Full wwPDB X-ray Structure Validation Report (i)

Mar 12, 2026 – 12:43 PM UTC

PDB ID	:	4ENS / pdb_00004ens
Title	:	Structure of E530Q variant of E. coli KatE
Authors	:	Loewen, P.C.; Jha, V.
Deposited on	:	2012-04-13
Resolution	:	1.60 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 (i) 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 (i)) were used in the production of this report:

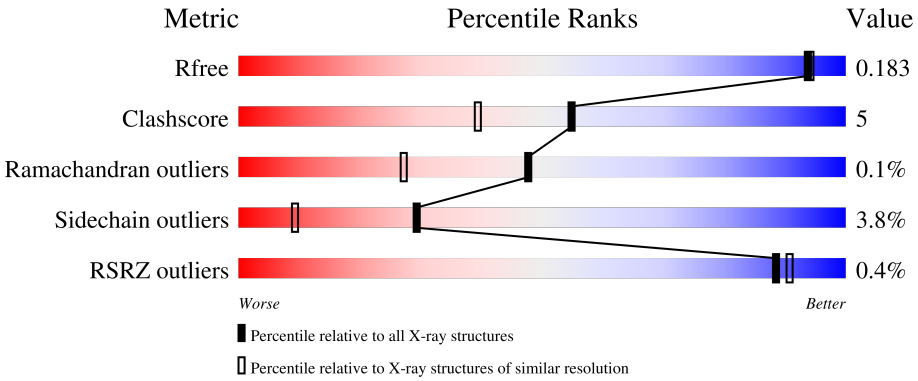
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal 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 (i)

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

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	83% 13% • •
1	B	753	82% 12% • •
1	C	753	81% 13% • •
1	D	753	% 81% 14% • •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 26323 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.

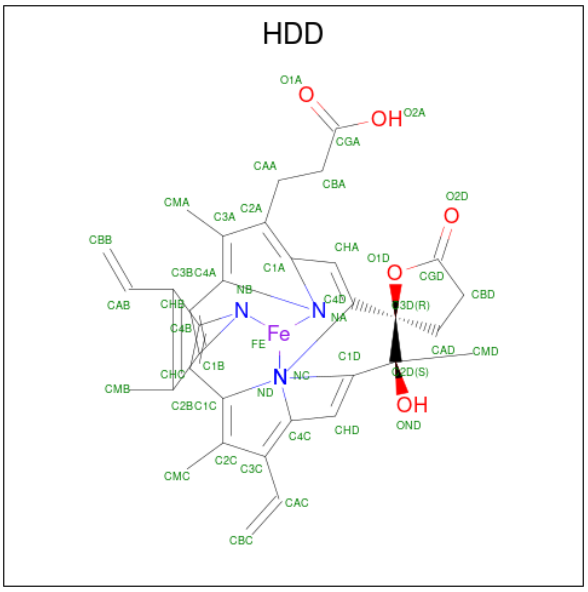
- Molecule 1 is a protein called Catalase HPII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	4	0
			5755	3655	1007	1081	12			
1	B	726	Total	C	N	O	S	0	4	0
			5758	3658	1008	1080	12			
1	C	726	Total	C	N	O	S	0	3	0
			5756	3658	1008	1078	12			
1	D	726	Total	C	N	O	S	0	4	0
			5758	3657	1008	1081	12			

There are 4 discrepancies between the modelled and reference sequences:

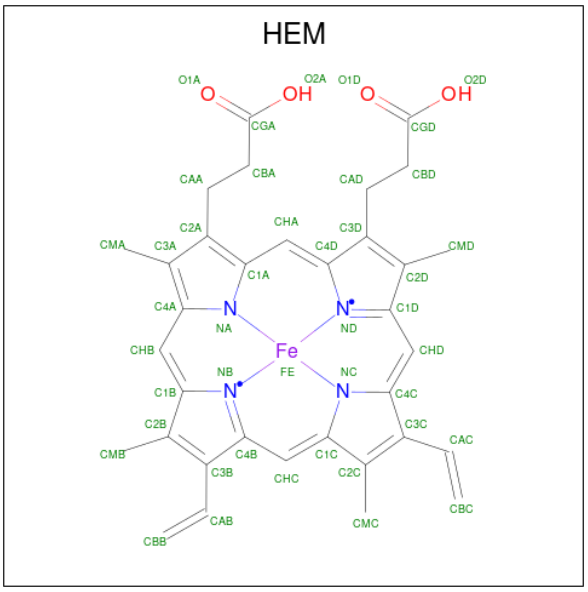
Chain	Residue	Modelled	Actual	Comment	Reference
A	530	GLN	GLU	engineered mutation	UNP P21179
B	530	GLN	GLU	engineered mutation	UNP P21179
C	530	GLN	GLU	engineered mutation	UNP P21179
D	530	GLN	GLU	engineered mutation	UNP P21179

- Molecule 2 is CIS-HEME D HYDROXYCHLORIN GAMMA-SPIROLACTONE (CCD ID: HDD) (formula: $C_{34}H_{32}FeN_4O_5$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	B	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	C	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		
2	D	1	Total	C	Fe	N	O	0	1
			44	34	1	4	5		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 4 is water.

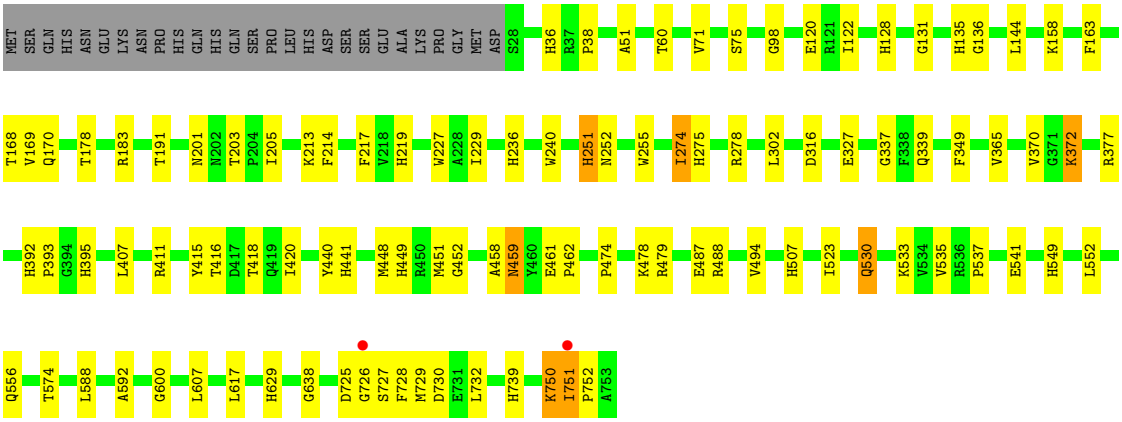
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	769	Total	O	0	0
			769	769		
4	B	696	Total	O	0	0
			696	696		
4	C	709	Total	O	0	0
			709	709		
4	D	774	Total	O	0	0
			774	774		

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.

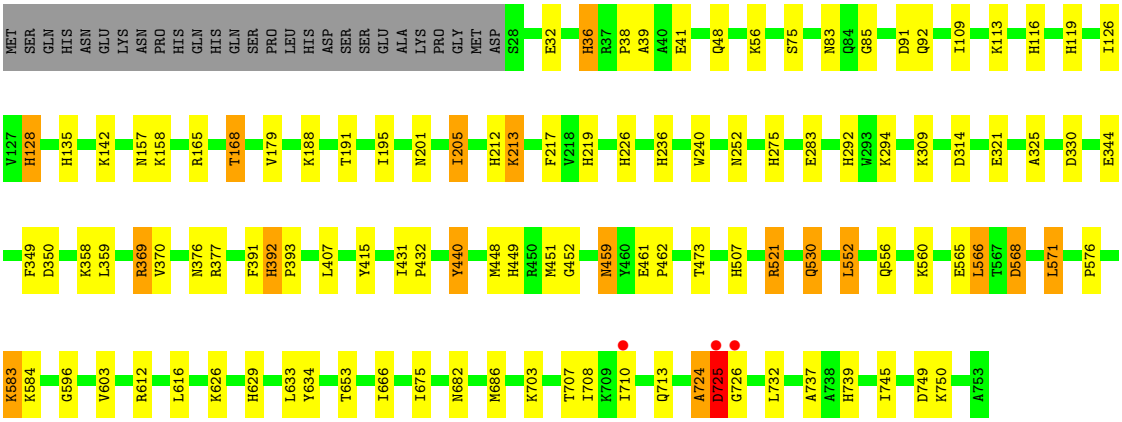
• Molecule 1: Catalase HPII

Chain A:



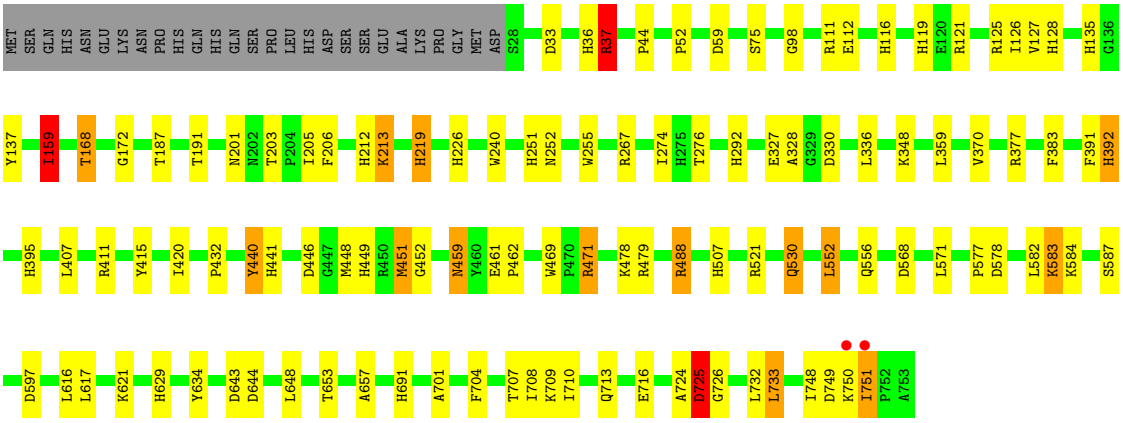
• Molecule 1: Catalase HPII

Chain B:



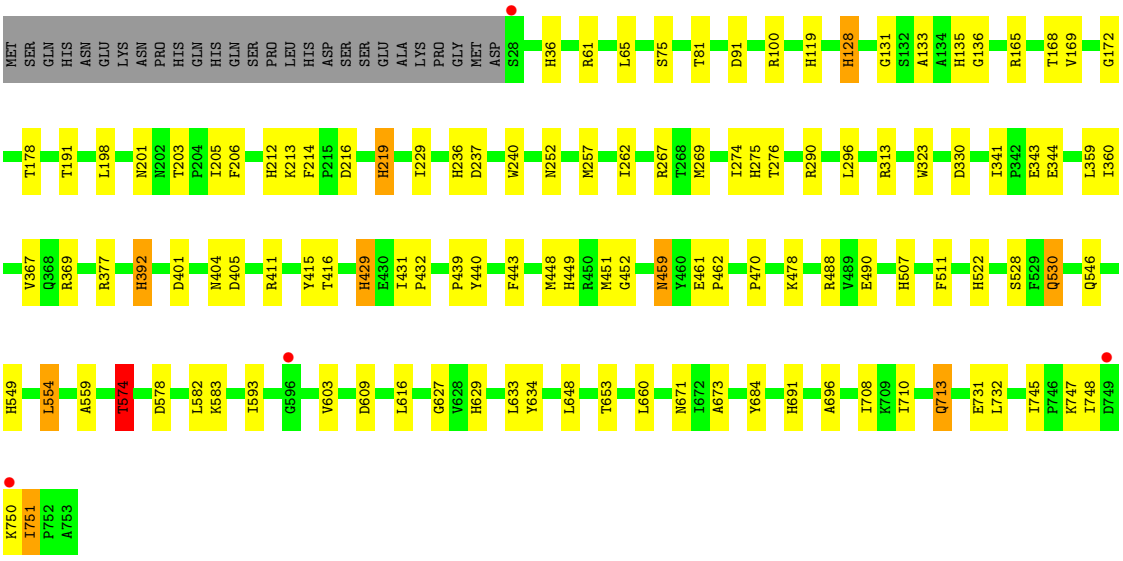
• Molecule 1: Catalase HPII

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	93.45Å 133.40Å 123.24Å 90.00° 109.18° 90.00°	Depositor
Resolution (Å)	32.19 – 1.60 32.19 – 1.60	Depositor EDS
% Data completeness (in resolution range)	91.8 (32.19-1.60) 91.8 (32.19-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 1.60Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.151 , 0.184 0.149 , 0.183	Depositor DCC
R_{free} test set	17269 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	13.1	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 39.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	26323	wwPDB-VP
Average B, all atoms (Å^2)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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

5.1 Standard geometry

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

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	1.64	49/5924 (0.8%)	1.36	12/8054 (0.1%)
1	B	1.60	39/5927 (0.7%)	1.33	20/8058 (0.2%)
1	C	1.57	41/5922 (0.7%)	1.34	23/8050 (0.3%)
1	D	1.64	47/5927 (0.8%)	1.35	12/8058 (0.1%)
All	All	1.61	176/23700 (0.7%)	1.35	67/32220 (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	B	0	1
1	C	0	2
All	All	0	3

