



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:35 PM UTC

PDB ID : 3TTW / pdb_00003ttw
Title : Structure of the F413E variant of E. coli KatE
Authors : Loewen, P.C.; Jha, V.
Deposited on : 2011-09-15
Resolution : 1.62 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

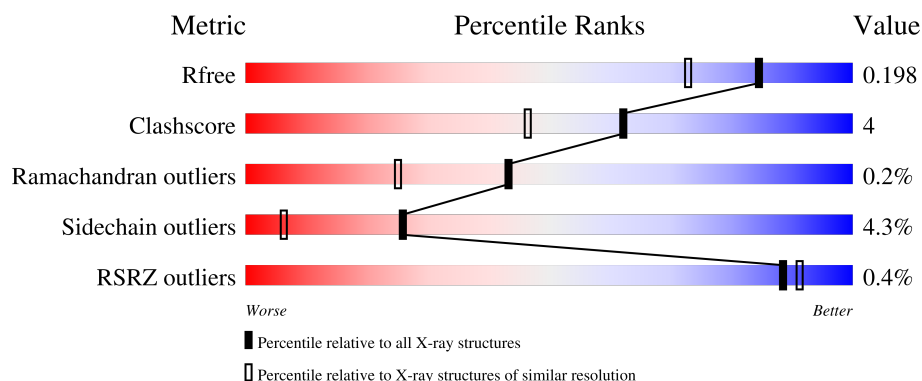
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.62 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	6728 (1.64-1.60)
Clashscore	190562	7023 (1.64-1.60)
Ramachandran outliers	187476	6898 (1.64-1.60)
Sidechain outliers	187428	6896 (1.64-1.60)
RSRZ outliers	180081	6727 (1.64-1.60)

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	% 84% 11% . .
1	B	753	 83% 12% . .
1	C	753	 83% 11% . .
1	D	753	% 85% 10% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25988 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	3643	1006	1084	12			
1	B	726	Total	C	N	O	S	0	1	0
			5746	3644	1006	1084	12			
1	C	726	Total	C	N	O	S	0	1	0
			5745	3643	1006	1084	12			
1	D	726	Total	C	N	O	S	0	1	0
			5746	3644	1006	1084	12			

There are 4 discrepancies between the modelled and reference sequences:

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

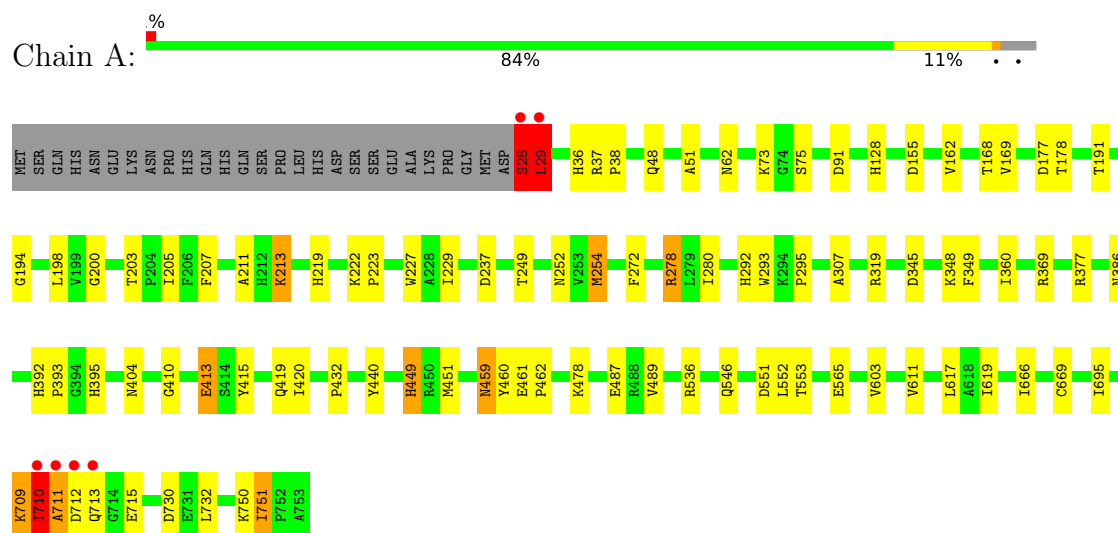
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	768	Total	O	0	0
			768	768		
3	B	643	Total	O	0	0
			643	643		
3	C	693	Total	O	0	0
			693	693		
3	D	730	Total	O	0	0
			730	730		

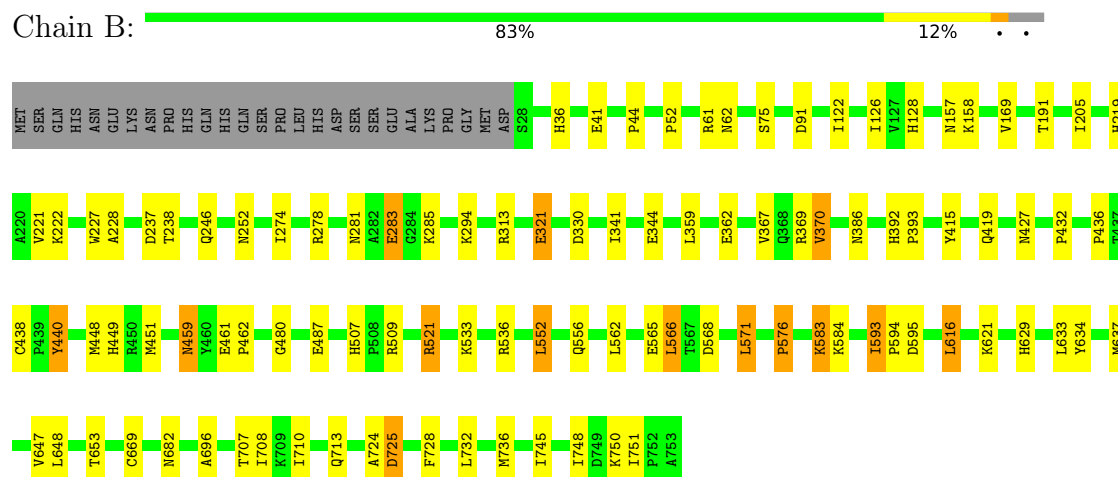
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

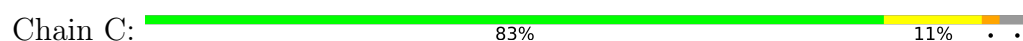
• Molecule 1: Catalase HPII

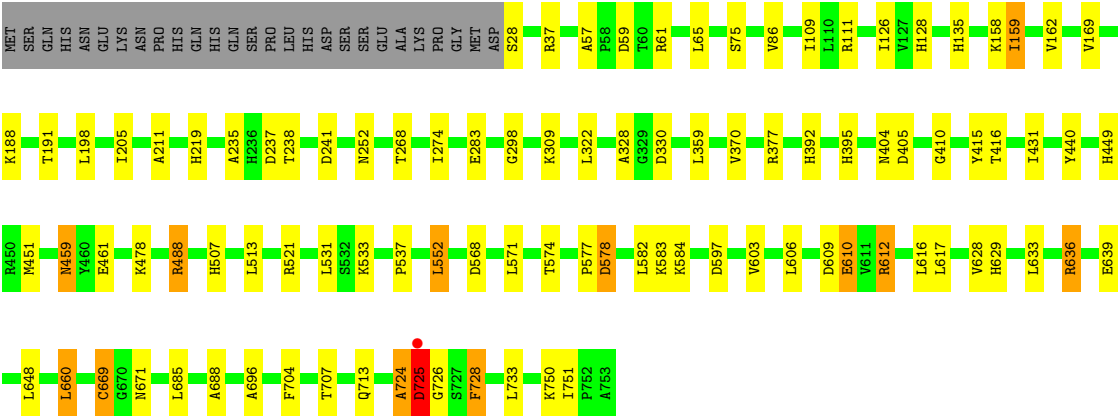


• Molecule 1: Catalase HPII

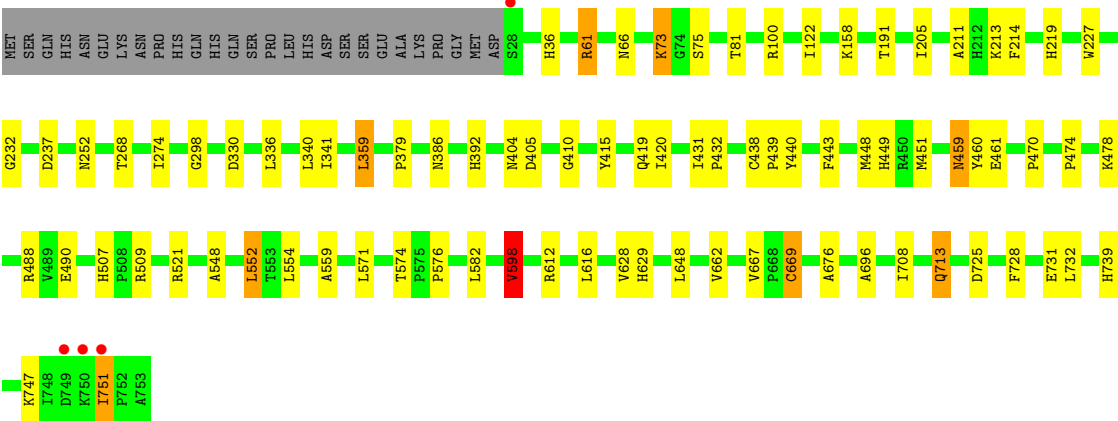
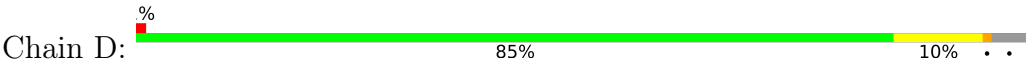


