Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2023 – 06:34 AM EDT

PDB ID	:	3TTW
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:

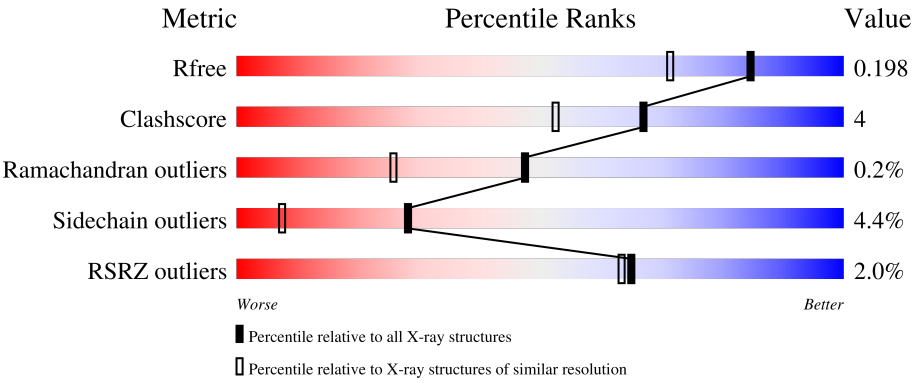
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.62 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}	130704	4693 (1.64-1.60)
Clashscore	141614	5002 (1.64-1.60)
Ramachandran outliers	138981	4888 (1.64-1.60)
Sidechain outliers	138945	4887 (1.64-1.60)
RSRZ outliers	127900	4609 (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 <=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	3% 84% 11%
1	C	753	3% 84% 10%
1	D	753	86% 9%

2 Entry composition (i)

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.

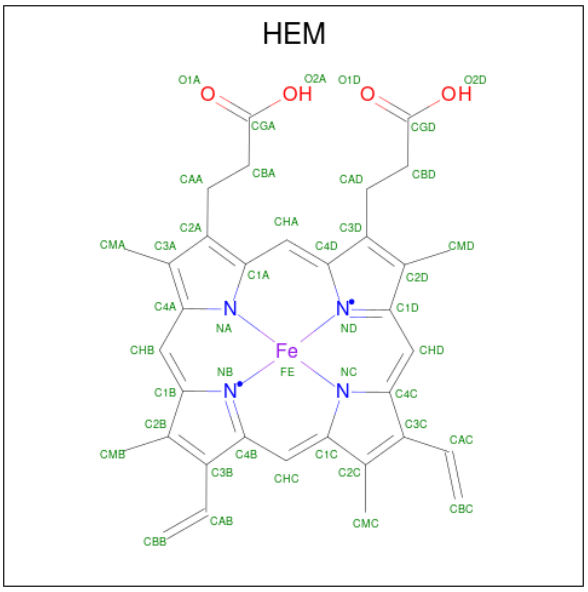
- Molecule 1 is a protein called Catalase HPII.

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 (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is water.

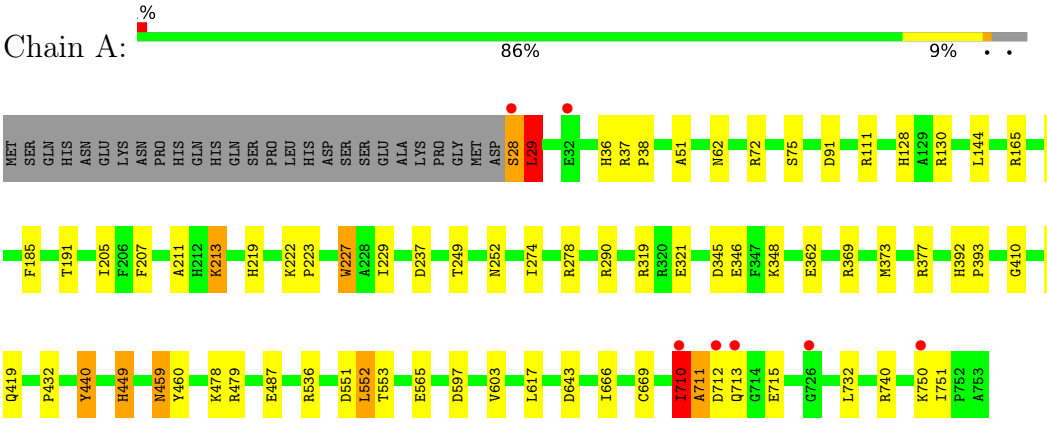
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	768	Total	O	0	0
			768	768		
3	B	643	Total	O	0	0
			643	643		
3	C	693	Total	O	0	0
			693	693		
3	D	730	Total	O	0	0
			730	730		

3 Residue-property plots (i)

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

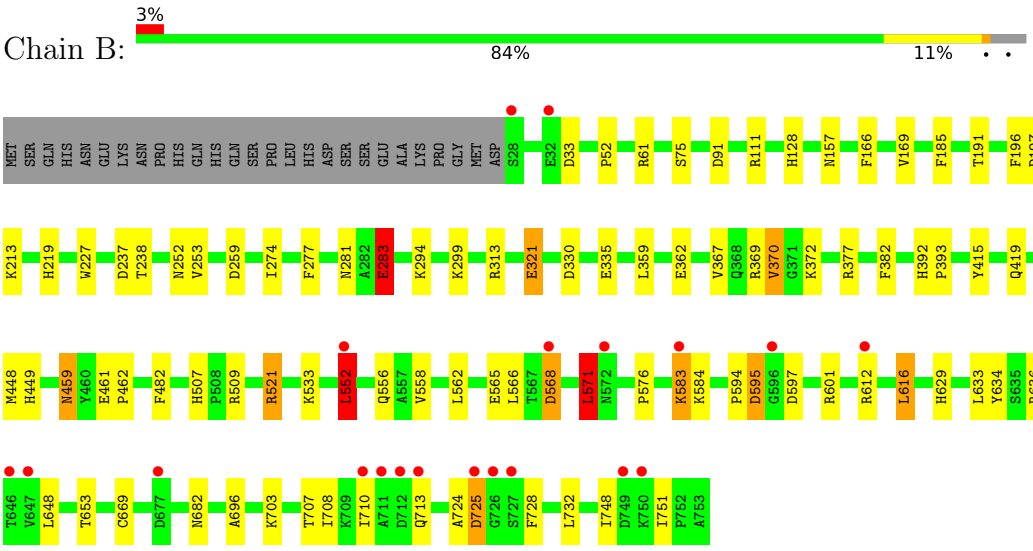
• Molecule 1: Catalase HPII

Chain A:



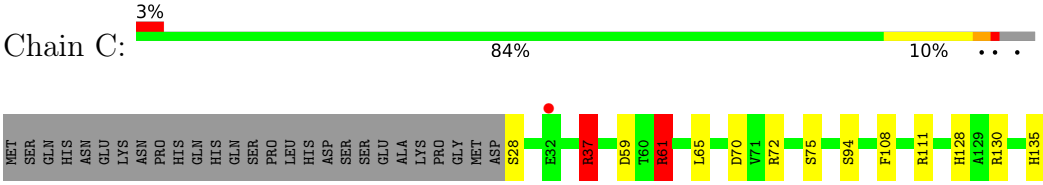
• Molecule 1: Catalase HPII

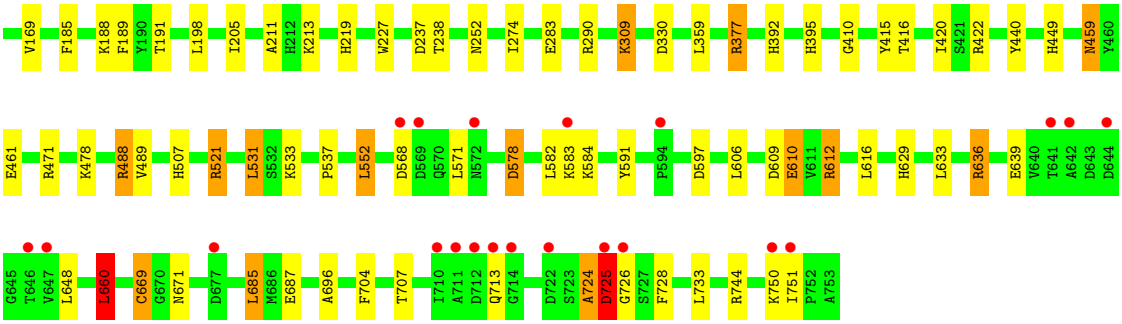
Chain B:



• Molecule 1: Catalase HPII

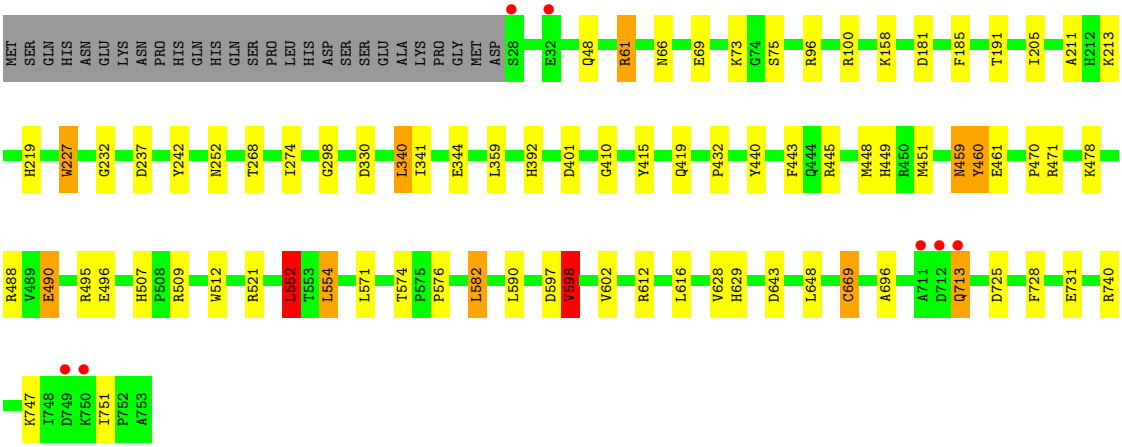
Chain C:





- Molecule 1: Catalase HPII

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 , 42.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	1.22	6/5895 (0.1%)	1.11	27/8013 (0.3%)
1	B	1.21	14/5895 (0.2%)	1.08	23/8013 (0.3%)
1	C	1.20	6/5895 (0.1%)	1.07	24/8013 (0.3%)
1	D	1.23	11/5895 (0.2%)	1.10	21/8013 (0.3%)
All	All	1.21	37/23580 (0.2%)	1.09	95/32052 (0.3%)

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 (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	321	GLU	CB-CG	10.32	1.71	1.52
1	B	157	ASN	CB-CG	7.22	1.67	1.51
1	A	440	TYR	CE1-CZ	7.17	1.47	1.38
1	B	321	GLU	CG-CD	-6.85	1.41	1.51
1	B	283	GLU	CG-CD	6.67	1.61	1.51
1	C	108	PHE	CE2-CZ	6.55	1.49	1.37
1	A	29	LEU	N-CA	-6.53	1.33	1.46
1	D	602	VAL	CB-CG1	-6.50	1.39	1.52
1	B	335	GLU	CB-CG	-6.04	1.40	1.52
1	D	100	ARG	CB-CG	-5.99	1.36	1.52
1	C	687	GLU	CB-CG	5.78	1.63	1.52
1	D	460	TYR	CG-CD1	5.78	1.46	1.39
1	B	482	PHE	CE2-CZ	5.74	1.48	1.37
1	B	382	PHE	CE1-CZ	5.74	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	591	TYR	CD2-CE2	5.64	1.47	1.39
1	D	496	GLU	CG-CD	5.64	1.60	1.51
1	A	415	TYR	CD2-CE2	-5.54	1.31	1.39
1	D	232	GLY	N-CA	5.49	1.54	1.46
1	C	59	ASP	CB-CG	5.41	1.63	1.51
1	C	309	LYS	CB-CG	-5.40	1.38	1.52
1	D	61	ARG	CZ-NH2	5.39	1.40	1.33
1	B	558	VAL	CB-CG1	5.38	1.64	1.52
1	D	69	GLU	CG-CD	5.36	1.59	1.51
1	D	344	GLU	CD-OE2	5.35	1.31	1.25
1	A	362	GLU	CD-OE2	5.34	1.31	1.25
1	B	196	PHE	CE1-CZ	5.28	1.47	1.37
1	D	242	TYR	CE2-CZ	5.27	1.45	1.38
1	B	166	PHE	CD1-CE1	5.25	1.49	1.39
1	D	512	TRP	CG-CD1	5.22	1.44	1.36
1	D	490	GLU	CG-CD	5.21	1.59	1.51
1	B	253	VAL	CB-CG2	5.18	1.63	1.52
1	B	166	PHE	CE1-CZ	5.09	1.47	1.37
1	A	346	GLU	CB-CG	5.07	1.61	1.52
1	B	277	PHE	CD1-CE1	5.05	1.49	1.39
1	C	94	SER	CB-OG	5.05	1.48	1.42
1	A	321	GLU	CD-OE1	5.04	1.31	1.25
1	B	568	ASP	CB-CG	5.03	1.62	1.51

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	61	ARG	NE-CZ-NH2	14.05	127.33	120.30
1	A	740	ARG	NE-CZ-NH1	10.29	125.44	120.30
1	D	61	ARG	NE-CZ-NH1	-10.22	115.19	120.30
1	A	377	ARG	NE-CZ-NH2	-9.12	115.74	120.30
1	B	521	ARG	NE-CZ-NH2	8.91	124.75	120.30
1	C	37	ARG	NE-CZ-NH1	8.37	124.48	120.30
1	D	340	LEU	CB-CG-CD1	8.13	124.81	111.00
1	D	495	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	A	740	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	A	130	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	D	213	LYS	CD-CE-NZ	-7.62	94.17	111.70
1	A	536	ARG	NE-CZ-NH1	-7.55	116.53	120.30
1	C	531	LEU	CB-CG-CD2	7.37	123.53	111.00
1	C	59	ASP	CB-CG-OD1	7.34	124.90	118.30
1	B	521	ARG	NE-CZ-NH1	-7.23	116.69	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	479	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	A	710	ILE	C-N-CA	7.12	139.51	121.70
1	C	685	LEU	CB-CG-CD1	7.02	122.93	111.00
1	A	536	ARG	NE-CZ-NH2	6.89	123.74	120.30
1	D	554	LEU	CB-CG-CD2	6.82	122.59	111.00
1	B	370	VAL	CG1-CB-CG2	6.77	121.74	110.90
1	B	552	LEU	CA-CB-CG	6.71	130.73	115.30
1	C	471	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	D	598	VAL	CA-CB-CG2	6.54	120.71	110.90
1	A	552	LEU	CB-CG-CD1	6.53	122.10	111.00
1	B	299	LYS	CD-CE-NZ	-6.44	96.90	111.70
1	B	643	ASP	CB-CG-OD1	6.39	124.06	118.30
1	A	144	LEU	CB-CG-CD1	-6.39	100.13	111.00
1	C	213	LYS	CD-CE-NZ	-6.38	97.03	111.70
1	B	377	ARG	NE-CZ-NH1	-6.35	117.13	120.30
1	D	590	LEU	CB-CG-CD2	-6.35	100.21	111.00
1	A	165	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	D	598	VAL	CG1-CB-CG2	6.33	121.03	110.90
1	B	197	ASP	CB-CG-OD1	-6.30	112.63	118.30
1	C	159	ILE	CB-CG1-CD1	-6.25	96.39	113.90
1	B	213	LYS	CD-CE-NZ	-6.17	97.51	111.70
1	C	660	LEU	CB-CG-CD1	6.17	121.49	111.00
1	C	37	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	D	100	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	C	552	LEU	CB-CG-CD1	-6.09	100.65	111.00
1	A	72	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	A	419	GLN	CB-CA-C	6.07	122.55	110.40
1	D	582	LEU	CB-CG-CD1	6.03	121.25	111.00
1	D	419	GLN	CB-CA-C	5.89	122.18	110.40
1	B	111	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	C	552	LEU	CB-CG-CD2	5.78	120.83	111.00
1	C	377	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	C	130	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	B	571	LEU	CA-CB-CG	5.75	128.51	115.30
1	D	597	ASP	CB-CG-OD1	5.72	123.45	118.30
1	D	445	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	C	72	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	C	61	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	A	181	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	595	ASP	CB-CG-OD1	5.58	123.33	118.30
1	D	96	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	C	130	ARG	NE-CZ-NH2	-5.55	117.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	29	LEU	CB-CA-C	5.52	120.69	110.20
1	C	660	LEU	CB-CG-CD2	5.52	120.38	111.00
1	D	401	ASP	CB-CG-OD2	5.45	123.21	118.30
1	C	290	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	D	471	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	A	479	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	B	419	GLN	CB-CA-C	5.35	121.10	110.40
1	C	744	ARG	NE-CZ-NH2	-5.35	117.63	120.30
1	D	740	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	A	290	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	259	ASP	CB-CG-OD1	-5.34	113.50	118.30
1	A	597	ASP	CB-CG-OD2	5.34	123.10	118.30
1	B	601	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	597	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	373	MET	CG-SD-CE	5.30	108.69	100.20
1	D	643	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	372	LYS	CD-CE-NZ	-5.29	99.54	111.70
1	A	710	ILE	O-C-N	5.25	131.10	122.70
1	A	377	ARG	CG-CD-NE	-5.23	100.81	111.80
1	C	531	LEU	CB-CG-CD1	5.22	119.88	111.00
1	A	711	ALA	N-CA-C	5.21	125.06	111.00
1	A	111	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	643	ASP	CB-CG-OD1	5.18	122.96	118.30
1	D	181	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	710	ILE	N-CA-C	5.17	124.96	111.00
1	A	449[A]	HIS	CB-CA-C	5.17	120.73	110.40
1	A	449[B]	HIS	CB-CA-C	5.17	120.73	110.40
1	B	196	PHE	CB-CG-CD2	-5.15	117.19	120.80
1	C	420	ILE	CG1-CB-CG2	-5.13	100.12	111.40
1	B	33	ASP	CB-CG-OD1	5.12	122.91	118.30
1	B	636	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	C	422	ARG	NE-CZ-NH1	-5.09	117.76	120.30
1	C	70	ASP	CB-CG-OD1	-5.07	113.74	118.30
1	B	321	GLU	CG-CD-OE2	-5.04	108.23	118.30
1	D	552	LEU	CB-CG-CD2	5.03	119.55	111.00
1	C	189	PHE	CB-CG-CD2	-5.03	117.28	120.80
1	B	198	LEU	CB-CG-CD2	-5.03	102.46	111.00
1	B	370	VAL	CA-CB-CG1	5.01	118.42	110.90