All (176) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	212	HIS	ND1-CE1	9.60	1.42	1.32
1	D	392	HIS	ND1-CE1	9.52	1.42	1.32
1	C	219	HIS	ND1-CE1	9.48	1.42	1.32
1	A	275	HIS	ND1-CE1	8.38	1.41	1.32
1	C	116	HIS	ND1-CE1	8.35	1.41	1.32
1	D	452	GLY	C-O	8.26	1.32	1.24
1	A	452	GLY	C-O	8.06	1.31	1.24
1	A	629	HIS	ND1-CE1	7.51	1.40	1.32
1	D	262	ILE	CA-C	7.27	1.60	1.52
1	B	85	GLY	N-CA	7.24	1.56	1.45
1	A	420	ILE	CA-CB	7.20	1.63	1.54
1	D	216	ASP	N-CA	7.18	1.54	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	392	HIS	ND1-CE1	7.13	1.39	1.32
1	A	178	THR	N-CA	6.94	1.53	1.46
1	B	675	ILE	N-CA	6.86	1.52	1.46
1	B	128	HIS	ND1-CE1	6.83	1.39	1.32
1	A	251	HIS	ND1-CE1	6.80	1.39	1.32
1	D	214	PHE	C-O	-6.74	1.18	1.24
1	D	511	PHE	C-O	6.64	1.31	1.24
1	D	219	HIS	CG-CD2	6.62	1.43	1.35
1	B	109	ILE	C-O	6.62	1.31	1.24
1	B	116	HIS	ND1-CE1	6.59	1.39	1.32
1	C	370	VAL	CA-CB	6.58	1.63	1.54
1	C	159	ILE	CB-CG1	-6.54	1.40	1.53
1	D	178	THR	N-CA	6.52	1.54	1.46
1	D	275	HIS	ND1-CE1	6.52	1.39	1.32
1	B	219	HIS	ND1-CE1	6.45	1.39	1.32
1	C	441	HIS	ND1-CE1	6.39	1.39	1.32
1	C	212	HIS	ND1-CE1	6.39	1.39	1.32
1	A	739	HIS	ND1-CE1	6.37	1.39	1.32
1	A	122	ILE	CA-CB	6.31	1.62	1.54
1	B	226	HIS	ND1-CE1	6.25	1.38	1.32
1	D	128	HIS	ND1-CE1	6.25	1.38	1.32
1	C	328	ALA	C-O	6.23	1.32	1.24
1	A	163	PHE	N-CA	6.18	1.53	1.46
1	C	36	HIS	CE1-NE2	6.16	1.38	1.32
1	C	127	VAL	C-O	6.15	1.30	1.23
1	C	116	HIS	CG-CD2	6.15	1.42	1.35
1	D	131	GLY	N-CA	6.11	1.51	1.45
1	C	292	HIS	CE1-NE2	6.11	1.38	1.32
1	C	420	ILE	CA-CB	6.10	1.62	1.54
1	D	367	VAL	C-O	6.10	1.30	1.24
1	A	458	ALA	C-O	6.08	1.31	1.23
1	B	113	LYS	CA-C	6.06	1.60	1.52
1	D	198	LEU	C-O	6.06	1.31	1.23
1	C	44	PRO	CA-C	6.05	1.57	1.52
1	B	739	HIS	CG-CD2	6.04	1.42	1.35
1	D	236	HIS	ND1-CE1	6.03	1.38	1.32
1	B	219	HIS	CG-CD2	6.02	1.42	1.35
1	B	119	HIS	ND1-CE1	5.99	1.38	1.32
1	D	276	THR	C-O	5.98	1.31	1.24
1	A	337	GLY	N-CA	5.97	1.51	1.45
1	A	170	GLN	C-O	-5.93	1.16	1.24
1	D	627	GLY	N-CA	5.93	1.53	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	429	HIS	CG-ND1	-5.92	1.31	1.38
1	C	121	ARG	C-N	5.92	1.39	1.33
1	D	343	GLU	C-O	5.90	1.31	1.24
1	B	473	THR	C-N	5.89	1.38	1.33
1	B	452	GLY	C-O	5.89	1.29	1.23
1	C	276	THR	N-CA	5.89	1.53	1.46
1	D	257	MET	C-O	5.88	1.31	1.24
1	C	292	HIS	CG-CD2	5.88	1.42	1.35
1	B	576	PRO	CA-C	5.86	1.57	1.52
1	B	393	PRO	CA-CB	5.85	1.62	1.53
1	A	339	GLN	N-CA	5.84	1.53	1.46
1	A	135	HIS	CE1-NE2	5.81	1.38	1.32
1	B	292	HIS	ND1-CE1	5.80	1.38	1.32
1	D	431	ILE	CA-C	5.78	1.58	1.52
1	A	377	ARG	CZ-NH1	5.78	1.40	1.32
1	D	269	MET	N-CA	5.76	1.53	1.45
1	A	549	HIS	CG-CD2	5.76	1.42	1.35
1	C	135	HIS	ND1-CE1	5.76	1.38	1.32
1	B	56	LYS	C-O	5.75	1.30	1.24
1	B	376	ASN	N-CA	5.73	1.52	1.46
1	B	275	HIS	CE1-NE2	5.72	1.38	1.32
1	A	494	VAL	C-O	5.72	1.29	1.24
1	D	236	HIS	CG-ND1	-5.68	1.31	1.38
1	D	219	HIS	ND1-CE1	5.67	1.38	1.32
1	A	600	GLY	N-CA	5.66	1.53	1.45
1	B	431	ILE	CA-C	5.66	1.58	1.53
1	B	226	HIS	CE1-NE2	5.66	1.38	1.32
1	A	592	ALA	N-CA	5.64	1.53	1.46
1	A	588	LEU	N-CA	5.63	1.53	1.46
1	D	133	ALA	N-CA	5.61	1.53	1.45
1	D	439	PRO	N-CA	5.60	1.53	1.47
1	B	36	HIS	CE1-NE2	5.60	1.38	1.32
1	C	691	HIS	CE1-NE2	5.59	1.38	1.32
1	B	165	ARG	CZ-NH1	5.55	1.40	1.32
1	C	187	THR	N-CA	5.54	1.52	1.46
1	D	528	SER	N-CA	5.53	1.53	1.46
1	C	452	GLY	N-CA	5.53	1.53	1.45
1	B	358	LYS	N-CA	5.52	1.52	1.46
1	C	203	THR	CA-C	5.52	1.57	1.52
1	B	391	PHE	C-O	5.50	1.30	1.23
1	A	365	VAL	CA-C	5.48	1.58	1.52
1	A	474	PRO	CA-CB	5.48	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	125	ARG	CD-NE	5.46	1.53	1.46
1	C	59	ASP	C-O	-5.46	1.16	1.24
1	A	327	GLU	N-CA	5.45	1.53	1.46
1	B	283	GLU	N-CA	5.43	1.53	1.46
1	A	730	ASP	C-O	5.42	1.30	1.24
1	D	216	ASP	C-O	5.41	1.30	1.24
1	C	395	HIS	ND1-CE1	5.41	1.38	1.32
1	A	255	TRP	CD2-CE2	5.40	1.50	1.41
1	C	327	GLU	N-CA	5.38	1.53	1.46
1	D	401	ASP	N-CA	5.38	1.52	1.46
1	C	119	HIS	ND1-CE1	5.38	1.38	1.32
1	D	691	HIS	CE1-NE2	5.38	1.38	1.32
1	A	316	ASP	N-CA	5.37	1.52	1.46
1	A	523	ILE	N-CA	5.36	1.52	1.46
1	B	219	HIS	CE1-NE2	5.36	1.38	1.32
1	B	188	LYS	CA-CB	5.35	1.60	1.53
1	B	205	ILE	CA-C	-5.34	1.47	1.52
1	C	112	GLU	N-CA	5.33	1.52	1.46
1	B	236	HIS	ND1-CE1	5.33	1.37	1.32
1	A	60	THR	CA-CB	5.32	1.60	1.53
1	D	603	VAL	C-O	5.32	1.29	1.24
1	A	183	ARG	CD-NE	5.32	1.53	1.46
1	A	214	PHE	N-CA	5.31	1.51	1.46
1	A	418	THR	CA-C	5.31	1.59	1.52
1	B	135	HIS	CG-ND1	-5.31	1.32	1.38
1	B	168	THR	N-CA	5.30	1.52	1.45
1	C	226	HIS	CG-CD2	5.29	1.41	1.35
1	D	119	HIS	CE1-NE2	5.29	1.37	1.32
1	B	314	ASP	N-CA	5.28	1.52	1.46
1	A	71	VAL	CA-CB	5.27	1.60	1.54
1	D	81	THR	C-O	5.27	1.30	1.23
1	A	131	GLY	N-CA	5.26	1.50	1.45
1	C	336	LEU	N-CA	5.24	1.52	1.46
1	C	135	HIS	CG-CD2	5.24	1.41	1.35
1	D	237	ASP	N-CA	5.23	1.52	1.46
1	D	212	HIS	ND1-CE1	5.22	1.37	1.32
1	C	716	GLU	CA-C	5.22	1.59	1.52
1	A	629	HIS	CG-CD2	5.20	1.41	1.35
1	C	657	ALA	C-O	-5.20	1.18	1.24
1	C	701	ALA	N-CA	5.20	1.52	1.46
1	A	607	LEU	N-CA	5.19	1.52	1.45
1	A	441	HIS	ND1-CE1	5.19	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	684	TYR	N-CA	5.19	1.52	1.46
1	D	203	THR	CA-C	5.19	1.57	1.52
1	C	219	HIS	N-CA	5.18	1.52	1.46
1	D	172	GLY	N-CA	5.18	1.51	1.45
1	C	255	TRP	CZ2-CH2	5.17	1.47	1.37
1	D	522	HIS	CG-ND1	-5.17	1.32	1.38
1	A	203	THR	C-N	5.17	1.37	1.33
1	B	392	HIS	ND1-CE1	5.17	1.37	1.32
1	B	142	LYS	N-CA	5.16	1.52	1.46
1	C	383	PHE	C-O	5.15	1.30	1.24
1	A	227	TRP	CD2-CE2	5.14	1.50	1.41
1	A	727	SER	CA-C	5.14	1.59	1.52
1	D	136	GLY	N-CA	5.14	1.51	1.45
1	B	369	ARG	C-O	5.13	1.30	1.24
1	C	587	SER	CA-C	5.13	1.59	1.52
1	A	251	HIS	CG-CD2	5.13	1.41	1.35
1	B	440	TYR	CE1-CZ	5.13	1.50	1.38
1	D	275	HIS	CG-CD2	5.13	1.41	1.35
1	D	165	ARG	CD-NE	5.12	1.53	1.46
1	A	302	LEU	N-CA	5.12	1.52	1.45
1	A	395	HIS	CE1-NE2	5.11	1.37	1.32
1	A	274	ILE	N-CA	5.11	1.52	1.46
1	B	217	PHE	CA-CB	5.09	1.61	1.53
1	A	275	HIS	CG-CD2	5.08	1.41	1.35
1	C	391	PHE	N-CA	5.08	1.51	1.45
1	C	733	LEU	CA-C	5.06	1.59	1.52
1	D	290	ARG	N-CA	5.05	1.52	1.46
1	A	136	GLY	N-CA	5.04	1.51	1.45
1	D	377	ARG	CZ-NH1	5.04	1.39	1.32
1	A	217	PHE	CA-CB	5.04	1.61	1.53
1	A	488	ARG	N-CA	5.03	1.52	1.46
1	A	236	HIS	ND1-CE1	5.03	1.37	1.32
1	D	323	TRP	NE1-CE2	5.03	1.43	1.37
1	A	729	MET	N-CA	5.02	1.52	1.46
1	D	549	HIS	CE1-NE2	5.02	1.37	1.32
1	D	559	ALA	C-O	-5.02	1.18	1.24
1	C	172	GLY	N-CA	5.01	1.51	1.45
1	D	696	ALA	N-CA	5.00	1.52	1.46

All (67) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	159	ILE	CB-CG1-CD1	-9.81	93.20	113.80
1	B	745	ILE	CA-C-N	-8.95	110.52	119.56
1	B	745	ILE	C-N-CA	-8.95	110.52	119.56
1	D	574	THR	CA-C-N	8.48	125.85	119.66
1	D	574	THR	C-N-CA	8.48	125.85	119.66
1	A	574	THR	CA-C-N	8.45	125.83	119.66
1	A	574	THR	C-N-CA	8.45	125.83	119.66
1	B	521	ARG	NE-CZ-NH2	8.01	126.41	119.20
1	C	159	ILE	CB-CA-C	7.34	121.96	110.81
1	A	533	LYS	CG-CD-CE	-7.17	94.81	111.30
1	C	725	ASP	N-CA-C	6.70	125.08	110.80
1	D	360	ILE	N-CA-C	-6.65	100.49	107.60
1	C	348	LYS	CA-CB-CG	-6.59	100.92	114.10
1	D	61	ARG	NE-CZ-NH2	6.50	125.06	119.20
1	B	126	ILE	CB-CA-C	-6.40	103.50	112.14
1	D	377	ARG	NH1-CZ-NH2	6.34	127.54	119.30
1	C	37	ARG	CA-C-N	6.29	126.24	119.76
1	C	37	ARG	C-N-CA	6.29	126.24	119.76
1	C	749	ASP	N-CA-C	6.27	118.92	111.71
1	B	750	LYS	CB-CA-C	-6.24	101.09	110.88
1	A	349	PHE	CA-C-N	-6.23	111.84	122.56
1	A	349	PHE	C-N-CA	-6.23	111.84	122.56
1	B	349	PHE	CA-C-N	-6.23	112.70	122.73
1	B	349	PHE	C-N-CA	-6.23	112.70	122.73
1	C	159	ILE	CA-CB-CG2	6.05	120.79	110.50
1	A	377	ARG	CG-CD-NE	-5.90	99.02	112.00
1	B	568	ASP	N-CA-C	5.80	118.34	111.33
1	A	372	LYS	CD-CE-NZ	-5.79	93.36	111.90
1	C	377	ARG	NE-CZ-NH1	-5.76	115.74	121.50
1	C	111	ARG	NE-CZ-NH1	-5.72	115.78	121.50
1	C	377	ARG	CG-CD-NE	-5.71	99.44	112.00
1	D	745	ILE	CA-C-N	-5.64	113.81	119.56
1	D	745	ILE	C-N-CA	-5.64	113.81	119.56
1	C	471	ARG	NE-CZ-NH2	-5.59	114.17	119.20
1	C	451	MET	CA-C-N	-5.58	114.62	120.31
1	C	451	MET	C-N-CA	-5.58	114.62	120.31
1	B	521	ARG	NE-CZ-NH1	-5.58	115.92	121.50
1	B	195	ILE	CB-CA-C	-5.55	103.89	111.33
1	A	120	GLU	N-CA-C	5.54	118.25	111.82
1	D	229	ILE	N-CA-CB	-5.53	105.72	111.64
1	D	431	ILE	N-CA-C	-5.47	103.93	109.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	479	ARG	CA-C-N	-5.46	115.38	121.83
1	C	479	ARG	C-N-CA	-5.46	115.38	121.83
1	D	574	THR	CB-CA-C	5.44	118.23	109.41
1	C	98	GLY	N-CA-C	-5.43	105.92	112.48
1	C	446	ASP	CB-CA-C	-5.43	108.73	115.89
1	B	686	MET	N-CA-C	5.42	116.87	111.07
1	A	98	GLY	N-CA-C	-5.36	105.93	112.68
1	B	38	PRO	CB-CA-C	-5.36	103.96	110.98
1	C	168	THR	CA-C-N	-5.32	117.71	123.08
1	C	168	THR	C-N-CA	-5.32	117.71	123.08
1	C	488	ARG	N-CA-CB	-5.28	102.09	110.06
1	A	638	GLY	N-CA-C	-5.28	104.96	111.45
1	B	377	ARG	CG-CD-NE	-5.28	100.39	112.00
1	B	725	ASP	N-CA-C	5.23	121.94	110.80
1	D	732	LEU	N-CA-C	-5.17	105.72	111.36
1	B	325	ALA	N-CA-C	-5.15	105.67	111.28
1	B	350	ASP	CB-CA-C	5.12	119.39	110.94
1	C	126	ILE	CB-CA-C	-5.12	105.23	112.14
1	A	229	ILE	N-CA-CB	-5.12	104.05	111.21
1	A	750	LYS	N-CA-C	-5.11	105.62	111.14
1	B	48	GLN	CA-C-N	-5.10	114.70	119.85
1	B	48	GLN	C-N-CA	-5.10	114.70	119.85
1	B	377	ARG	NE-CZ-NH1	-5.06	116.44	121.50
1	C	33	ASP	N-CA-C	5.03	119.29	113.20
1	B	179	VAL	CB-CA-C	-5.03	105.82	111.45
1	D	554	LEU	CD1-CG-CD2	5.02	121.84	110.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	724	ALA	Peptide
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	5755	0	5599	37	0
1	B	5758	0	5605	60	0
1	C	5756	0	5606	54	0
1	D	5758	0	5602	62	0
2	A	44	0	31	1	0
2	B	44	0	31	1	0
2	C	44	0	31	2	0
2	D	44	0	31	4	0
3	A	43	0	30	13	0
3	B	43	0	30	12	0
3	C	43	0	30	13	0
3	D	43	0	30	8	0
4	A	769	0	0	9	0
4	B	696	0	0	11	0
4	C	709	0	0	9	0
4	D	774	0	0	16	0
All	All	26323	0	22656	219	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 5.