• Molecule 1: Catalase HPII





● 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	93.49Å 132.85Å 122.68Å 90.00° 109.36° 90.00°	Depositor
Resolution (Å)	31.25 – 1.62 31.25 – 1.62	Depositor EDS
% Data completeness (in resolution range)	87.1 (31.25-1.62) 87.1 (31.25-1.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 1.62Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.156 , 0.199 0.155 , 0.198	Depositor DCC
R_{free} test set	15716 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	15.0	Xtriage
Anisotropy	0.043	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	25988	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OCS, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.44	23/5895 (0.4%)	1.28	27/8013 (0.3%)
1	B	1.40	14/5895 (0.2%)	1.25	20/8013 (0.2%)
1	C	1.40	15/5895 (0.3%)	1.22	14/8013 (0.2%)
1	D	1.43	20/5895 (0.3%)	1.24	10/8013 (0.1%)
All	All	1.42	72/23580 (0.3%)	1.25	71/32052 (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 (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	LEU	N-CA	-8.51	1.33	1.46
1	C	57	ALA	CA-CB	7.93	1.62	1.53
1	B	438	CYS	C-O	7.87	1.32	1.23
1	D	438	CYS	C-O	7.50	1.31	1.23
1	A	420	ILE	CA-CB	6.80	1.63	1.54
1	B	480	GLY	N-CA	6.72	1.51	1.44
1	C	370	VAL	CA-CB	6.63	1.64	1.55
1	C	603	VAL	CA-CB	6.46	1.62	1.54
1	B	321	GLU	CB-CG	6.43	1.71	1.52
1	A	194	GLY	N-CA	6.41	1.51	1.45
1	B	341	ILE	CA-C	-6.38	1.47	1.52
1	A	611	VAL	CA-CB	6.36	1.60	1.54
1	B	157	ASN	CB-CG	6.25	1.67	1.52
1	D	232	GLY	N-CA	6.22	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	474	PRO	CA-C	6.18	1.55	1.51
1	C	577	PRO	C-O	6.15	1.31	1.23
1	A	272	PHE	N-CA	6.10	1.53	1.46
1	C	241	ASP	C-O	6.00	1.31	1.24
1	B	221	VAL	CA-CB	5.99	1.62	1.54
1	C	235	ALA	CA-CB	5.97	1.60	1.52
1	D	420	ILE	CA-CB	5.76	1.61	1.54
1	C	628	VAL	CA-CB	5.73	1.61	1.54
1	B	228	ALA	CA-CB	5.73	1.62	1.53
1	A	292	HIS	C-O	5.71	1.30	1.23
1	D	431	ILE	CA-C	5.64	1.58	1.53
1	D	336	LEU	N-CA	5.60	1.52	1.46
1	A	489	VAL	C-O	-5.59	1.18	1.24
1	A	278	ARG	N-CA	5.58	1.52	1.46
1	C	86	VAL	N-CA	5.55	1.53	1.46
1	B	321	GLU	N-CA	5.54	1.52	1.46
1	A	695	ILE	C-O	5.53	1.29	1.24
1	D	122	ILE	CA-CB	5.53	1.59	1.55
1	B	222	LYS	CA-CB	5.51	1.60	1.53
1	D	676	ALA	CA-CB	5.47	1.62	1.53
1	D	214	PHE	C-O	-5.46	1.19	1.24
1	D	739	HIS	N-CA	5.44	1.53	1.46
1	B	440	TYR	N-CA	5.42	1.52	1.46
1	D	419	GLN	CA-CB	5.40	1.62	1.53
1	C	298	GLY	N-CA	5.40	1.50	1.45
1	C	328	ALA	C-O	5.38	1.31	1.24
1	D	100	ARG	CB-CG	-5.36	1.36	1.52
1	A	360	ILE	N-CA	5.34	1.50	1.46
1	C	688	ALA	CA-CB	5.34	1.61	1.53
1	A	254	MET	C-O	5.33	1.30	1.24
1	B	122	ILE	CA-C	5.33	1.56	1.52
1	D	359	LEU	N-CA	5.33	1.52	1.45
1	A	711	ALA	N-CA	5.32	1.53	1.46
1	A	546	GLN	C-O	5.32	1.30	1.24
1	A	162	VAL	N-CA	5.31	1.51	1.46
1	B	427	ASN	N-CA	5.30	1.52	1.46
1	C	59	ASP	CG-OD1	5.27	1.35	1.25
1	D	667	VAL	CA-CB	-5.27	1.48	1.53
1	A	200	GLY	N-CA	5.27	1.49	1.44
1	A	280	ILE	C-O	-5.27	1.18	1.24
1	D	81	THR	C-O	5.25	1.30	1.23
1	D	548	ALA	CA-CB	5.25	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	246	GLN	C-O	-5.24	1.18	1.24
1	D	439	PRO	N-CA	5.23	1.53	1.47
1	A	307	ALA	CA-CB	5.23	1.61	1.53
1	B	576	PRO	CA-C	5.22	1.57	1.52
1	A	395	HIS	CA-C	-5.21	1.46	1.53
1	A	203	THR	CA-CB	5.19	1.60	1.54
1	C	86	VAL	CA-CB	5.15	1.60	1.54
1	A	419	GLN	CA-CB	5.14	1.62	1.53
1	C	322	LEU	C-O	5.11	1.29	1.24
1	A	178	THR	N-CA	5.10	1.52	1.46
1	D	662	VAL	CA-CB	5.09	1.62	1.54
1	D	61	ARG	CZ-NH2	5.08	1.40	1.33
1	A	730	ASP	C-O	5.08	1.30	1.24
1	A	293	TRP	N-CA	5.07	1.52	1.46
1	D	559	ALA	C-O	-5.07	1.18	1.24
1	C	268	THR	CA-CB	5.05	1.62	1.53

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	710	ILE	CA-C-N	9.41	139.51	121.54
1	A	710	ILE	C-N-CA	9.41	139.51	121.54
1	D	61	ARG	NE-CZ-NH2	9.03	127.33	119.20
1	C	159	ILE	CB-CG1-CD1	-8.29	96.39	113.80
1	B	438	CYS	CA-C-N	-7.63	112.14	119.85
1	B	438	CYS	C-N-CA	-7.63	112.14	119.85
1	A	710	ILE	N-CA-C	7.51	124.96	109.34
1	A	28	SER	CA-C-N	-7.26	109.67	123.32
1	A	28	SER	C-N-CA	-7.26	109.67	123.32
1	B	370	VAL	N-CA-CB	-7.14	102.48	112.12
1	B	237	ASP	N-CA-C	7.05	119.86	111.33
1	B	745	ILE	CA-C-N	-6.97	112.52	119.56
1	B	745	ILE	C-N-CA	-6.97	112.52	119.56
1	A	237	ASP	N-CA-C	6.85	119.33	111.11
1	A	710	ILE	O-C-N	6.83	131.10	122.57
1	A	711	ALA	N-CA-C	6.70	125.06	110.80
1	C	552	LEU	N-CA-C	6.67	118.55	111.28
1	A	449[A]	HIS	CB-CA-C	6.34	120.73	111.73
1	A	449[B]	HIS	CB-CA-C	6.34	120.73	111.73
1	D	61	ARG	NE-CZ-NH1	-6.31	115.19	121.50
1	B	536	ARG	CA-C-N	-6.27	112.55	119.19
1	B	536	ARG	C-N-CA	-6.27	112.55	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	709	LYS	CA-C-N	-6.22	110.78	121.97
1	A	709	LYS	C-N-CA	-6.22	110.78	121.97
1	B	521	ARG	NE-CZ-NH2	6.17	124.75	119.20
1	C	158	LYS	CA-C-N	-6.09	115.24	123.10
1	C	158	LYS	C-N-CA	-6.09	115.24	123.10
1	D	598	VAL	CA-CB-CG2	6.07	120.71	110.40
1	C	574	THR	CA-C-N	-6.00	114.20	120.38
1	C	574	THR	C-N-CA	-6.00	114.20	120.38
1	B	593	ILE	CA-C-N	5.96	127.29	119.84
1	B	593	ILE	C-N-CA	5.96	127.29	119.84
1	C	513	LEU	N-CA-C	-5.92	105.54	112.89
1	C	126	ILE	CB-CA-C	-5.90	104.17	112.14
1	D	122	ILE	CA-C-N	-5.86	113.75	119.78
1	D	122	ILE	C-N-CA	-5.86	113.75	119.78
1	A	349	PHE	CA-C-N	-5.85	112.49	122.56
1	A	349	PHE	C-N-CA	-5.85	112.49	122.56
1	B	227	TRP	O-C-N	5.81	128.57	122.23
1	C	725	ASP	N-CA-C	5.80	123.15	110.80
1	A	419	GLN	CB-CA-C	5.79	122.55	110.32
1	C	109	ILE	N-CA-C	-5.72	105.27	110.82
1	B	321	GLU	CB-CG-CD	-5.69	102.93	112.60
1	C	159	ILE	CA-CB-CG2	5.68	120.16	110.50
1	D	751	ILE	N-CA-CB	5.68	115.84	109.99
1	D	419	GLN	CB-CA-C	5.68	122.18	110.31
1	C	237	ASP	N-CA-C	5.64	117.11	111.07
1	D	213	LYS	CD-CE-NZ	-5.54	94.17	111.90
1	B	41	GLU	CA-C-N	-5.51	114.25	119.76
1	B	41	GLU	C-N-CA	-5.51	114.25	119.76
1	A	177	ASP	N-CA-C	5.44	118.38	111.69
1	D	237	ASP	N-CA-C	5.40	117.59	111.11
1	A	48	GLN	CA-C-N	-5.40	114.22	119.78
1	A	48	GLN	C-N-CA	-5.40	114.22	119.78
1	A	404	ASN	N-CA-C	5.37	119.70	113.20
1	B	736	MET	N-CA-C	-5.25	105.73	111.82
1	C	728	PHE	N-CA-C	-5.21	105.69	111.36
1	A	295	PRO	CB-CA-C	-5.19	106.68	111.40
1	B	126	ILE	CB-CA-C	-5.16	105.17	112.14
1	B	419	GLN	CB-CA-C	5.16	121.10	110.31
1	B	44	PRO	N-CA-C	5.12	116.95	110.70
1	A	413	GLU	CA-CB-CG	5.11	124.31	114.10
1	D	379	PRO	CB-CA-C	-5.10	103.55	111.40
1	B	436	PRO	CB-CA-C	-5.09	104.55	111.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	377	ARG	CG-CD-NE	-5.08	100.81	112.00
1	C	431	ILE	N-CA-C	-5.08	103.43	108.96
1	A	619	ILE	N-CA-C	-5.07	105.55	110.42
1	A	536	ARG	NE-CZ-NH2	5.05	123.74	119.20
1	A	751	ILE	N-CA-CB	5.01	114.74	110.08
1	A	155	ASP	CA-C-N	-5.00	114.92	119.82
1	A	155	ASP	C-N-CA	-5.00	114.92	119.82

