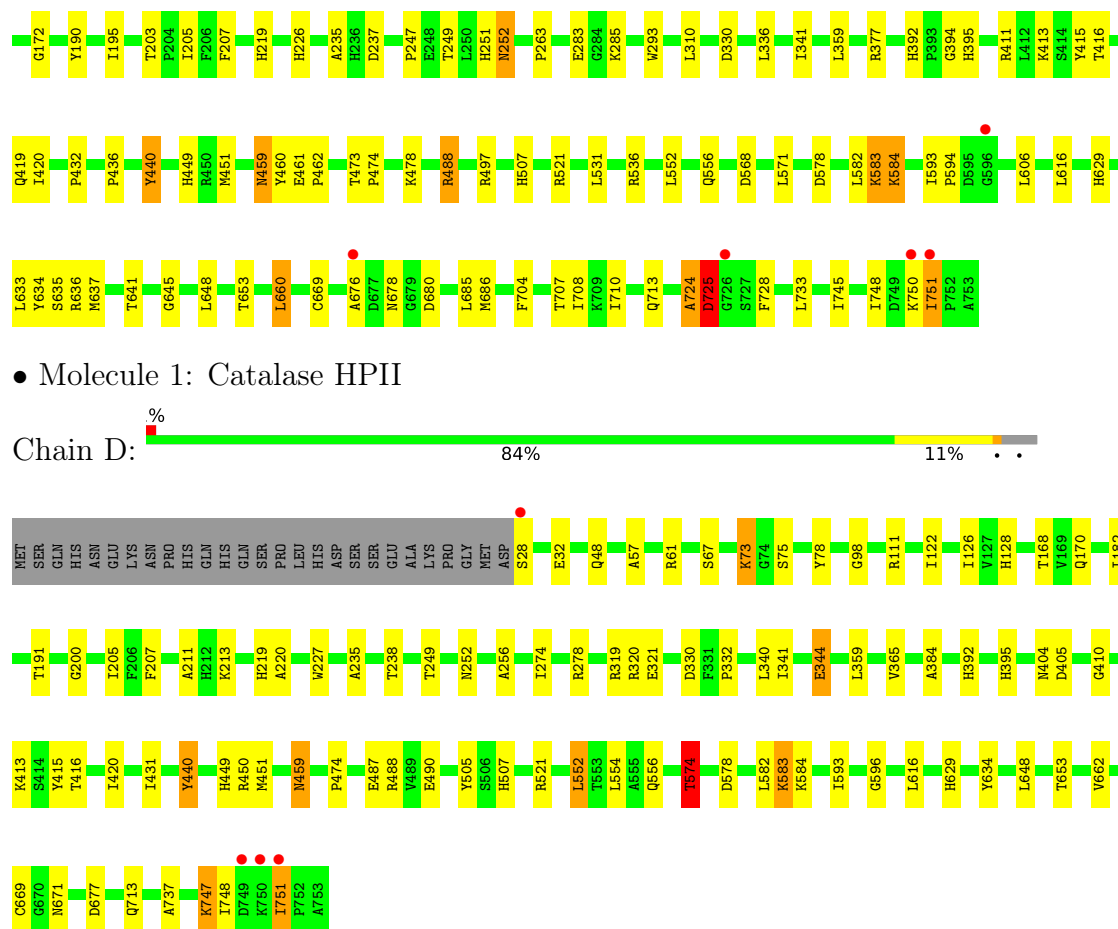


• Molecule 1: Catalase HP11



• Molecule 1: Catalase HP11





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.50Å 132.96Å 122.03Å 90.00° 109.69° 90.00°	Depositor
Resolution (Å)	35.18 – 1.74 35.18 – 1.74	Depositor EDS
% Data completeness (in resolution range)	97.0 (35.18-1.74) 97.0 (35.18-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 1.74Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.146 , 0.185 0.146 , 0.184	Depositor DCC
R_{free} test set	14075 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	12.3	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	26010	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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, OCS

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	1.46	12/5895 (0.2%)	1.21	17/8012 (0.2%)
1	B	1.43	7/5895 (0.1%)	1.21	15/8012 (0.2%)
1	C	1.41	13/5895 (0.2%)	1.19	13/8012 (0.2%)
1	D	1.45	20/5895 (0.3%)	1.19	10/8012 (0.1%)
All	All	1.44	52/23580 (0.2%)	1.20	55/32048 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	745	ILE	CA-CB	8.16	1.58	1.54
1	D	57	ALA	CA-CB	8.11	1.62	1.53
1	A	341	ILE	CA-C	-7.30	1.46	1.52
1	A	235	ALA	CA-CB	7.06	1.62	1.52
1	A	29	LEU	N-CA	-6.74	1.36	1.46
1	C	341	ILE	CA-CB	-6.67	1.49	1.54
1	D	122	ILE	CA-CB	6.32	1.60	1.55
1	B	262	ILE	CA-CB	6.31	1.62	1.54
1	D	200	GLY	N-CA	6.30	1.50	1.44
1	A	135	HIS	N-CA	6.29	1.53	1.45
1	B	497	ARG	CZ-NH2	6.21	1.41	1.33
1	C	235	ALA	CA-CB	5.98	1.59	1.52
1	A	447	GLY	N-CA	5.92	1.51	1.45
1	D	320	ARG	CZ-NH1	5.89	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	263	PRO	C-O	5.88	1.30	1.23
1	D	256	ALA	CA-CB	5.87	1.62	1.53
1	D	220	ALA	CA-C	5.86	1.60	1.52
1	D	235	ALA	C-O	5.78	1.30	1.23
1	A	445	ARG	CD-NE	5.71	1.54	1.46
1	B	568	ASP	CB-CG	5.63	1.66	1.52
1	A	433	ILE	CA-CB	5.55	1.62	1.54
1	C	474	PRO	C-O	-5.55	1.20	1.25
1	D	420	ILE	CA-CB	5.52	1.61	1.54
1	A	411	ARG	CZ-NH1	5.52	1.40	1.32
1	D	431	ILE	CA-C	5.51	1.59	1.52
1	D	593	ILE	CA-CB	5.50	1.59	1.53
1	A	186	ALA	N-CA	5.48	1.52	1.46
1	B	420	ILE	CA-CB	5.45	1.61	1.54
1	C	419	GLN	CB-CG	5.44	1.68	1.52
1	A	181	ASP	C-O	5.42	1.29	1.23
1	C	497	ARG	CZ-NH2	5.40	1.40	1.33
1	C	190	TYR	C-O	5.37	1.30	1.23
1	D	365	VAL	N-CA	5.35	1.53	1.46
1	D	170	GLN	C-O	5.31	1.30	1.24
1	B	427	ASN	N-CA	5.31	1.52	1.46
1	D	319	ARG	C-O	5.30	1.30	1.24
1	C	172	GLY	N-CA	5.29	1.52	1.45
1	D	67	SER	N-CA	5.27	1.53	1.46
1	C	473	THR	C-N	5.23	1.38	1.33
1	C	473	THR	CA-C	-5.22	1.48	1.52
1	D	332	PRO	N-CA	5.20	1.53	1.47
1	C	169	VAL	N-CA	5.13	1.50	1.46
1	D	450	ARG	C-O	-5.09	1.18	1.24
1	D	384	ALA	CA-CB	5.08	1.61	1.53
1	D	505	TYR	CA-CB	5.08	1.61	1.54
1	C	203	THR	CA-C	5.07	1.57	1.52
1	C	247	PRO	CA-CB	5.06	1.60	1.53
1	A	125	ARG	N-CA	5.05	1.52	1.46
1	D	78	TYR	N-CA	5.04	1.51	1.45
1	B	356	PRO	CA-C	5.02	1.57	1.52
1	D	662	VAL	CA-CB	5.01	1.62	1.54
1	A	274	ILE	N-CA	5.01	1.52	1.46