All (219) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:HIS:ND1	1:D:415:TYR:CB	1.69	1.52
1:C:392:HIS:ND1	1:C:415:TYR:CB	1.72	1.51
1:A:392:HIS:ND1	1:A:415:TYR:CB	1.75	1.50
1:B:392:HIS:ND1	1:B:415:TYR:CB	1.70	1.49
1:B:157:ASN:HB2	4:B:1578:HOH:O	1.28	1.30
1:D:392:HIS:CE1	1:D:415:TYR:HB2	1.71	1.24
1:D:449[B]:HIS:NE2	4:D:1534:HOH:O	1.66	1.21
1:B:392:HIS:CE1	1:B:415:TYR:HB2	1.76	1.19
1:A:392:HIS:CE1	1:A:415:TYR:HB2	1.80	1.17
1:C:392:HIS:CE1	1:C:415:TYR:HB2	1.84	1.13
1:C:440:TYR:CD1	4:C:1370:HOH:O	2.00	1.13
1:A:392:HIS:ND1	1:A:415:TYR:HB2	0.80	1.13
3:A:802[B]:HEM:HMC2	3:A:802[B]:HEM:HBC2	1.22	1.13
1:B:451:MET:HE2	1:D:451:MET:HE2	1.19	1.11
1:D:546:GLN:HG3	4:D:1590:HOH:O	1.50	1.11
1:D:392:HIS:ND1	1:D:415:TYR:HB2	0.78	1.11
1:A:451:MET:HE2	1:C:451:MET:HE2	1.22	1.10
1:C:392:HIS:ND1	1:C:415:TYR:HB2	0.77	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:HIS:ND1	1:B:415:TYR:HB2	0.76	1.09
1:C:583[A]:LYS:H	1:C:583[A]:LYS:HE2	1.06	1.06
1:C:440:TYR:HD1	4:C:1370:HOH:O	1.35	1.04
1:A:541:GLU:OE2	4:A:1540:HOH:O	1.76	1.01
1:B:369:ARG:HG2	4:B:1302:HOH:O	1.64	0.96
1:C:392:HIS:CG	1:C:415:TYR:HB2	2.04	0.93
3:C:802[B]:HEM:HBC2	3:C:802[B]:HEM:HMC2	1.52	0.89
1:D:449[B]:HIS:CE1	4:D:1534:HOH:O	2.18	0.84
1:D:267:ARG:HG3	4:D:1384:HOH:O	1.79	0.83
1:C:578:ASP:HB2	1:C:582:LEU:O	1.77	0.83
1:C:201:ASN:CG	3:C:802[B]:HEM:HMB2	2.04	0.82
1:A:392:HIS:CG	1:A:415:TYR:HB2	2.07	0.82
1:B:407:LEU:CD2	3:B:802[B]:HEM:HBB1	2.11	0.81
1:B:708:ILE:HD12	1:B:710:ILE:HD11	1.63	0.80
1:C:583[A]:LYS:H	1:C:583[A]:LYS:CE	1.91	0.80
2:C:801[A]:HDD:HMB1	2:C:801[A]:HDD:HBB1	1.66	0.76
3:A:802[B]:HEM:HBC2	3:A:802[B]:HEM:CMC	2.00	0.75
1:D:490:GLU:OE1	4:D:1482:HOH:O	2.02	0.75
2:D:801[A]:HDD:HMB1	2:D:801[A]:HDD:HBB1	1.69	0.75
1:C:748:ILE:O	1:C:751:ILE:HG22	1.86	0.75
1:C:440:TYR:CE1	4:C:1370:HOH:O	2.33	0.74
1:D:731:GLU:OE2	4:D:1653:HOH:O	2.06	0.74
1:D:546:GLN:CG	4:D:1590:HOH:O	2.19	0.73
1:D:341:ILE:HG13	4:D:1651:HOH:O	1.87	0.73
1:B:451:MET:CE	1:D:451:MET:HE2	2.12	0.72
1:D:392:HIS:ND1	1:D:415:TYR:CG	2.58	0.70
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.74	0.70
1:C:201:ASN:ND2	3:C:802[B]:HEM:CMB	2.55	0.70
1:C:206:PHE:CG	3:C:802[B]:HEM:HAB	2.27	0.69
1:C:392:HIS:ND1	1:C:415:TYR:CG	2.59	0.69
1:A:201:ASN:CG	3:A:802[B]:HEM:HMB2	2.16	0.69
1:A:392:HIS:ND1	1:A:415:TYR:CG	2.60	0.68
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.75	0.68
1:D:201:ASN:CG	3:D:802[B]:HEM:HMB2	2.19	0.68
1:B:407:LEU:HD21	3:B:802[B]:HEM:HBB1	1.74	0.68
1:D:546:GLN:CD	4:D:1590:HOH:O	2.33	0.67
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.78	0.67
2:A:801[A]:HDD:HBB1	2:A:801[A]:HDD:HMB1	1.75	0.66
1:B:157:ASN:CB	4:B:1578:HOH:O	2.07	0.66
1:B:407:LEU:HD23	3:B:802[B]:HEM:HBB1	1.76	0.66
1:B:392:HIS:ND1	1:B:415:TYR:CG	2.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:GLN:HG2	1:B:566:LEU:HD23	1.78	0.64
1:A:416[B]:THR:HG22	4:A:1016:HOH:O	1.97	0.64
1:B:521:ARG:HD3	4:B:1566:HOH:O	1.97	0.64
2:B:801[A]:HDD:HBB1	2:B:801[A]:HDD:HMB1	1.78	0.64
1:D:629:HIS:HD2	4:D:1267:HOH:O	1.81	0.64
2:D:801[A]:HDD:HMC1	2:D:801[A]:HDD:HBC1	1.79	0.64
1:D:206:PHE:HB2	3:D:802[B]:HEM:HBB1	1.79	0.64
1:C:206:PHE:CD2	3:C:802[B]:HEM:HAB	2.33	0.63
1:A:36:HIS:CD2	1:A:36:HIS:H	2.17	0.62
1:B:201:ASN:CG	3:B:802[B]:HEM:HMB2	2.25	0.62
1:D:574:THR:HG22	4:D:1313:HOH:O	2.00	0.61
4:C:1452:HOH:O	1:D:488:ARG:HD2	2.01	0.60
1:C:201:ASN:ND2	3:C:802[B]:HEM:HMB1	2.16	0.60
1:D:392:HIS:ND1	1:D:415:TYR:HB3	2.02	0.60
1:C:629:HIS:HD2	4:C:1210:HOH:O	1.84	0.59
1:B:294:LYS:HB2	4:B:1189:HOH:O	2.01	0.59
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.85	0.59
1:A:240:TRP:HE1	1:A:530:GLN:HE21	1.51	0.59
1:B:359:LEU:H	1:B:507:HIS:HD2	1.50	0.59
1:D:448:MET:O	1:D:449[A]:HIS:HB2	2.03	0.58
1:C:201:ASN:CG	3:C:802[B]:HEM:CMB	2.76	0.58
1:B:552:LEU:HD22	1:B:556:GLN:HG3	1.83	0.58
1:D:206:PHE:CG	3:D:802[B]:HEM:HAB	2.37	0.57
1:B:521:ARG:CD	4:B:1566:HOH:O	2.52	0.57
1:B:708:ILE:CD1	1:B:710:ILE:HD11	2.34	0.57
1:B:725:ASP:OD1	1:B:725:ASP:C	2.46	0.57
1:B:201:ASN:CG	3:B:802[B]:HEM:CMB	2.79	0.56
1:D:274:ILE:HD12	3:D:802[B]:HEM:HMB1	1.88	0.56
1:A:448:MET:O	1:A:449[B]:HIS:HB2	2.06	0.56
1:D:359:LEU:H	1:D:507:HIS:HD2	1.53	0.56
1:B:583:LYS:H	1:B:583:LYS:NZ	2.04	0.56
1:A:479:ARG:NH2	4:A:1549:HOH:O	2.04	0.56
1:C:201:ASN:ND2	3:C:802[B]:HEM:HMB2	2.19	0.55
1:A:274:ILE:HD12	3:A:802[B]:HEM:HMB1	1.88	0.55
1:D:713:GLN:O	1:D:713:GLN:HG2	2.07	0.55
1:B:407:LEU:HD21	3:B:802[B]:HEM:CBB	2.36	0.55
2:D:801[A]:HDD:HMC1	2:D:801[A]:HDD:CBC	2.36	0.54
1:B:629:HIS:HD2	4:B:1157:HOH:O	1.89	0.54
1:D:708:ILE:HG13	1:D:710:ILE:HG12	1.89	0.54
1:D:206:PHE:HB2	3:D:802[B]:HEM:CBB	2.38	0.54
1:D:416[B]:THR:CG2	4:D:1169:HOH:O	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:TRP:HE1	1:B:530:GLN:HE21	1.57	0.53
4:A:1169:HOH:O	1:D:100:ARG:HG3	2.08	0.53
1:D:609:ASP:O	4:D:1345:HOH:O	2.18	0.53
1:B:201:ASN:ND2	3:B:802[B]:HEM:HMB1	2.25	0.52
1:D:411:ARG:HG2	3:D:802[B]:HEM:C2C	2.44	0.52
1:D:478:LYS:NZ	4:D:1005:HOH:O	2.42	0.52
1:A:407:LEU:CD2	3:A:802[B]:HEM:HBB1	2.39	0.52
1:B:634:TYR:O	1:B:653:THR:HA	2.08	0.52
4:B:1339:HOH:O	1:D:449[A]:HIS:HE1	1.92	0.52
1:B:36:HIS:H	1:B:36:HIS:HD1	1.58	0.52
1:B:392:HIS:ND1	1:B:415:TYR:HB3	2.06	0.52
1:A:407:LEU:HD23	3:A:802[B]:HEM:HBB1	1.92	0.52
1:C:621:LYS:HE3	4:C:1595:HOH:O	2.09	0.52
1:B:407:LEU:CD2	3:B:802[B]:HEM:CBB	2.86	0.52
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.92	0.52
4:B:1139:HOH:O	1:D:449[B]:HIS:HD2	1.93	0.52
1:C:411:ARG:HG2	3:C:802[B]:HEM:C2C	2.45	0.52
4:A:1344:HOH:O	1:C:449[B]:HIS:HE1	1.93	0.51
1:B:461:GLU:HA	1:B:462:PRO:C	2.34	0.51
1:B:583:LYS:O	1:B:584:LYS:HB3	2.10	0.51
4:A:1047:HOH:O	1:C:52:PRO:HG3	2.09	0.51
1:D:748:ILE:O	1:D:751:ILE:HG22	2.10	0.51
1:B:521:ARG:NE	4:B:1566:HOH:O	2.43	0.51
1:D:671:ASN:HD21	1:D:673:ALA:HB3	1.76	0.50
1:D:416[B]:THR:HG22	4:D:1169:HOH:O	2.11	0.50
1:C:240:TRP:HE1	1:C:530:GLN:HE21	1.60	0.50
1:A:201:ASN:CG	3:A:802[B]:HEM:CMB	2.85	0.50
1:C:359:LEU:H	1:C:507:HIS:HD2	1.60	0.50
1:A:219:HIS:HB3	1:B:459:ASN:ND2	2.28	0.49
1:A:372:LYS:NZ	4:A:1629:HOH:O	2.44	0.49
1:B:359:LEU:H	1:B:507:HIS:CD2	2.29	0.49
3:A:802[B]:HEM:HMC2	3:A:802[B]:HEM:CBC	2.15	0.49
3:B:802[B]:HEM:HMC2	3:B:802[B]:HEM:HBC2	1.96	0.48
3:A:802[B]:HEM:CMC	3:A:802[B]:HEM:CBC	2.80	0.48
1:C:704:PHE:O	1:C:707:THR:HG22	2.12	0.48
1:C:577:PRO:HG2	4:C:1495:HOH:O	2.13	0.48
1:D:240:TRP:HE1	1:D:530:GLN:HE21	1.61	0.48
1:A:411:ARG:HD2	3:A:802[B]:HEM:HBB2	1.96	0.48
3:B:802[B]:HEM:HBC2	3:B:802[B]:HEM:CMC	2.44	0.47
1:C:597:ASP:OD2	4:C:1417:HOH:O	2.20	0.47
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:801[A]:HDD:HBC1	2:D:801[A]:HDD:CMC	2.44	0.47
1:D:461:GLU:HA	1:D:462:PRO:C	2.41	0.46
3:A:802[B]:HEM:HHC	3:A:802[B]:HEM:CBB	2.44	0.46
1:B:461:GLU:OE1	1:D:91:ASP:OD1	2.34	0.46
1:B:724:ALA:O	1:B:726:GLY:N	2.45	0.46
1:B:448:MET:O	1:B:449[B]:HIS:HB2	2.15	0.46
1:C:359:LEU:H	1:C:507:HIS:CD2	2.34	0.46
1:A:36:HIS:H	1:A:36:HIS:HD2	1.62	0.46
3:C:802[B]:HEM:HMC2	3:C:802[B]:HEM:CBC	2.35	0.46
1:A:726:GLY:HA2	4:A:1492:HOH:O	2.16	0.45
1:C:37:ARG:HD3	4:C:1509:HOH:O	2.16	0.45
1:D:634:TYR:O	1:D:653:THR:HA	2.15	0.45
1:D:128:HIS:HA	1:D:168:THR:O	2.17	0.45
1:B:201:ASN:ND2	3:B:802[B]:HEM:CMB	2.80	0.45
1:B:39:ALA:HB1	1:B:41:GLU:HG2	1.98	0.45
1:D:359:LEU:H	1:D:507:HIS:CD2	2.31	0.45
1:A:144:LEU:HD11	1:A:370:VAL:HG13	1.97	0.45
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.47	0.45
1:B:92:GLN:HA	1:C:213:LYS:HD2	1.99	0.44
3:A:802[B]:HEM:CBB	3:A:802[B]:HEM:CHC	2.94	0.44
1:D:404:ASN:O	1:D:405:ASP:C	2.59	0.44
1:A:128:HIS:HA	1:A:168:THR:O	2.18	0.44
1:B:128:HIS:HA	1:B:168:THR:O	2.17	0.44
1:A:128:HIS:CE1	1:A:169:VAL:HG22	2.53	0.44
1:B:530:GLN:HE21	1:B:530:GLN:HB3	1.63	0.44
1:B:157:ASN:CA	4:B:1578:HOH:O	2.58	0.43
1:B:201:ASN:OD1	3:B:802[B]:HEM:HMB2	2.16	0.43
1:A:201:ASN:ND2	3:A:802[B]:HEM:CMB	2.81	0.43
1:B:603:VAL:HG11	1:B:666:ILE:HD12	2.00	0.43
1:C:201:ASN:OD1	3:C:802[B]:HEM:HMB2	2.16	0.43
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.53	0.43
1:D:359:LEU:HD21	4:D:1643:HOH:O	2.19	0.43
1:C:461:GLU:HB2	1:C:462:PRO:HA	2.01	0.43
1:A:393:PRO:HD2	1:A:415:TYR:CD2	2.54	0.43
1:D:201:ASN:ND2	3:D:802[B]:HEM:CMB	2.82	0.43
1:B:213:LYS:HB3	1:B:213:LYS:HE3	1.82	0.43
1:B:556:GLN:HG2	1:B:566:LEU:CD2	2.47	0.43
1:C:448:MET:O	1:C:449[B]:HIS:HB2	2.19	0.43
1:C:274:ILE:HD12	3:C:802[B]:HEM:HMB1	2.01	0.43
1:A:449[B]:HIS:CG	1:C:449[B]:HIS:CG	2.36	0.42
1:A:459:ASN:HD22	1:A:459:ASN:H	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ASN:HB3	1:D:429:HIS:CD2	2.54	0.42
1:A:535:VAL:O	1:A:537:PRO:HD3	2.20	0.42
1:C:643:ASP:OD1	1:C:644:ASP:N	2.52	0.42
1:D:206:PHE:CG	3:D:802[B]:HEM:CAB	3.02	0.42
1:B:459:ASN:H	1:B:459:ASN:HD22	1.66	0.42
1:C:251:HIS:CE1	1:C:507:HIS:HB3	2.54	0.42
2:C:801[A]:HDD:HMD3	2:C:801[A]:HDD:HAD2	1.88	0.42
1:D:65:LEU:HD21	1:D:135:HIS:CG	2.54	0.42
1:D:448:MET:O	1:D:449[A]:HIS:CB	2.67	0.42
1:D:578:ASP:OD1	1:D:583:LYS:HE3	2.20	0.42
1:B:91:ASP:OD1	1:D:461:GLU:OE1	2.38	0.41
1:B:583:LYS:H	1:B:583:LYS:HZ2	1.68	0.41
1:D:36:HIS:H	1:D:36:HIS:HD1	1.67	0.41
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.35	0.41
1:A:251:HIS:CE1	1:A:507:HIS:HB3	2.55	0.41
1:C:407:LEU:HD23	3:C:802[B]:HEM:HBB1	2.03	0.41
1:C:725:ASP:HB3	1:C:726:GLY:H	1.65	0.41
1:A:751:ILE:HA	1:A:752:PRO:HD3	1.73	0.41
1:A:725:ASP:H	1:A:728:PHE:HB3	1.85	0.41
1:D:313:ARG:HG3	1:D:660:LEU:HD12	2.03	0.41
1:A:38:PRO:HG2	1:A:51:ALA:HB2	2.03	0.41
1:A:461:GLU:HA	1:A:462:PRO:C	2.45	0.41
1:B:552:LEU:HD21	1:B:571:LEU:HD12	2.03	0.41
1:C:128:HIS:HA	1:C:168:THR:O	2.20	0.41
1:C:469:TRP:CE3	1:C:471:ARG:HG3	2.56	0.41
1:B:596:GLY:HA3	1:B:737:ALA:O	2.22	0.40
1:C:634:TYR:O	1:C:653:THR:HA	2.21	0.40
1:D:296:LEU:HD23	1:D:296:LEU:HA	1.93	0.40
1:C:552:LEU:HD22	1:C:556:GLN:HG3	2.03	0.40
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.29	0.40
1:C:267:ARG:HH11	1:C:267:ARG:HD2	1.63	0.40
1:A:449[B]:HIS:HE1	4:A:1344:HOH:O	2.03	0.40
1:B:83:ASN:HB3	1:D:429:HIS:CG	2.56	0.40
1:B:626:LYS:HA	1:B:626:LYS:HD3	1.69	0.40
1:D:443:PHE:CZ	1:D:470:PRO:HD2	2.56	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	728/753 (97%)	710 (98%)	17 (2%)	1 (0%)	48 27
1	B	728/753 (97%)	714 (98%)	13 (2%)	1 (0%)	48 27
1	C	727/753 (96%)	709 (98%)	17 (2%)	1 (0%)	48 27
1	D	728/753 (97%)	715 (98%)	12 (2%)	1 (0%)	48 27
All	All	2911/3012 (97%)	2848 (98%)	59 (2%)	4 (0%)	48 27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	SER
1	B	75	SER
1	C	75	SER
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	615/636 (97%)	600 (98%)	15 (2%)	43 19
1	B	615/636 (97%)	585 (95%)	30 (5%)	22 5
1	C	614/636 (96%)	586 (95%)	28 (5%)	24 6
1	D	615/636 (97%)	594 (97%)	21 (3%)	32 11
All	All	2459/2544 (97%)	2365 (96%)	94 (4%)	29 9

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	158	LYS
1	A	191	THR
1	A	205	ILE
1	A	213	LYS
1	A	252	ASN
1	A	440	TYR
1	A	459	ASN
1	A	478	LYS
1	A	530	GLN
1	A	552	LEU
1	A	556	GLN
1	A	617	LEU
1	A	732	LEU
1	A	750	LYS
1	A	751	ILE
1	B	32	GLU
1	B	158	LYS
1	B	191	THR
1	B	205	ILE
1	B	213	LYS
1	B	252	ASN
1	B	309	LYS
1	B	321	GLU
1	B	344	GLU
1	B	370[A]	VAL
1	B	370[B]	VAL
1	B	432	PRO
1	B	440	TYR
1	B	459	ASN
1	B	530	GLN
1	B	552	LEU
1	B	560	LYS
1	B	565	GLU
1	B	566	LEU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	612	ARG
1	B	616	LEU
1	B	633	LEU
1	B	703	LYS
1	B	713	GLN

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Mol	Chain	Res	Type
1	B	725	ASP
1	B	732	LEU
1	B	749	ASP
1	C	37	ARG
1	C	159	ILE
1	C	191	THR
1	C	205	ILE
1	C	213	LYS
1	C	252	ASN
1	C	432	PRO
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS
1	C	488	ARG
1	C	521	ARG
1	C	530	GLN
1	C	552	LEU
1	C	568	ASP
1	C	571	LEU
1	C	583[A]	LYS
1	C	583[B]	LYS
1	C	616	LEU
1	C	617	LEU
1	C	648	LEU
1	C	709	LYS
1	C	713	GLN
1	C	725	ASP
1	C	732	LEU
1	C	733	LEU
1	C	750	LYS
1	C	751	ILE
1	D	191	THR
1	D	205	ILE
1	D	213	LYS
1	D	252	ASN
1	D	344	GLU
1	D	369	ARG
1	D	432	PRO
1	D	440	TYR
1	D	459	ASN
1	D	530	GLN
1	D	554	LEU

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Mol	Chain	Res	Type
1	D	574	THR
1	D	582	LEU
1	D	593	ILE
1	D	616	LEU
1	D	633	LEU
1	D	648	LEU
1	D	713	GLN
1	D	747	LYS
1	D	750	LYS
1	D	751	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	66	ASN
1	A	201	ASN
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	A	530	GLN
1	A	556	GLN
1	A	713	GLN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	530	GLN
1	B	629	HIS
1	B	713	GLN
1	C	201	ASN
1	C	252	ASN
1	C	419	GLN
1	C	459	ASN
1	C	507	HIS
1	C	530	GLN
1	C	572	ASN
1	C	629	HIS
1	C	682	ASN
1	C	713	GLN
1	D	48	GLN
1	D	252	ASN
1	D	419	GLN

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Mol	Chain	Res	Type
1	D	459	ASN
1	D	507	HIS
1	D	530	GLN
1	D	556	GLN
1	D	629	HIS
1	D	671	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