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	5572	50	0
1	B	5746	0	5577	52	0
1	C	5745	0	5573	50	0
1	D	5746	0	5577	46	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	768	0	0	4	0
3	B	643	0	0	10	0
3	C	693	0	0	19	0
3	D	730	0	0	10	0
All	All	25988	0	22419	186	0

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

All (186) 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:392:HIS:ND1	1:A:415:TYR:CB	1.67	1.54
1:B:392:HIS:ND1	1:B:415:TYR:CB	1.70	1.52
1:D:392:HIS:ND1	1:D:415:TYR:CB	1.69	1.51
1:C:392:HIS:ND1	1:C:415:TYR:CB	1.70	1.48
1:D:392:HIS:CE1	1:D:415:TYR:HB2	1.63	1.31
1:C:392:HIS:CE1	1:C:415:TYR:HB2	1.67	1.28
1:B:392:HIS:CE1	1:B:415:TYR:HB2	1.68	1.26
1:A:392:HIS:CE1	1:A:415:TYR:HB2	1.69	1.26
1:D:341:ILE:HG13	3:D:3022:HOH:O	1.42	1.20
1:D:392:HIS:ND1	1:D:415:TYR:HB2	0.79	1.12
1:B:392:HIS:ND1	1:B:415:TYR:HB2	0.79	1.11
1:C:392:HIS:ND1	1:C:415:TYR:HB2	0.80	1.11
1:B:451:MET:HE2	1:D:451:MET:HE2	1.30	1.09
1:A:451:MET:HE2	1:C:451:MET:HE2	1.27	1.06
1:A:392:HIS:ND1	1:A:415:TYR:HB2	0.74	1.06
1:A:710:ILE:HG12	1:A:715:GLU:OE1	1.64	0.97
1:A:392:HIS:CG	1:A:415:TYR:HB2	2.04	0.91
1:A:29:LEU:HD22	3:C:2405:HOH:O	1.71	0.90
1:D:521:ARG:HD3	3:D:3252:HOH:O	1.78	0.82
1:B:533:LYS:HE2	3:B:3100:HOH:O	1.79	0.82
1:B:521:ARG:HD3	3:B:3047:HOH:O	1.77	0.81
1:A:28:SER:OG	1:A:28:SER:O	1.98	0.80
1:B:583:LYS:H	1:B:583:LYS:NZ	1.82	0.78
1:D:451:MET:SD	3:D:3264:HOH:O	2.42	0.77
1:B:392:HIS:ND1	1:B:415:TYR:HB3	1.99	0.75
1:C:37:ARG:NH1	3:C:1870:HOH:O	2.19	0.74
3:B:2705:HOH:O	1:D:73:LYS:HD3	1.87	0.73
1:A:713:GLN:HG2	3:A:2153:HOH:O	1.90	0.71
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.73	0.71
1:C:597:ASP:OD2	3:C:2146:HOH:O	2.09	0.69
1:B:294:LYS:HB2	3:B:1081:HOH:O	1.92	0.69
1:A:392:HIS:ND1	1:A:415:TYR:CG	2.60	0.68
1:A:751:ILE:O	1:A:751:ILE:HD12	1.94	0.68
1:D:392:HIS:ND1	1:D:415:TYR:HB3	1.98	0.67
1:A:478:LYS:HG2	3:A:1955:HOH:O	1.94	0.67
1:C:578:ASP:HB3	3:C:2919:HOH:O	1.93	0.67
1:C:283:GLU:OE1	3:C:2292:HOH:O	2.13	0.66
1:A:36:HIS:CD2	1:A:36:HIS:H	2.13	0.66
1:D:341:ILE:CG1	3:D:3022:HOH:O	2.19	0.65
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.79	0.65
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.04	0.65
2:A:760:HEM:HBB2	2:A:760:HEM:HMB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:HIS:ND1	1:A:415:TYR:HB3	2.03	0.64
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.81	0.63
3:B:2705:HOH:O	1:D:73:LYS:CD	2.44	0.62
1:D:488:ARG:NH1	1:D:490:GLU:OE1	2.31	0.62
1:B:724:ALA:O	1:B:725:ASP:O	2.18	0.62
1:C:392:HIS:ND1	1:C:415:TYR:HB3	2.01	0.62
1:C:533:LYS:NZ	3:C:2231:HOH:O	2.28	0.61
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.83	0.61
1:D:392:HIS:ND1	1:D:415:TYR:CG	2.63	0.60
1:D:392:HIS:CE1	1:D:415:TYR:CB	2.55	0.57
1:D:158:LYS:NZ	3:D:2950:HOH:O	2.35	0.57
1:B:583:LYS:H	1:B:583:LYS:HZ3	1.52	0.57
3:B:2705:HOH:O	1:D:73:LYS:CE	2.51	0.57
1:D:359:LEU:H	1:D:507:HIS:HD2	1.53	0.57
1:D:629:HIS:HD2	3:D:1554:HOH:O	1.88	0.57
1:A:710:ILE:CG1	1:A:715:GLU:OE1	2.46	0.57
1:A:449[A]:HIS:CD2	1:C:449[A]:HIS:CD2	2.92	0.57
1:C:724:ALA:O	1:C:725:ASP:HB2	2.05	0.56
1:D:478:LYS:NZ	3:D:892:HOH:O	2.14	0.56
1:C:578:ASP:HB2	1:C:582:LEU:O	2.06	0.56
1:C:392:HIS:ND1	1:C:415:TYR:CG	2.65	0.55
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.89	0.55
1:A:710:ILE:HG12	1:A:715:GLU:CD	2.31	0.55
1:C:416:THR:HG21	3:C:3270:HOH:O	2.06	0.55
1:A:29:LEU:HB2	3:C:2405:HOH:O	2.07	0.54
1:C:636:ARG:NH2	1:C:639:GLU:O	2.41	0.54
1:B:583:LYS:H	1:B:583:LYS:HZ2	1.52	0.53
1:B:629:HIS:HD2	3:B:1051:HOH:O	1.92	0.53
1:C:395:HIS:HE1	3:C:3269:HOH:O	1.91	0.52
1:B:359:LEU:H	1:B:507:HIS:HD2	1.56	0.52
1:C:609:ASP:HB3	3:C:3175:HOH:O	2.08	0.52
1:C:238:THR:HB	1:D:460:TYR:CE2	2.45	0.52
1:D:61:ARG:HH11	1:D:66:ASN:HA	1.76	0.51
1:B:583:LYS:O	1:B:584:LYS:HB3	2.10	0.51
1:C:704:PHE:O	1:C:707:THR:HG22	2.10	0.51
1:B:52:PRO:HG3	3:D:1451:HOH:O	2.11	0.51
1:C:533:LYS:HG3	3:C:2231:HOH:O	2.11	0.50
1:B:392:HIS:ND1	1:B:415:TYR:CG	2.69	0.50
1:B:616:LEU:CD1	1:B:648:LEU:HD22	2.42	0.50
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.47	0.49
1:B:552:LEU:HD22	1:B:556:GLN:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:731:GLU:OE2	3:D:3028:HOH:O	2.18	0.49
1:A:449[B]:HIS:CG	1:C:449[B]:HIS:CG	2.45	0.49
1:D:713:GLN:O	1:D:713:GLN:HG2	2.12	0.49
1:A:345:ASP:HA	1:A:348:LYS:HD2	1.96	0.48
1:A:211:ALA:CB	1:A:410:GLY:HA3	2.43	0.48
1:D:36:HIS:H	1:D:36:HIS:HD1	1.60	0.48
2:B:760:HEM:HMC2	2:B:760:HEM:HBC2	1.96	0.48
1:C:696:ALA:HB1	1:C:728:PHE:CZ	2.49	0.48
1:B:449[A]:HIS:CG	1:D:449[A]:HIS:CG	2.42	0.48
1:C:629:HIS:HD2	3:C:1129:HOH:O	1.96	0.48
1:D:274:ILE:HD12	2:D:760:HEM:HMB1	1.95	0.48
1:D:552:LEU:HD11	1:D:571:LEU:HA	1.96	0.48
1:A:38:PRO:HG2	1:A:51:ALA:HB2	1.94	0.48
1:C:610:GLU:HB3	1:C:671:ASN:HB2	1.96	0.48
1:C:28:SER:N	3:C:2523:HOH:O	2.47	0.47
1:A:36:HIS:H	1:A:36:HIS:HD2	1.62	0.47
1:C:211:ALA:CB	1:C:410:GLY:HA3	2.44	0.47
1:C:274:ILE:HD12	2:C:760:HEM:HMB1	1.96	0.47
1:B:461:GLU:HA	1:B:462:PRO:C	2.38	0.47
1:A:29:LEU:CB	3:C:2405:HOH:O	2.62	0.47
1:B:61:ARG:HG2	3:B:2908:HOH:O	2.15	0.47