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 (i)

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	49	0
1	B	5746	0	5577	46	0
1	C	5745	0	5573	52	0
1	D	5746	0	5577	41	0
2	A	43	0	30	2	0
2	B	43	0	30	1	0
2	C	43	0	30	2	0
2	D	43	0	30	1	0
3	A	768	0	0	6	0
3	B	643	0	0	9	0
3	C	693	0	0	21	0
3	D	730	0	0	10	0
All	All	25988	0	22419	177	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 (177) 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:C:449[A]:HIS:CE1	3:C:3266:HOH:O	1.71	1.31
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:A:449[A]:HIS:CE1	3:A:3268:HOH:O	1.68	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:449[A]:HIS:NE2	3:A:3268:HOH:O	1.95	0.68
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:C:533:LYS:NZ	3:C:2231:HOH:O	2.28	0.67
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: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:B:330:ASP:OD1	1:B:629:HIS:HE1	1.83	0.61
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.04	0.61
1:D:392:HIS:ND1	1:D:415:TYR:CG	2.63	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ILE:HD12	2:A:760:HEM:HMB1	1.84	0.59
1:D:392:HIS:CE1	1:D:415:TYR:CB	2.55	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: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:C:449[A]:HIS:NE2	3:C:3266:HOH:O	2.07	0.50
1:B:392:HIS:ND1	1:B:415:TYR:CG	2.69	0.50
1:A:710:ILE:HG12	1:A:715:GLU:CD	2.31	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:158:LYS:NZ	3:D:2950:HOH:O	2.35	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: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: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
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
2:A:760:HEM:HMB1	2:A:760:HEM:HBB2	2.00	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:C:521:ARG:NH1	1:C:521:ARG:HG2	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:461:GLU:HA	1:B:462:PRO:C	2.38	0.43
1:D:509:ARG:HD2	1:D:576:PRO:HD2	2.00	0.43
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:A:62:ASN:OD1	1:A:62:ASN:C	2.58	0.41
1:A:213:LYS:HB3	1:A:213:LYS:HE3	1.81	0.41
1:B:313:ARG:NH2	1:C:309:LYS:HD2	2.34	0.41
1:C:488:ARG:HG3	1:C:489:VAL:N	2.35	0.41
1:C:416:THR:CG2	3:C:3270:HOH:O	2.67	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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	41	21
1	B	724/753 (96%)	701 (97%)	21 (3%)	2 (0%)	41	21
1	C	724/753 (96%)	703 (97%)	19 (3%)	2 (0%)	41	21
1	D	724/753 (96%)	707 (98%)	16 (2%)	1 (0%)	51	28
All	All	2896/3012 (96%)	2817 (97%)	72 (2%)	7 (0%)	47	26

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 (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	611/635 (96%)	590 (97%)	21 (3%)	37 12
1	B	611/635 (96%)	584 (96%)	27 (4%)	28 7
1	C	611/635 (96%)	573 (94%)	38 (6%)	18 3
1	D	611/635 (96%)	589 (96%)	22 (4%)	35 11
All	All	2444/2540 (96%)	2336 (96%)	108 (4%)	28 7

All (108) 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	185	PHE
1	A	191	THR
1	A	205	ILE
1	A	213	LYS
1	A	227	TRP
1	A	237	ASP
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	710	ILE
1	A	712	ASP
1	A	732	LEU
1	A	750	LYS
1	B	185	PHE
1	B	191	THR
1	B	205	ILE
1	B	227	TRP
1	B	237	ASP
1	B	252	ASN
1	B	283	GLU

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Mol	Chain	Res	Type
1	B	321	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	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	594	PRO
1	B	595	ASP
1	B	612	ARG
1	B	616	LEU
1	B	633	LEU
1	B	703	LYS
1	B	713	GLN
1	B	732	LEU
1	C	37	ARG
1	C	61	ARG
1	C	159	ILE
1	C	185	PHE
1	C	191	THR
1	C	198	LEU
1	C	205	ILE
1	C	227	TRP
1	C	237	ASP
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

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Mol	Chain	Res	Type
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	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	48	GLN
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	227	TRP
1	D	237	ASP
1	D	252	ASN
1	D	340	LEU
1	D	432	PRO
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	598	VAL
1	D	616	LEU
1	D	648	LEU
1	D	713	GLN
1	D	725	ASP
1	D	747	LYS
1	D	751	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) 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	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	556	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	556	GLN
1	D	629	HIS
1	D	671	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	7,8,9	0.70	0	6,11,13	2.21	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	OCS	B	669	1	7,8,9	1.06	0	6,11,13	1.44	1 (16%)
1	OCS	C	669	1	7,8,9	0.80	0	6,11,13	2.42	2 (33%)
1	OCS	D	669	1	7,8,9	0.94	0	6,11,13	1.39	1 (16%)

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	-	4/4/7/9	-
1	OCS	B	669	1	-	1/4/7/9	-
1	OCS	C	669	1	-	3/4/7/9	-
1	OCS	D	669	1	-	1/4/7/9	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	669	OCS	OD1-SG-CB	4.65	112.47	106.94
1	C	669	OCS	OD3-SG-CB	4.52	112.31	106.94
1	C	669	OCS	OD1-SG-CB	-3.43	102.86	106.94
1	B	669	OCS	OD3-SG-CB	-3.25	103.08	106.94
1	D	669	OCS	OD2-SG-OD3	2.24	116.75	111.27

There are no chirality outliers.