8 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	HDD	D	801[A]	4,1	46,52,52	1.98	16 (34%)	62,89,89	3.07	26 (41%)
3	HEM	A	802[B]	4,1	50,50,50	2.41	21 (42%)	67,82,82	2.71	30 (44%)
3	HEM	B	802[B]	4	50,50,50	2.52	22 (44%)	67,82,82	2.77	33 (49%)
2	HDD	C	801[A]	4,1	46,52,52	1.96	13 (28%)	62,89,89	2.38	23 (37%)
3	HEM	D	802[B]	4,1	50,50,50	2.59	21 (42%)	67,82,82	2.84	31 (46%)
3	HEM	C	802[B]	-	50,50,50	2.46	23 (46%)	67,82,82	2.91	32 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HDD	B	801[A]	4,1	46,52,52	1.94	14 (30%)	62,89,89	3.07	22 (35%)
2	HDD	A	801[A]	4,1	46,52,52	1.94	13 (28%)	62,89,89	3.05	24 (38%)

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	HDD	D	801[A]	4,1	-	2/9/89/89	0/1/9/9
3	HEM	A	802[B]	4,1	-	3/14/54/54	-
3	HEM	B	802[B]	4	-	2/14/54/54	-
2	HDD	C	801[A]	4,1	-	2/9/89/89	0/1/9/9
3	HEM	D	802[B]	4,1	-	3/14/54/54	-
3	HEM	C	802[B]	-	-	4/14/54/54	-
2	HDD	B	801[A]	4,1	-	3/9/89/89	0/1/9/9
2	HDD	A	801[A]	4,1	-	3/9/89/89	0/1/9/9

All (143) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802[B]	HEM	FE-ND	5.95	2.13	1.94
3	D	802[B]	HEM	FE-ND	5.49	2.11	1.94
3	C	802[B]	HEM	FE-ND	5.39	2.11	1.94
3	C	802[B]	HEM	FE-NB	5.26	2.11	1.94
3	B	802[B]	HEM	FE-ND	5.23	2.11	1.94
2	B	801[A]	HDD	C4C-NC	-5.20	1.29	1.39
3	D	802[B]	HEM	FE-NB	5.18	2.10	1.94
3	C	802[B]	HEM	C1C-NC	5.10	1.49	1.39
2	A	801[A]	HDD	CHB-C1B	5.06	1.48	1.38
3	B	802[B]	HEM	C1C-NC	4.93	1.48	1.39
3	D	802[B]	HEM	C1C-NC	4.92	1.48	1.39
3	D	802[B]	HEM	C4C-NC	4.91	1.48	1.39
2	C	801[A]	HDD	C1A-NA	-4.81	1.30	1.39
3	B	802[B]	HEM	C1A-NA	4.81	1.48	1.39
3	B	802[B]	HEM	FE-NB	4.77	2.09	1.94
2	B	801[A]	HDD	C4D-ND	4.74	1.45	1.37
3	B	802[B]	HEM	C4A-NA	4.74	1.48	1.39
3	A	802[B]	HEM	C1C-NC	4.64	1.48	1.39
2	D	801[A]	HDD	O1D-CGD	4.53	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801[A]	HDD	CHB-C1B	4.48	1.47	1.38
3	D	802[B]	HEM	C1A-NA	4.36	1.47	1.39
3	C	802[B]	HEM	C4C-NC	4.31	1.47	1.39
2	A	801[A]	HDD	CHC-C4B	4.28	1.46	1.38
2	C	801[A]	HDD	CHC-C4B	4.27	1.46	1.38
3	A	802[B]	HEM	FE-NB	4.23	2.07	1.94
2	C	801[A]	HDD	CHB-C4A	4.23	1.48	1.39
3	A	802[B]	HEM	C4A-NA	4.22	1.47	1.39
3	A	802[B]	HEM	CHA-C4D	4.20	1.46	1.38
3	D	802[B]	HEM	C3D-C2D	4.16	1.45	1.36
2	B	801[A]	HDD	CHB-C1B	4.14	1.46	1.38
3	B	802[B]	HEM	CHA-C4D	4.11	1.46	1.38
3	B	802[B]	HEM	CHC-C1C	4.10	1.46	1.38
2	C	801[A]	HDD	CHC-C1C	4.09	1.48	1.39
3	C	802[B]	HEM	CHD-C4C	4.07	1.46	1.38
3	C	802[B]	HEM	C3C-C2C	4.07	1.45	1.37
3	D	802[B]	HEM	CHA-C4D	4.04	1.46	1.38
3	D	802[B]	HEM	CHD-C1D	4.04	1.48	1.39
3	C	802[B]	HEM	CHD-C1D	4.03	1.48	1.39
3	A	802[B]	HEM	C1A-NA	4.02	1.47	1.39
3	C	802[B]	HEM	CHA-C4D	4.00	1.46	1.38
3	B	802[B]	HEM	C3C-C2C	3.98	1.45	1.37
3	A	802[B]	HEM	C3C-C2C	3.98	1.45	1.37
2	A	801[A]	HDD	OND-C2D	3.97	1.50	1.42
3	D	802[B]	HEM	C3C-C2C	3.94	1.45	1.37
3	C	802[B]	HEM	C3D-C2D	3.90	1.45	1.36
3	A	802[B]	HEM	CHC-C1C	3.89	1.46	1.38
2	A	801[A]	HDD	C4C-NC	-3.84	1.32	1.39
3	A	802[B]	HEM	CHD-C1D	3.81	1.47	1.39
3	A	802[B]	HEM	C3D-C2D	3.80	1.45	1.36
3	A	802[B]	HEM	C4C-NC	3.73	1.46	1.39
3	D	802[B]	HEM	C4A-NA	3.70	1.46	1.39
3	A	802[B]	HEM	C1B-NB	-3.66	1.33	1.40
2	D	801[A]	HDD	CHA-C1A	3.60	1.47	1.39
3	C	802[B]	HEM	CHC-C1C	3.58	1.45	1.38
3	D	802[B]	HEM	CHA-C1A	3.58	1.47	1.39
2	D	801[A]	HDD	C4C-NC	-3.55	1.32	1.39
3	B	802[B]	HEM	CHC-C4B	3.53	1.47	1.39
3	C	802[B]	HEM	C4A-NA	3.48	1.46	1.39
2	C	801[A]	HDD	CHB-C1B	3.47	1.45	1.38
3	C	802[B]	HEM	C3B-C2B	3.37	1.44	1.37
3	D	802[B]	HEM	C3B-C2B	3.33	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	802[B]	HEM	C1A-NA	3.32	1.45	1.39
3	B	802[B]	HEM	C1B-NB	-3.32	1.34	1.40
2	D	801[A]	HDD	C1A-NA	-3.31	1.33	1.39
3	D	802[B]	HEM	C1C-C2C	3.30	1.51	1.45
3	D	802[B]	HEM	CHC-C4B	3.29	1.46	1.39
3	B	802[B]	HEM	CHD-C4C	3.27	1.44	1.38
2	C	801[A]	HDD	C4C-NC	-3.25	1.33	1.39
3	B	802[B]	HEM	CHD-C1D	3.24	1.46	1.39
2	B	801[A]	HDD	O1D-C3D	3.19	1.51	1.46
3	D	802[B]	HEM	CHD-C4C	3.18	1.44	1.38
2	A	801[A]	HDD	CAD-C3D	-3.15	1.48	1.53
2	D	801[A]	HDD	OND-C2D	3.14	1.48	1.42
3	B	802[B]	HEM	C4C-NC	3.13	1.45	1.39
2	A	801[A]	HDD	CHB-C4A	3.07	1.46	1.39
2	B	801[A]	HDD	O1D-CGD	3.04	1.40	1.35
3	C	802[B]	HEM	C4D-ND	-3.03	1.35	1.40
2	B	801[A]	HDD	C4A-C3A	3.01	1.50	1.43
2	A	801[A]	HDD	O1D-C3D	3.01	1.51	1.46
3	B	802[B]	HEM	C3D-C2D	2.95	1.43	1.36
3	B	802[B]	HEM	C3B-C2B	2.94	1.43	1.37
2	B	801[A]	HDD	CHB-C4A	2.93	1.46	1.39
3	D	802[B]	HEM	CHB-C1B	2.93	1.44	1.38
2	B	801[A]	HDD	CHA-C1A	2.91	1.45	1.39
3	D	802[B]	HEM	C4D-ND	-2.90	1.35	1.40
3	B	802[B]	HEM	C2A-C3A	2.86	1.46	1.38
3	A	802[B]	HEM	C2A-C3A	2.85	1.46	1.38
2	D	801[A]	HDD	CMC-C2C	2.84	1.56	1.50
3	B	802[B]	HEM	C1A-C2A	2.82	1.50	1.44
2	C	801[A]	HDD	O1A-CGA	2.81	1.31	1.22
3	B	802[B]	HEM	C1C-C2C	2.81	1.50	1.45
3	C	802[B]	HEM	C2A-C3A	2.80	1.46	1.38
3	D	802[B]	HEM	C2A-C3A	2.76	1.46	1.38
3	A	802[B]	HEM	CHB-C1B	2.75	1.44	1.38
3	D	802[B]	HEM	CHC-C1C	2.74	1.43	1.38
2	A	801[A]	HDD	C3B-C2B	2.72	1.42	1.37
2	D	801[A]	HDD	C1C-NC	-2.68	1.34	1.39
2	D	801[A]	HDD	CHC-C4B	2.66	1.43	1.38
3	D	802[B]	HEM	C1B-NB	-2.65	1.35	1.40
2	C	801[A]	HDD	CHA-C1A	2.63	1.45	1.39
2	C	801[A]	HDD	C4A-NA	-2.63	1.34	1.39
3	D	802[B]	HEM	C1A-C2A	2.62	1.49	1.44
3	A	802[B]	HEM	CHC-C4B	2.60	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801[A]	HDD	O1D-CGD	2.60	1.39	1.35
2	D	801[A]	HDD	CMA-C3A	2.59	1.56	1.50
3	C	802[B]	HEM	C1A-C2A	2.58	1.49	1.44
2	A	801[A]	HDD	CHA-C1A	2.58	1.45	1.39
2	D	801[A]	HDD	CMD-C2D	2.56	1.56	1.53
2	D	801[A]	HDD	C1B-C2B	2.53	1.50	1.45
3	A	802[B]	HEM	C1A-C2A	2.50	1.49	1.44
3	B	802[B]	HEM	CHA-C1A	2.48	1.45	1.39
2	C	801[A]	HDD	O1D-C3D	2.48	1.50	1.46
3	B	802[B]	HEM	C4A-C3A	2.47	1.48	1.43
3	A	802[B]	HEM	CHB-C4A	2.46	1.44	1.39
2	B	801[A]	HDD	CHC-C1C	2.45	1.44	1.39
2	A	801[A]	HDD	CHC-C1C	2.44	1.44	1.39
3	C	802[B]	HEM	C4A-C3A	2.43	1.48	1.43
3	A	802[B]	HEM	CHD-C4C	2.42	1.43	1.38
2	D	801[A]	HDD	CHD-C4C	2.40	1.44	1.39
3	A	802[B]	HEM	CHA-C1A	2.39	1.44	1.39
3	B	802[B]	HEM	CHB-C1B	2.38	1.43	1.38
2	B	801[A]	HDD	CHC-C4B	2.34	1.43	1.38
2	D	801[A]	HDD	C1C-C2C	2.34	1.48	1.43
2	D	801[A]	HDD	CHB-C4A	2.34	1.44	1.39
2	B	801[A]	HDD	C1C-NC	-2.32	1.35	1.39
2	B	801[A]	HDD	C4B-NB	-2.32	1.35	1.39
3	C	802[B]	HEM	CHA-C1A	2.27	1.44	1.39
2	A	801[A]	HDD	C1C-C2C	2.26	1.48	1.43
2	B	801[A]	HDD	CHD-C4C	2.25	1.44	1.39
3	C	802[B]	HEM	C1B-NB	-2.23	1.36	1.40
3	C	802[B]	HEM	CHB-C4A	2.23	1.44	1.39
2	A	801[A]	HDD	C1A-NA	-2.20	1.35	1.39
3	C	802[B]	HEM	O1A-CGA	2.18	1.29	1.22
3	A	802[B]	HEM	C3B-C2B	2.18	1.41	1.37
2	D	801[A]	HDD	CBA-CAA	2.13	1.59	1.51
3	A	802[B]	HEM	C4D-ND	-2.12	1.36	1.40
3	C	802[B]	HEM	CHB-C1B	2.11	1.42	1.38
3	C	802[B]	HEM	CHC-C4B	2.08	1.43	1.39
2	C	801[A]	HDD	C1B-C2B	2.07	1.49	1.45
2	C	801[A]	HDD	C2A-C3A	2.05	1.44	1.38
3	B	802[B]	HEM	CHB-C4A	2.04	1.44	1.39
2	B	801[A]	HDD	C3B-C2B	2.04	1.41	1.37
2	A	801[A]	HDD	C2A-C3A	2.03	1.44	1.38