1:B:533:LYS:HE3	3:C:2623:HOH:O	2.14	0.47
1:C:61:ARG:HG3	3:C:2648:HOH:O	2.14	0.47
1:B:274:ILE:HD12	2:B:760:HEM:HMB1	1.96	0.47
1:B:509:ARG:HD2	1:B:576:PRO:HD2	1.97	0.47
1:B:281:ASN:OD1	1:B:283:GLU:HG3	2.15	0.46
1:B:533:LYS:CE	3:C:2623:HOH:O	2.63	0.46
2:C:760:HEM:CMB	2:C:760:HEM:HBB2	2.45	0.46
1:D:359:LEU:H	1:D:507:HIS:CD2	2.30	0.46
1:A:62:ASN:OD1	1:A:62:ASN:C	2.58	0.46
1:B:521:ARG:CD	3:B:3047:HOH:O	2.50	0.46
1:C:612:ARG:NH2	1:C:669:OCS:OD1	2.47	0.46
1:D:612:ARG:NH1	1:D:669:OCS:OD2	2.44	0.46
1:A:91:ASP:OD1	1:C:461:GLU:OE1	2.32	0.46
1:A:392:HIS:CG	1:A:415:TYR:CB	2.79	0.46
1:A:254:MET:HE3	1:A:254:MET:HB3	1.88	0.45
1:C:128:HIS:CE1	1:C:169:VAL:HG22	2.51	0.45
1:A:128:HIS:HA	1:A:168:THR:O	2.17	0.45
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.32	0.45
1:D:448:MET:O	1:D:449[A]:HIS:HB2	2.16	0.45
1:B:459:ASN:H	1:B:459:ASN:HD22	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:ASN:O	1:C:405:ASP:C	2.59	0.44
1:A:128:HIS:CE1	1:A:169:VAL:HG22	2.53	0.44
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.33	0.44
1:D:341:ILE:CD1	3:D:3022:HOH:O	2.60	0.44
1:B:696:ALA:HB1	1:B:728:PHE:CZ	2.53	0.44
1:C:392:HIS:CE1	1:C:415:TYR:CB	2.59	0.44
1:B:278:ARG:HH22	1:B:487:GLU:CD	2.26	0.44
1:D:598:VAL:HG13	1:D:628:VAL:CG2	2.48	0.44
1:C:725:ASP:HB3	1:C:726:GLY:H	1.68	0.44
1:A:710:ILE:HD13	3:A:3248:HOH:O	2.17	0.43
1:D:459:ASN:HD22	1:D:459:ASN:H	1.66	0.43
1:A:36:HIS:CD2	1:A:36:HIS:N	2.84	0.43
1:A:603:VAL:HG11	1:A:666:ILE:HD12	2.00	0.43
1:A:460:TYR:CE2	1:B:238:THR:HB	2.53	0.43
1:B:748:ILE:O	1:B:751:ILE:HG22	2.18	0.43
1:B:128:HIS:CE1	1:B:169:VAL:HG22	2.54	0.43
1:D:509:ARG:HD2	1:D:576:PRO:HD2	2.00	0.43
1:B:62:ASN:OD1	1:B:62:ASN:C	2.62	0.42
1:B:359:LEU:H	1:B:507:HIS:CD2	2.36	0.42
1:C:111:ARG:CZ	1:C:111:ARG:HB2	2.49	0.42
1:C:359:LEU:H	1:C:507:HIS:HD2	1.67	0.42
1:C:488:ARG:HD3	3:C:2379:HOH:O	2.19	0.42
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.49	0.42
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.34	0.42
1:D:696:ALA:HB1	1:D:728:PHE:CZ	2.54	0.42
1:B:708:ILE:HG13	1:B:710:ILE:HG12	2.00	0.42
1:A:459:ASN:HD22	1:A:459:ASN:H	1.66	0.42
1:C:459:ASN:H	1:C:459:ASN:HD22	1.67	0.42
1:B:362:GLU:HG2	1:B:367:VAL:HG23	2.02	0.42
1:A:319:ARG:HD3	1:D:227:TRP:O	2.18	0.42
1:B:556:GLN:HG2	1:B:566:LEU:HD23	2.01	0.42
1:C:309:LYS:HB3	1:C:660:LEU:HD21	2.02	0.42
1:B:637:MET:HE3	3:B:2035:HOH:O	2.20	0.42
1:A:213:LYS:HB3	1:A:213:LYS:HE3	1.81	0.41
1:A:461:GLU:HA	1:A:462:PRO:C	2.43	0.41
1:B:313:ARG:NH2	1:C:309:LYS:HD2	2.34	0.41
1:C:416:THR:CG2	3:C:3270:HOH:O	2.67	0.41
1:A:386:ASN:OD1	1:A:386:ASN:C	2.63	0.41
1:A:603:VAL:HG11	1:A:666:ILE:CD1	2.50	0.41
1:A:617:LEU:HD11	3:A:3081:HOH:O	2.20	0.41
1:B:386:ASN:OD1	1:B:386:ASN:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:VAL:HA	1:C:188:LYS:O	2.21	0.41
1:A:227:TRP:CE3	1:A:229:ILE:HD12	2.55	0.41
1:B:91:ASP:OD1	1:D:461:GLU:OE1	2.38	0.41
1:D:725:ASP:OD1	1:D:725:ASP:C	2.62	0.41
1:B:448:MET:HG3	1:B:449[A]:HIS:CD2	2.55	0.41
1:D:268:THR:HA	1:D:298:GLY:O	2.21	0.41
1:A:222:LYS:HB3	1:A:223:PRO:HD2	2.02	0.41
1:B:36:HIS:HD1	1:B:36:HIS:H	1.68	0.41
1:D:386:ASN:OD1	1:D:386:ASN:C	2.64	0.41
1:A:393:PRO:HD2	1:A:415:TYR:CD2	2.56	0.41
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.56	0.40
1:C:65:LEU:HD21	1:C:135:HIS:CG	2.56	0.40
1:C:330:ASP:OD1	1:C:629:HIS:CE1	2.63	0.40
1:C:359:LEU:H	1:C:507:HIS:CD2	2.40	0.40
1:D:404:ASN:O	1:D:405:ASP:C	2.63	0.40
1:A:551:ASP:OD1	1:A:553:THR:HB	2.21	0.40
1:C:392:HIS:HB3	1:C:395:HIS:CE1	2.56	0.40
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.37	0.40
1:A:207:PHE:O	1:A:249:THR:HA	2.21	0.40
1:A:222:LYS:HB3	1:A:223:PRO:CD	2.52	0.40
1:B:634:TYR:O	1:B:653:THR:HA	2.21	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	724/753 (96%)	706 (98%)	16 (2%)	2 (0%)	36	20
1	B	724/753 (96%)	701 (97%)	21 (3%)	2 (0%)	36	20
1	C	724/753 (96%)	703 (97%)	19 (3%)	2 (0%)	36	20
1	D	724/753 (96%)	707 (98%)	16 (2%)	1 (0%)	48	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2896/3012 (96%)	2817 (97%)	72 (2%)	7 (0%)	43 25

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	711	ALA
1	B	725	ASP
1	A	75	SER
1	B	75	SER
1	C	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%)	590 (97%)	21 (3%)	32 10
1	B	611/635 (96%)	581 (95%)	30 (5%)	22 5
1	C	611/635 (96%)	577 (94%)	34 (6%)	19 3
1	D	611/635 (96%)	591 (97%)	20 (3%)	33 11
All	All	2444/2540 (96%)	2339 (96%)	105 (4%)	26 6

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	198	LEU
1	A	205	ILE
1	A	213	LYS

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Mol	Chain	Res	Type
1	A	252	ASN
1	A	369	ARG
1	A	413	GLU
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	565	GLU
1	A	709	LYS
1	A	710	ILE
1	A	712	ASP
1	A	732	LEU
1	A	750	LYS
1	B	158	LYS
1	B	191	THR
1	B	205	ILE
1	B	252	ASN
1	B	283	GLU
1	B	285	LYS
1	B	321	GLU
1	B	344	GLU
1	B	369	ARG
1	B	370	VAL
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	593	ILE
1	B	594	PRO
1	B	595	ASP
1	B	616	LEU
1	B	621	LYS
1	B	633	LEU
1	B	647	VAL
1	B	713	GLN
1	B	732	LEU