All (55) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	710	ILE	N-CA-C	8.33	126.66	109.34
1	B	521	ARG	NE-CZ-NH2	7.28	125.75	119.20
1	B	536	ARG	CA-C-N	-6.83	111.95	119.19
1	B	536	ARG	C-N-CA	-6.83	111.95	119.19
1	B	111	ARG	NE-CZ-NH1	-6.79	114.71	121.50
1	C	725	ASP	N-CA-C	6.68	125.03	110.80
1	C	111	ARG	NE-CZ-NH1	-6.68	114.82	121.50
1	D	126	ILE	CB-CA-C	-6.51	103.35	112.14
1	D	431	ILE	N-CA-C	-6.36	102.03	108.96
1	A	751	ILE	N-CA-CB	6.27	115.91	110.08
1	D	182	ILE	N-CA-C	-6.23	103.26	110.05
1	C	159	ILE	CB-CG1-CD1	-6.19	100.80	113.80
1	C	237	ASP	N-CA-C	6.19	118.54	111.11
1	A	420	ILE	CB-CG1-CD1	6.14	126.69	113.80
1	A	111	ARG	NE-CZ-NH2	-6.10	113.71	119.20
1	C	226	HIS	N-CA-C	-6.05	104.60	111.14
1	C	41	GLU	N-CA-C	-5.88	102.93	108.22
1	B	595	ASP	CA-C-N	5.87	125.56	119.92
1	B	595	ASP	C-N-CA	5.87	125.56	119.92
1	C	676	ALA	N-CA-C	5.81	119.85	112.87
1	B	270	GLU	CA-C-N	5.71	126.00	121.61
1	B	270	GLU	C-N-CA	5.71	126.00	121.61
1	B	596	GLY	N-CA-C	5.67	117.99	111.36
1	D	574	THR	CA-C-N	5.64	123.78	119.66
1	D	574	THR	C-N-CA	5.64	123.78	119.66
1	A	449[A]	HIS	CB-CA-C	5.61	119.69	111.73
1	A	449[B]	HIS	CB-CA-C	5.61	119.69	111.73
1	D	61	ARG	NE-CZ-NH2	5.59	124.24	119.20
1	C	536	ARG	CA-C-N	-5.57	113.93	119.56
1	C	536	ARG	C-N-CA	-5.57	113.93	119.56
1	A	648	LEU	CA-C-N	-5.54	114.27	120.14
1	A	648	LEU	C-N-CA	-5.54	114.27	120.14
1	D	344	GLU	CA-CB-CG	5.53	125.17	114.10
1	B	419	GLN	CB-CA-C	5.51	121.82	110.31
1	A	709	LYS	CA-C-N	-5.50	112.07	121.97
1	A	709	LYS	C-N-CA	-5.50	112.07	121.97
1	C	158	LYS	CA-C-N	-5.44	116.45	123.19
1	C	158	LYS	C-N-CA	-5.44	116.45	123.19
1	D	98	GLY	N-CA-C	-5.42	105.92	112.48
1	A	377	ARG	CG-CD-NE	-5.35	100.23	112.00
1	D	474	PRO	CA-C-N	-5.34	114.74	120.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	474	PRO	C-N-CA	-5.34	114.74	120.03
1	A	419	GLN	CB-CA-C	5.21	121.19	110.31
1	B	474	PRO	CA-C-N	-5.19	114.89	120.03
1	B	474	PRO	C-N-CA	-5.19	114.89	120.03
1	C	745	ILE	O-C-N	5.17	123.73	120.42
1	A	745	ILE	O-C-N	5.14	123.71	120.42
1	B	283	GLU	CB-CG-CD	5.14	121.33	112.60
1	A	350	ASP	CB-CA-C	5.13	119.49	110.37
1	A	596	GLY	N-CA-C	5.11	117.34	111.36
1	C	100	ARG	CB-CA-C	-5.10	102.76	111.02
1	B	163	PHE	N-CA-C	-5.09	100.16	108.76
1	B	111	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	A	349	PHE	CA-C-N	-5.03	113.91	122.56
1	A	349	PHE	C-N-CA	-5.03	113.91	122.56

There are no chirality outliers.

All (2) planarity outliers are listed below:

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

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5745	0	5579	44	1
1	B	5746	0	5584	55	1
1	C	5745	0	5580	62	0
1	D	5746	0	5584	51	0
2	A	43	0	30	2	0
2	B	43	0	30	4	0
2	C	43	0	30	4	0
2	D	43	0	30	1	0
3	A	771	0	0	14	0
3	B	650	0	0	12	0
3	C	690	0	0	15	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	745	0	0	11	1
All	All	26010	0	22447	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:392:HIS:ND1	1:D:415:TYR:CB	1.69	1.52
1:B:392:HIS:ND1	1:B:415:TYR:CB	1.71	1.49
1:C:392:HIS:ND1	1:C:415:TYR:CB	1.84	1.40
1:D:392:HIS:CE1	1:D:415:TYR:HB2	1.64	1.29
1:B:392:HIS:CE1	1:B:415:TYR:HB2	1.71	1.24
1:C:392:HIS:ND1	1:C:415:TYR:HB2	0.91	1.23
1:A:713:GLN:HG2	3:A:2153:HOH:O	1.40	1.19
1:B:392:HIS:ND1	1:B:415:TYR:HB2	0.80	1.12
1:D:392:HIS:ND1	1:D:415:TYR:HB2	0.80	1.11
1:B:451:MET:HE2	1:D:451:MET:HE2	1.25	1.11
1:A:451:MET:HE2	1:C:451:MET:HE2	1.20	1.10
1:D:451:MET:SD	3:D:3264:HOH:O	2.07	1.10
1:C:392:HIS:CE1	1:C:415:TYR:HB2	1.88	1.07
1:A:710:ILE:HG12	1:A:715:GLU:OE1	1.55	1.05
1:B:267:ARG:HG3	3:B:3310:HOH:O	1.64	0.97
1:A:111:ARG:HB2	3:A:3292:HOH:O	1.68	0.92
1:D:521:ARG:HD3	3:D:3252:HOH:O	1.78	0.82
2:C:760:HEM:HMB2	2:C:760:HEM:HBB2	1.63	0.81
1:A:28:SER:OG	1:A:28:SER:O	1.98	0.80
1:C:416:THR:HG21	3:C:3270:HOH:O	1.81	0.79
1:B:521:ARG:HD3	3:B:3047:HOH:O	1.81	0.79
3:B:2705:HOH:O	1:D:73:LYS:CD	2.30	0.79
3:B:2705:HOH:O	1:D:73:LYS:HE3	1.87	0.75
3:B:2705:HOH:O	1:D:73:LYS:CE	2.34	0.74
1:D:552:LEU:HD23	1:D:552:LEU:O	1.87	0.74
3:B:2705:HOH:O	1:D:73:LYS:HD3	1.89	0.72
1:C:704:PHE:O	1:C:707:THR:HG22	1.90	0.72
1:D:629:HIS:HD2	3:D:1554:HOH:O	1.74	0.71
1:D:321:GLU:HG3	3:D:2151:HOH:O	1.92	0.70
1:C:283:GLU:OE1	3:C:2292:HOH:O	2.09	0.69
2:C:760:HEM:HBC2	2:C:760:HEM:HMC2	1.75	0.69
1:B:533:LYS:HE2	3:B:3100:HOH:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:HIS:ND1	1:D:415:TYR:HB3	1.99	0.68
1:A:479:ARG:NH2	3:A:2607:HOH:O	2.08	0.67
1:C:416:THR:CG2	3:C:3270:HOH:O	2.40	0.66
1:B:583:LYS:H	1:B:583:LYS:NZ	1.95	0.65
1:D:677:ASP:HB2	3:D:3247:HOH:O	1.95	0.65
1:A:29:LEU:HB2	3:C:2405:HOH:O	1.98	0.63
1:B:392:HIS:ND1	1:B:415:TYR:CG	2.63	0.63
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.80	0.63
1:B:281:ASN:OD1	1:B:283:GLU:HG3	1.99	0.63
1:A:751:ILE:O	1:A:751:ILE:HD12	1.97	0.62
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.82	0.62
1:C:488:ARG:HD2	3:C:2379:HOH:O	1.98	0.62
1:A:111:ARG:HD3	3:A:3287:HOH:O	1.99	0.62
1:B:111:ARG:HB2	3:B:3290:HOH:O	1.99	0.61
1:B:449[A]:HIS:CG	1:D:449[A]:HIS:CG	2.44	0.61
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.83	0.60
1:A:395:HIS:HE1	3:A:3308:HOH:O	1.84	0.60
1:B:392:HIS:ND1	1:B:415:TYR:HB3	2.04	0.60
1:D:416:THR:HG21	3:D:3280:HOH:O	2.00	0.60
1:D:552:LEU:CD2	1:D:556:GLN:NE2	2.65	0.59
1:B:583:LYS:O	1:B:584:LYS:HB3	2.02	0.59
1:D:392:HIS:ND1	1:D:415:TYR:CG	2.64	0.59
1:A:29:LEU:HD22	3:C:2405:HOH:O	2.02	0.58
1:A:274:ILE:HD12	2:A:760:HEM:HMB1	1.87	0.57
1:B:612:ARG:HB2	1:B:612:ARG:NH1	2.20	0.57
1:B:359:LEU:H	1:B:507:HIS:HD2	1.52	0.57
1:C:583:LYS:O	1:C:584:LYS:HB3	2.04	0.57
1:D:111:ARG:HD3	3:D:3305:HOH:O	2.05	0.57
1:C:556:GLN:NE2	3:C:2533:HOH:O	2.37	0.56
1:A:416:THR:HG21	3:A:3307:HOH:O	2.05	0.56
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.87	0.56
1:A:451:MET:CE	1:C:451:MET:HE2	2.14	0.56
2:B:760:HEM:CMC	2:B:760:HEM:HBC2	2.35	0.56
1:B:416:THR:HG21	3:B:3285:HOH:O	2.05	0.55
1:B:678:ASN:OD1	1:B:680:ASP:HB2	2.06	0.55
1:C:678:ASN:OD1	1:C:680:ASP:HB2	2.06	0.55
1:D:274:ILE:HD12	2:D:760:HEM:HMB1	1.87	0.55
1:A:36:HIS:HE1	3:A:1872:HOH:O	1.89	0.55
1:A:533:LYS:NZ	3:A:2232:HOH:O	2.38	0.55
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.89	0.55
1:B:629:HIS:HD2	3:B:1055:HOH:O	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.89	0.55
1:C:488:ARG:CD	3:C:2379:HOH:O	2.52	0.54
1:B:612:ARG:O	1:B:612:ARG:HG3	2.06	0.54
1:B:634:TYR:O	1:B:653:THR:HA	2.07	0.54
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.23	0.54
1:B:395:HIS:HE1	3:B:3300:HOH:O	1.91	0.54
1:B:38:PRO:HG2	1:B:51:ALA:HB2	1.91	0.53
1:C:578:ASP:HB2	1:C:582:LEU:O	2.07	0.53
1:D:578:ASP:CG	1:D:583:LYS:HG2	2.33	0.53
1:D:747:LYS:H	1:D:747:LYS:HD2	1.74	0.53
1:D:552:LEU:HD23	1:D:552:LEU:C	2.33	0.53
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.39	0.52
1:D:341:ILE:HG13	3:D:3022:HOH:O	2.09	0.52
1:A:682:ASN:HB3	1:A:707:THR:HG21	1.92	0.52
1:A:111:ARG:NH2	3:A:3292:HOH:O	2.43	0.52
1:C:359:LEU:H	1:C:507:HIS:HD2	1.58	0.52
2:C:760:HEM:HBB2	2:C:760:HEM:CMB	2.38	0.52
1:B:448:MET:HG3	1:B:449[A]:HIS:CD2	2.45	0.51
1:B:725:ASP:OD2	1:B:727:SER:HB3	2.11	0.51
1:A:111:ARG:CD	3:A:3287:HOH:O	2.58	0.51
1:B:449[B]:HIS:CD2	1:D:449[B]:HIS:CD2	2.99	0.50
1:C:724:ALA:O	1:C:725:ASP:HB2	2.11	0.50
1:C:629:HIS:HD2	3:C:1129:HOH:O	1.95	0.50
1:C:748:ILE:O	1:C:751:ILE:HG22	2.12	0.50
1:B:686:MET:HB3	1:B:751:ILE:HD11	1.93	0.50
1:B:37:ARG:HD3	3:B:2886:HOH:O	2.12	0.49
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.43	0.49
2:B:760:HEM:HMB1	2:B:760:HEM:HBB2	1.94	0.49
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.21	0.49
1:D:552:LEU:HD22	1:D:556:GLN:NE2	2.27	0.49
1:B:556:GLN:HG2	1:B:566:LEU:HD23	1.94	0.49
2:B:760:HEM:HBB2	2:B:760:HEM:CMB	2.43	0.49
1:D:634:TYR:O	1:D:653:THR:HA	2.14	0.48
1:C:111:ARG:HD3	3:C:3296:HOH:O	2.13	0.48
1:C:686:MET:HB3	1:C:751:ILE:HD11	1.94	0.48
1:D:552:LEU:CD2	1:D:552:LEU:C	2.86	0.48
1:A:469:TRP:CE3	1:A:471:ARG:HG3	2.48	0.48
1:B:344:GLU:H	1:B:344:GLU:CD	2.21	0.48
1:B:392:HIS:CG	1:B:415:TYR:CB	2.83	0.48
1:A:111:ARG:CZ	3:A:3292:HOH:O	2.62	0.48
1:D:671:ASN:ND2	3:D:2248:HOH:O	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:760:HEM:HBC2	2:B:760:HEM:HMC1	1.95	0.47
1:D:574:THR:HG23	3:D:1614:HOH:O	2.14	0.47
1:B:583:LYS:H	1:B:583:LYS:HZ3	1.63	0.46
1:A:128:HIS:CE1	1:A:169:VAL:HG22	2.51	0.46
1:B:207:PHE:O	1:B:249:THR:HA	2.16	0.46
1:C:395:HIS:HE1	3:C:3269:HOH:O	1.99	0.46
1:D:128:HIS:HA	1:D:168:THR:O	2.15	0.46
1:D:395:HIS:HE1	3:D:3303:HOH:O	1.98	0.46
1:D:488:ARG:NH1	1:D:490:GLU:OE1	2.46	0.46
1:B:732:LEU:C	1:B:732:LEU:HD13	2.41	0.46
1:D:552:LEU:HD21	1:D:556:GLN:CD	2.41	0.46
1:A:449[A]:HIS:CD2	1:C:449[A]:HIS:CD2	3.03	0.46
1:C:111:ARG:CD	3:C:3296:HOH:O	2.64	0.46
1:C:195:ILE:HD11	1:C:436:PRO:HA	1.98	0.46
1:D:404:ASN:O	1:D:405:ASP:C	2.59	0.45
1:A:36:HIS:CD2	1:A:36:HIS:H	2.35	0.45
1:B:562:LEU:HA	1:C:637:MET:HB2	1.99	0.45
1:C:359:LEU:H	1:C:507:HIS:CD2	2.35	0.45
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.52	0.45
1:B:392:HIS:CD2	1:B:394:GLY:H	2.34	0.44
1:C:634:TYR:O	1:C:653:THR:HA	2.17	0.44
1:D:278:ARG:HH12	1:D:487:GLU:CD	2.25	0.44
1:D:552:LEU:HD21	1:D:556:GLN:NE2	2.32	0.44
3:A:3250:HOH:O	1:C:111:ARG:HD3	2.16	0.44
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.99	0.44
1:C:51:ALA:HB1	1:C:52:PRO:HD2	2.00	0.44
1:C:359:LEU:HD12	1:C:359:LEU:C	2.43	0.44
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.52	0.44
1:B:440:TYR:CD2	1:B:440:TYR:C	2.95	0.44
1:A:607:LEU:HD11	1:A:632:LEU:HB3	1.99	0.44
1:C:28:SER:N	3:C:2523:HOH:O	2.50	0.44
1:A:449[B]:HIS:CG	1:C:449[B]:HIS:CG	2.54	0.44
1:B:359:LEU:H	1:B:507:HIS:CD2	2.35	0.44
1:B:612:ARG:HB2	1:B:612:ARG:HH11	1.82	0.44
1:C:459:ASN:H	1:C:459:ASN:HD22	1.66	0.44
1:D:359:LEU:H	1:D:507:HIS:HD2	1.66	0.44
1:C:411:ARG:HG2	2:C:760:HEM:C2C	2.53	0.43
1:A:252:ASN:HD22	1:A:252:ASN:HA	1.70	0.43
1:A:448:MET:O	1:A:449[B]:HIS:HB2	2.18	0.43
1:C:310:LEU:HD13	1:C:660:LEU:HB3	1.99	0.43
1:A:144:LEU:HD11	1:A:370:VAL:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:359:LEU:HD12	1:B:359:LEU:C	2.43	0.43
1:D:440:TYR:CD2	1:D:440:TYR:C	2.96	0.43
1:C:252:ASN:HD22	1:C:252:ASN:HA	1.65	0.43
1:A:38:PRO:HG2	1:A:51:ALA:HB2	2.00	0.43
1:A:319:ARG:HD3	1:D:227:TRP:O	2.18	0.43
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.54	0.43
1:B:725:ASP:OD2	1:B:727:SER:N	2.49	0.43
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.33	0.43
1:B:97:ALA:O	1:B:101:GLY:HA3	2.18	0.43
1:C:207:PHE:O	1:C:249:THR:HA	2.18	0.43
1:A:416:THR:HB	3:A:3250:HOH:O	2.18	0.43
1:B:583:LYS:H	1:B:583:LYS:HZ2	1.63	0.43
1:C:634:TYR:CG	1:C:635:SER:N	2.87	0.43
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.34	0.42
1:A:92:GLN:HA	1:D:213:LYS:HD3	2.00	0.42
1:D:748:ILE:HA	1:D:751:ILE:HG23	2.01	0.42
1:C:460:TYR:CE2	1:D:238:THR:HB	2.54	0.42
1:C:724:ALA:O	1:C:725:ASP:CB	2.67	0.42
1:A:411:ARG:HG2	2:A:760:HEM:C2C	2.54	0.42
1:A:460:TYR:CE2	1:B:238:THR:HB	2.54	0.42
1:B:558:VAL:HG12	1:B:562:LEU:HD22	2.01	0.42
1:C:459:ASN:HD22	1:C:459:ASN:C	2.27	0.42
1:C:392:HIS:CD2	1:C:394:GLY:H	2.37	0.42
1:B:38:PRO:HA	1:B:48:GLN:OE1	2.20	0.42
1:C:251:HIS:CE1	1:C:507:HIS:HB3	2.55	0.42
1:C:583:LYS:HE2	1:C:583:LYS:HB2	1.76	0.42
1:C:461:GLU:HA	1:C:462:PRO:C	2.44	0.41
1:A:136:GLY:C	1:A:162:VAL:HG22	2.45	0.41
1:C:593:ILE:HA	1:C:594:PRO:HD2	1.92	0.41
1:B:278:ARG:HH22	1:B:487:GLU:CD	2.28	0.41
1:C:440:TYR:CD2	1:C:440:TYR:C	2.98	0.41
1:D:48:GLN:HE21	1:D:48:GLN:HB3	1.74	0.41
1:C:293:TRP:CZ3	1:C:336:LEU:HB2	2.56	0.41
1:D:207:PHE:O	1:D:249:THR:HA	2.20	0.41
1:A:128:HIS:HA	1:A:168:THR:O	2.21	0.41
1:A:461:GLU:HA	1:A:462:PRO:C	2.45	0.41
1:C:725:ASP:HA	1:C:728:PHE:HB3	2.03	0.41
1:D:596:GLY:HA3	1:D:737:ALA:O	2.21	0.41
3:A:938:HOH:O	1:C:52:PRO:HG3	2.20	0.41
1:A:104:LEU:HB3	3:C:775:HOH:O	2.21	0.40
1:A:393:PRO:HD2	1:A:415:TYR:CG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:PRO:HG2	1:C:51:ALA:HB2	2.03	0.40
1:C:748:ILE:O	1:C:751:ILE:CG2	2.69	0.40
1:C:128:HIS:HA	1:C:168:THR:O	2.20	0.40
1:B:461:GLU:HA	1:B:462:PRO:C	2.45	0.40
1:C:61:ARG:HG3	3:C:2648:HOH:O	2.20	0.40
1:B:521:ARG:HD2	1:B:745:ILE:HG21	2.03	0.40
1:C:133:ALA:HA	1:C:164:VAL:O	2.22	0.40
1:C:641:THR:CG2	1:C:645:GLY:HA2	2.51	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:OD1	1:B:369:ARG:NH1[2_545]	2.10	0.10
3:C:2040:HOH:O	3:D:2980:HOH:O[2_545]	2.13	0.07