All (221) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801[A]	HDD	O1D-CGD-CBD	-10.34	100.74	110.17
2	B	801[A]	HDD	O1D-CGD-O2D	10.04	129.27	120.81
2	D	801[A]	HDD	C3D-O1D-CGD	9.48	119.98	111.14
2	B	801[A]	HDD	OND-C2D-CMD	-9.16	91.74	109.45
2	A	801[A]	HDD	O1D-CGD-O2D	8.75	128.18	120.81
2	D	801[A]	HDD	O1D-CGD-O2D	8.69	128.13	120.81
2	A	801[A]	HDD	C3C-C2C-C1C	-8.04	97.70	107.17
2	B	801[A]	HDD	C3C-C2C-C1C	-7.84	97.93	107.17
3	A	802[B]	HEM	C3B-C2B-C1B	-7.73	100.61	106.41
2	B	801[A]	HDD	O1D-CGD-CBD	-7.65	103.20	110.17
3	C	802[B]	HEM	C3B-C4B-NB	7.64	114.96	109.47
2	A	801[A]	HDD	C3D-O1D-CGD	7.51	118.15	111.14
3	D	802[B]	HEM	C2B-C1B-NB	7.50	118.47	109.84
3	D	802[B]	HEM	C3B-C2B-C1B	-7.08	101.09	106.41
2	B	801[A]	HDD	C3D-O1D-CGD	7.08	117.74	111.14
3	C	802[B]	HEM	C3B-C2B-C1B	-6.86	101.26	106.41
2	D	801[A]	HDD	C3C-C2C-C1C	-6.80	99.15	107.17
3	B	802[B]	HEM	C2B-C1B-NB	6.77	117.62	109.84
3	D	802[B]	HEM	C4C-NC-C1C	-6.44	95.32	105.82
3	B	802[B]	HEM	C3B-C2B-C1B	-6.40	101.60	106.41
3	A	802[B]	HEM	C2B-C1B-NB	6.39	117.18	109.84
3	A	802[B]	HEM	C3D-C4D-ND	6.26	117.04	110.17
3	C	802[B]	HEM	C2B-C1B-NB	6.21	116.98	109.84
2	D	801[A]	HDD	O1D-CGD-CBD	-6.19	104.53	110.17
3	C	802[B]	HEM	C3D-C4D-ND	6.01	116.76	110.17
3	B	802[B]	HEM	C2D-C1D-ND	5.99	116.83	109.90
2	D	801[A]	HDD	C3B-C2B-C1B	-5.98	101.39	107.05
3	D	802[B]	HEM	C3B-C4B-NB	5.95	113.74	109.47
2	D	801[A]	HDD	CMC-C2C-C1C	5.91	134.42	125.42
3	D	802[B]	HEM	C3D-C4D-ND	5.89	116.63	110.17
2	C	801[A]	HDD	C3C-C2C-C1C	-5.85	100.27	107.17
3	A	802[B]	HEM	C2D-C1D-ND	5.83	116.64	109.90
3	B	802[B]	HEM	C3C-C2C-C1C	-5.70	101.65	107.05
2	C	801[A]	HDD	O1D-CGD-O2D	5.68	125.60	120.81
2	C	801[A]	HDD	OND-C2D-CMD	-5.64	98.54	109.45
3	C	802[B]	HEM	C2D-C1D-ND	5.62	116.39	109.90
2	A	801[A]	HDD	C3B-C2B-C1B	-5.40	101.93	107.05
3	B	802[B]	HEM	C3D-C4D-ND	5.34	116.02	110.17
2	D	801[A]	HDD	CBD-CAD-C3D	5.34	111.59	103.98
2	C	801[A]	HDD	C3B-C2B-C1B	-5.32	102.01	107.05
3	D	802[B]	HEM	C2D-C1D-ND	5.20	115.91	109.90
2	C	801[A]	HDD	C3C-C4C-NC	5.14	114.12	109.80
3	D	802[B]	HEM	CMC-C2C-C1C	5.11	133.72	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801[A]	HDD	C3B-C2B-C1B	-5.00	102.32	107.05
3	D	802[B]	HEM	C3C-C2C-C1C	-4.99	102.32	107.05
3	D	802[B]	HEM	CHD-C4C-C3C	-4.94	116.87	125.21
3	C	802[B]	HEM	C1D-C2D-C3D	-4.94	101.78	106.98
2	D	801[A]	HDD	C3C-C4C-NC	4.82	113.86	109.80
3	C	802[B]	HEM	C3C-C2C-C1C	-4.81	102.50	107.05
2	D	801[A]	HDD	CAA-CBA-CGA	-4.71	101.17	113.67
2	B	801[A]	HDD	C4A-C3A-C2A	-4.68	101.45	106.82
2	B	801[A]	HDD	CAA-CBA-CGA	-4.64	101.35	113.67
2	A	801[A]	HDD	C2C-C1C-NC	4.62	117.54	110.14
3	C	802[B]	HEM	C2A-C1A-NA	4.56	115.21	110.15
3	B	802[B]	HEM	C4A-NA-C1A	-4.55	98.40	105.82
3	A	802[B]	HEM	C3C-C2C-C1C	-4.54	102.75	107.05
3	C	802[B]	HEM	CHC-C1C-C2C	-4.52	116.08	125.49
2	C	801[A]	HDD	C2D-C1D-CHD	-4.46	117.34	124.27
3	A	802[B]	HEM	C3B-C4B-NB	4.44	112.66	109.47
3	D	802[B]	HEM	C2C-C1C-NC	4.42	117.82	109.64
2	A	801[A]	HDD	OND-C2D-CMD	-4.33	101.07	109.45
2	C	801[A]	HDD	CBD-CAD-C3D	4.31	110.13	103.98
2	B	801[A]	HDD	CMC-C2C-C1C	4.28	131.94	125.42
2	A	801[A]	HDD	C3C-C4C-NC	4.25	113.38	109.80
3	C	802[B]	HEM	C4C-NC-C1C	-4.22	98.94	105.82
3	B	802[B]	HEM	C2A-C1A-NA	4.17	114.78	110.15
3	A	802[B]	HEM	C1D-C2D-C3D	-4.13	102.63	106.98
3	B	802[B]	HEM	C4C-NC-C1C	-4.13	99.09	105.82
3	B	802[B]	HEM	CMC-C2C-C1C	4.12	131.99	124.73
3	A	802[B]	HEM	C4D-ND-C1D	-4.11	100.34	105.21
3	D	802[B]	HEM	C1D-C2D-C3D	-4.10	102.67	106.98
2	A	801[A]	HDD	O1D-C3D-CAD	-4.06	95.55	103.06
2	C	801[A]	HDD	CAA-CBA-CGA	-4.06	102.90	113.67
2	A	801[A]	HDD	CMC-C2C-C1C	4.01	131.52	125.42
3	C	802[B]	HEM	C2C-C1C-NC	3.97	116.99	109.64
3	A	802[B]	HEM	C4C-NC-C1C	-3.95	99.38	105.82
3	B	802[B]	HEM	C4D-ND-C1D	-3.94	100.54	105.21
2	D	801[A]	HDD	C2C-C1C-NC	3.93	116.44	110.14
2	B	801[A]	HDD	C2C-C1C-NC	3.89	116.39	110.14
2	D	801[A]	HDD	OND-C2D-CMD	-3.89	101.93	109.45
3	A	802[B]	HEM	CAA-CBA-CGA	-3.88	103.36	113.67
3	C	802[B]	HEM	C4A-NA-C1A	-3.73	99.74	105.82
2	A	801[A]	HDD	CHC-C1C-C2C	-3.72	116.64	127.43
2	A	801[A]	HDD	CAA-C2A-C1A	3.70	132.17	124.94
3	C	802[B]	HEM	C1C-CHC-C4B	-3.69	118.17	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	801[A]	HDD	C2C-C1C-NC	3.65	115.98	110.14
3	B	802[B]	HEM	C1D-C2D-C3D	-3.62	103.17	106.98
3	B	802[B]	HEM	CHB-C1B-C2B	-3.57	116.81	126.95
3	B	802[B]	HEM	CMB-C2B-C3B	3.56	137.05	128.43
3	B	802[B]	HEM	CHA-C4D-C3D	-3.54	118.71	125.23
3	C	802[B]	HEM	C4D-ND-C1D	-3.53	101.03	105.21
2	B	801[A]	HDD	CHB-C1B-NB	-3.52	120.62	124.45
2	D	801[A]	HDD	CAA-C2A-C1A	3.49	131.76	124.94
2	A	801[A]	HDD	CHB-C1B-C2B	-3.46	118.28	125.49
3	B	802[B]	HEM	CBD-CAD-C3D	-3.46	102.97	112.53
2	A	801[A]	HDD	CAA-CBA-CGA	-3.46	104.50	113.67
3	B	802[B]	HEM	C3A-C4A-NA	3.45	115.68	110.14
3	C	802[B]	HEM	CHC-C4B-C3B	-3.43	118.22	125.07
2	D	801[A]	HDD	CHC-C4B-NB	-3.43	120.71	124.45
3	D	802[B]	HEM	C1B-NB-C4B	-3.43	101.14	105.21
3	C	802[B]	HEM	C1B-NB-C4B	-3.43	101.15	105.21
2	B	801[A]	HDD	CBD-CAD-C3D	3.42	108.85	103.98
3	B	802[B]	HEM	C2C-C1C-NC	3.40	115.93	109.64
3	A	802[B]	HEM	CMB-C2B-C1B	3.40	130.35	125.03
3	A	802[B]	HEM	CHC-C1C-C2C	-3.36	118.49	125.49
3	B	802[B]	HEM	CHB-C4A-C3A	-3.35	117.71	127.43
2	C	801[A]	HDD	CMC-C2C-C1C	3.33	130.49	125.42
3	D	802[B]	HEM	CHB-C1B-C2B	-3.25	117.70	126.95
3	A	802[B]	HEM	C4A-NA-C1A	-3.25	100.52	105.82
3	C	802[B]	HEM	CBD-CAD-C3D	-3.23	103.60	112.53
3	A	802[B]	HEM	CHD-C1D-C2D	-3.22	119.94	125.03
3	A	802[B]	HEM	C2C-C1C-NC	3.20	115.56	109.64
3	A	802[B]	HEM	C4A-CHB-C1B	-3.19	118.75	126.25
2	D	801[A]	HDD	O1D-C3D-CAD	-3.16	97.21	103.06
3	A	802[B]	HEM	CBB-CAB-C3B	-3.16	111.73	127.53
3	C	802[B]	HEM	CHB-C1B-C2B	-3.15	117.99	126.95
3	A	802[B]	HEM	CHB-C4A-C3A	-3.15	118.28	127.43
2	B	801[A]	HDD	CMD-C2D-C3D	3.15	123.39	115.11
3	A	802[B]	HEM	CHB-C1B-C2B	-3.06	118.24	126.95
3	D	802[B]	HEM	CAD-C3D-C2D	3.06	133.60	127.87
2	D	801[A]	HDD	C1C-CHC-C4B	3.04	134.04	124.66
3	C	802[B]	HEM	CHA-C1A-C2A	-3.02	118.68	125.30
2	C	801[A]	HDD	C4A-C3A-C2A	-3.00	103.38	106.82
3	D	802[B]	HEM	C4D-ND-C1D	-2.99	101.67	105.21
2	B	801[A]	HDD	CAD-CBD-CGD	2.98	108.91	104.48
3	C	802[B]	HEM	C4A-CHB-C1B	-2.96	119.28	126.25
3	D	802[B]	HEM	CHD-C1D-C2D	-2.96	120.36	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	802[B]	HEM	CBB-CAB-C3B	-2.95	112.81	127.53
3	B	802[B]	HEM	C3B-C4B-NB	2.94	111.58	109.47
3	B	802[B]	HEM	CAA-C2A-C1A	2.94	130.68	124.94
3	A	802[B]	HEM	C2A-C1A-NA	2.91	113.38	110.15
3	B	802[B]	HEM	CHD-C1D-C2D	-2.87	120.49	125.03
2	D	801[A]	HDD	CHB-C1B-NB	-2.85	121.35	124.45
3	C	802[B]	HEM	CHA-C4D-C3D	-2.83	120.00	125.23
3	C	802[B]	HEM	C3A-C4A-NA	2.82	114.67	110.14
3	D	802[B]	HEM	CHC-C1C-C2C	-2.82	119.61	125.49
2	B	801[A]	HDD	CMA-C3A-C2A	2.82	131.60	125.62
3	A	802[B]	HEM	CHA-C4D-C3D	-2.80	120.06	125.23
2	D	801[A]	HDD	C2D-C1D-CHD	-2.79	119.93	124.27
3	B	802[B]	HEM	CHD-C4C-C3C	-2.79	120.51	125.21
3	D	802[B]	HEM	C4A-CHB-C1B	-2.79	119.70	126.25
2	A	801[A]	HDD	C2B-C1B-NB	2.78	114.78	109.64
3	B	802[B]	HEM	CHC-C1C-NC	-2.77	121.43	124.45
3	D	802[B]	HEM	CMB-C2B-C3B	2.77	135.13	128.43
3	D	802[B]	HEM	C4C-CHD-C1D	-2.77	120.14	126.02
3	A	802[B]	HEM	CMC-C2C-C1C	2.76	129.59	124.73
2	C	801[A]	HDD	C4B-C3B-C2B	2.71	109.17	106.81
2	B	801[A]	HDD	CBA-CAA-C2A	-2.71	105.04	112.53
3	C	802[B]	HEM	C4C-C3C-C2C	2.70	109.15	106.81
2	B	801[A]	HDD	C2B-C1B-NB	2.68	114.60	109.64
3	C	802[B]	HEM	CHD-C1D-C2D	-2.68	120.79	125.03
3	C	802[B]	HEM	CMC-C2C-C1C	2.66	129.41	124.73
3	C	802[B]	HEM	C4C-CHD-C1D	-2.66	120.37	126.02
3	D	802[B]	HEM	C4D-C3D-C2D	-2.61	103.09	106.89
3	A	802[B]	HEM	CAA-C2A-C1A	2.60	130.03	124.94
3	D	802[B]	HEM	CBD-CAD-C3D	-2.59	105.38	112.53
3	D	802[B]	HEM	C1C-CHC-C4B	-2.57	120.56	126.02
3	B	802[B]	HEM	C4C-C3C-C2C	2.53	109.01	106.81
2	C	801[A]	HDD	CMD-C2D-C3D	2.53	121.78	115.11
3	C	802[B]	HEM	CHB-C4A-C3A	-2.53	120.09	127.43
3	A	802[B]	HEM	C4D-C3D-C2D	-2.52	103.22	106.89
2	D	801[A]	HDD	O2A-CGA-CBA	2.52	121.96	114.00
3	A	802[B]	HEM	C1B-NB-C4B	-2.51	102.24	105.21
3	B	802[B]	HEM	O2A-CGA-O1A	-2.51	116.88	123.33
3	B	802[B]	HEM	C4D-C3D-C2D	-2.48	103.28	106.89
3	B	802[B]	HEM	C4A-CHB-C1B	-2.48	120.42	126.25
3	B	802[B]	HEM	C1A-CHA-C4D	-2.46	120.45	126.25
2	A	801[A]	HDD	C2A-C1A-NA	2.46	112.89	110.15
2	B	801[A]	HDD	CHC-C1C-C2C	-2.46	120.29	127.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	802[B]	HEM	CAA-CBA-CGA	-2.43	107.21	113.67
2	C	801[A]	HDD	CAA-C2A-C1A	2.43	129.69	124.94
2	D	801[A]	HDD	C3D-C4D-CHA	-2.43	117.09	124.14
2	A	801[A]	HDD	C4C-NC-C1C	-2.39	101.92	105.82
3	B	802[B]	HEM	CAD-C3D-C2D	2.38	132.32	127.87
2	C	801[A]	HDD	CHD-C1D-ND	2.38	127.56	124.28
3	A	802[B]	HEM	C3A-C4A-NA	2.37	113.94	110.14
3	B	802[B]	HEM	CMB-C2B-C1B	-2.37	121.33	125.03
2	B	801[A]	HDD	C3D-C4D-CHA	-2.36	117.30	124.14
3	A	802[B]	HEM	C4C-CHD-C1D	-2.35	121.02	126.02
3	C	802[B]	HEM	CAA-C2A-C1A	2.34	129.51	124.94
2	A	801[A]	HDD	O2A-CGA-CBA	2.33	121.35	114.00
2	C	801[A]	HDD	CHC-C1C-C2C	-2.31	120.72	127.43
2	C	801[A]	HDD	CBA-CAA-C2A	-2.31	106.16	112.53
2	D	801[A]	HDD	C2B-C1B-NB	2.29	113.88	109.64
2	D	801[A]	HDD	CMA-C3A-C2A	2.29	130.48	125.62
2	D	801[A]	HDD	OND-C2D-C3D	-2.29	105.10	110.46
3	D	802[B]	HEM	CHA-C4D-C3D	-2.28	121.02	125.23
3	C	802[B]	HEM	CMD-C2D-C3D	2.28	132.31	126.15
2	D	801[A]	HDD	CHB-C4A-C3A	-2.26	120.86	127.43
2	A	801[A]	HDD	C1A-C2A-C3A	-2.26	103.37	106.87
2	A	801[A]	HDD	CHB-C1B-NB	2.26	126.91	124.45
3	C	802[B]	HEM	CHC-C1C-NC	2.26	126.91	124.45
2	C	801[A]	HDD	C3D-O1D-CGD	2.25	113.24	111.14
3	D	802[B]	HEM	C4A-NA-C1A	-2.25	102.16	105.82
2	C	801[A]	HDD	C2B-C1B-NB	2.24	113.79	109.64
2	D	801[A]	HDD	CBA-CAA-C2A	-2.23	106.38	112.53
2	C	801[A]	HDD	O2A-CGA-CBA	2.23	121.03	114.00
3	A	802[B]	HEM	C1C-CHC-C4B	-2.22	121.29	126.02
2	D	801[A]	HDD	CHC-C1C-C2C	-2.22	120.99	127.43
3	D	802[B]	HEM	O2A-CGA-CBA	2.20	120.96	114.00
3	D	802[B]	HEM	CHB-C4A-C3A	-2.20	121.03	127.43
2	B	801[A]	HDD	CBC-CAC-C3C	-2.19	116.60	127.53
2	A	801[A]	HDD	C3D-C4D-CHA	-2.18	117.81	124.14
3	B	802[B]	HEM	CMD-C2D-C1D	2.18	128.44	125.03
3	D	802[B]	HEM	CMD-C2D-C3D	2.17	132.03	126.15
3	C	802[B]	HEM	C4D-C3D-C2D	-2.16	103.75	106.89
2	A	801[A]	HDD	C2D-C1D-CHD	-2.15	120.93	124.27
2	B	801[A]	HDD	C4C-C3C-C2C	2.14	109.96	107.30
2	A	801[A]	HDD	CMA-C3A-C4A	2.10	128.61	125.42
2	C	801[A]	HDD	CHB-C4A-C3A	-2.09	121.37	127.43
3	A	802[B]	HEM	CHB-C4A-NA	2.08	127.64	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	802[B]	HEM	CBB-CAB-C3B	-2.08	117.11	127.53
3	D	802[B]	HEM	C2A-C1A-NA	2.08	112.46	110.15
2	D	801[A]	HDD	C4C-NC-C1C	-2.07	102.44	105.82
2	A	801[A]	HDD	CMD-C2D-C3D	2.06	120.53	115.11
2	C	801[A]	HDD	CMA-C3A-C2A	2.06	129.99	125.62
2	C	801[A]	HDD	CMB-C2B-C3B	2.04	133.37	128.43
3	D	802[B]	HEM	CHC-C4B-C3B	-2.03	121.02	125.07
2	B	801[A]	HDD	CHB-C4A-C3A	-2.02	121.56	127.43
3	A	802[B]	HEM	C4C-C3C-C2C	2.02	108.56	106.81
3	B	802[B]	HEM	CMA-C3A-C2A	2.01	129.89	125.62

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	802[B]	HEM	C2B-C3B-CAB-CBB
3	C	802[B]	HEM	C4B-C3B-CAB-CBB
2	B	801[A]	HDD	CAA-CBA-CGA-O2A
3	A	802[B]	HEM	CAA-CBA-CGA-O2A
2	A	801[A]	HDD	CAA-CBA-CGA-O1A
2	B	801[A]	HDD	CAA-CBA-CGA-O1A
3	C	802[B]	HEM	CAA-CBA-CGA-O1A
3	C	802[B]	HEM	CAA-CBA-CGA-O2A
2	C	801[A]	HDD	CAA-CBA-CGA-O2A
2	D	801[A]	HDD	CAA-CBA-CGA-O1A
3	D	802[B]	HEM	CAA-CBA-CGA-O2A
2	A	801[A]	HDD	C2C-C3C-CAC-CBC
2	A	801[A]	HDD	CAA-CBA-CGA-O2A
2	C	801[A]	HDD	CAA-CBA-CGA-O1A
2	D	801[A]	HDD	CAA-CBA-CGA-O2A
3	D	802[B]	HEM	CAA-CBA-CGA-O1A
3	B	802[B]	HEM	CAA-CBA-CGA-O2A
3	A	802[B]	HEM	CAA-CBA-CGA-O1A
3	B	802[B]	HEM	CAA-CBA-CGA-O1A
2	B	801[A]	HDD	C2C-C3C-CAC-CBC
3	A	802[B]	HEM	C2B-C3B-CAB-CBB
3	D	802[B]	HEM	C2B-C3B-CAB-CBB

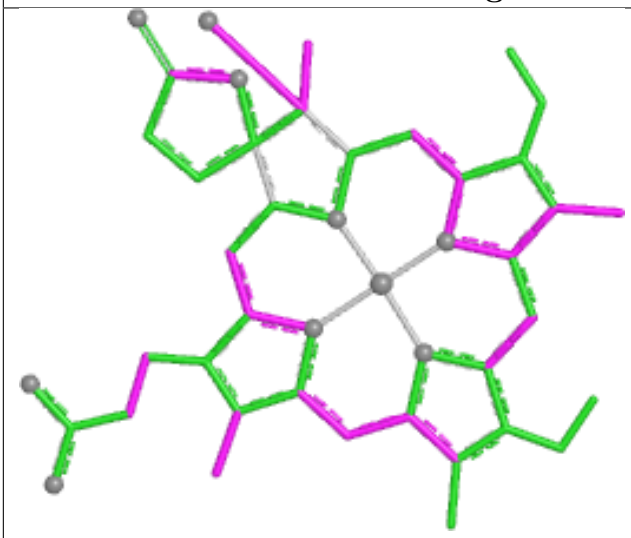
There are no ring outliers.