All (9) 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	A	669	OCS	CA-CB-SG-OD2
1	C	669	OCS	CA-CB-SG-OD2
1	C	669	OCS	CA-CB-SG-OD3

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 monosaccharides 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	41,50,50	1.60	10 (24%)	45,82,82	2.44	17 (37%)
2	HEM	B	760	1	41,50,50	1.78	9 (21%)	45,82,82	2.29	18 (40%)
2	HEM	A	760	1	41,50,50	1.73	9 (21%)	45,82,82	2.39	20 (44%)
2	HEM	D	760	1	41,50,50	1.77	10 (24%)	45,82,82	2.35	19 (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
2	HEM	C	760	1	-	2/12/54/54	-
2	HEM	B	760	1	-	2/12/54/54	-
2	HEM	A	760	1	-	2/12/54/54	-
2	HEM	D	760	1	-	2/12/54/54	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HEM	C3D-C2D	5.60	1.48	1.36
2	D	760	HEM	C3D-C2D	5.56	1.48	1.36
2	B	760	HEM	C3D-C2D	4.74	1.46	1.36
2	B	760	HEM	C3C-C2C	-4.34	1.34	1.40
2	C	760	HEM	C3D-C2D	4.15	1.45	1.36
2	A	760	HEM	C3C-C2C	-3.74	1.35	1.40
2	B	760	HEM	CHA-C4D	3.41	1.43	1.35
2	A	760	HEM	CMB-C2B	3.41	1.58	1.50
2	D	760	HEM	CAB-C3B	3.40	1.56	1.47
2	C	760	HEM	C3C-CAC	3.38	1.54	1.47
2	D	760	HEM	CMC-C2C	3.10	1.59	1.51
2	D	760	HEM	FE-ND	2.97	2.11	1.96
2	A	760	HEM	CMC-C2C	2.94	1.58	1.51
2	D	760	HEM	FE-NB	2.75	2.10	1.96
2	D	760	HEM	C1A-NA	2.71	1.41	1.36
2	C	760	HEM	CAA-C2A	2.69	1.56	1.52
2	A	760	HEM	C1A-NA	2.65	1.41	1.36
2	B	760	HEM	FE-NB	2.62	2.09	1.96
2	C	760	HEM	O2A-CGA	-2.61	1.22	1.30
2	A	760	HEM	CHA-C4D	2.57	1.41	1.35
2	C	760	HEM	FE-ND	2.47	2.09	1.96
2	B	760	HEM	CMB-C2B	2.47	1.56	1.50
2	C	760	HEM	C1A-NA	2.46	1.41	1.36
2	D	760	HEM	CBA-CGA	2.45	1.56	1.50
2	B	760	HEM	CAA-C2A	2.44	1.55	1.52
2	B	760	HEM	C1B-NB	-2.41	1.36	1.40
2	B	760	HEM	CAB-C3B	2.34	1.53	1.47
2	B	760	HEM	C3C-CAC	2.34	1.52	1.47
2	A	760	HEM	C3C-CAC	2.30	1.52	1.47
2	A	760	HEM	O2A-CGA	-2.28	1.23	1.30
2	C	760	HEM	FE-NB	2.25	2.08	1.96
2	C	760	HEM	CBD-CAD	2.21	1.59	1.52
2	C	760	HEM	CMA-C3A	2.15	1.56	1.51
2	D	760	HEM	O1A-CGA	2.10	1.29	1.22
2	A	760	HEM	C1B-C2B	2.06	1.48	1.44
2	C	760	HEM	CAB-C3B	2.06	1.53	1.47
2	D	760	HEM	C3C-C2C	-2.03	1.37	1.40
2	D	760	HEM	CHA-C4D	2.00	1.40	1.35

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	760	HEM	CBD-CAD-C3D	-7.07	92.98	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	760	HEM	CBD-CAD-C3D	-7.06	93.00	112.63
2	D	760	HEM	CBD-CAD-C3D	-6.59	94.33	112.63
2	C	760	HEM	C1B-NB-C4B	6.16	111.43	105.07
2	B	760	HEM	CBD-CAD-C3D	-5.62	97.01	112.63
2	B	760	HEM	C1B-NB-C4B	5.05	110.29	105.07
2	A	760	HEM	C4B-C3B-C2B	4.98	111.07	107.11
2	C	760	HEM	C2B-C1B-NB	-4.70	104.27	109.84
2	D	760	HEM	C1B-NB-C4B	4.66	109.89	105.07
2	A	760	HEM	C2C-C3C-C4C	4.60	110.11	106.90
2	D	760	HEM	C4D-ND-C1D	4.30	109.52	105.07
2	B	760	HEM	CHA-C4D-ND	4.20	129.57	124.38
2	C	760	HEM	CHB-C1B-NB	4.16	129.52	124.38
2	B	760	HEM	C2C-C3C-C4C	4.08	109.75	106.90
2	B	760	HEM	C4D-ND-C1D	4.01	109.22	105.07
2	C	760	HEM	CMA-C3A-C4A	-3.88	122.50	128.46
2	D	760	HEM	CMD-C2D-C1D	3.88	130.94	125.04
2	B	760	HEM	O2D-CGD-O1D	-3.80	113.83	123.30
2	B	760	HEM	O2D-CGD-CBD	3.70	125.93	114.03
2	D	760	HEM	CMA-C3A-C4A	-3.68	122.81	128.46
2	A	760	HEM	CMA-C3A-C4A	-3.57	122.97	128.46
2	D	760	HEM	O2D-CGD-CBD	3.53	125.36	114.03
2	D	760	HEM	CAA-CBA-CGA	-3.48	104.01	113.76
2	A	760	HEM	O2D-CGD-O1D	-3.46	114.68	123.30
2	A	760	HEM	C1D-C2D-C3D	-3.42	103.37	106.96
2	A	760	HEM	CAD-CBD-CGD	-3.35	106.40	113.60
2	A	760	HEM	CAA-CBA-CGA	-3.33	104.41	113.76
2	C	760	HEM	C4A-C3A-C2A	3.33	109.31	107.00
2	D	760	HEM	C3B-C2B-C1B	3.31	108.94	106.49
2	C	760	HEM	C4B-C3B-C2B	3.31	109.74	107.11
2	D	760	HEM	O2D-CGD-O1D	-3.29	115.11	123.30
2	B	760	HEM	CAA-CBA-CGA	-3.22	104.74	113.76
2	C	760	HEM	CAA-CBA-CGA	-3.21	104.76	113.76
2	C	760	HEM	C2C-C3C-C4C	3.21	109.14	106.90
2	C	760	HEM	C4D-ND-C1D	3.19	108.37	105.07
2	D	760	HEM	C2B-C1B-NB	-3.18	106.06	109.84
2	A	760	HEM	O2D-CGD-CBD	3.10	123.98	114.03
2	D	760	HEM	O1A-CGA-CBA	-3.05	113.28	123.08
2	A	760	HEM	CHB-C1B-NB	3.02	128.11	124.38
2	A	760	HEM	C2D-C1D-ND	2.92	113.38	109.88
2	C	760	HEM	CAD-CBD-CGD	-2.86	107.44	113.60
2	B	760	HEM	CAD-CBD-CGD	-2.83	107.52	113.60
2	D	760	HEM	CAD-CBD-CGD	-2.81	107.56	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	760	HEM	C3D-C4D-ND	-2.78	107.07	110.17
2	B	760	HEM	C4B-C3B-C2B	2.73	109.28	107.11
2	D	760	HEM	C1D-C2D-C3D	-2.70	104.11	106.96
2	B	760	HEM	C3C-C4C-NC	-2.67	105.90	110.94
2	D	760	HEM	CHB-C1B-NB	2.62	127.61	124.38
2	A	760	HEM	CHD-C1D-C2D	-2.61	120.91	124.98
2	A	760	HEM	C1B-NB-C4B	2.58	107.74	105.07
2	B	760	HEM	C2B-C1B-NB	-2.58	106.79	109.84
2	C	760	HEM	O2D-CGD-CBD	2.57	122.29	114.03
2	D	760	HEM	CHD-C1D-ND	2.51	127.16	124.43
2	D	760	HEM	C4B-CHC-C1C	2.50	125.86	122.56
2	A	760	HEM	CMC-C2C-C3C	2.42	129.21	124.68
2	C	760	HEM	C3B-C2B-C1B	2.42	108.28	106.49
2	A	760	HEM	CHC-C4B-NB	2.40	127.03	124.43
2	B	760	HEM	CMA-C3A-C4A	-2.39	124.79	128.46
2	A	760	HEM	C3B-C2B-C1B	-2.38	104.72	106.49
2	D	760	HEM	CMB-C2B-C1B	-2.38	121.41	125.04
2	D	760	HEM	CHC-C4B-C3B	2.38	128.21	124.57
2	A	760	HEM	CMD-C2D-C1D	2.32	128.57	125.04
2	B	760	HEM	C4B-CHC-C1C	2.30	125.59	122.56
2	B	760	HEM	C1D-C2D-C3D	-2.30	104.54	106.96
2	D	760	HEM	CMA-C3A-C2A	2.28	129.23	124.94
2	A	760	HEM	O1A-CGA-CBA	-2.25	115.86	123.08
2	A	760	HEM	C3C-C4C-NC	-2.23	106.74	110.94
2	B	760	HEM	CHB-C1B-NB	2.22	127.13	124.38
2	C	760	HEM	C3C-C4C-NC	-2.20	106.78	110.94
2	C	760	HEM	C4C-CHD-C1D	2.18	125.43	122.56
2	B	760	HEM	CHC-C4B-C3B	2.16	127.88	124.57
2	C	760	HEM	CHC-C4B-NB	2.16	126.78	124.43
2	C	760	HEM	CMC-C2C-C3C	2.15	128.71	124.68
2	A	760	HEM	C4A-C3A-C2A	2.09	108.45	107.00