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Mol	Chain	Res	Type
1	B	750	LYS
1	C	159	ILE
1	C	191	THR
1	C	198	LEU
1	C	205	ILE
1	C	252	ASN
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	537	PRO
1	C	552	LEU
1	C	568	ASP
1	C	571	LEU
1	C	578	ASP
1	C	583	LYS
1	C	584	LYS
1	C	606	LEU
1	C	610	GLU
1	C	612	ARG
1	C	616	LEU
1	C	617	LEU
1	C	633	LEU
1	C	636	ARG
1	C	648	LEU
1	C	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	73	LYS
1	D	191	THR
1	D	205	ILE
1	D	252	ASN
1	D	340	LEU
1	D	432	PRO
1	D	440	TYR

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Mol	Chain	Res	Type
1	D	459	ASN
1	D	552	LEU
1	D	554	LEU
1	D	574	THR
1	D	582	LEU
1	D	598	VAL
1	D	616	LEU
1	D	648	LEU
1	D	708	ILE
1	D	713	GLN
1	D	732	LEU
1	D	747	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	66	ASN
1	A	77	ASN
1	A	139	GLN
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	A	546	GLN
1	B	77	ASN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	C	252	ASN
1	C	459	ASN
1	C	486	GLN
1	C	507	HIS
1	C	556	GLN
1	C	629	HIS
1	C	671	ASN
1	C	682	ASN
1	D	48	GLN
1	D	77	ASN
1	D	252	ASN
1	D	459	ASN

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Mol	Chain	Res	Type
1	D	507	HIS
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	B	669	1	6,8,9	1.06	0	7,11,13	1.23	1 (14%)
1	OCS	A	669	1	6,8,9	0.71	0	7,11,13	1.79	1 (14%)
1	OCS	C	669	1	6,8,9	0.68	0	7,11,13	2.08	3 (42%)
1	OCS	D	669	1	6,8,9	0.91	0	7,11,13	1.30	1 (14%)

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	B	669	1	-	1/4/7/9	-
1	OCS	A	669	1	-	4/4/7/9	-
1	OCS	C	669	1	-	4/4/7/9	-
1	OCS	D	669	1	-	2/4/7/9	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	669	OCS	OD1-SG-CB	3.83	112.47	106.76
1	C	669	OCS	OD3-SG-CB	3.72	112.31	106.76
1	C	669	OCS	OD1-SG-CB	-2.61	102.86	106.76
1	C	669	OCS	CA-CB-SG	2.59	117.45	113.61
1	B	669	OCS	OD3-SG-CB	-2.46	103.08	106.76
1	D	669	OCS	OD2-SG-OD3	2.14	116.75	111.40

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	669	OCS	1	0
1	D	669	OCS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	C	760	1	50,50,50	1.74	11 (22%)	67,82,82	2.12	20 (29%)
2	HEM	B	760	1	50,50,50	1.77	10 (20%)	67,82,82	1.96	19 (28%)
2	HEM	A	760	1	50,50,50	1.68	9 (18%)	67,82,82	2.05	22 (32%)
2	HEM	D	760	1	50,50,50	1.89	9 (18%)	67,82,82	2.02	19 (28%)

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

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

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HEM	C3D-C2D	5.50	1.48	1.36
2	D	760	HEM	C3D-C2D	5.46	1.48	1.36
2	D	760	HEM	FE-ND	5.41	2.11	1.94
2	D	760	HEM	FE-NB	5.05	2.10	1.94
2	B	760	HEM	FE-NB	4.84	2.09	1.94
2	B	760	HEM	C3D-C2D	4.65	1.46	1.36
2	C	760	HEM	FE-ND	4.60	2.09	1.94
2	C	760	HEM	FE-NB	4.24	2.08	1.94
2	C	760	HEM	C3D-C2D	4.07	1.45	1.36
2	D	760	HEM	CMC-C2C	3.99	1.59	1.50
2	A	760	HEM	FE-NC	3.83	2.07	1.95
2	A	760	HEM	CMC-C2C	3.81	1.58	1.50
2	A	760	HEM	CMB-C2B	3.53	1.58	1.50
2	D	760	HEM	CAB-C3B	3.49	1.56	1.47
2	C	760	HEM	FE-NC	3.35	2.06	1.95
2	B	760	HEM	FE-NC	3.29	2.06	1.95
2	B	760	HEM	FE-ND	3.19	2.04	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HEM	FE-ND	3.06	2.04	1.94
2	D	760	HEM	FE-NC	2.79	2.04	1.95
2	C	760	HEM	CAC-C3C	2.76	1.54	1.47
2	B	760	HEM	FE-NA	2.69	2.04	1.95
2	C	760	HEM	O2A-CGA	-2.67	1.22	1.30
2	B	760	HEM	CHA-C4D	2.61	1.43	1.38
2	C	760	HEM	CMA-C3A	2.61	1.56	1.50
2	B	760	HEM	CMB-C2B	2.56	1.56	1.50
2	D	760	HEM	CBA-CGA	2.47	1.56	1.50
2	B	760	HEM	CAB-C3B	2.41	1.53	1.47
2	B	760	HEM	CMC-C2C	2.40	1.55	1.50
2	D	760	HEM	FE-NA	2.39	2.03	1.95
2	B	760	HEM	C1B-NB	-2.36	1.36	1.40
2	A	760	HEM	O2A-CGA	-2.34	1.23	1.30
2	C	760	HEM	FE-NA	2.31	2.02	1.95
2	A	760	HEM	C4C-NC	-2.24	1.35	1.39
2	C	760	HEM	C4C-NC	-2.19	1.35	1.39
2	A	760	HEM	FE-NA	2.17	2.02	1.95
2	A	760	HEM	CMA-C3A	2.17	1.55	1.50
2	D	760	HEM	O1A-CGA	2.15	1.29	1.22
2	C	760	HEM	CAB-C3B	2.12	1.53	1.47
2	C	760	HEM	CBD-CAD	2.05	1.59	1.51

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	760	HEM	CBD-CAD-C3D	-7.07	92.98	112.53
2	A	760	HEM	CBD-CAD-C3D	-7.06	93.00	112.53
2	D	760	HEM	CBD-CAD-C3D	-6.58	94.33	112.53
2	B	760	HEM	CBD-CAD-C3D	-5.62	97.01	112.53
2	C	760	HEM	C1B-NB-C4B	5.26	111.43	105.21
2	B	760	HEM	C3B-C4B-NB	-4.88	105.96	109.47
2	C	760	HEM	C2B-C1B-NB	-4.85	104.27	109.84
2	C	760	HEM	C3B-C4B-NB	-4.81	106.01	109.47
2	D	760	HEM	C2A-C1A-NA	-4.45	105.21	110.15
2	B	760	HEM	C1B-NB-C4B	4.30	110.29	105.21
2	B	760	HEM	CHA-C4D-ND	4.20	129.57	124.37
2	C	760	HEM	CHB-C1B-NB	4.17	129.52	124.37
2	A	760	HEM	C4B-C3B-C2B	4.12	111.07	107.28
2	D	760	HEM	C1B-NB-C4B	3.95	109.89	105.21
2	A	760	HEM	C4C-C3C-C2C	3.80	110.11	106.81
2	D	760	HEM	CMD-C2D-C1D	3.78	130.94	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	760	HEM	O2D-CGD-CBD	3.78	125.93	114.00
2	B	760	HEM	O2D-CGD-O1D	-3.70	113.83	123.33
2	D	760	HEM	C4D-ND-C1D	3.64	109.52	105.21
2	D	760	HEM	CAA-CBA-CGA	-3.64	104.01	113.67
2	C	760	HEM	CHC-C1C-NC	3.60	128.37	124.45
2	D	760	HEM	O2D-CGD-CBD	3.60	125.36	114.00
2	A	760	HEM	CAA-CBA-CGA	-3.49	104.41	113.67
2	C	760	HEM	CHA-C1A-NA	3.44	130.09	123.86
2	A	760	HEM	C1D-C2D-C3D	-3.44	103.37	106.98
2	B	760	HEM	C4D-ND-C1D	3.39	109.22	105.21
2	B	760	HEM	C4C-C3C-C2C	3.38	109.75	106.81
2	D	760	HEM	C3B-C2B-C1B	3.37	108.94	106.41
2	B	760	HEM	CAA-CBA-CGA	-3.36	104.74	113.67
2	A	760	HEM	O2D-CGD-O1D	-3.36	114.68	123.33
2	C	760	HEM	CAA-CBA-CGA	-3.36	104.76	113.67
2	D	760	HEM	C2B-C1B-NB	-3.28	106.06	109.84
2	D	760	HEM	CHD-C4C-NC	3.28	128.02	124.45
2	B	760	HEM	CHC-C1C-NC	3.21	127.95	124.45
2	D	760	HEM	O2D-CGD-O1D	-3.20	115.11	123.33
2	A	760	HEM	CHD-C4C-NC	3.19	127.93	124.45
2	A	760	HEM	O2D-CGD-CBD	3.16	123.98	114.00
2	D	760	HEM	O1A-CGA-CBA	-3.09	113.28	123.09
2	A	760	HEM	C3B-C4B-NB	-3.08	107.26	109.47
2	A	760	HEM	C2A-C1A-NA	-3.05	106.76	110.15
2	B	760	HEM	CHD-C4C-NC	3.03	127.75	124.45
2	A	760	HEM	CHB-C1B-NB	3.03	128.11	124.37
2	A	760	HEM	C2D-C1D-ND	3.01	113.38	109.90
2	B	760	HEM	C3D-C4D-ND	-2.82	107.07	110.17
2	C	760	HEM	C2A-C1A-NA	-2.79	107.05	110.15
2	D	760	HEM	CHC-C1C-NC	2.78	127.48	124.45
2	A	760	HEM	CAD-CBD-CGD	-2.74	106.40	113.67
2	D	760	HEM	C1D-C2D-C3D	-2.72	104.11	106.98
2	C	760	HEM	C4C-C3C-C2C	2.68	109.14	106.81
2	C	760	HEM	C4B-C3B-C2B	2.68	109.74	107.28
2	C	760	HEM	C4D-ND-C1D	2.67	108.37	105.21
2	B	760	HEM	C2B-C1B-NB	-2.66	106.79	109.84
2	D	760	HEM	CHB-C1B-NB	2.63	127.61	124.37
2	C	760	HEM	O2D-CGD-CBD	2.62	122.29	114.00
2	A	760	HEM	CHD-C1D-C2D	-2.61	120.91	125.03
2	D	760	HEM	CHD-C1D-ND	2.54	127.16	124.42
2	C	760	HEM	C3B-C2B-C1B	2.49	108.28	106.41
2	A	760	HEM	CHC-C4B-NB	2.43	127.03	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	760	HEM	C4C-NC-C1C	2.39	109.72	105.82
2	C	760	HEM	CAD-CBD-CGD	-2.35	107.44	113.67
2	A	760	HEM	CHA-C1A-NA	2.32	128.07	123.86
2	B	760	HEM	C1D-C2D-C3D	-2.32	104.54	106.98
2	B	760	HEM	CAD-CBD-CGD	-2.32	107.52	113.67
2	D	760	HEM	CMB-C2B-C1B	-2.32	121.41	125.03
2	D	760	HEM	CAD-CBD-CGD	-2.30	107.56	113.67
2	C	760	HEM	C4C-NC-C1C	2.29	109.56	105.82
2	A	760	HEM	O1A-CGA-CBA	-2.28	115.86	123.09
2	A	760	HEM	CMD-C2D-C1D	2.26	128.57	125.03
2	A	760	HEM	C3B-C2B-C1B	-2.26	104.72	106.41
2	B	760	HEM	CHB-C1B-NB	2.23	127.13	124.37
2	A	760	HEM	CBC-CAC-C3C	-2.20	116.52	127.53
2	D	760	HEM	CHA-C1A-NA	2.19	127.84	123.86
2	C	760	HEM	CHC-C4B-NB	2.19	126.78	124.42
2	C	760	HEM	C4A-C3A-C2A	2.18	109.31	106.82
2	B	760	HEM	C4B-C3B-C2B	2.17	109.28	107.28
2	C	760	HEM	CBC-CAC-C3C	-2.16	116.73	127.53
2	A	760	HEM	C1B-NB-C4B	2.14	107.74	105.21
2	C	760	HEM	CAC-C3C-C4C	-2.09	119.83	124.82
2	A	760	HEM	C4A-CHB-C1B	-2.07	121.38	126.25
2	B	760	HEM	CHA-C1A-NA	2.04	127.55	123.86