8 monomers are involved in 54 short contacts:

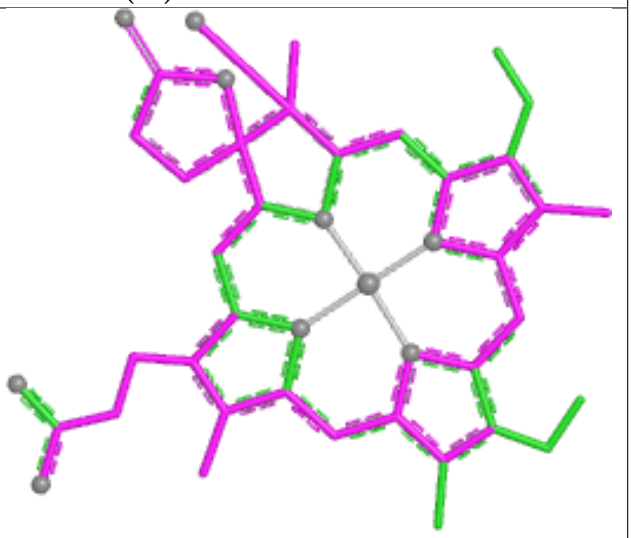
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801[A]	HDD	4	0
3	A	802[B]	HEM	13	0
3	B	802[B]	HEM	12	0
2	C	801[A]	HDD	2	0
3	D	802[B]	HEM	8	0
3	C	802[B]	HEM	13	0
2	B	801[A]	HDD	1	0
2	A	801[A]	HDD	1	0

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.

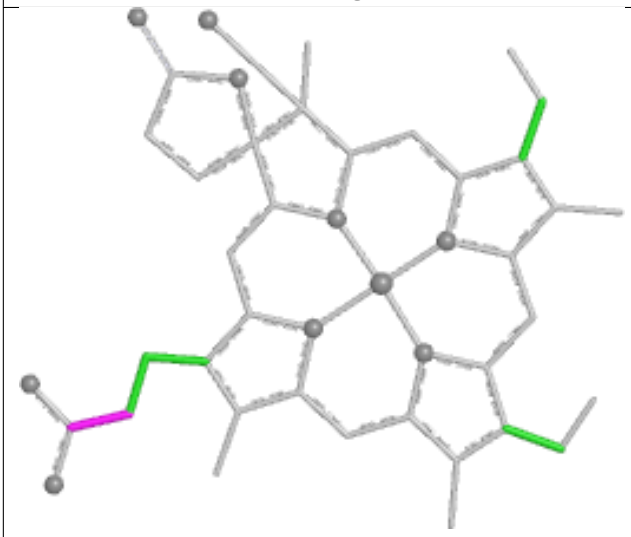
Ligand HDD D 801 (A)



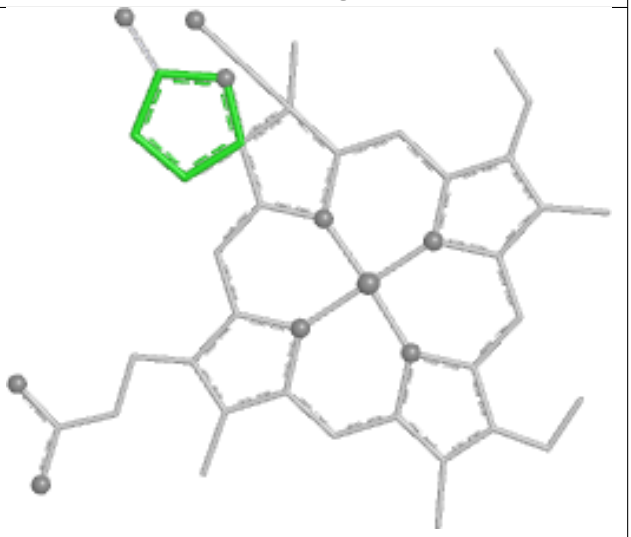
Bond lengths



Bond angles

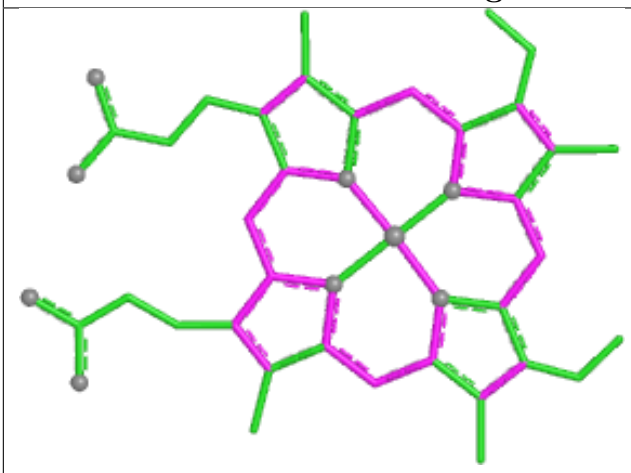


Torsions

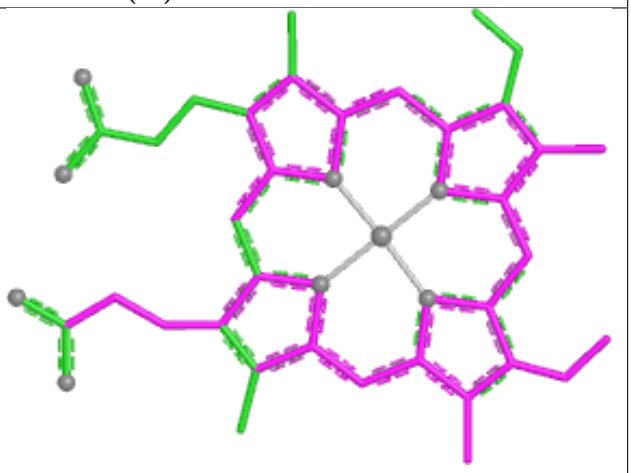


Rings

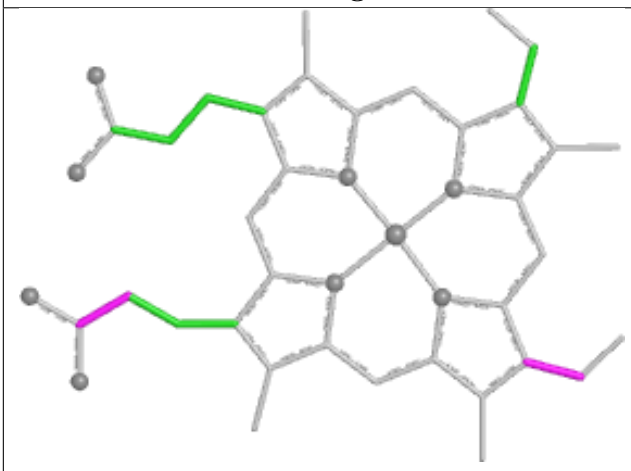
Ligand HEM A 802 (B)



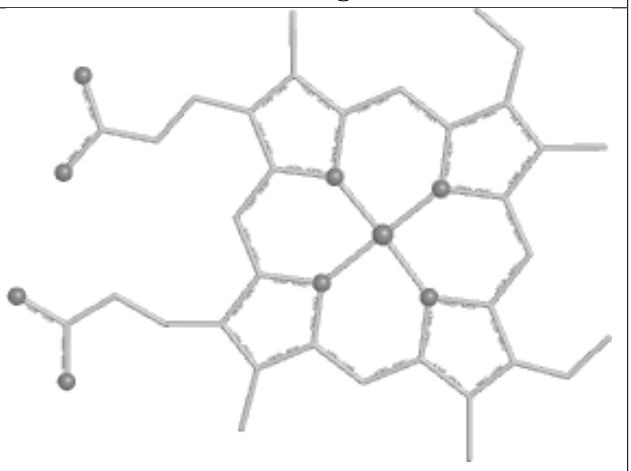
Bond lengths



Bond angles

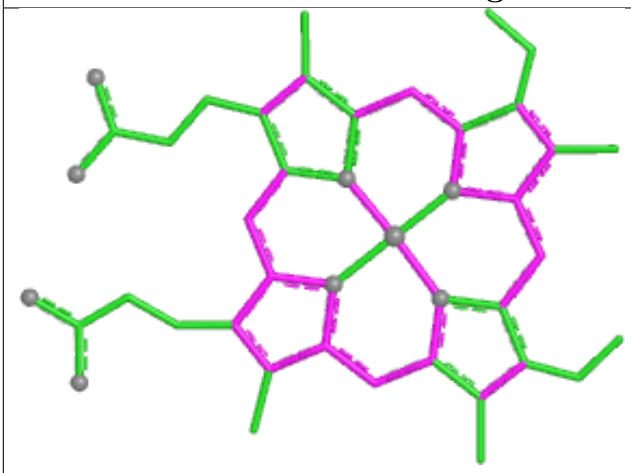


Torsions

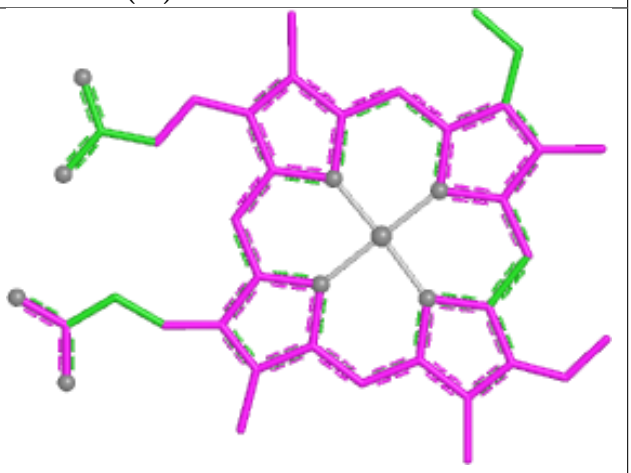


Rings

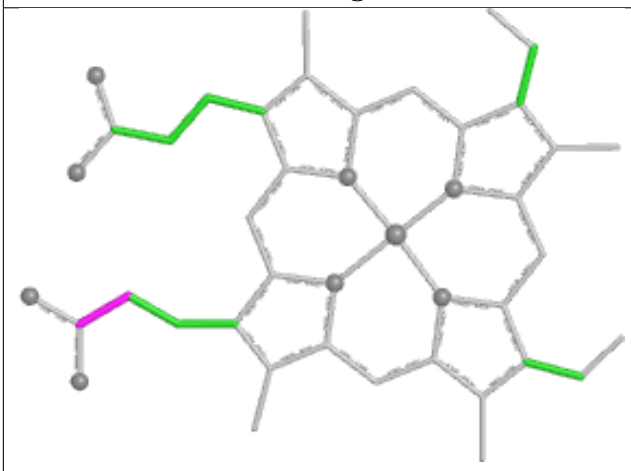
Ligand HEM B 802 (B)



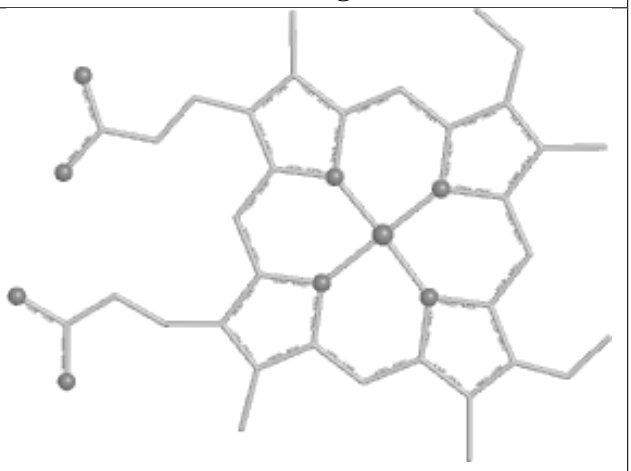
Bond lengths



Bond angles

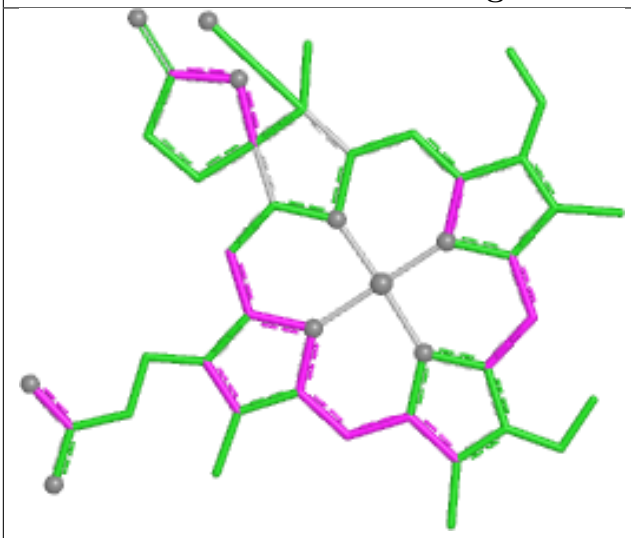


Torsions

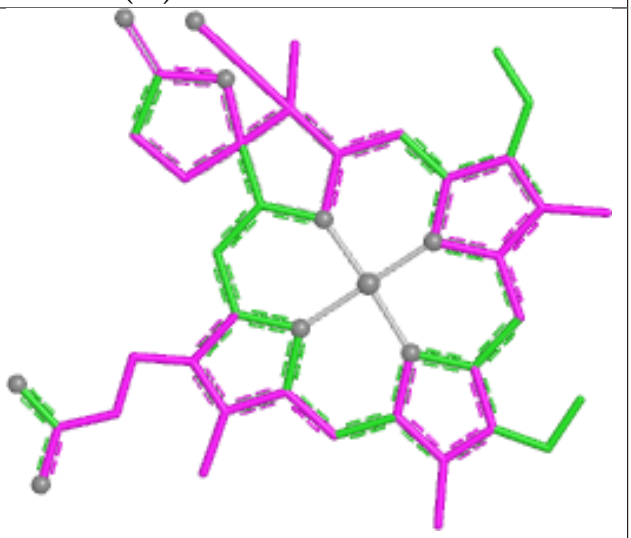


Rings

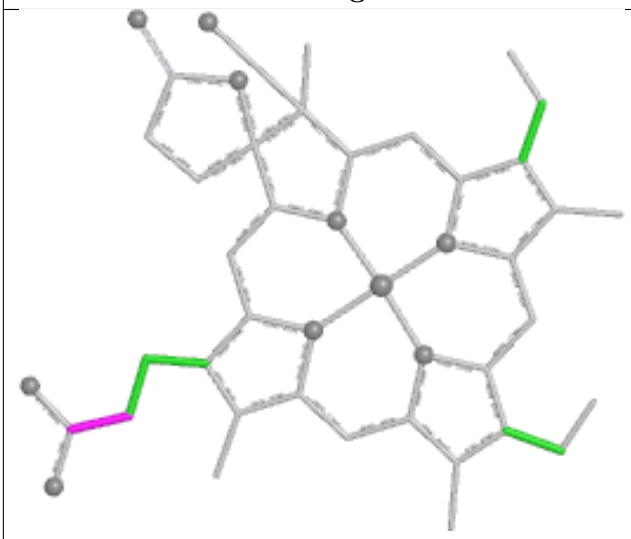
Ligand HDD C 801 (A)



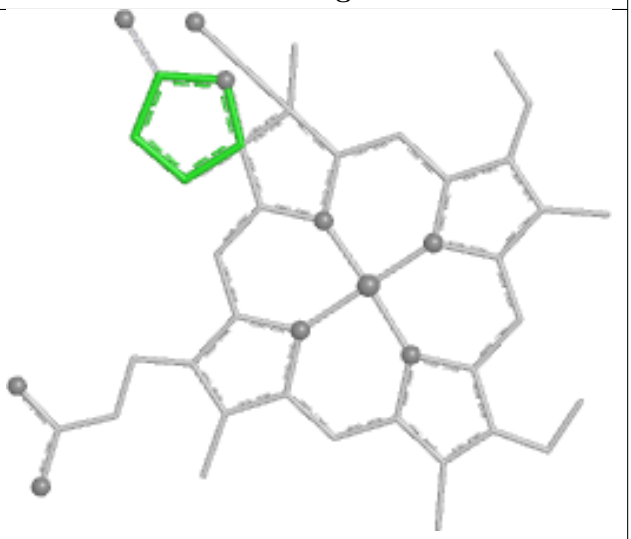
Bond lengths



Bond angles

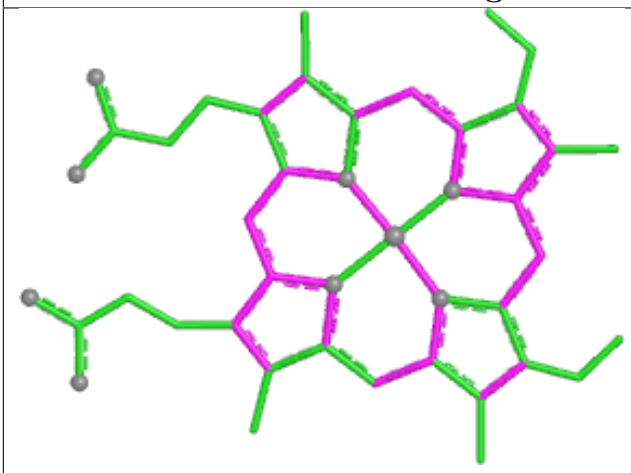


Torsions

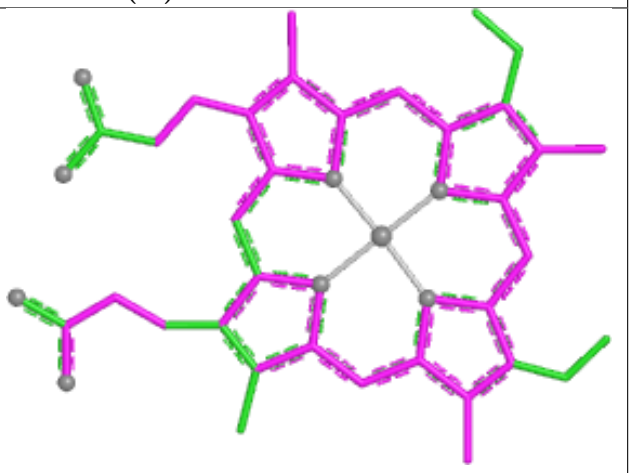


Rings

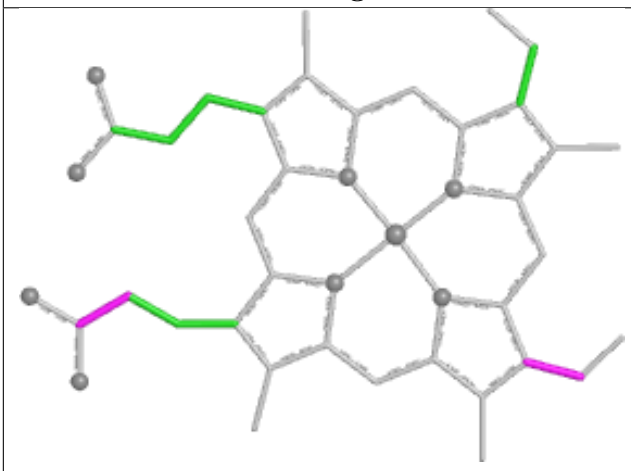
Ligand HEM D 802 (B)



