



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2025 – 06:31 PM EDT

PDB ID : 4ENT
Title : Structure of the S234A variant of E. coli KatE
Authors : Loewen, P.C.; Jha, V.
Deposited on : 2012-04-13
Resolution : 1.70 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

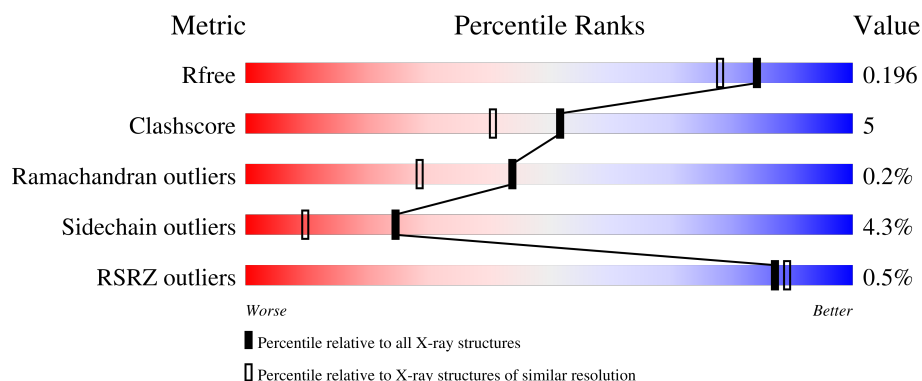
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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}	164625	5161 (1.70-1.70)
Clashscore	180529	5671 (1.70-1.70)
Ramachandran outliers	177936	5594 (1.70-1.70)
Sidechain outliers	177891	5594 (1.70-1.70)
RSRZ outliers	164620	5159 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	753	<div> <div>%</div> <div> <div></div> <div>87%</div> <div>8%</div> <div>..</div> </div> </div>
1	B	753	<div> <div></div> <div>83%</div> <div>12%</div> <div>..</div> </div>
1	C	753	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>12%</div> <div>..</div> </div> </div>
1	D	753	<div> <div></div> <div>85%</div> <div>10%</div> <div>..</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 26312 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

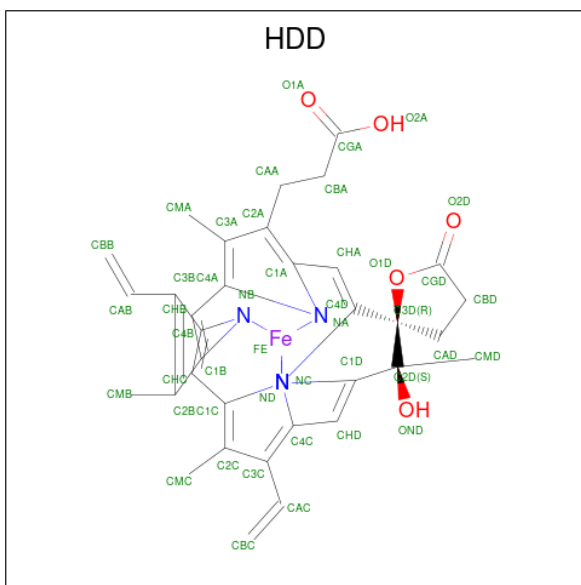
- Molecule 1 is a protein called Catalase HP11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	3	0
			5753	3652	1007	1082	12			
1	B	726	Total	C	N	O	S	0	0	0
			5740	3643	1004	1081	12			
1	C	726	Total	C	N	O	S	0	2	0
			5755	3654	1007	1082	12			
1	D	726	Total	C	N	O	S	0	2	0
			5749	3649	1005	1083	12			

There are 4 discrepancies between the modelled and reference sequences:

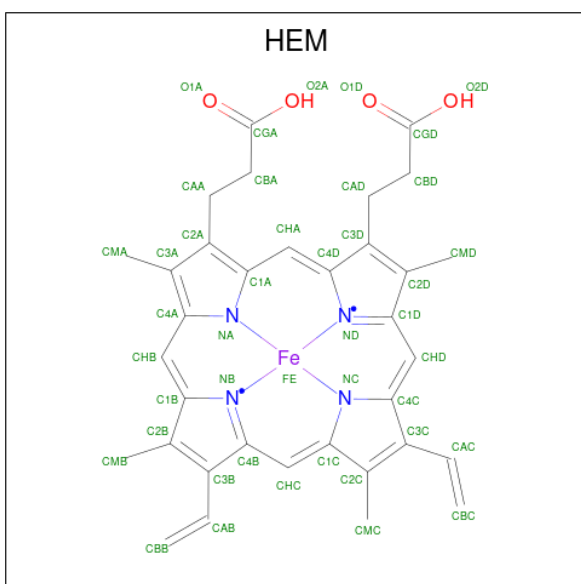
Chain	Residue	Modelled	Actual	Comment	Reference
A	234	ALA	SER	engineered mutation	UNP P21179
B	234	ALA	SER	engineered mutation	UNP P21179
C	234	ALA	SER	engineered mutation	UNP P21179
D	234	ALA	SER	engineered mutation	UNP P21179

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



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

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



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

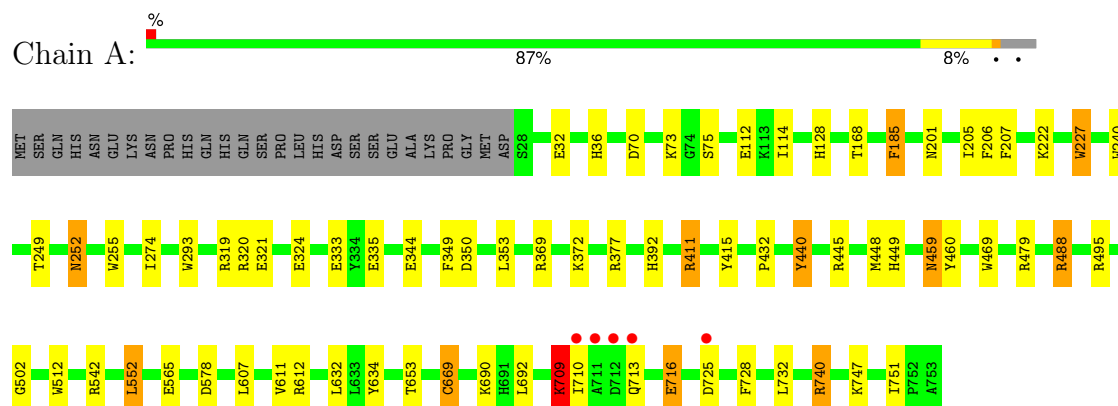
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	779	Total 779	O 779	0	0
4	B	679	Total 679	O 679	0	0
4	C	741	Total 741	O 741	0	0
4	D	768	Total 768	O 768	0	0