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

4 monomers are involved in 6 short contacts:

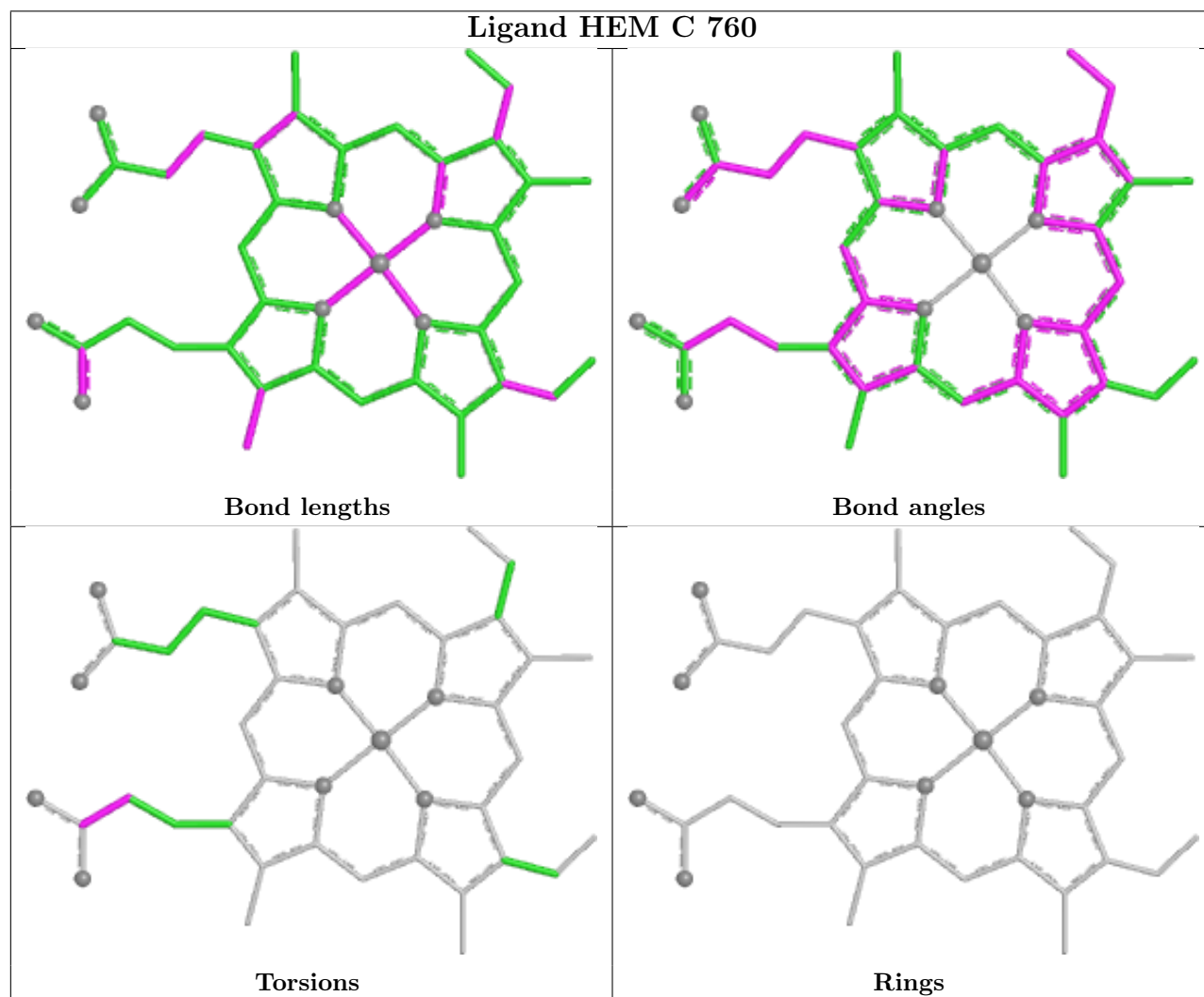
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	760	HEM	2	0