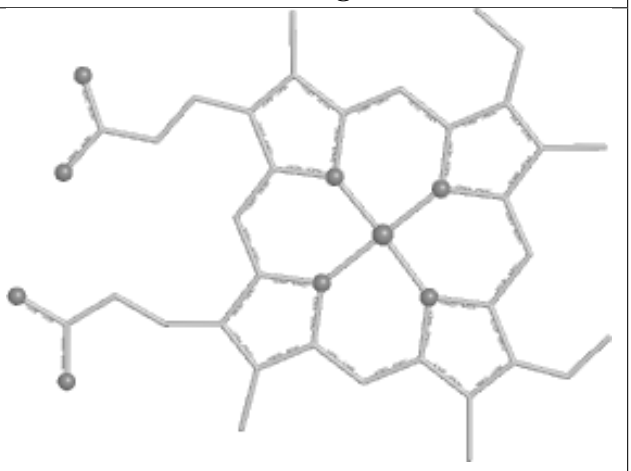
Bond lengths



Bond angles

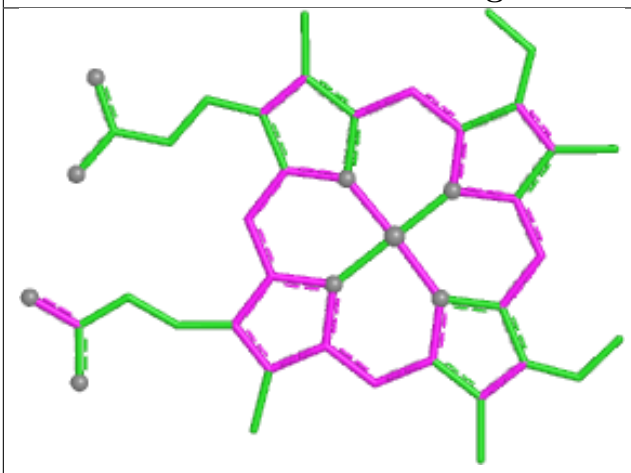


Torsions

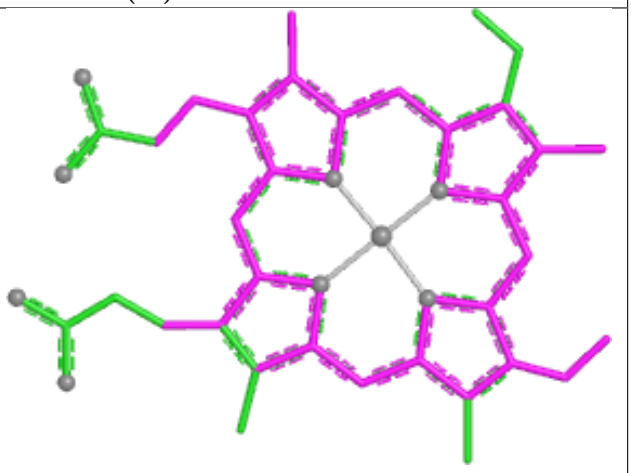


Rings

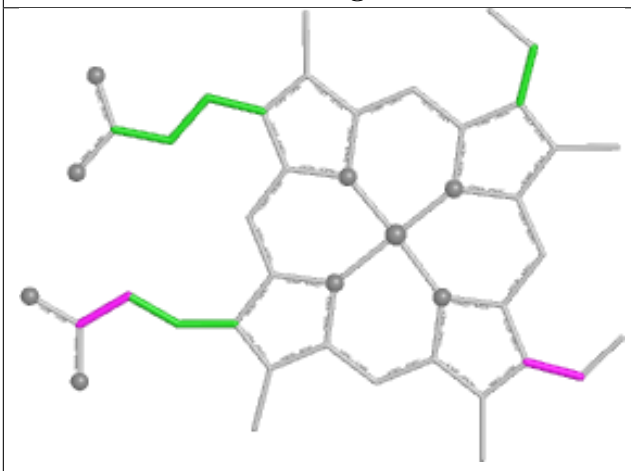
Ligand HEM C 802 (B)



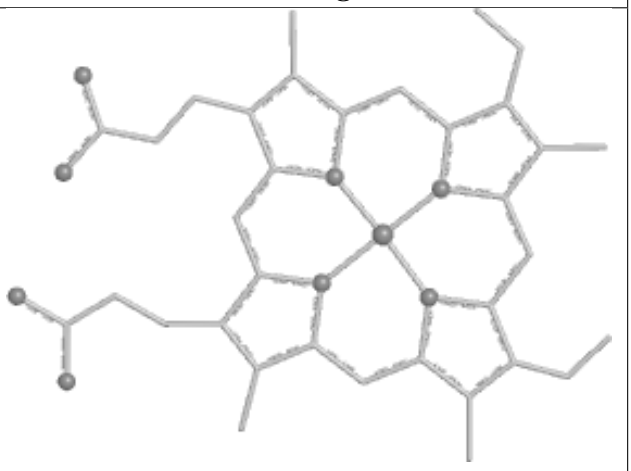
Bond lengths



Bond angles

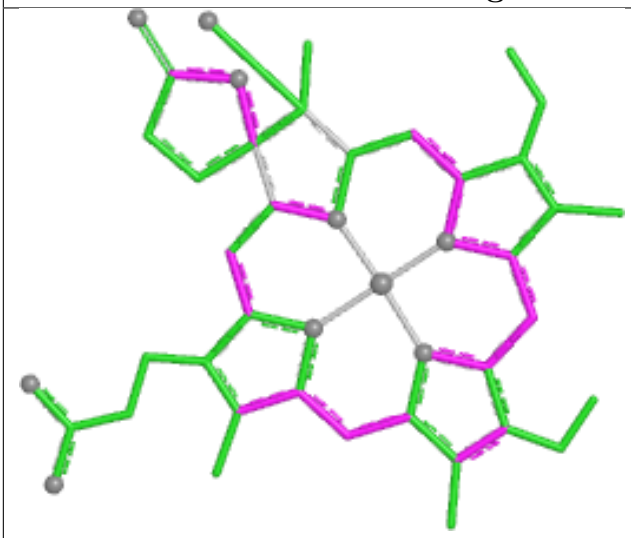


Torsions

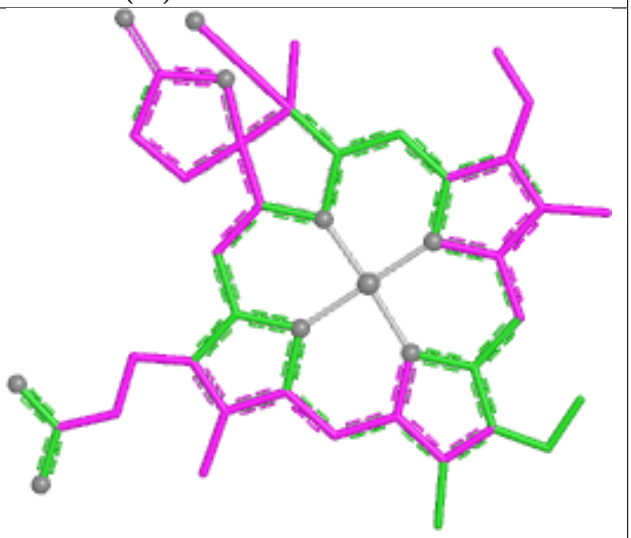


Rings

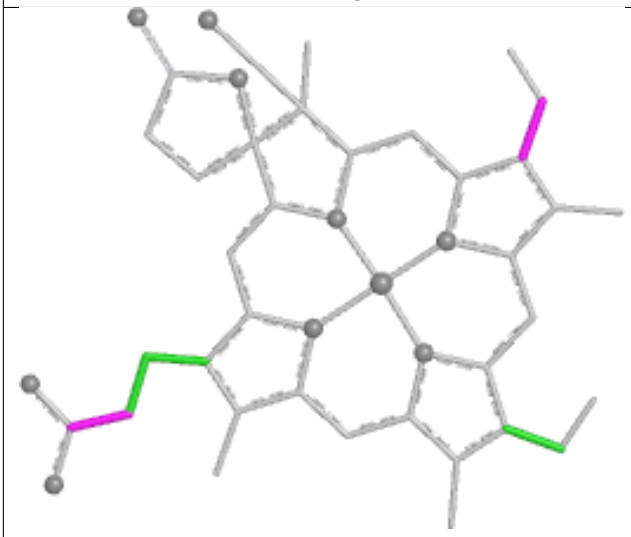
Ligand HDD B 801 (A)



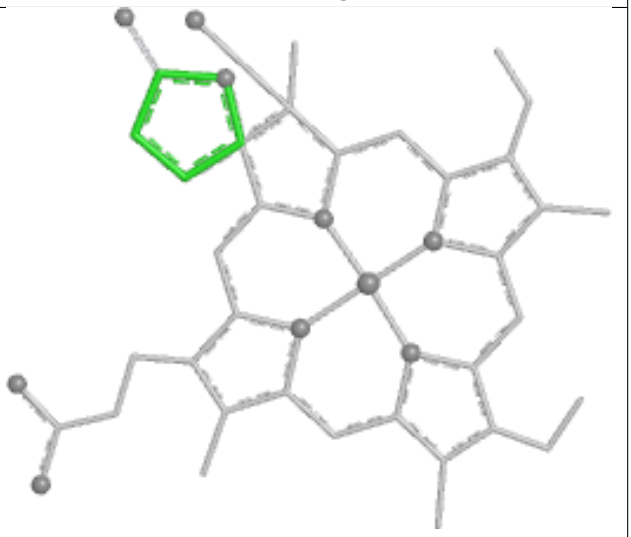
Bond lengths



Bond angles

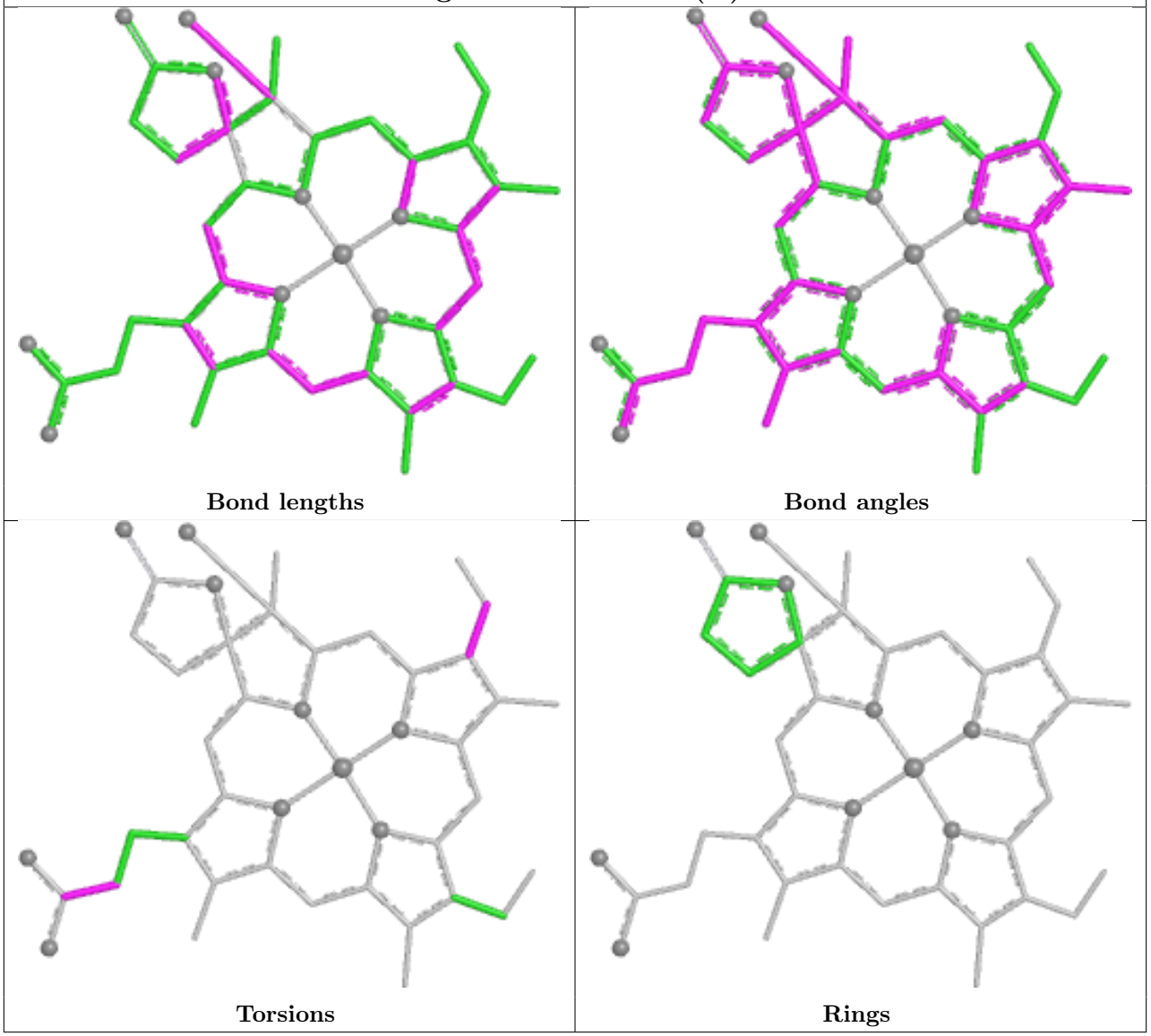


Torsions



Rings

Ligand HDD A 801 (A)



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	726/753 (96%)	-0.70	2 (0%)	90	91	6, 12, 26, 58	5 (0%)
1	B	726/753 (96%)	-0.55	3 (0%)	88	91	6, 13, 36, 65	5 (0%)
1	C	726/753 (96%)	-0.56	2 (0%)	90	91	5, 13, 36, 62	4 (0%)
1	D	726/753 (96%)	-0.60	4 (0%)	85	88	5, 12, 32, 62	5 (0%)
All	All	2904/3012 (96%)	-0.60	11 (0%)	88	91	5, 13, 33, 65	19 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	GLY	3.9
1	C	751	ILE	3.0
1	D	28	SER	3.0
1	D	750	LYS	2.8
1	B	710	ILE	2.7
1	D	749	ASP	2.7
1	C	750	LYS	2.6
1	D	596	GLY	2.3
1	B	725	ASP	2.3
1	A	726	GLY	2.2
1	A	751	ILE	2.1

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands (i)

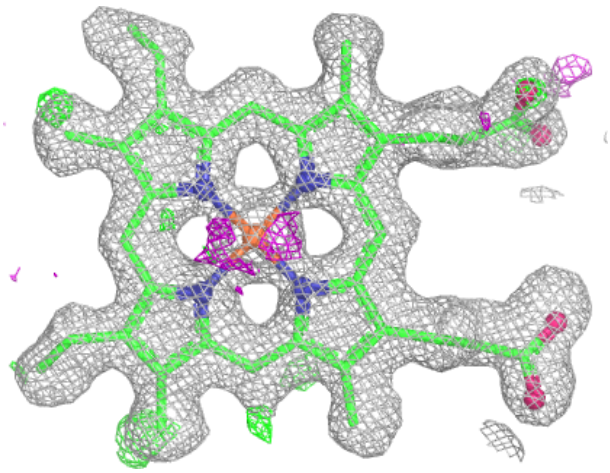
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

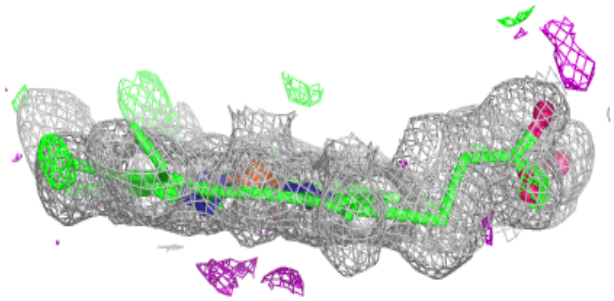
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HEM	D	802[B]	43/43	0.97	0.06	4,6,8,9	43
2	HDD	B	801[A]	44/44	0.98	0.05	6,7,14,18	44
2	HDD	C	801[A]	44/44	0.98	0.05	6,7,14,18	44
2	HDD	D	801[A]	44/44	0.98	0.05	5,7,12,16	44
3	HEM	A	802[B]	43/43	0.98	0.05	3,5,6,7	43
3	HEM	B	802[B]	43/43	0.98	0.05	4,7,8,8	43
3	HEM	C	802[B]	43/43	0.98	0.06	4,6,8,9	43
2	HDD	A	801[A]	44/44	0.98	0.05	5,6,12,15	44