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	724/753 (96%)	703 (97%)	19 (3%)	2 (0%)	36	23
1	B	724/753 (96%)	703 (97%)	19 (3%)	2 (0%)	36	23
1	C	724/753 (96%)	701 (97%)	21 (3%)	2 (0%)	36	23
1	D	724/753 (96%)	708 (98%)	15 (2%)	1 (0%)	48	34
All	All	2896/3012 (96%)	2815 (97%)	74 (3%)	7 (0%)	43	29

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	711	ALA

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Mol	Chain	Res	Type
1	B	725	ASP
1	A	75	SER
1	C	75	SER
1	B	75	SER
1	C	725	ASP
1	D	75	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	611/635 (96%)	594 (97%)	17 (3%)	38	15
1	B	611/635 (96%)	585 (96%)	26 (4%)	26	6
1	C	611/635 (96%)	578 (95%)	33 (5%)	20	4
1	D	611/635 (96%)	589 (96%)	22 (4%)	31	9
All	All	2444/2540 (96%)	2346 (96%)	98 (4%)	28	7

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	73	LYS
1	A	158	LYS
1	A	185	PHE
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	617	LEU
1	A	707	THR

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Mol	Chain	Res	Type
1	A	732	LEU
1	A	750	LYS
1	B	142	LYS
1	B	205	ILE
1	B	252	ASN
1	B	285	LYS
1	B	321	GLU
1	B	344	GLU
1	B	369	ARG
1	B	370	VAL
1	B	413	LYS
1	B	432	PRO
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	565	GLU
1	B	566	LEU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	595	ASP
1	B	612	ARG
1	B	621	LYS
1	B	633	LEU
1	B	707	THR
1	B	713	GLN
1	B	751	ILE
1	C	32	GLU
1	C	37	ARG
1	C	159	ILE
1	C	205	ILE
1	C	252	ASN
1	C	285	LYS
1	C	377	ARG
1	C	413	LYS
1	C	420	ILE
1	C	432	PRO
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG

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Mol	Chain	Res	Type
1	C	521	ARG
1	C	531	LEU
1	C	552	LEU
1	C	568	ASP
1	C	571	LEU
1	C	583	LYS
1	C	584	LYS
1	C	606	LEU
1	C	616	LEU
1	C	633	LEU
1	C	636	ARG
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU
1	C	713	GLN
1	C	725	ASP
1	C	733	LEU
1	C	750	LYS
1	C	751	ILE
1	D	28	SER
1	D	32	GLU
1	D	73	LYS
1	D	191	THR
1	D	205	ILE
1	D	252	ASN
1	D	340	LEU
1	D	344	GLU
1	D	413	LYS
1	D	440	TYR
1	D	459	ASN
1	D	552	LEU
1	D	554	LEU
1	D	574	THR
1	D	582	LEU
1	D	583	LYS
1	D	584	LYS
1	D	616	LEU
1	D	648	LEU
1	D	713	GLN
1	D	747	LYS
1	D	751	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	A	713	GLN
1	B	66	ASN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	C	252	ASN
1	C	459	ASN
1	C	507	HIS
1	C	546	GLN
1	C	556	GLN
1	C	629	HIS
1	C	682	ASN
1	C	713	GLN
1	D	48	GLN
1	D	77	ASN
1	D	212	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 ⓘ

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	OCS	A	669	1	6,8,9	0.98	0	7,11,13	1.13	1 (14%)
1	OCS	D	669	1	6,8,9	1.27	0	7,11,13	1.49	1 (14%)
1	OCS	C	669	1	6,8,9	1.50	1 (16%)	7,11,13	1.43	1 (14%)
1	OCS	B	669	1	6,8,9	2.03	1 (16%)	7,11,13	2.18	3 (42%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OCS	A	669	1	-	3/4/7/9	-
1	OCS	D	669	1	-	1/4/7/9	-
1	OCS	C	669	1	-	1/4/7/9	-
1	OCS	B	669	1	-	1/4/7/9	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	669	OCS	CB-CA	-4.67	1.50	1.53
1	C	669	OCS	CB-CA	-2.45	1.51	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	669	OCS	OD1-SG-CB	4.02	112.75	106.76
1	D	669	OCS	OD1-SG-CB	3.24	111.59	106.76
1	B	669	OCS	CA-CB-SG	2.62	117.50	113.61
1	C	669	OCS	CA-CB-SG	2.29	117.01	113.61
1	A	669	OCS	CA-CB-SG	2.16	116.82	113.61
1	B	669	OCS	OD2-SG-CB	-2.02	102.07	105.97

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	669	OCS	N-CA-CB-SG

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

There are no ring outliers.

No monomer is involved in short contacts.