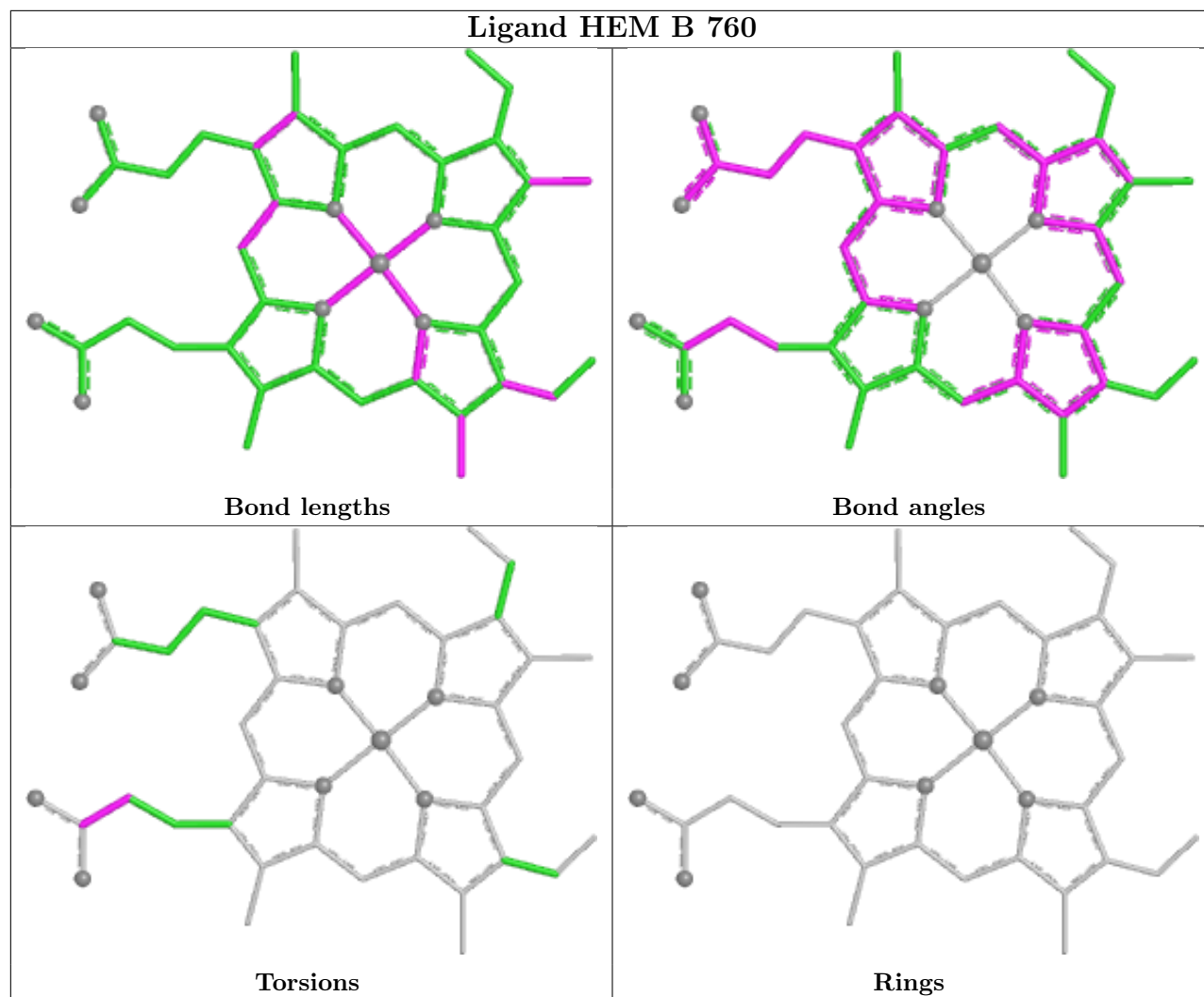
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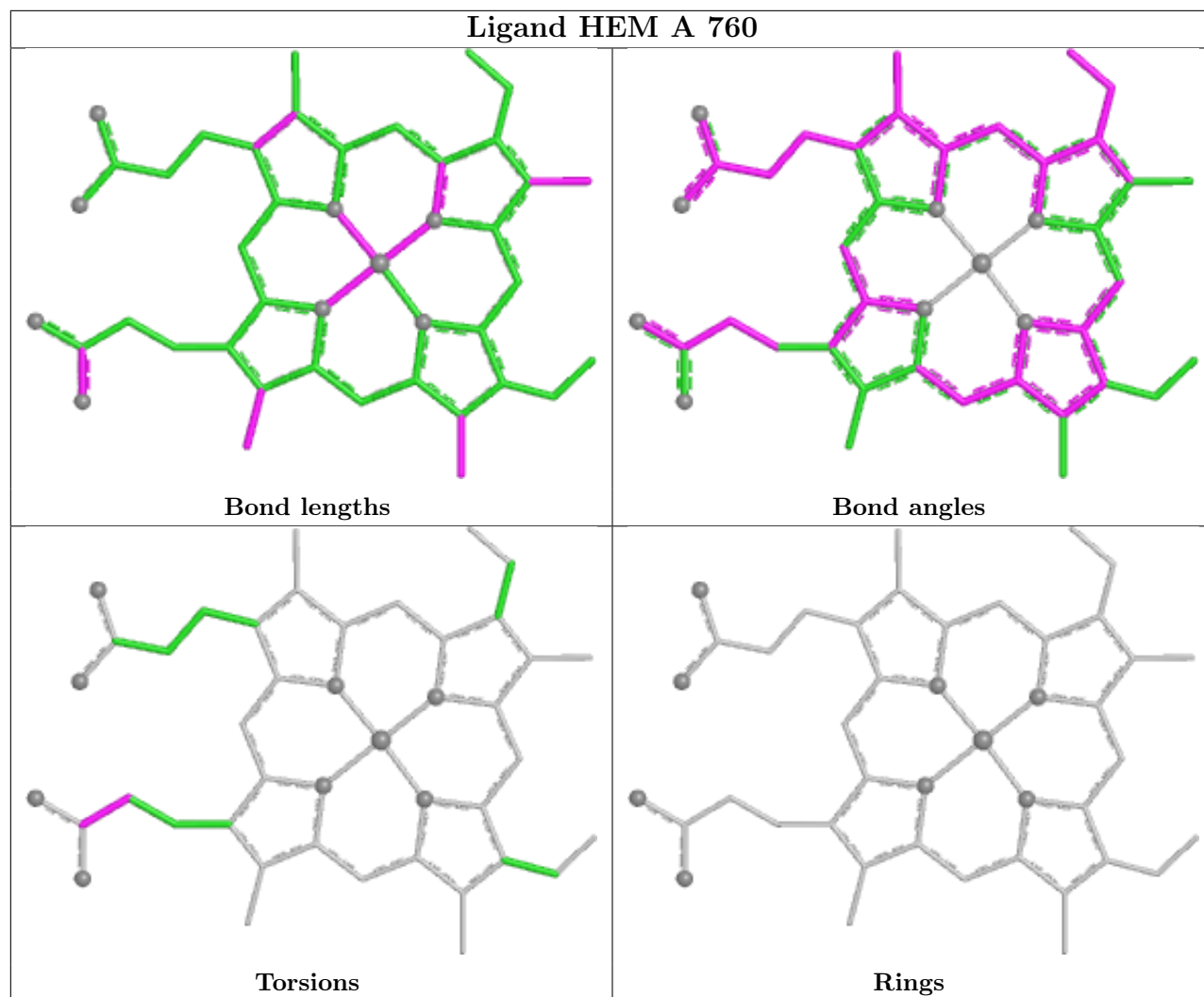
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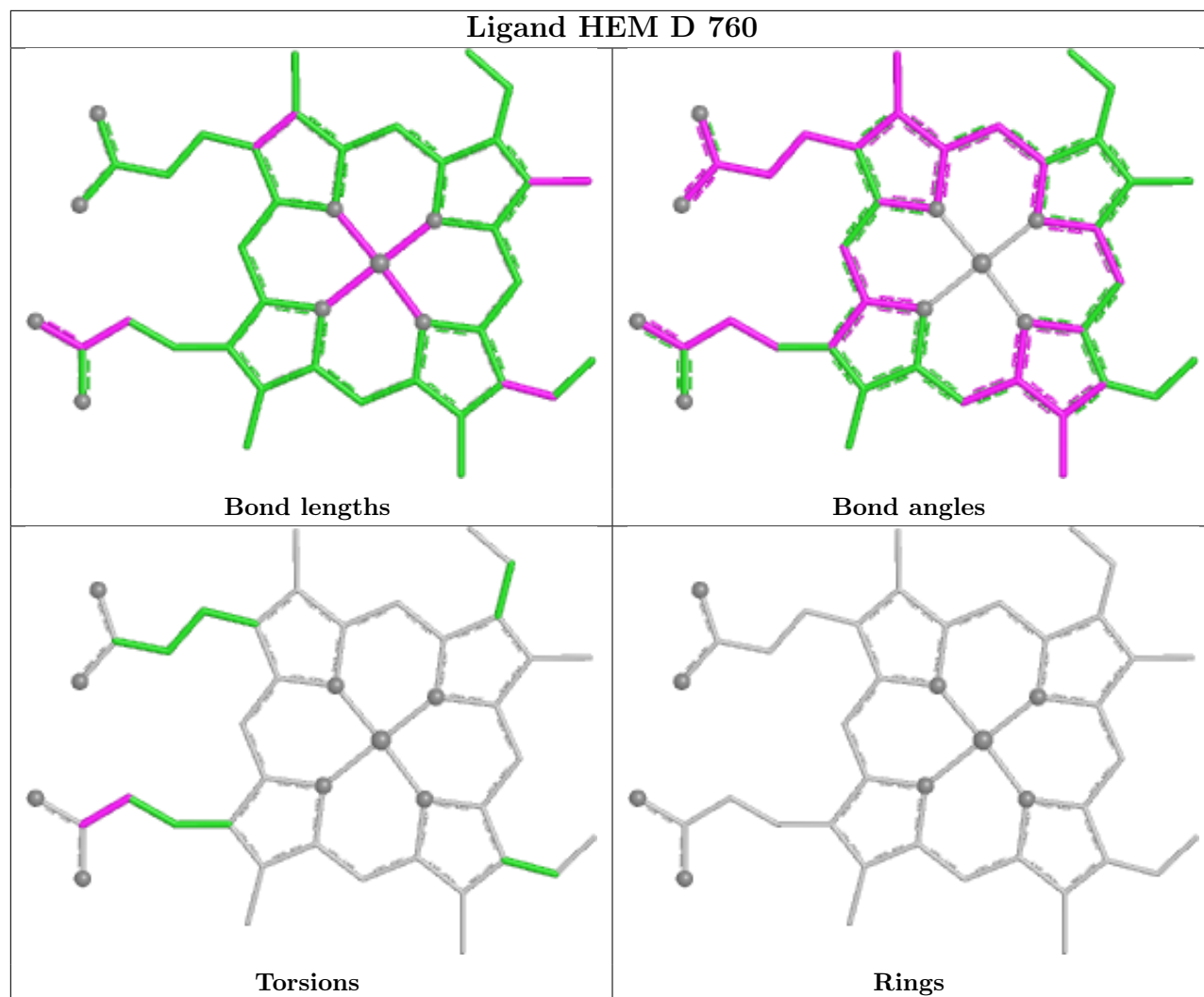
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	760	HEM	2	0
2	A	760	HEM	1	0
2	D	760	HEM	1	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	725/753 (96%)	-0.62	6 (0%) 82 86	7, 13, 28, 45	2 (0%)
1	B	725/753 (96%)	-0.52	0 100 100	6, 15, 33, 48	2 (0%)
1	C	725/753 (96%)	-0.51	1 (0%) 92 93	7, 15, 34, 48	2 (0%)
1	D	725/753 (96%)	-0.61	4 (0%) 85 89	6, 13, 30, 47	2 (0%)
All	All	2900/3012 (96%)	-0.57	11 (0%) 88 91	6, 14, 31, 48	8 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	710	ILE	5.2
1	A	28	SER	3.8
1	A	712	ASP	2.8
1	A	713	GLN	2.6
1	D	28	SER	2.4
1	A	711	ALA	2.4
1	D	751	ILE	2.3
1	D	750	LYS	2.3
1	C	725	ASP	2.1
1	A	29	LEU	2.0
1	D	749	ASP	2.0