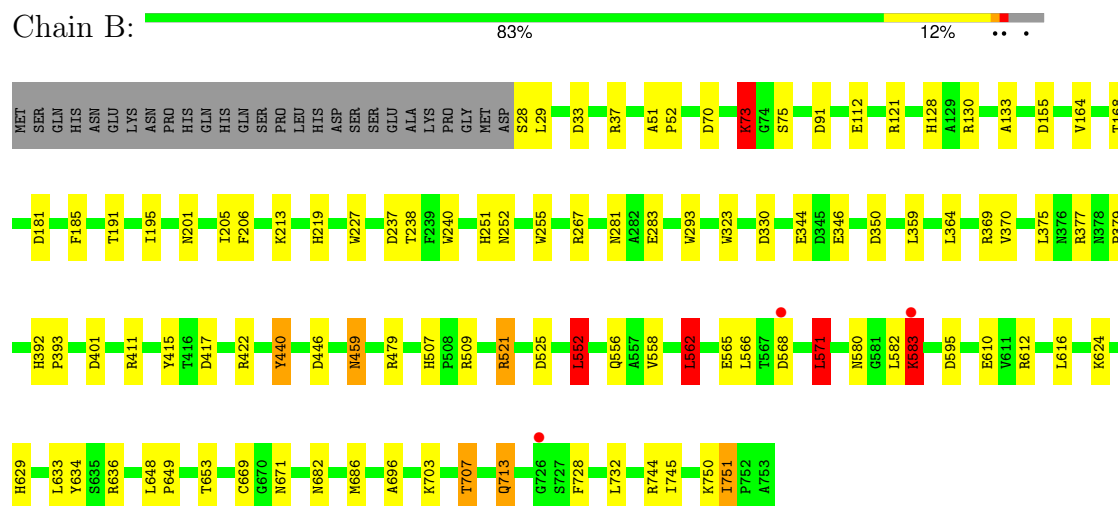
3 Residue-property plots

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

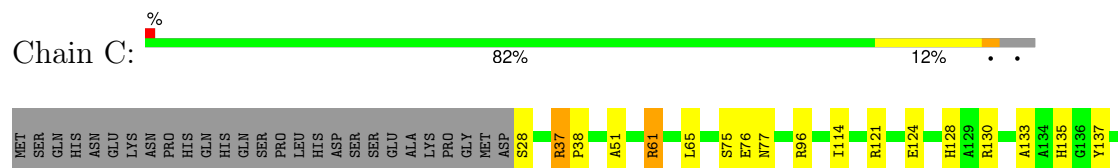
• Molecule 1: Catalase HP11

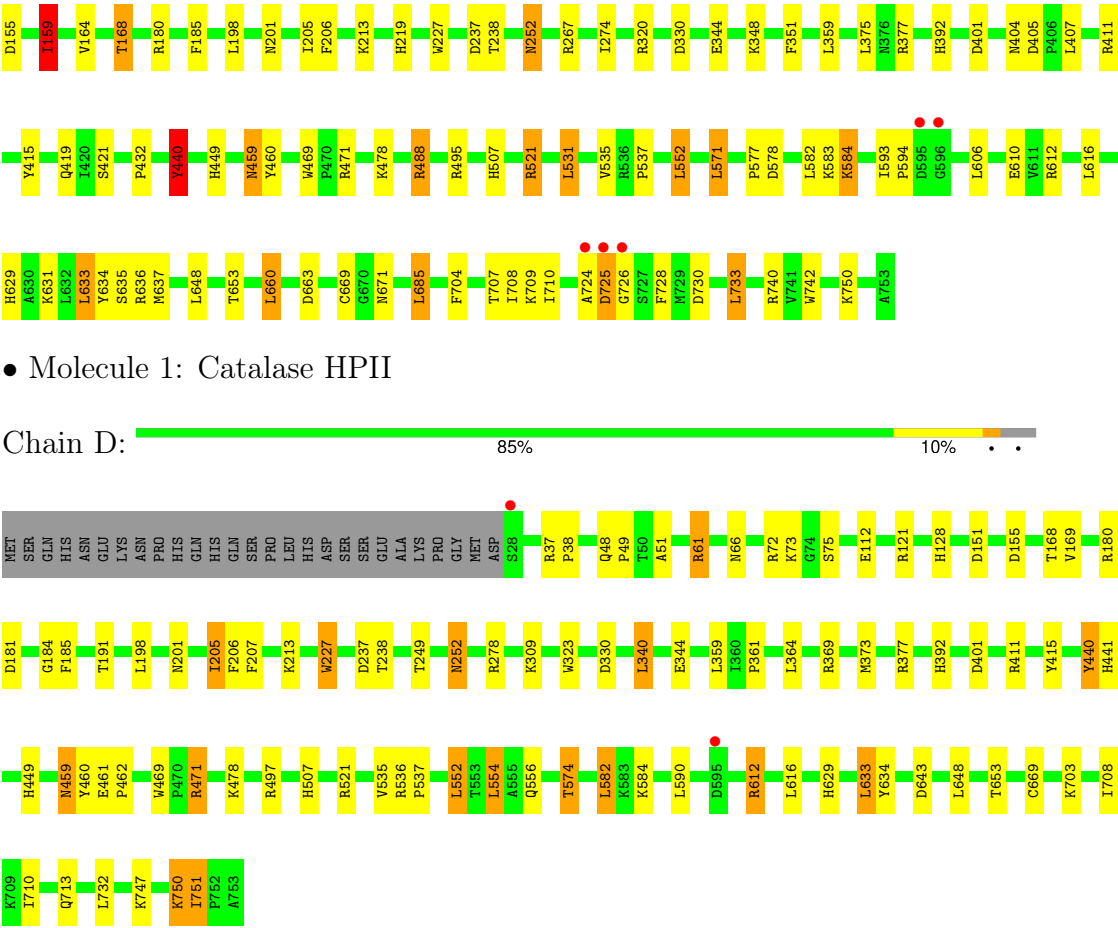


• Molecule 1: Catalase HP11



• Molecule 1: Catalase HP11





● Molecule 1: Catalase HP11

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.46Å 133.05Å 122.19Å 90.00° 109.58° 90.00°	Depositor
Resolution (Å)	33.26 – 1.70 33.26 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.1 (33.26-1.70) 98.1 (33.26-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 1.70Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.158 , 0.197 0.158 , 0.196	Depositor DCC
R_{free} test set	15289 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	12.2	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26312	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.16	13/5912 (0.2%)	1.08	14/8035 (0.2%)
1	B	1.13	9/5886 (0.2%)	1.08	23/8001 (0.3%)
1	C	1.11	9/5905 (0.2%)	1.07	25/8027 (0.3%)
1	D	1.17	7/5901 (0.1%)	1.12	26/8021 (0.3%)
All	All	1.14	38/23604 (0.2%)	1.09	88/32084 (0.3%)

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	324	GLU	CD-OE2	7.92	1.34	1.25
1	B	323	TRP	CD2-CE2	7.90	1.50	1.41
1	B	346	GLU	CD-OE1	7.69	1.34	1.25