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	C	760	1,3	50,50,50	1.89	11 (22%)	67,82,82	2.21	20 (29%)
2	HEM	D	760	1,3	50,50,50	1.78	11 (22%)	67,82,82	2.25	16 (23%)
2	HEM	B	760	1,3	50,50,50	2.18	12 (24%)	67,82,82	2.63	21 (31%)
2	HEM	A	760	1,3	50,50,50	1.93	11 (22%)	67,82,82	2.36	22 (32%)

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	C	760	1,3	-	3/14/54/54	-
2	HEM	D	760	1,3	-	2/14/54/54	-

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

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HEM	C3D-C2D	6.40	1.50	1.36
2	B	760	HEM	FE-NC	6.32	2.16	1.95
2	B	760	HEM	C3D-C2D	6.19	1.50	1.36
2	D	760	HEM	C3D-C2D	6.03	1.49	1.36
2	B	760	HEM	FE-NB	5.80	2.12	1.94
2	C	760	HEM	C3D-C2D	5.69	1.49	1.36
2	C	760	HEM	FE-ND	5.54	2.12	1.94
2	A	760	HEM	CMC-C2C	5.01	1.61	1.50
2	D	760	HEM	FE-NA	4.85	2.11	1.95
2	B	760	HEM	FE-ND	4.59	2.09	1.94
2	C	760	HEM	FE-NB	4.11	2.07	1.94
2	D	760	HEM	FE-NB	4.04	2.07	1.94
2	A	760	HEM	FE-ND	3.75	2.06	1.94
2	A	760	HEM	C3C-C2C	-3.59	1.29	1.37
2	A	760	HEM	FE-NB	3.57	2.05	1.94
2	B	760	HEM	C1B-NB	-3.55	1.34	1.40
2	C	760	HEM	CMC-C2C	3.44	1.57	1.50
2	D	760	HEM	FE-ND	3.35	2.05	1.94
2	C	760	HEM	CAB-C3B	3.25	1.56	1.47
2	B	760	HEM	CMA-C3A	3.21	1.57	1.50
2	A	760	HEM	CMB-C2B	3.06	1.57	1.50
2	D	760	HEM	FE-NC	3.04	2.05	1.95
2	B	760	HEM	O1A-CGA	3.01	1.31	1.22
2	C	760	HEM	CMB-C2B	2.96	1.56	1.50
2	D	760	HEM	CAB-C3B	2.82	1.54	1.47
2	C	760	HEM	FE-NC	2.80	2.04	1.95
2	B	760	HEM	CMC-C2C	2.74	1.56	1.50
2	B	760	HEM	C4C-NC	-2.67	1.34	1.39
2	C	760	HEM	C4D-ND	-2.66	1.35	1.40
2	D	760	HEM	CMC-C2C	2.57	1.56	1.50
2	C	760	HEM	CMA-C3A	2.51	1.55	1.50
2	B	760	HEM	CAB-C3B	2.50	1.54	1.47
2	D	760	HEM	CAC-C3C	2.48	1.54	1.47
2	B	760	HEM	C2A-C3A	-2.43	1.32	1.38
2	A	760	HEM	FE-NC	2.36	2.03	1.95
2	A	760	HEM	C4A-NA	2.35	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	760	HEM	CAA-C2A	2.32	1.57	1.51
2	A	760	HEM	CAC-C3C	2.29	1.53	1.47
2	D	760	HEM	CMB-C2B	2.28	1.55	1.50
2	D	760	HEM	CMA-C3A	2.24	1.55	1.50
2	D	760	HEM	CBD-CAD	2.21	1.59	1.51
2	B	760	HEM	CBA-CAA	2.15	1.59	1.51
2	C	760	HEM	CBD-CAD	2.06	1.59	1.51
2	A	760	HEM	CAB-C3B	2.02	1.52	1.47
2	A	760	HEM	O2A-CGA	-2.01	1.24	1.30

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	760	HEM	CBD-CAD-C3D	-9.61	85.97	112.53
2	D	760	HEM	CBD-CAD-C3D	-9.50	86.26	112.53
2	A	760	HEM	CBD-CAD-C3D	-8.61	88.72	112.53
2	B	760	HEM	CBD-CAD-C3D	-7.68	91.30	112.53
2	B	760	HEM	C3B-C4B-NB	-7.63	103.99	109.47
2	B	760	HEM	C1B-NB-C4B	6.76	113.22	105.21
2	B	760	HEM	CHA-C4D-ND	6.30	132.16	124.37
2	B	760	HEM	C4D-ND-C1D	5.97	112.27	105.21
2	A	760	HEM	CHD-C4C-NC	5.92	130.90	124.45
2	B	760	HEM	CHC-C4B-NB	5.33	130.16	124.42
2	D	760	HEM	CAD-CBD-CGD	-5.29	99.62	113.67
2	A	760	HEM	C3B-C4B-NB	-5.10	105.81	109.47
2	C	760	HEM	C4D-ND-C1D	5.01	111.14	105.21
2	D	760	HEM	C2A-C1A-NA	-4.81	104.82	110.15
2	B	760	HEM	CHD-C4C-NC	4.73	129.60	124.45
2	A	760	HEM	CAD-C3D-C4D	4.59	132.70	124.70
2	A	760	HEM	O2D-CGD-O1D	-4.58	111.54	123.33
2	C	760	HEM	CAD-CBD-CGD	-4.53	101.66	113.67
2	A	760	HEM	C1B-NB-C4B	4.35	110.36	105.21
2	B	760	HEM	C4C-NC-C1C	4.32	112.87	105.82
2	C	760	HEM	O2D-CGD-O1D	-4.24	112.44	123.33
2	A	760	HEM	CHB-C1B-NB	4.12	129.46	124.37
2	C	760	HEM	CHC-C1C-NC	4.10	128.92	124.45
2	D	760	HEM	CMD-C2D-C1D	4.06	131.38	125.03
2	B	760	HEM	CAA-CBA-CGA	-3.83	103.51	113.67
2	D	760	HEM	C4A-NA-C1A	3.83	112.06	105.82
2	B	760	HEM	O2D-CGD-O1D	-3.69	113.84	123.33
2	C	760	HEM	CHD-C4C-NC	3.65	128.42	124.45
2	A	760	HEM	C4D-ND-C1D	3.55	109.42	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	760	HEM	CAD-CBD-CGD	-3.53	104.31	113.67
2	D	760	HEM	O2D-CGD-CBD	3.51	125.10	114.00
2	B	760	HEM	O2D-CGD-CBD	3.49	125.03	114.00
2	D	760	HEM	CHB-C4A-NA	3.42	130.06	123.86
2	B	760	HEM	CAD-CBD-CGD	-3.38	104.70	113.67
2	C	760	HEM	CHD-C1D-ND	3.34	128.01	124.42
2	A	760	HEM	CAD-C3D-C2D	-3.33	121.63	127.87
2	D	760	HEM	O2D-CGD-O1D	-3.31	114.81	123.33
2	C	760	HEM	C4B-C3B-C2B	3.31	110.32	107.28
2	B	760	HEM	C2B-C1B-NB	-3.28	106.07	109.84
2	D	760	HEM	CAA-CBA-CGA	-3.20	105.18	113.67
2	B	760	HEM	C3D-C4D-ND	-3.17	106.70	110.17
2	D	760	HEM	CAD-C3D-C4D	3.15	130.19	124.70
2	D	760	HEM	C4D-ND-C1D	3.10	108.88	105.21
2	D	760	HEM	C3A-C4A-NA	-3.07	105.22	110.14
2	A	760	HEM	C4C-C3C-C2C	2.96	109.39	106.81
2	C	760	HEM	CAA-CBA-CGA	-2.95	105.83	113.67
2	A	760	HEM	O2D-CGD-CBD	2.95	123.32	114.00
2	B	760	HEM	CMD-C2D-C1D	2.87	129.52	125.03
2	A	760	HEM	C4B-C3B-C2B	2.85	109.90	107.28
2	C	760	HEM	C4C-C3C-C2C	2.83	109.27	106.81
2	A	760	HEM	CHC-C1C-NC	2.82	127.52	124.45
2	D	760	HEM	CHA-C4D-ND	2.80	127.83	124.37
2	C	760	HEM	C1B-NB-C4B	2.77	108.48	105.21
2	B	760	HEM	CAD-C3D-C4D	2.70	129.40	124.70
2	C	760	HEM	CAD-C3D-C4D	2.69	129.39	124.70
2	C	760	HEM	CHB-C1B-NB	2.65	127.64	124.37
2	C	760	HEM	C3B-C4B-NB	-2.64	107.58	109.47
2	D	760	HEM	CHD-C4C-NC	2.60	127.29	124.45
2	A	760	HEM	CMD-C2D-C1D	2.59	129.09	125.03
2	B	760	HEM	C4C-C3C-C2C	2.49	108.97	106.81
2	C	760	HEM	CBB-CAB-C3B	-2.40	115.51	127.53
2	A	760	HEM	CHD-C1D-ND	2.35	126.95	124.42
2	B	760	HEM	C1A-CHA-C4D	-2.33	120.76	126.25
2	C	760	HEM	C4C-NC-C1C	2.33	109.62	105.82
2	A	760	HEM	C2B-C1B-NB	-2.31	107.18	109.84
2	B	760	HEM	CHA-C4D-C3D	-2.31	120.97	125.23
2	D	760	HEM	C3B-C2B-C1B	2.28	108.12	106.41
2	B	760	HEM	C3B-C2B-C1B	2.28	108.12	106.41
2	C	760	HEM	CHA-C1A-NA	2.27	127.98	123.86
2	C	760	HEM	CAC-C3C-C4C	-2.22	119.52	124.82
2	A	760	HEM	CAA-CBA-CGA	-2.21	107.79	113.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	760	HEM	CBC-CAC-C3C	-2.19	116.56	127.53
2	C	760	HEM	CHC-C4B-NB	2.19	126.78	124.42
2	C	760	HEM	C2B-C1B-NB	-2.16	107.36	109.84
2	A	760	HEM	CHC-C4B-NB	2.16	126.75	124.42
2	A	760	HEM	CHA-C4D-ND	2.13	127.00	124.37
2	A	760	HEM	CAC-C3C-C4C	-2.05	119.92	124.82
2	B	760	HEM	CHB-C1B-NB	2.04	126.89	124.37
2	D	760	HEM	CMC-C2C-C3C	-2.01	123.56	128.43

There are no chirality outliers.