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

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

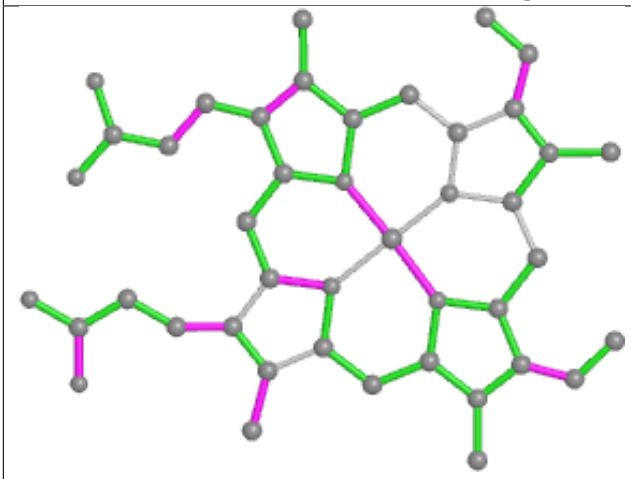
There are no ring outliers.

4 monomers are involved in 6 short contacts:

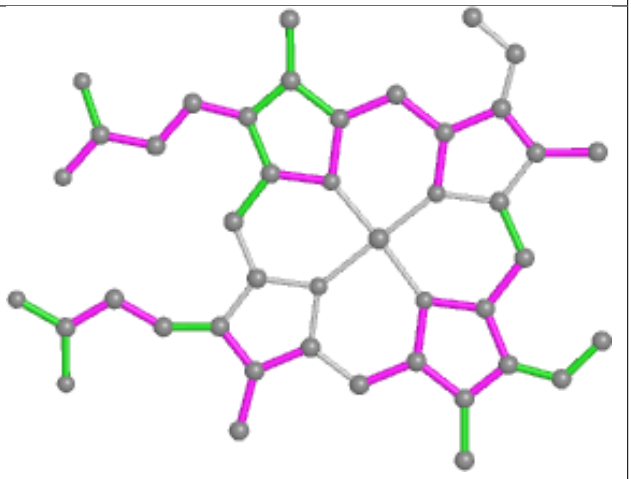
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	760	HEM	2	0
2	B	760	HEM	1	0
2	A	760	HEM	2	0
2	D	760	HEM	1	0

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 then 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.