1	B	440	TYR	CE1-CZ	7.42	1.48	1.38
1	D	440	TYR	CE1-CZ	7.03	1.47	1.38
1	A	440	TYR	CE1-CZ	6.47	1.47	1.38
1	B	181	ASP	CB-CG	6.46	1.65	1.51
1	C	469	TRP	CD2-CE2	6.31	1.49	1.41
1	A	512	TRP	CD2-CE2	6.27	1.48	1.41
1	C	124	GLU	CD-OE1	6.26	1.32	1.25
1	D	377	ARG	CZ-NH1	6.19	1.41	1.33
1	A	321	GLU	CD-OE1	6.14	1.32	1.25
1	C	344	GLU	CD-OE1	5.83	1.32	1.25
1	B	255	TRP	CD2-CE2	5.76	1.48	1.41
1	C	440	TYR	CE1-CZ	5.71	1.46	1.38
1	B	112	GLU	CD-OE2	5.70	1.31	1.25
1	A	240	TRP	CD2-CE2	5.69	1.48	1.41
1	D	377	ARG	CZ-NH2	5.67	1.40	1.33
1	B	70	ASP	CB-CG	5.67	1.63	1.51
1	C	742	TRP	CD2-CE2	5.63	1.48	1.41
1	A	293	TRP	CD2-CE2	5.58	1.48	1.41
1	A	227	TRP	CG-CD1	5.54	1.44	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	469	TRP	CD2-CE2	5.48	1.48	1.41
1	A	411	ARG	CZ-NH1	5.47	1.40	1.33
1	D	181	ASP	CB-CG	5.46	1.63	1.51
1	C	495	ARG	CZ-NH2	5.46	1.40	1.33
1	A	320	ARG	CZ-NH2	5.45	1.40	1.33
1	A	112	GLU	CD-OE2	5.42	1.31	1.25
1	D	112	GLU	CD-OE2	5.40	1.31	1.25
1	D	323	TRP	CD2-CE2	5.40	1.47	1.41
1	C	121	ARG	CZ-NH2	5.38	1.40	1.33
1	C	351	PHE	CG-CD2	5.30	1.46	1.38
1	A	255	TRP	CD2-CE2	5.17	1.47	1.41
1	B	293	TRP	CD2-CE2	5.10	1.47	1.41
1	A	502	GLY	N-CA	5.04	1.53	1.46
1	C	421	SER	CB-OG	5.04	1.48	1.42
1	B	240	TRP	CD2-CE2	5.03	1.47	1.41
1	D	478	LYS	CE-NZ	5.01	1.61	1.49