All (10) torsion outliers are listed below:

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

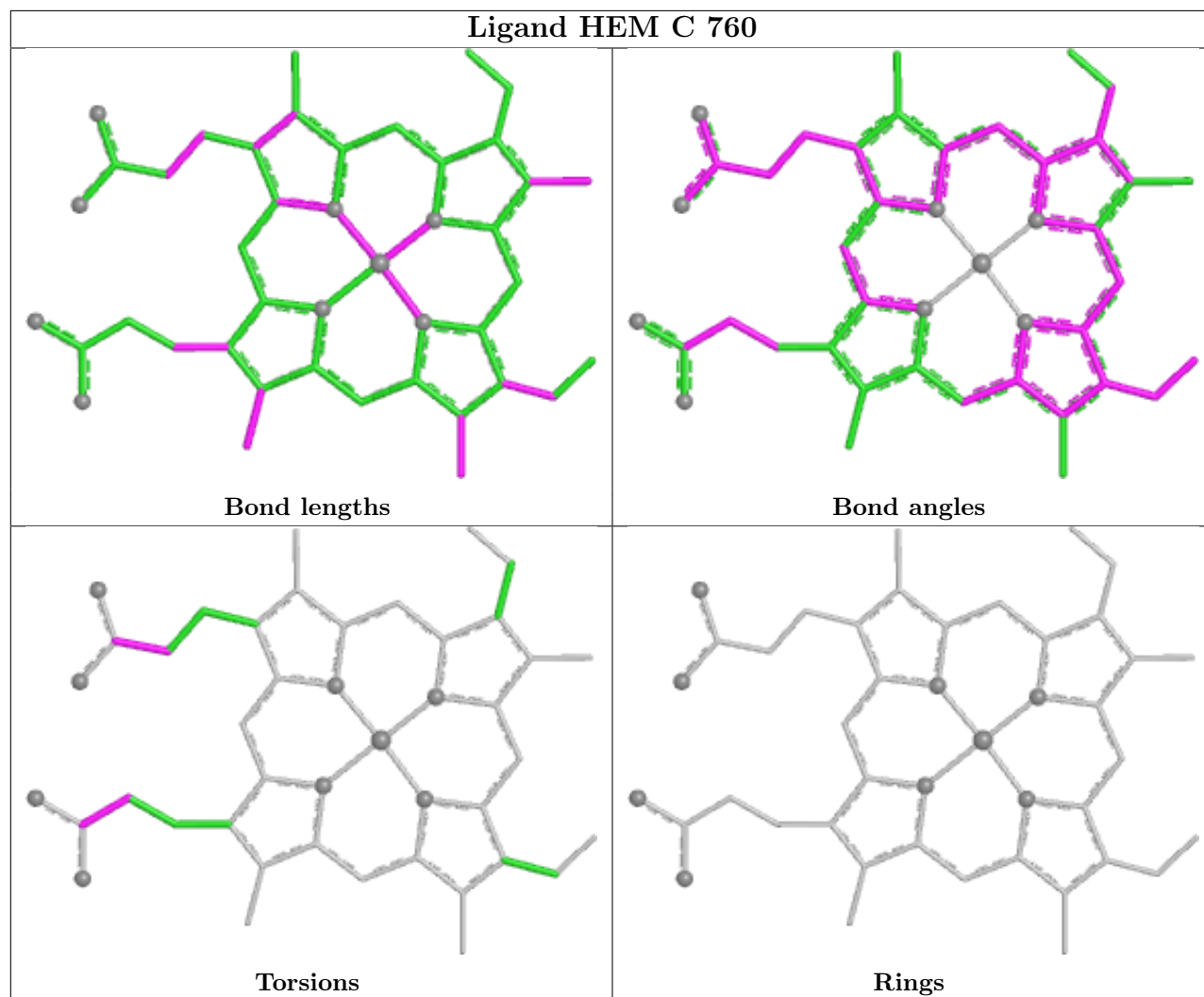
There are no ring outliers.

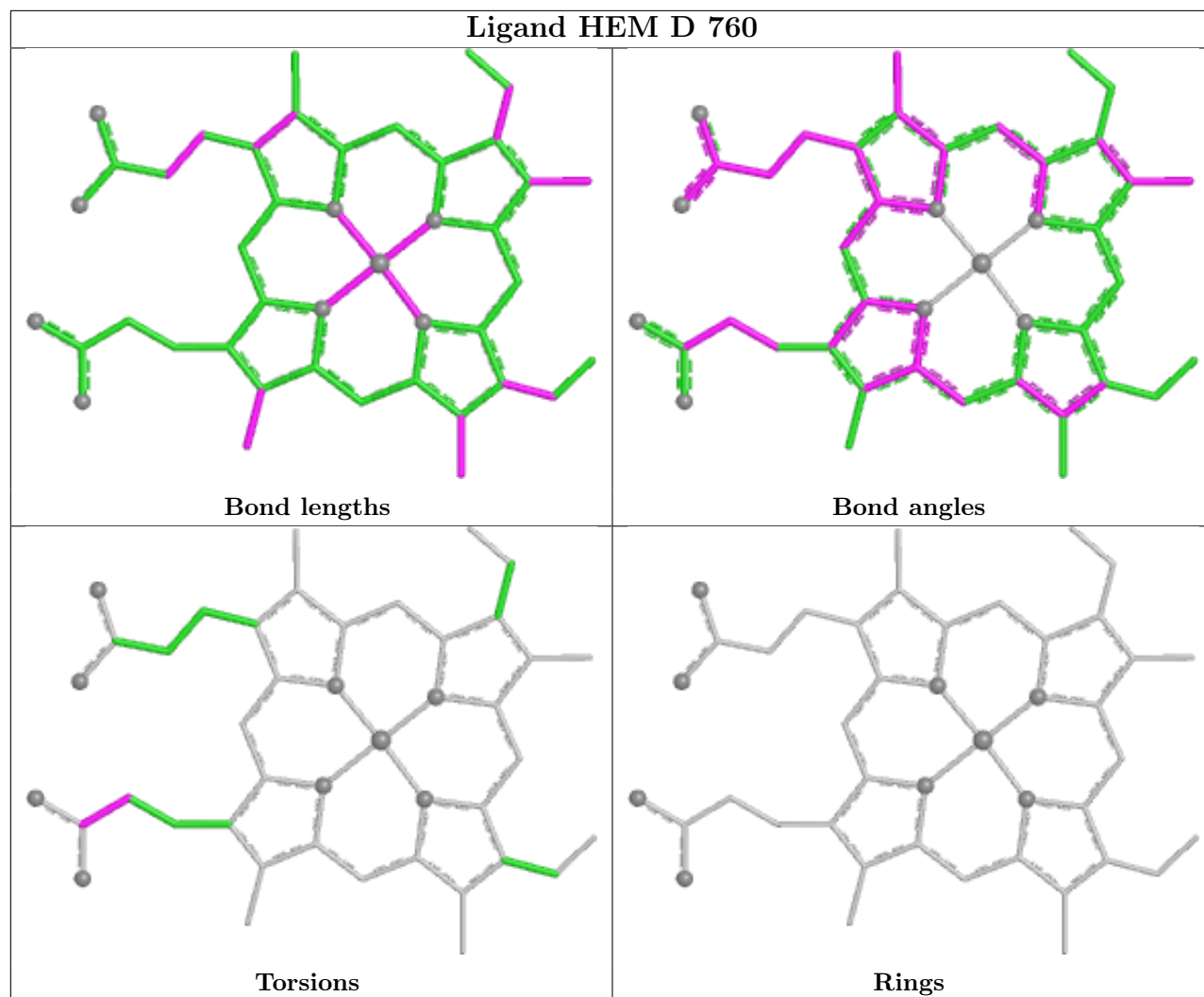
4 monomers are involved in 11 short contacts:

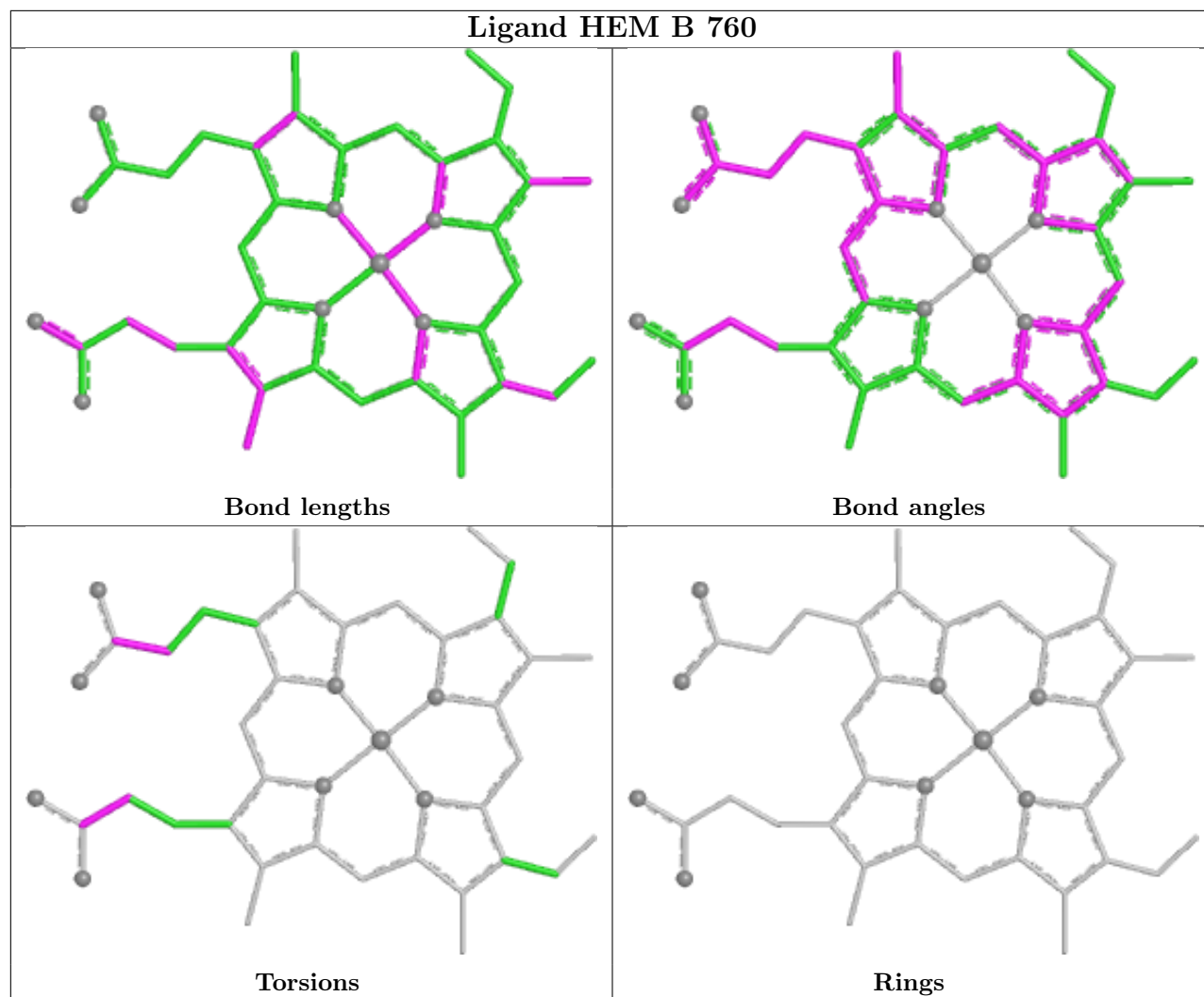
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	760	HEM	4	0
2	D	760	HEM	1	0
2	B	760	HEM	4	0
2	A	760	HEM	2	0

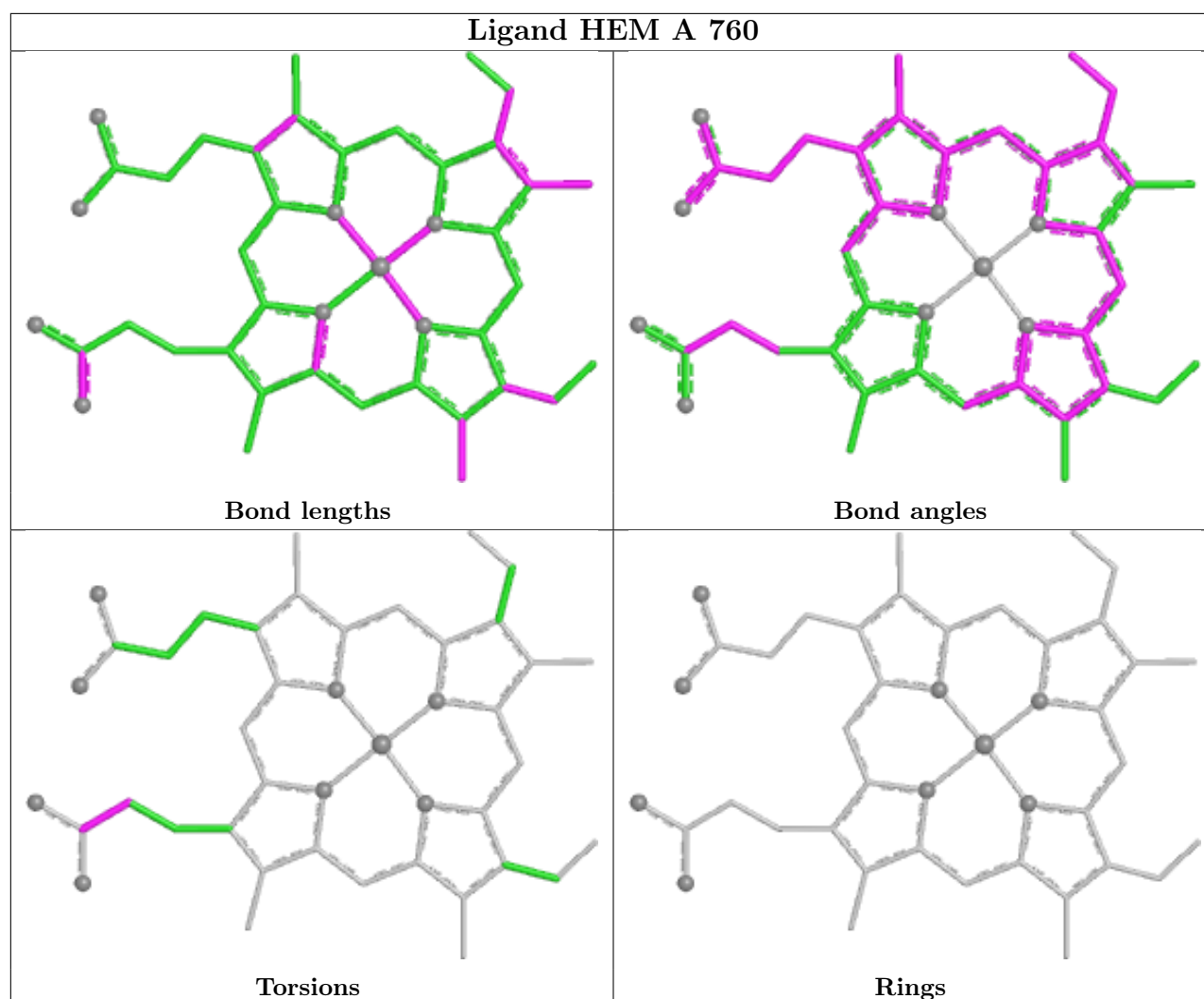
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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(Å²)	Q<0.9	
1	A	725/753 (96%)	-0.76	5 (0%)	84	89	4, 10, 27, 46	2 (0%)
1	B	725/753 (96%)	-0.62	4 (0%)	85	90	5, 12, 33, 48	2 (0%)
1	C	725/753 (96%)	-0.63	5 (0%)	84	89	5, 11, 32, 47	2 (0%)
1	D	725/753 (96%)	-0.76	4 (0%)	85	90	4, 10, 26, 46	2 (0%)
All	All	2900/3012 (96%)	-0.69	18 (0%)	85	90	4, 11, 31, 48	8 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	710	ILE	5.4
1	A	28	SER	4.4
1	B	726	GLY	3.7
1	A	711	ALA	3.4
1	D	28	SER	3.3
1	A	713	GLN	3.2
1	C	726	GLY	2.6
1	B	673	ALA	2.6
1	C	676	ALA	2.5
1	D	749	ASP	2.4
1	D	750	LYS	2.4
1	C	751	ILE	2.4
1	A	29	LEU	2.3
1	C	750	LYS	2.2
1	D	751	ILE	2.2
1	B	710	ILE	2.1
1	C	596	GLY	2.1
1	B	583	LYS	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	OCS	B	669	9/10	0.92	0.09	27,29,36,37	0
1	OCS	C	669	9/10	0.92	0.09	26,29,36,36	0
1	OCS	A	669	9/10	0.95	0.07	15,18,27,29	0
1	OCS	D	669	9/10	0.95	0.07	19,20,25,28	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