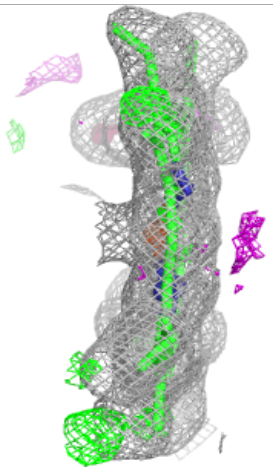
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HEM D 802 (B):

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

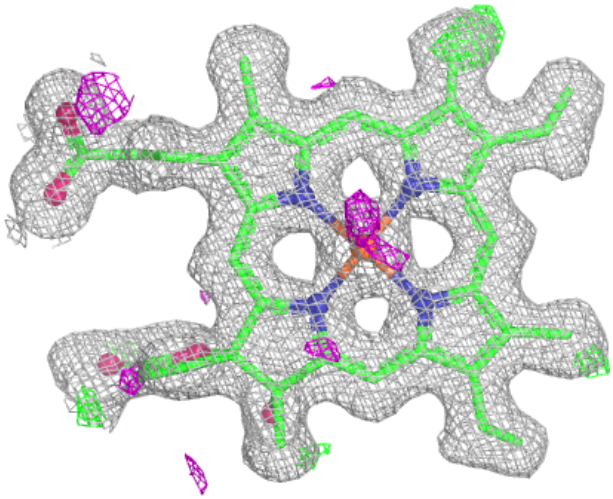


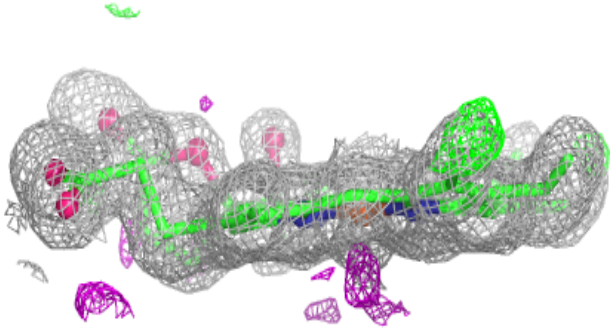


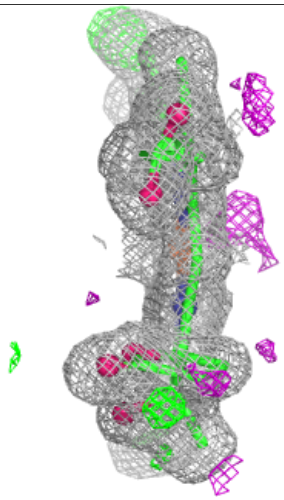


Electron density around HDD B 801 (A):

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

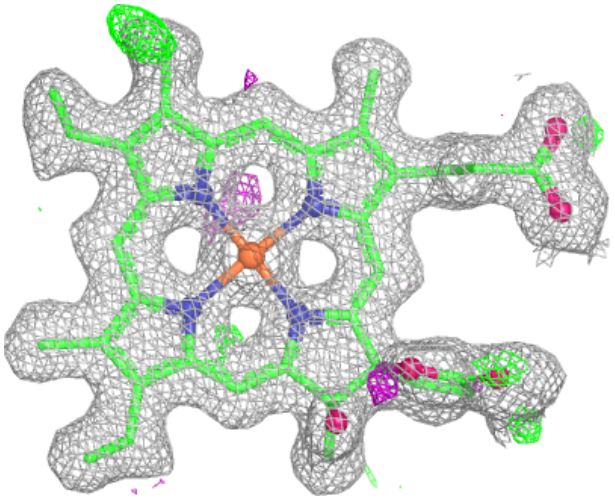


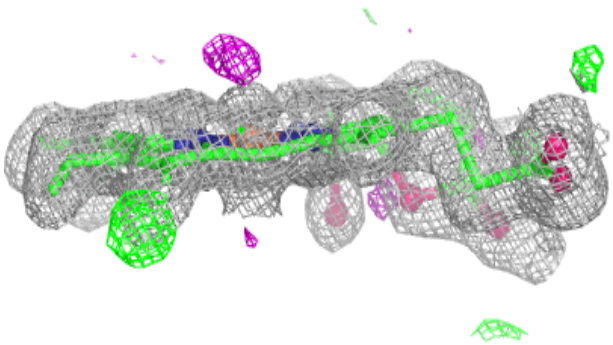


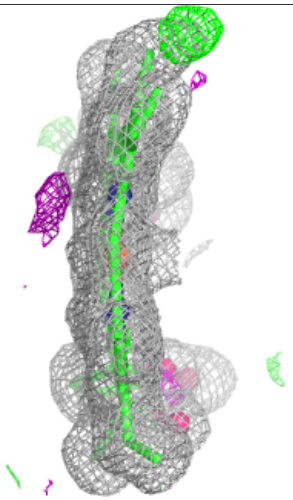


Electron density around HDD C 801 (A):

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

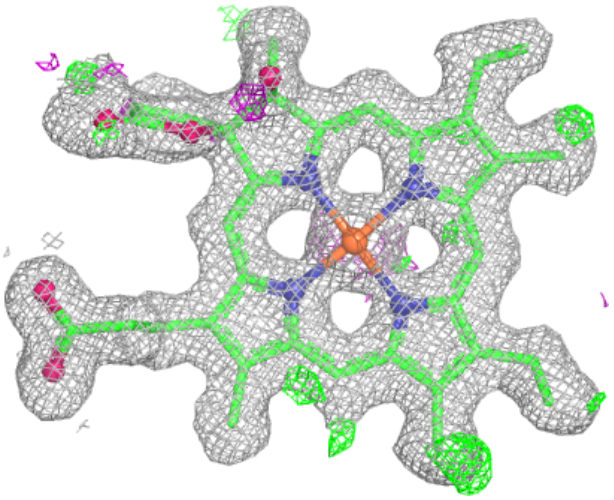


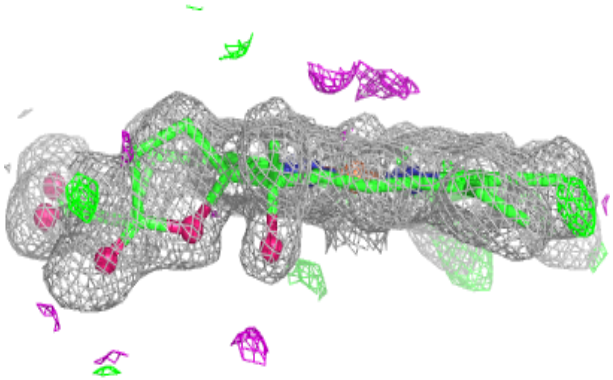


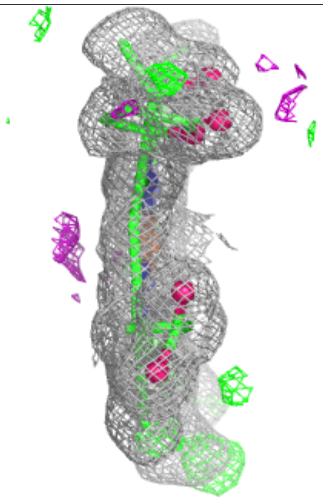


Electron density around HDD D 801 (A):

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

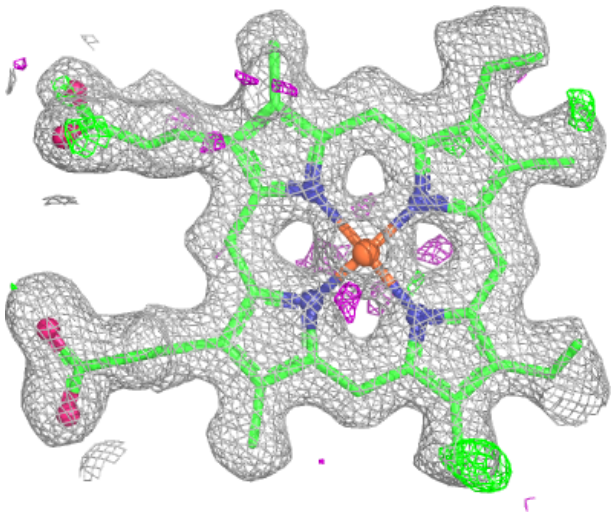


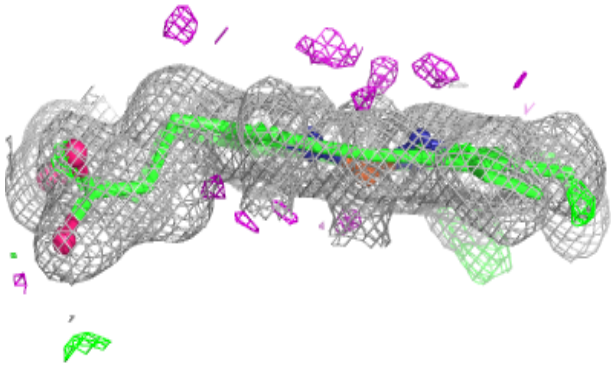


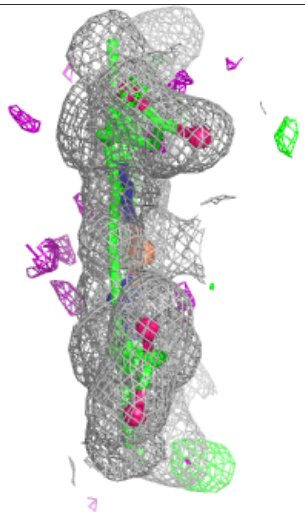


Electron density around HEM A 802 (B):

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

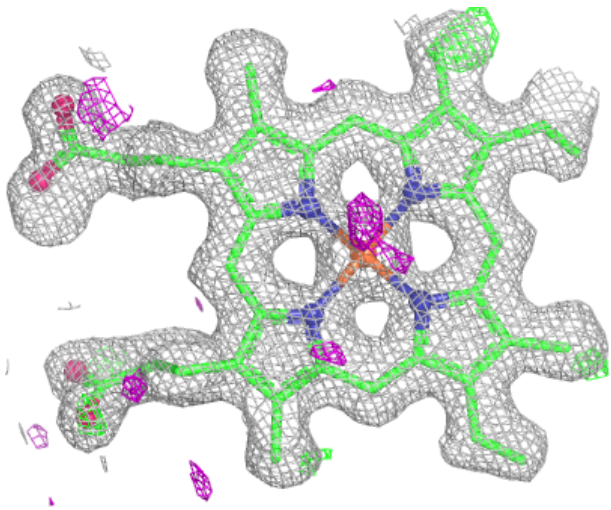


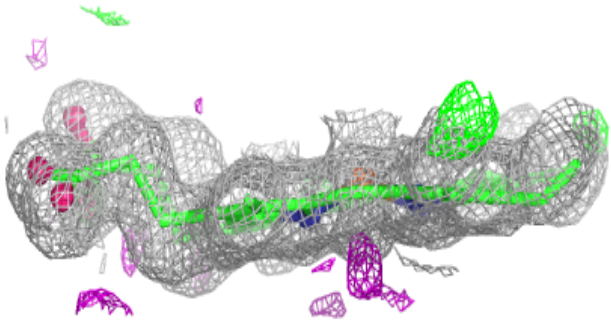


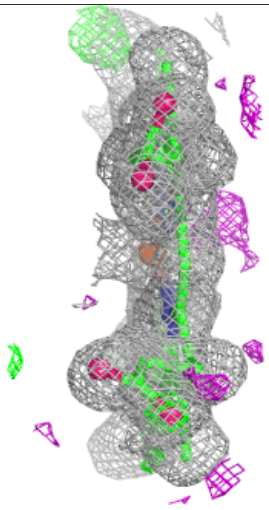


Electron density around HEM B 802 (B):

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

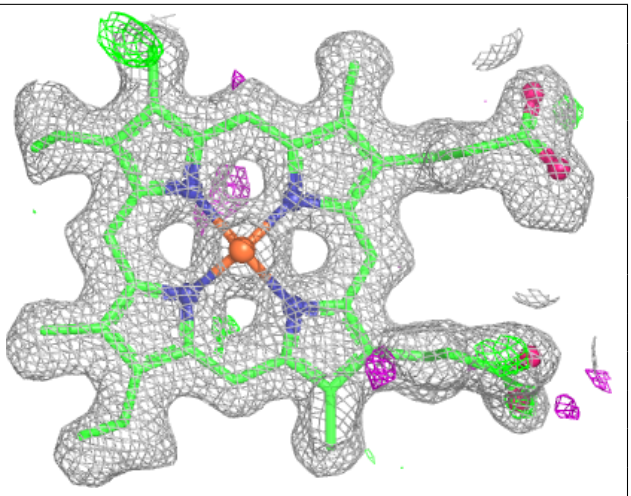


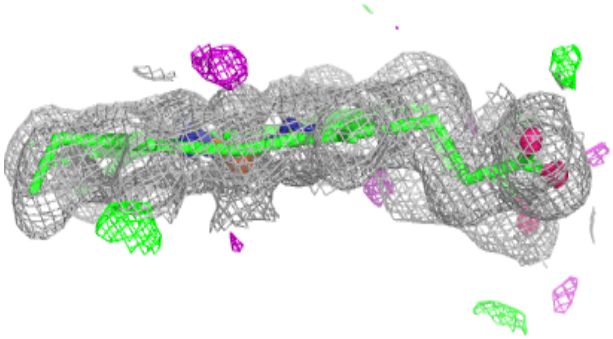


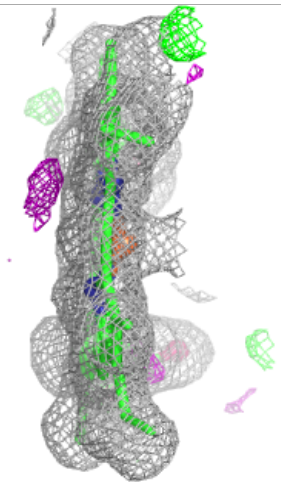


Electron density around HEM C 802 (B):

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

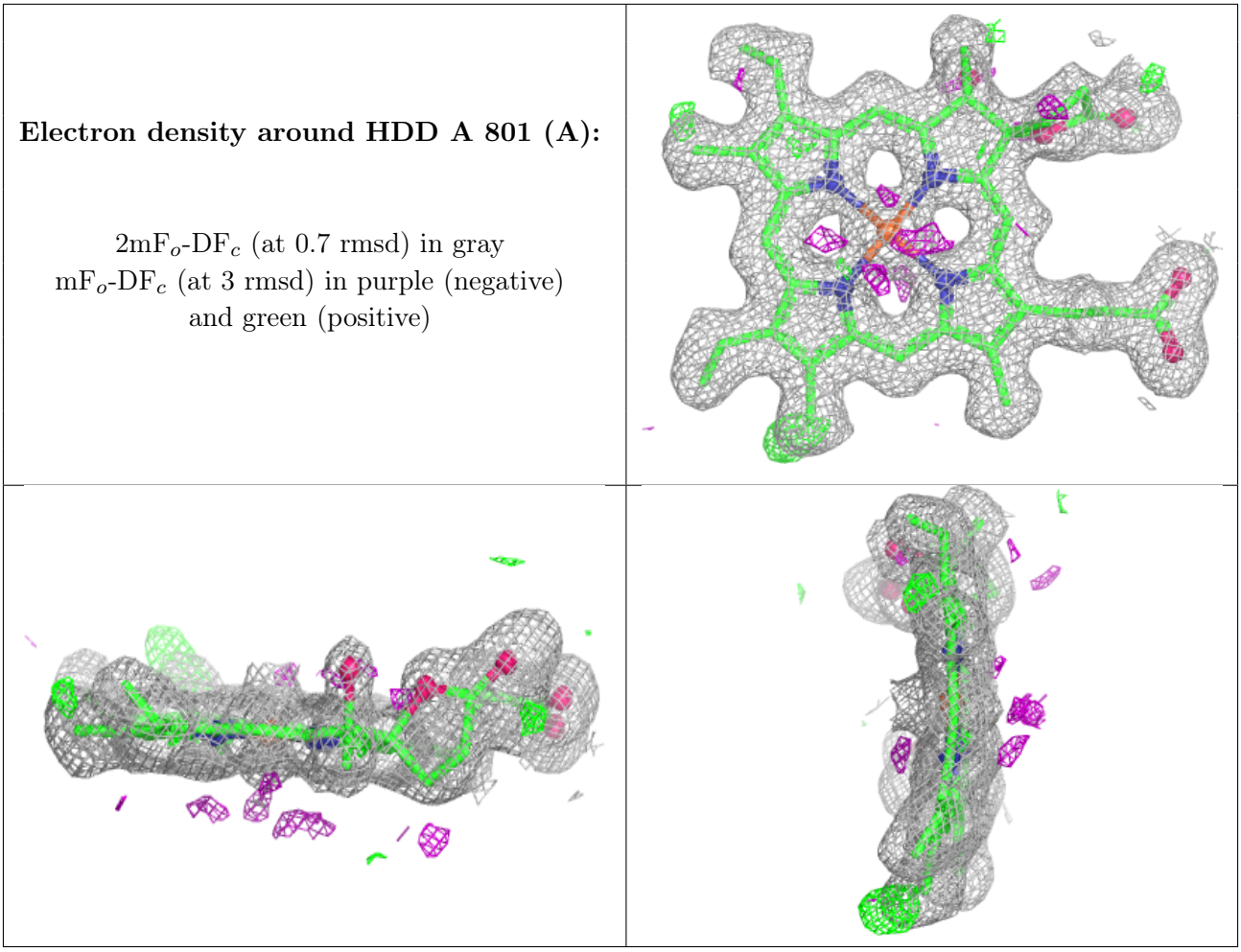






Electron density around HDD A 801 (A):

$2mF_o$-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.