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	478	LYS	CD-CE-NZ	11.18	137.40	111.70
1	D	377	ARG	NE-CZ-NH2	-10.34	115.13	120.30
1	B	521	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	A	552	LEU	CB-CG-CD1	9.05	126.39	111.00
1	C	213	LYS	CD-CE-NZ	-8.43	92.32	111.70
1	C	401	ASP	CB-CG-OD2	8.19	125.67	118.30
1	D	340	LEU	CB-CG-CD1	8.17	124.89	111.00
1	C	531	LEU	CB-CG-CD1	8.13	124.83	111.00
1	B	350	ASP	CB-CG-OD1	-8.10	111.01	118.30
1	C	660	LEU	CB-CG-CD1	8.06	124.70	111.00
1	D	198	LEU	CB-CG-CD2	-7.93	97.52	111.00
1	D	401	ASP	CB-CG-OD1	-7.71	111.36	118.30
1	B	417	ASP	CB-CG-OD2	-7.45	111.59	118.30
1	B	370	VAL	CG1-CB-CG2	7.33	122.63	110.90
1	C	37	ARG	NE-CZ-NH1	7.32	123.96	120.30
1	B	562	LEU	CB-CG-CD1	7.22	123.27	111.00
1	D	633	LEU	CB-CG-CD1	7.07	123.02	111.00
1	D	497	ARG	NE-CZ-NH1	6.99	123.79	120.30
1	B	121	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	B	422	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	B	377	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	D	643	ASP	CB-CG-OD1	6.75	124.37	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	583	LYS	N-CA-CB	-6.71	98.52	110.60
1	B	130	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	A	350	ASP	CB-CG-OD1	-6.69	112.28	118.30
1	C	348	LYS	CD-CE-NZ	-6.59	96.55	111.70
1	A	445	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	D	61	ARG	NE-CZ-NH2	6.49	123.54	120.30
1	D	401	ASP	CB-CG-OD2	6.44	124.09	118.30
1	A	542	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	C	552	LEU	CA-CB-CG	6.39	129.99	115.30
1	B	401	ASP	CB-CG-OD1	-6.36	112.58	118.30
1	A	495	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	D	278	ARG	NE-CZ-NH1	-6.19	117.20	120.30
1	D	121	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	C	96	ARG	NE-CZ-NH1	6.11	123.35	120.30
1	A	479	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	A	185	PHE	CB-CG-CD2	-6.06	116.56	120.80
1	C	180	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	D	180	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	C	61	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	121	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	B	33	ASP	CB-CG-OD1	5.89	123.60	118.30
1	B	509	ARG	NE-CZ-NH2	5.85	123.22	120.30
1	D	377	ARG	NH1-CZ-NH2	5.83	125.82	119.40
1	A	70	ASP	CB-CG-OD1	5.83	123.55	118.30
1	A	222	LYS	CD-CE-NZ	-5.75	98.48	111.70
1	D	155	ASP	CB-CG-OD2	5.74	123.47	118.30
1	D	309	LYS	CD-CE-NZ	-5.74	98.51	111.70
1	C	130	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	C	37	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	C	740	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	B	582	LEU	CB-CG-CD1	-5.65	101.39	111.00
1	D	151	ASP	CB-CG-OD2	5.64	123.38	118.30
1	D	213	LYS	CD-CE-NZ	-5.64	98.72	111.70
1	C	471	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	611	VAL	CG1-CB-CG2	-5.60	101.94	110.90
1	B	446	ASP	CB-CG-OD1	5.59	123.34	118.30