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

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	C	669	9/10	0.94	0.09	28,29,32,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	OCS	B	669	9/10	0.95	0.07	26,27,33,33	0
1	OCS	A	669	9/10	0.95	0.07	19,21,26,29	0
1	OCS	D	669	9/10	0.95	0.08	22,23,27,29	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

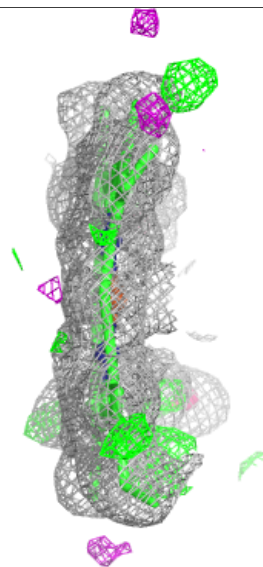
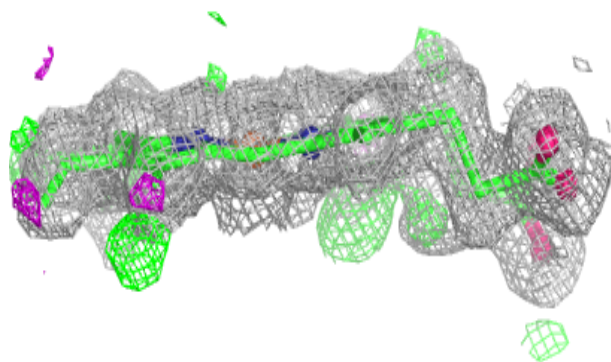
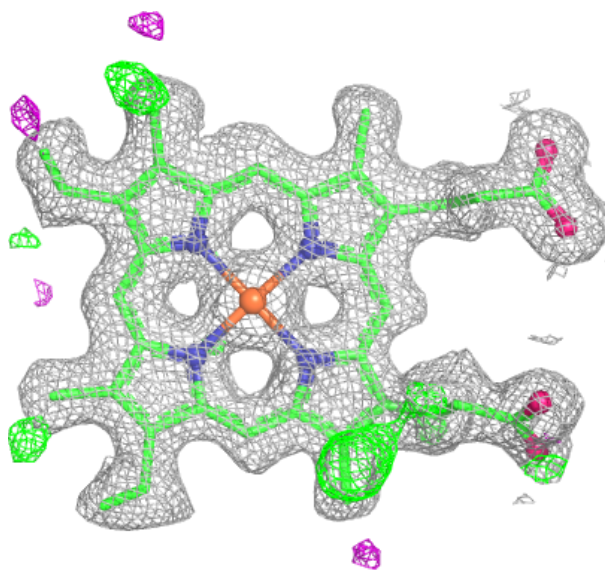
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	C	760	43/43	0.98	0.05	8,11,20,21	0
2	HEM	B	760	43/43	0.99	0.05	7,11,16,23	0
2	HEM	A	760	43/43	0.99	0.04	6,9,14,18	0
2	HEM	D	760	43/43	0.99	0.04	5,10,17,21	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.

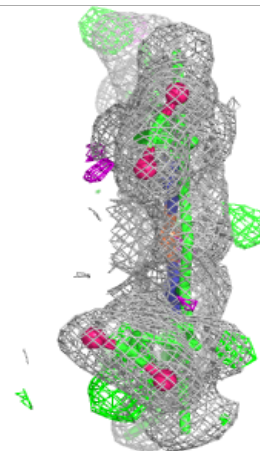
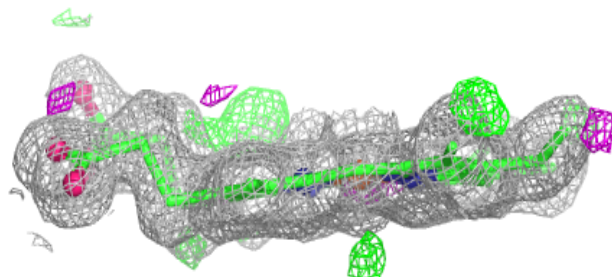
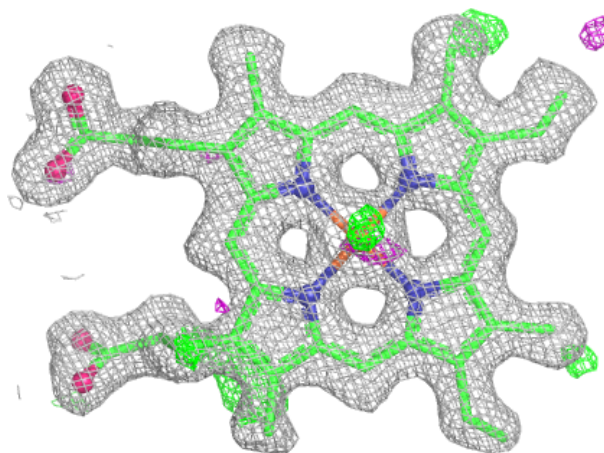
Electron density around HEM C 760:

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



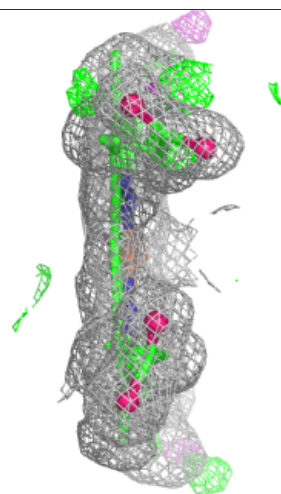
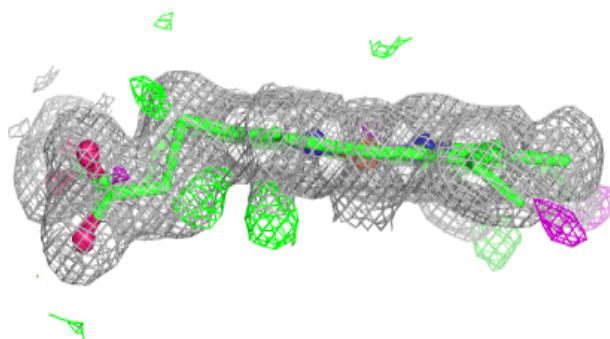
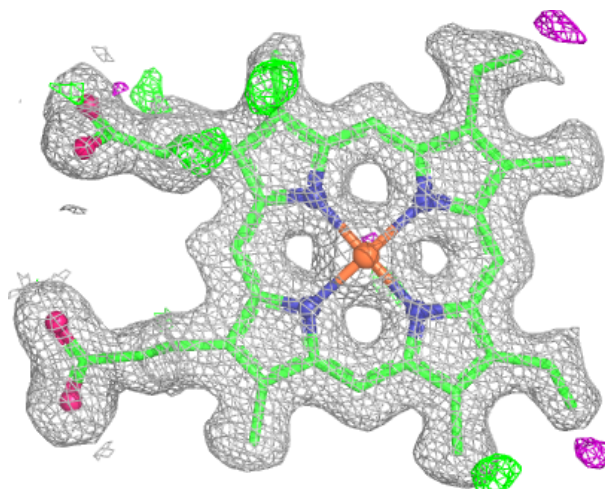
Electron density around HEM B 760:

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



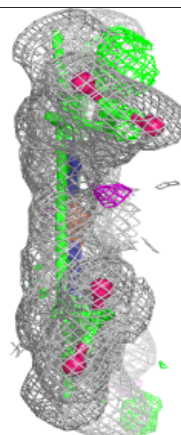
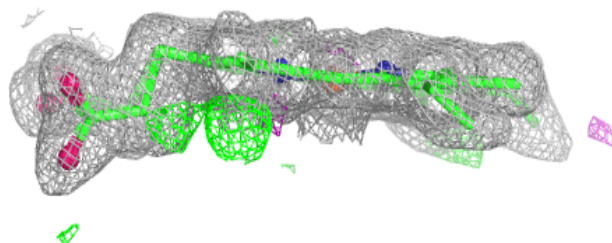
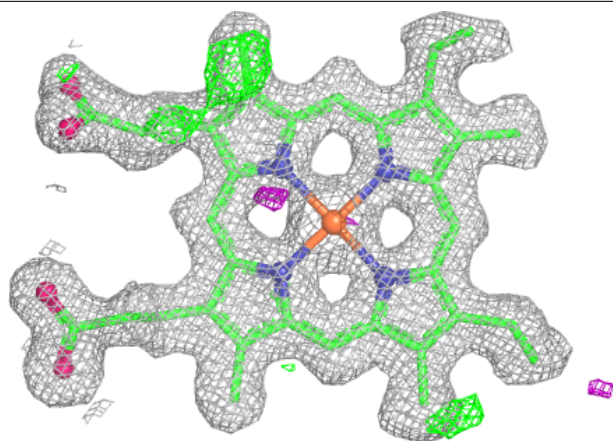
Electron density around HEM A 760:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.