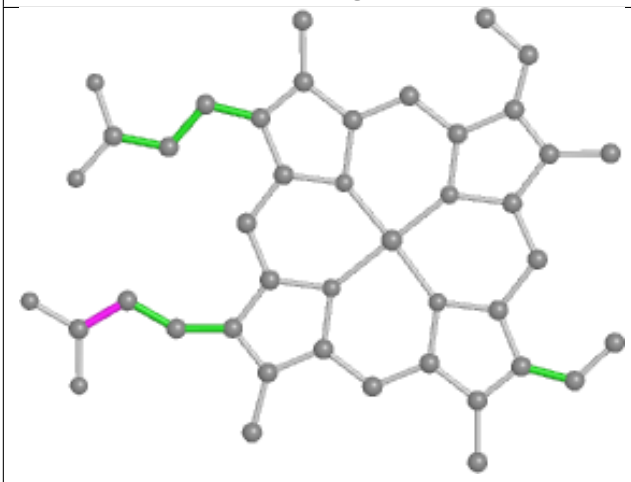
Ligand HEM C 760



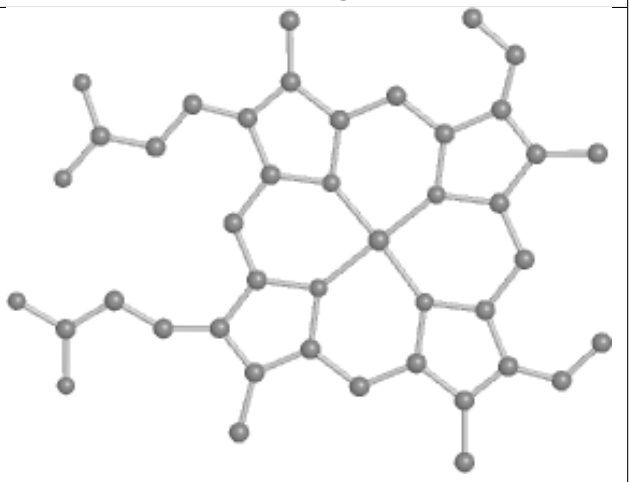
Bond lengths



Bond angles

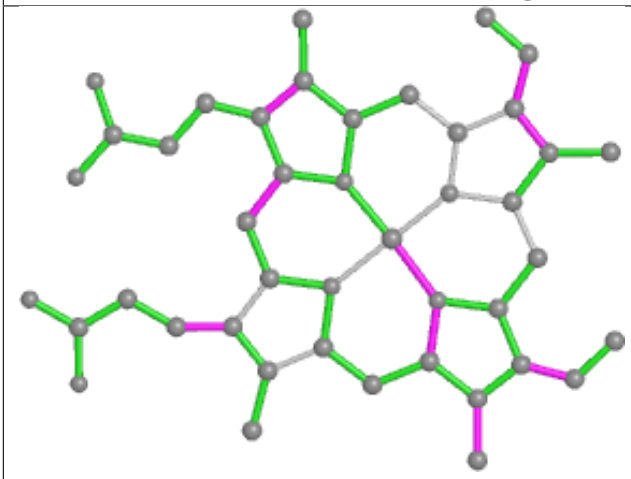


Torsions

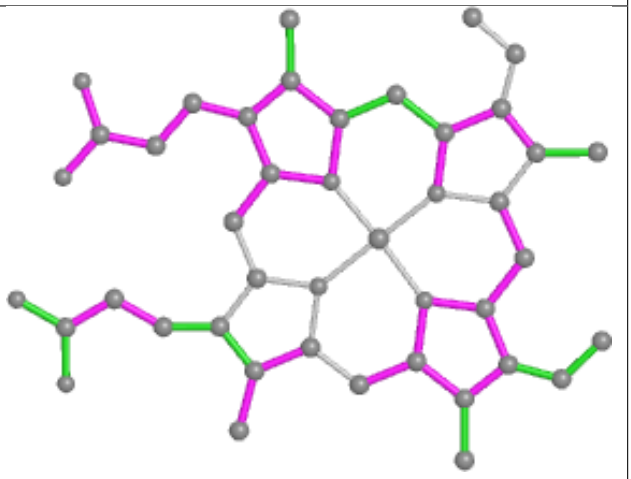


Rings

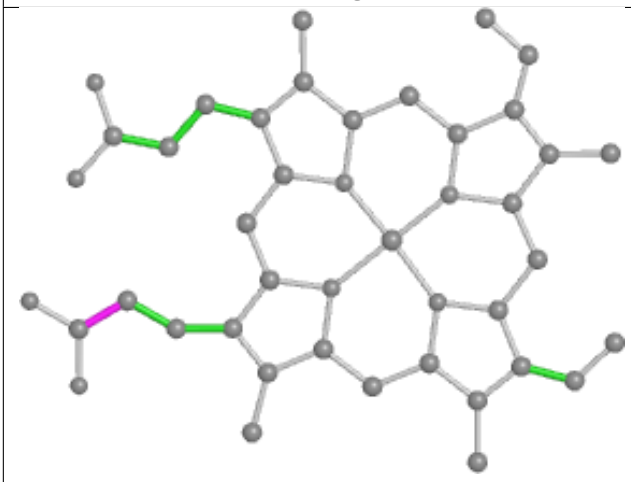
Ligand HEM B 760



Bond lengths



Bond angles



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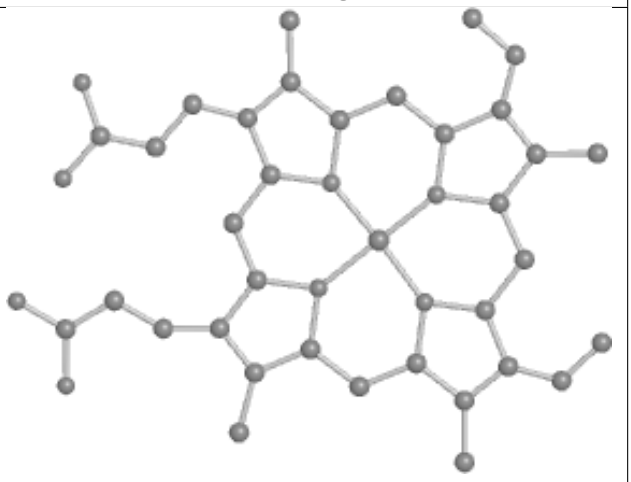
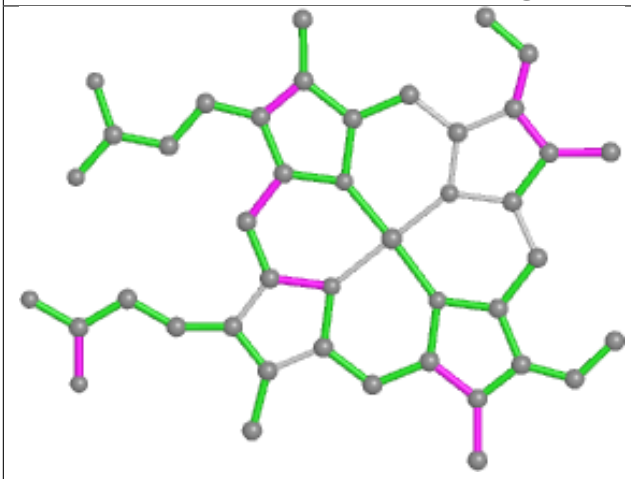
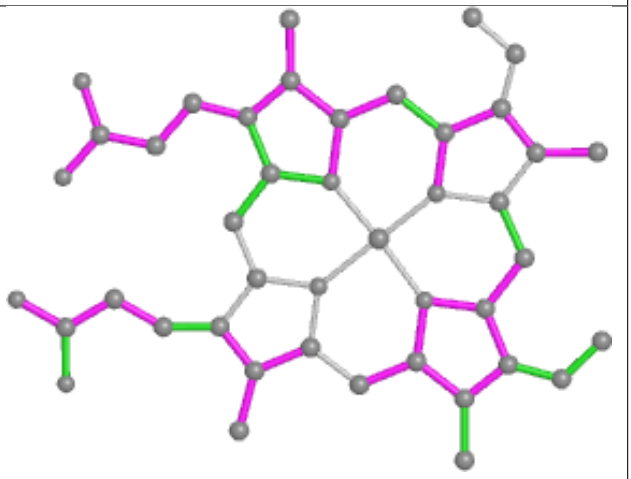