1	C	155	ASP	CB-CG-OD2	5.58	123.32	118.30
1	D	582	LEU	CB-CG-CD1	5.55	120.44	111.00
1	D	554	LEU	CB-CG-CD2	5.54	120.42	111.00
1	B	571	LEU	CA-CB-CG	5.45	127.84	115.30
1	C	401	ASP	CB-CG-OD1	-5.41	113.43	118.30
1	D	373	MET	CG-SD-CE	5.37	108.78	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	130	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	D	377	ARG	CG-CD-NE	-5.31	100.66	111.80
1	B	744	ARG	NE-CZ-NH2	5.31	122.95	120.30
1	D	536	ARG	NE-CZ-NH1	-5.27	117.66	120.30
1	C	320	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	D	471	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	B	375	LEU	CB-CG-CD1	-5.24	102.09	111.00
1	C	159[A]	ILE	CB-CG1-CD1	-5.21	99.31	113.90
1	C	159[B]	ILE	CB-CG1-CD1	-5.21	99.31	113.90
1	B	552	LEU	CA-CB-CG	5.20	127.26	115.30
1	B	479	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	C	663	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	D	72	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	353	LEU	CB-CG-CD1	-5.17	102.22	111.00
1	B	401	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	740	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	C	685	LEU	CB-CG-CD1	5.12	119.71	111.00
1	A	377	ARG	CG-CD-NE	-5.12	101.06	111.80
1	C	168	THR	CA-CB-CG2	-5.11	105.25	112.40
1	D	590	LEU	CB-CG-CD2	-5.09	102.34	111.00
1	A	488	ARG	NE-CZ-NH1	-5.06	117.77	120.30
1	C	733	LEU	CA-CB-CG	5.05	126.92	115.30
1	B	73	LYS	CD-CE-NZ	-5.01	100.17	111.70
1	C	440	TYR	CB-CG-CD2	-5.00	118.00	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5753	0	5591	44	0
1	B	5740	0	5574	50	0
1	C	5755	0	5591	77	0
1	D	5749	0	5587	50	0
2	A	44	0	31	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	44	0	31	3	0
2	C	44	0	31	2	0
2	D	44	0	31	4	0
3	A	43	0	30	8	0
3	B	43	0	30	6	0
3	C	43	0	30	15	0
3	D	43	0	30	9	0
4	A	779	0	0	9	0
4	B	679	0	0	15	0
4	C	741	0	0	12	0
4	D	768	0	0	8	0
All	All	26312	0	22587	230	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 (230) 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:B:392:HIS:ND1	1:B:415:TYR:CB	1.74	1.51
1:D:392:HIS:ND1	1:D:415:TYR:CB	1.73	1.49
1:A:392:HIS:ND1	1:A:415:TYR:CB	1.73	1.49
1:C:392:HIS:ND1	1:C:415:TYR:CB	1.77	1.47
1:B:369:ARG:HG2	4:B:1296:HOH:O	1.26	1.32
1:A:392:HIS:CE1	1:A:415:TYR:HB2	1.73	1.23
1:C:392:HIS:ND1	1:C:415:TYR:HB2	0.83	1.15
3:C:802[B]:HEM:HBC2	3:C:802[B]:HEM:HMC2	1.26	1.15
1:A:392:HIS:ND1	1:A:415:TYR:HB2	0.82	1.14
1:B:392:HIS:CE1	1:B:415:TYR:HB2	1.82	1.14
1:C:392:HIS:CE1	1:C:415:TYR:HB2	1.82	1.13
1:C:521:ARG:CG	1:C:521:ARG:HH11	1.58	1.13
1:D:392:HIS:CE1	1:D:415:TYR:HB2	1.82	1.12
1:B:392:HIS:ND1	1:B:415:TYR:HB2	0.79	1.12
1:D:392:HIS:ND1	1:D:415:TYR:HB2	0.78	1.10
1:A:716:GLU:HG3	4:A:1647:HOH:O	1.50	1.10
4:B:1574:HOH:O	1:D:73:LYS:HD3	1.57	1.04
1:C:521:ARG:NH1	1:C:521:ARG:HG2	1.41	1.03
1:A:369:ARG:NH2	4:A:1179:HOH:O	1.96	0.99
2:A:801[A]:HDD:HBB1	2:A:801[A]:HDD:HMB1	1.49	0.95
1:C:267:ARG:HG3	4:C:1555:HOH:O	1.67	0.94