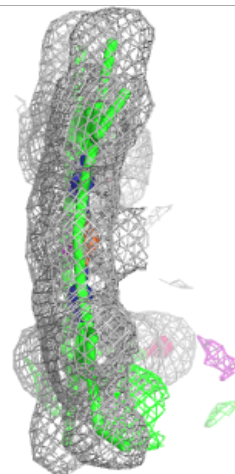
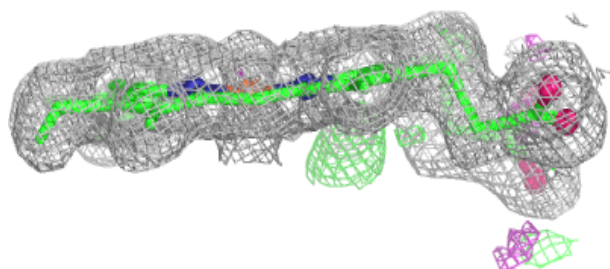
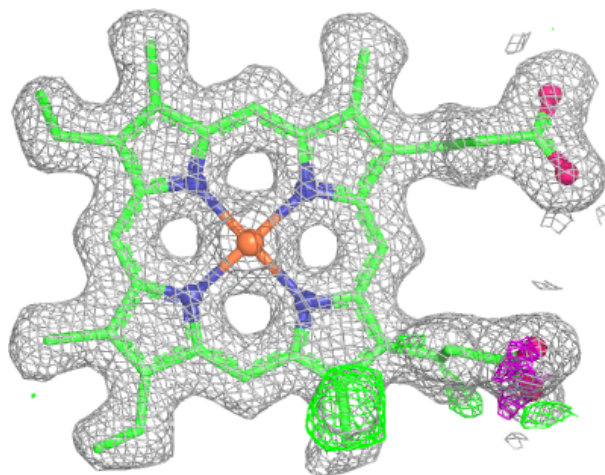
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	C	760	43/43	0.98	0.05	3,7,13,21	0
2	HEM	B	760	43/43	0.99	0.04	4,7,13,21	0
2	HEM	A	760	43/43	0.99	0.04	3,6,12,18	0
2	HEM	D	760	43/43	0.99	0.04	2,6,12,17	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.

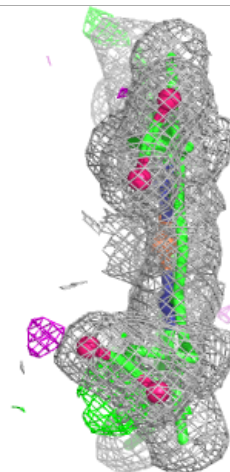
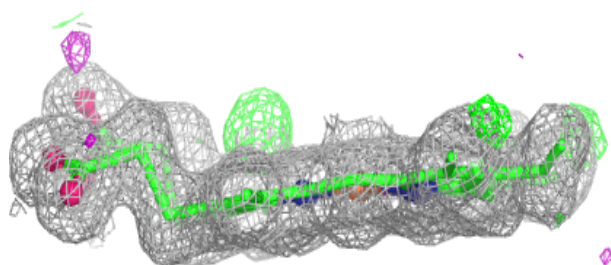
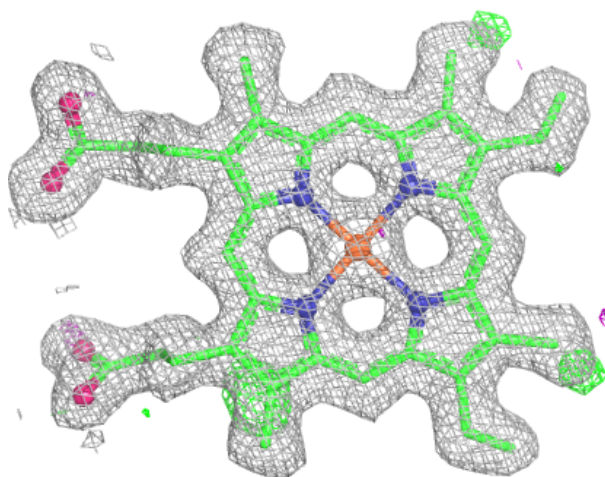
Electron density around HEM C 760:

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



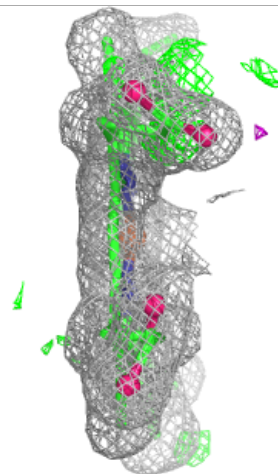
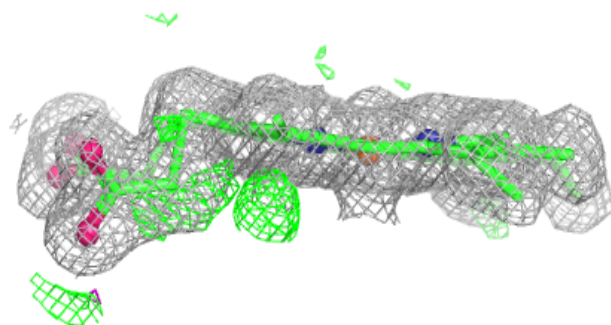
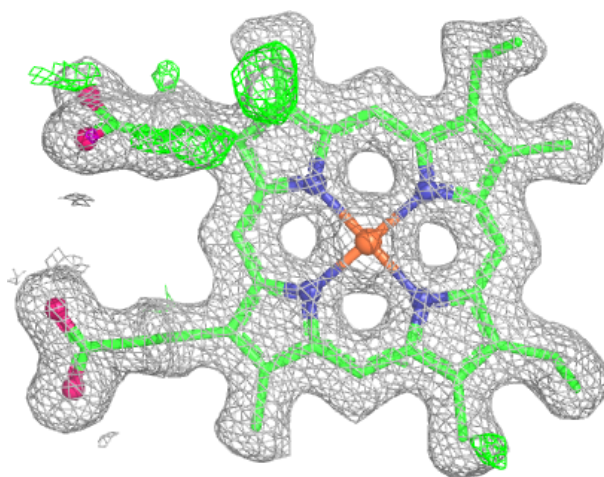
Electron density around HEM B 760:

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



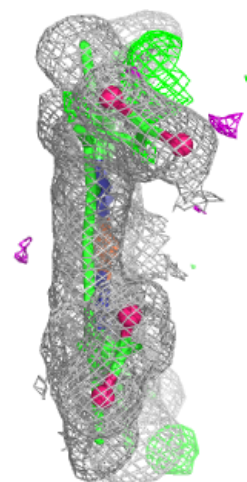
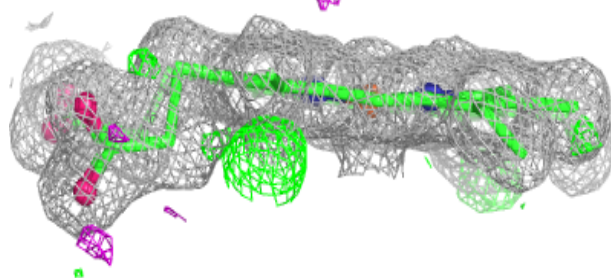
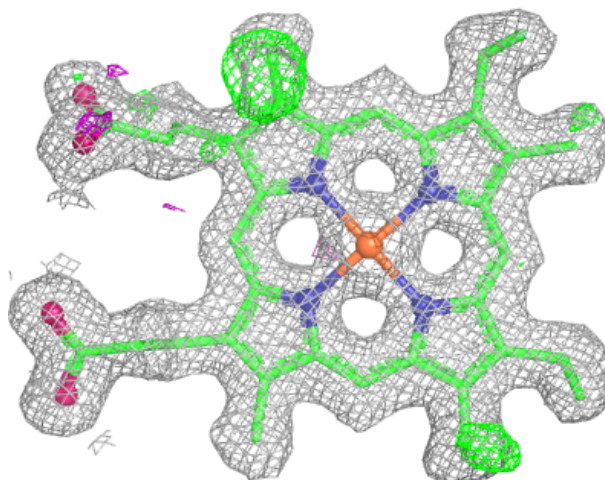
Electron density around HEM A 760:

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



Electron density around HEM D 760:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.