Rings

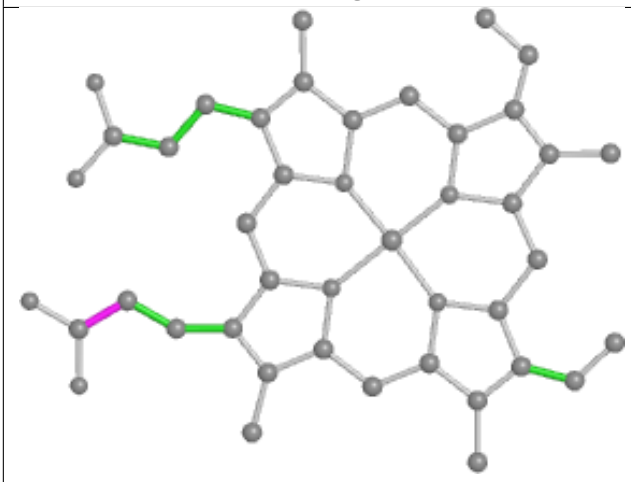
Ligand HEM A 760



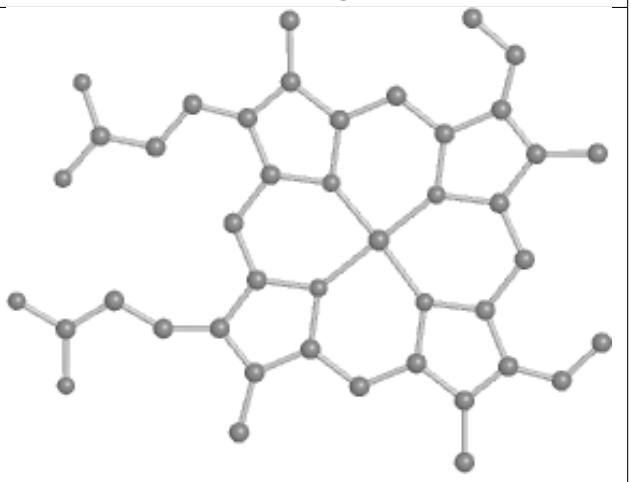
Bond lengths



Bond angles

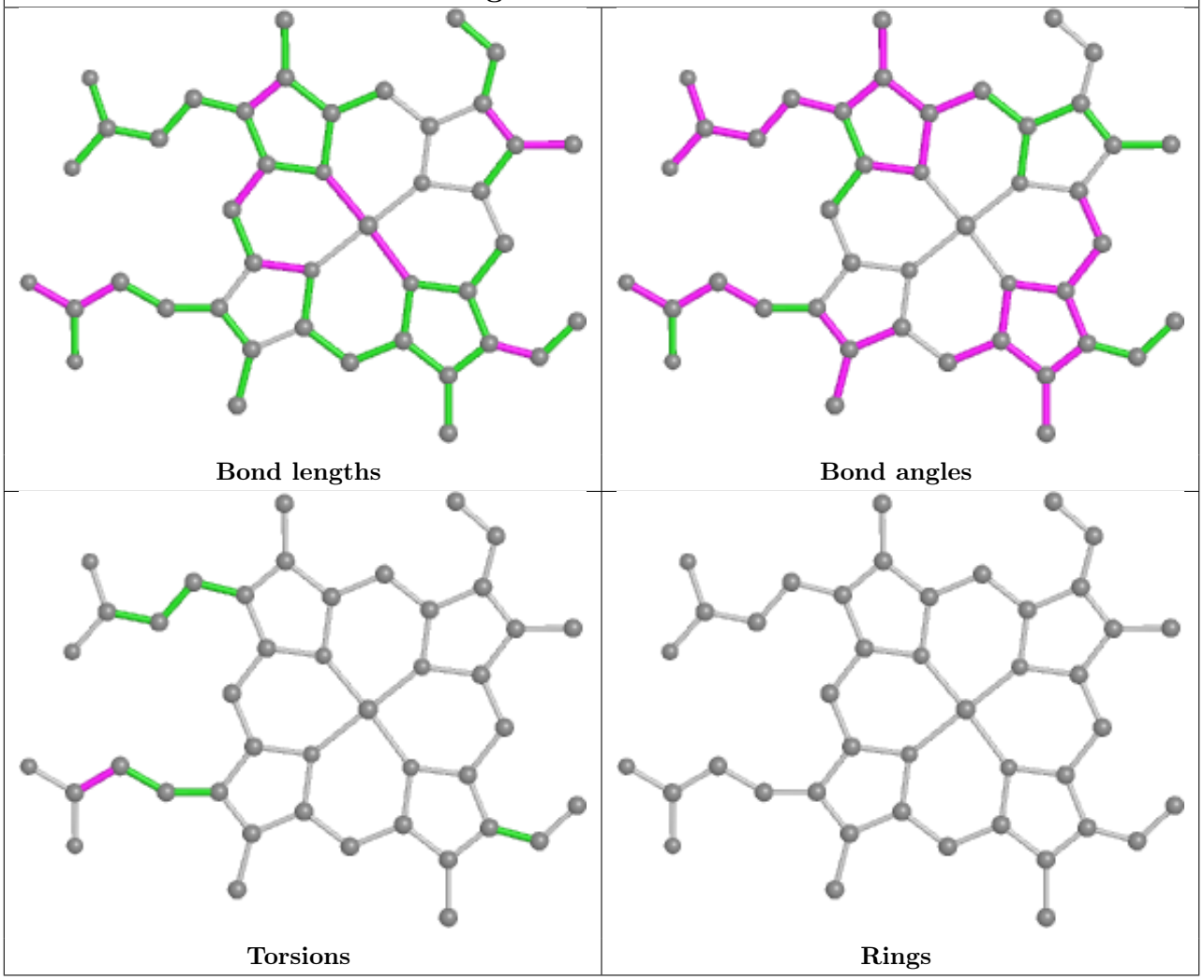


Torsions



Rings

Ligand HEM D 760



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, 95^{th} 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%)	-0.42	7 (0%)	82	82	7, 13, 28, 45	1 (0%)
1	B	725/753 (96%)	-0.31	21 (2%)	51	48	8, 15, 33, 48	1 (0%)
1	C	725/753 (96%)	-0.29	22 (3%)	50	47	8, 15, 34, 48	1 (0%)
1	D	725/753 (96%)	-0.39	7 (0%)	82	82	7, 13, 30, 47	1 (0%)
All	All	2900/3012 (96%)	-0.35	57 (1%)	65	63	7, 14, 31, 48	4 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	710	ILE	6.7
1	B	726	GLY	5.3
1	D	28	SER	4.3
1	C	711	ALA	3.9
1	B	713	GLN	3.8
1	D	713	GLN	3.7
1	C	647	VAL	3.7
1	C	712	ASP	3.5
1	C	726	GLY	3.5
1	B	750	LYS	3.4
1	B	32	GLU	3.4
1	D	750	LYS	3.2
1	B	712	ASP	3.1
1	D	712	ASP	3.1
1	C	642	ALA	3.1
1	C	750	LYS	3.1
1	B	749	ASP	3.1
1	C	646	THR	3.1
1	D	749	ASP	3.1
1	C	713	GLN	3.1
1	B	647	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	726	GLY	3.0
1	B	28	SER	3.0
1	B	646	THR	2.9
1	C	714	GLY	2.9
1	C	725	ASP	2.8
1	B	677	ASP	2.8
1	B	552	LEU	2.7
1	C	641	THR	2.7
1	A	32	GLU	2.7
1	B	596	GLY	2.7
1	A	28	SER	2.6
1	B	725	ASP	2.6
1	B	711	ALA	2.6
1	C	32	GLU	2.6
1	C	583	LYS	2.6
1	B	583	LYS	2.5
1	A	750	LYS	2.4
1	A	713	GLN	2.4
1	C	568	ASP	2.4
1	D	32	GLU	2.3
1	B	572	ASN	2.3
1	C	569	ASP	2.3
1	D	711	ALA	2.3
1	C	677	ASP	2.3
1	C	751	ILE	2.2
1	B	645	GLY	2.2
1	B	568	ASP	2.2
1	B	727	SER	2.2
1	C	594	PRO	2.1
1	B	612	ARG	2.1
1	C	710	ILE	2.1
1	B	710	ILE	2.1
1	C	644	ASP	2.1
1	A	712	ASP	2.1
1	C	722	ASP	2.0
1	C	572	ASN	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, 95^{th} 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	A	669	9/10	0.96	0.10	19,21,26,29	0
1	OCS	B	669	9/10	0.96	0.11	26,27,33,33	0
1	OCS	C	669	9/10	0.96	0.14	28,29,32,34	0
1	OCS	D	669	9/10	0.96	0.10	22,23,27,29	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

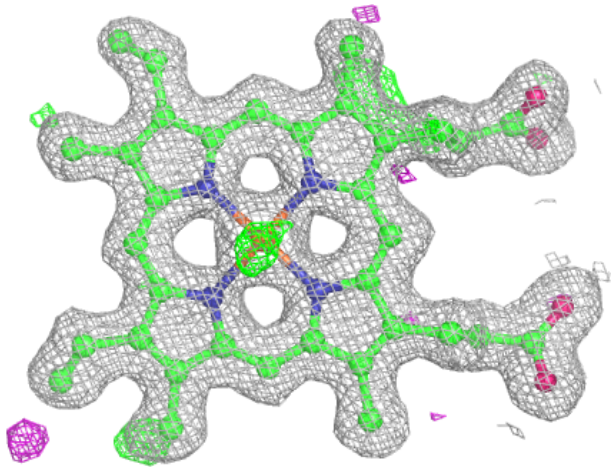
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

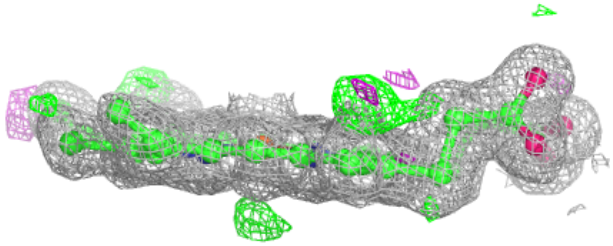
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	HEM	B	760	43/43	0.98	0.07	7,11,16,23	0
2	HEM	C	760	43/43	0.98	0.08	8,11,20,21	0
2	HEM	D	760	43/43	0.98	0.07	5,10,17,21	0
2	HEM	A	760	43/43	0.99	0.07	6,9,14,18	0

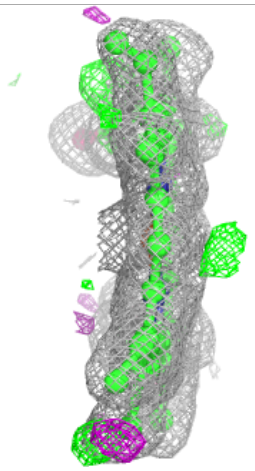
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HEM 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)

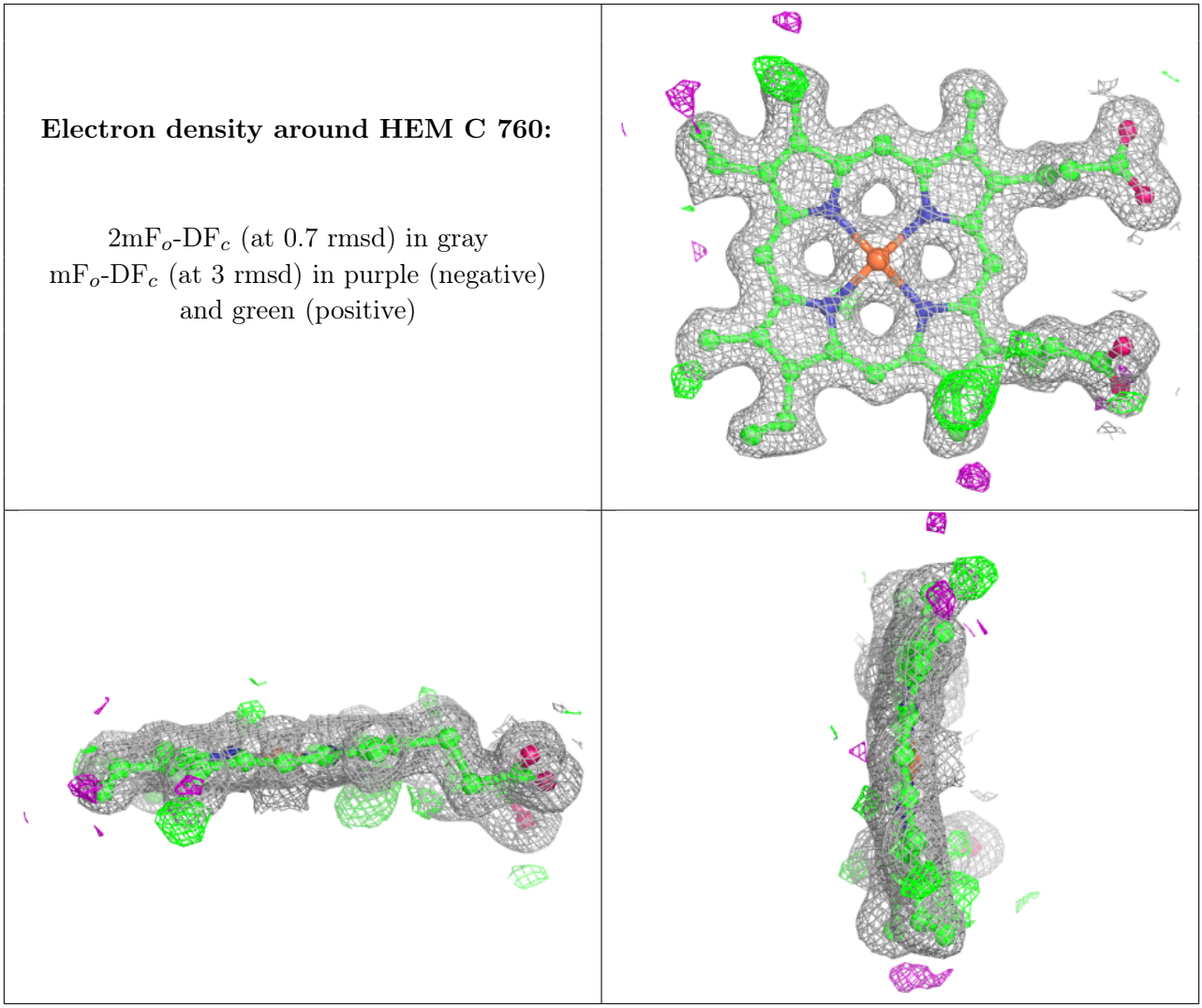






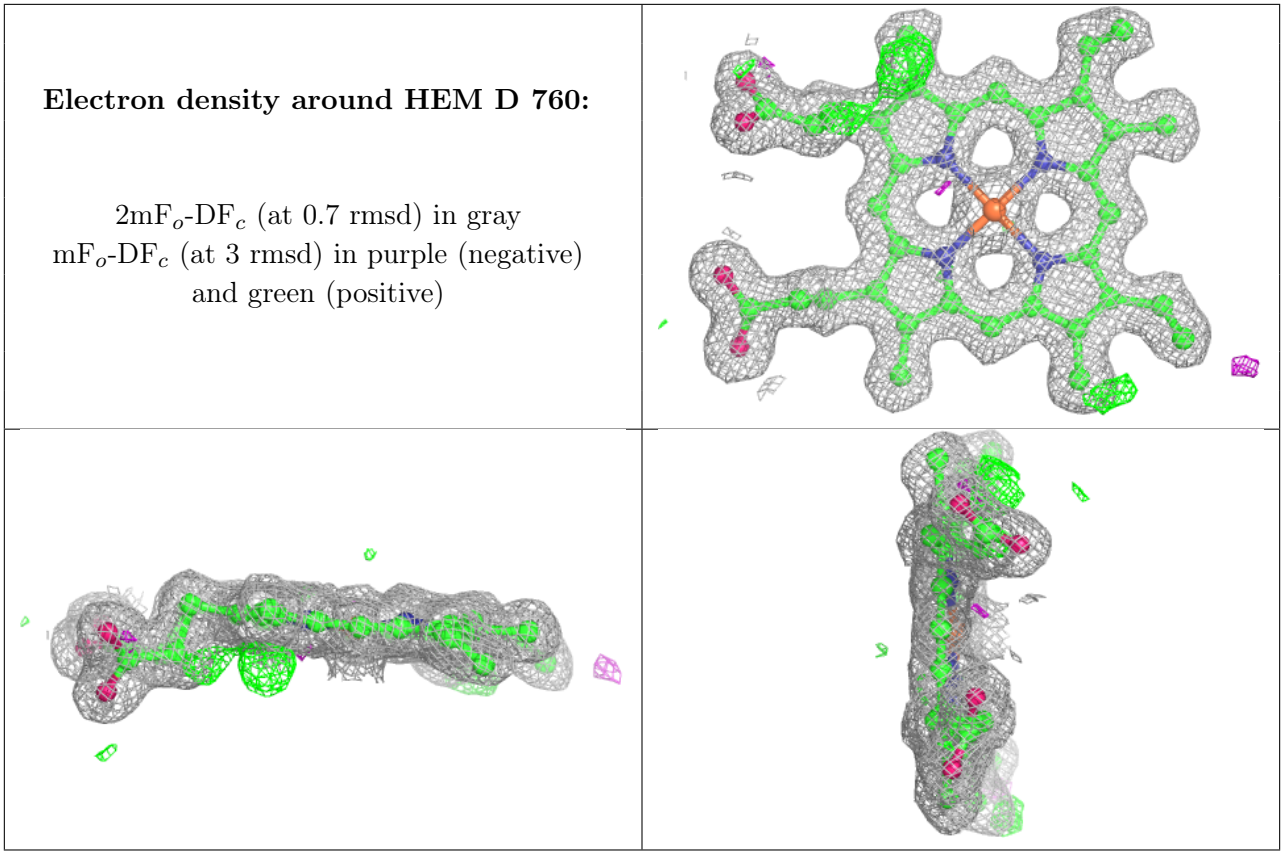
Electron density around HEM C 760:

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



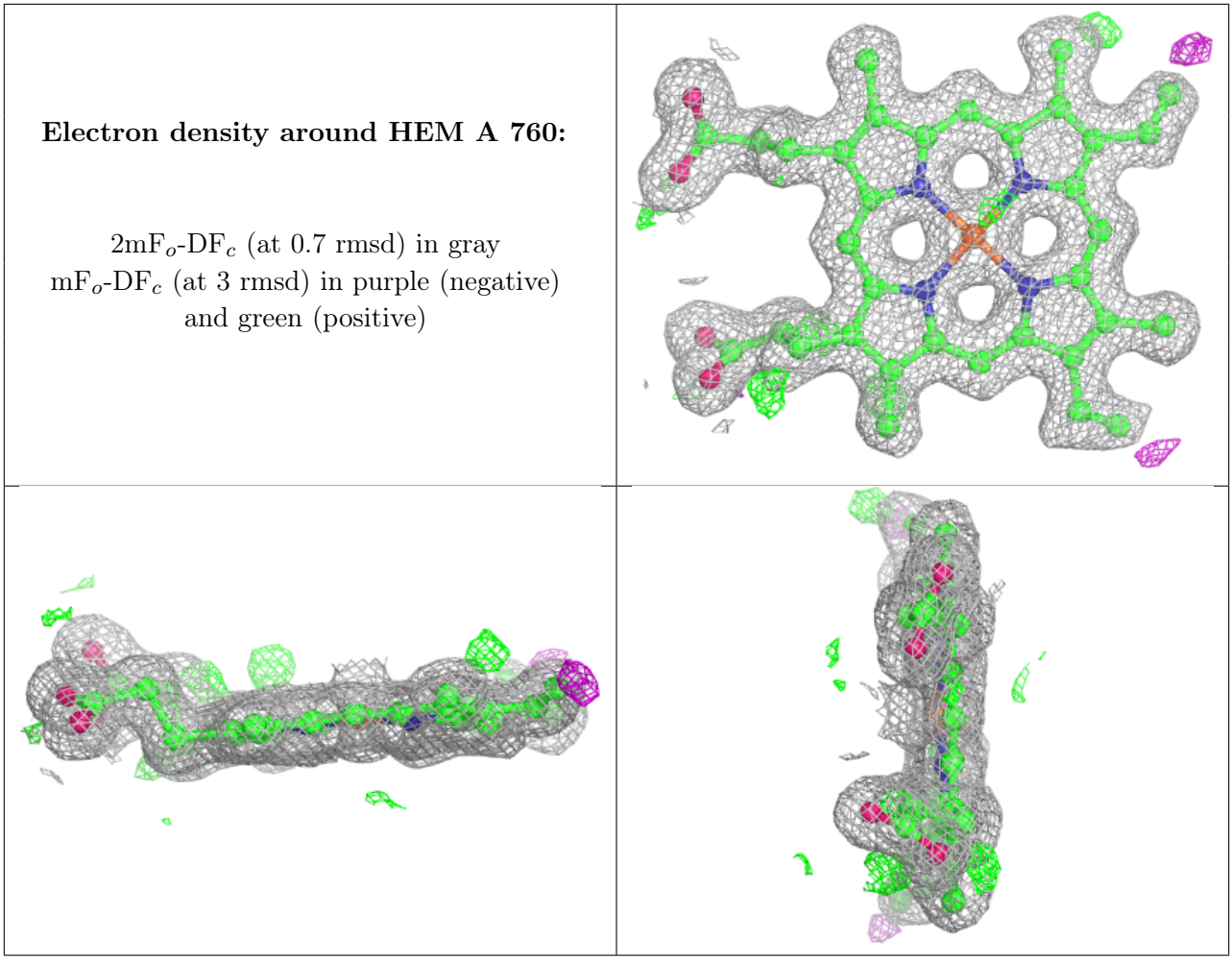
Electron density around HEM D 760:

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



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)



6.5 Other polymers (i)

There are no such residues in this entry.