1:B:392:HIS:CG	1:B:415:TYR:HB2	2.02	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:MET:HG3	1:A:449[A]:HIS:CD2	2.04	0.93
1:D:392:HIS:CG	1:D:415:TYR:HB2	2.03	0.90
1:A:206:PHE:CD2	3:A:802[B]:HEM:HAB	2.08	0.88
1:B:267:ARG:HG3	4:B:1362:HOH:O	1.74	0.88
1:A:344:GLU:HB3	4:A:1587:HOH:O	1.75	0.87
1:C:392:HIS:CG	1:C:415:TYR:HB2	2.08	0.86
3:D:802[B]:HEM:HBC2	3:D:802[B]:HEM:HMC2	1.55	0.85
1:C:521:ARG:HH11	1:C:521:ARG:HG2	1.02	0.85
1:C:440:TYR:HD1	4:C:1374:HOH:O	1.60	0.83
1:C:725:ASP:HB3	1:C:726:GLY:CA	2.10	0.82
1:C:521:ARG:HH11	1:C:521:ARG:CB	1.93	0.80
1:D:206:PHE:CG	3:D:802[B]:HEM:HAB	2.17	0.80
1:C:201:ASN:CG	3:C:802[B]:HEM:HMB2	2.03	0.79
1:C:725:ASP:HB3	1:C:726:GLY:C	2.02	0.78
1:C:206:PHE:CG	3:C:802[B]:HEM:HAB	2.19	0.78
1:C:440:TYR:CD1	4:C:1374:HOH:O	2.36	0.77
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.66	0.77
4:B:1574:HOH:O	1:D:73:LYS:CD	2.18	0.77
3:C:802[B]:HEM:HBC2	3:C:802[B]:HEM:CMC	2.06	0.76
2:B:801[A]:HDD:HBB1	2:B:801[A]:HDD:HMB1	1.69	0.75
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.69	0.74
1:A:449[A]:HIS:CG	1:C:449[A]:HIS:CG	2.62	0.73
1:D:703:LYS:HE2	4:D:1568:HOH:O	1.90	0.71
1:C:488:ARG:HD2	4:C:1460:HOH:O	1.90	0.71
1:A:206:PHE:CG	3:A:802[B]:HEM:HAB	2.25	0.71
1:B:206:PHE:CG	3:B:802[B]:HEM:HAB	2.26	0.71
1:B:392:HIS:ND1	1:B:415:TYR:CG	2.57	0.70
1:C:552:LEU:HD21	1:C:571:LEU:HD12	1.74	0.70
1:C:636:ARG:NH1	4:C:1525:HOH:O	2.25	0.68
1:D:629:HIS:HD2	4:D:1255:HOH:O	1.77	0.68
1:A:392:HIS:ND1	1:A:415:TYR:CG	2.61	0.68
1:C:206:PHE:CD2	3:C:802[B]:HEM:HAB	2.29	0.68
1:B:629:HIS:HD2	4:B:1160:HOH:O	1.77	0.67
1:D:750:LYS:HE2	1:D:751:ILE:HG22	1.75	0.67
1:A:448:MET:CG	1:A:449[A]:HIS:CD2	2.77	0.67
1:D:206:PHE:CD2	3:D:802[B]:HEM:HAB	2.29	0.67
1:A:709:LYS:N	1:A:709:LYS:HD3	2.09	0.67
1:D:392:HIS:ND1	1:D:415:TYR:CG	2.63	0.66
1:B:28:SER:HA	4:B:1464:HOH:O	1.95	0.65
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.79	0.65
1:C:704:PHE:O	1:C:707:THR:HG22	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:ARG:HH11	1:D:66:ASN:HA	1.62	0.65
1:C:392:HIS:ND1	1:C:415:TYR:CG	2.64	0.65
1:D:556:GLN:NE2	4:D:1571:HOH:O	2.31	0.63
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.81	0.62
1:D:469:TRP:CE3	1:D:471:ARG:HG3	2.36	0.60
1:B:281:ASN:OD1	1:B:283:GLU:HG2	2.01	0.60
1:C:359:LEU:H	1:C:507:HIS:HD2	1.49	0.60
1:D:201:ASN:CG	3:D:802[B]:HEM:HMB2	2.22	0.60
1:D:411:ARG:HG2	3:D:802[B]:HEM:C2C	2.36	0.60
1:A:449[B]:HIS:HD2	4:C:1195:HOH:O	1.83	0.60
1:A:612:ARG:HG3	4:A:1567:HOH:O	2.01	0.59
1:C:201:ASN:ND2	3:C:802[B]:HEM:CMB	2.66	0.59
1:B:359:LEU:H	1:B:507:HIS:HD2	1.50	0.59
1:C:578:ASP:HB2	1:C:582:LEU:O	2.03	0.58
1:B:201:ASN:CG	3:B:802[B]:HEM:HMB2	2.24	0.58
1:A:690:LYS:HB2	1:A:751:ILE:HD11	1.86	0.58
1:C:137:TYR:HB2	1:C:159[A]:ILE:CD1	2.34	0.58
1:D:732:LEU:C	1:D:732:LEU:HD13	2.25	0.57
1:C:634:TYR:O	1:C:653:THR:HA	2.03	0.57
1:B:73:LYS:HD3	1:D:441:HIS:CD2	2.39	0.57
1:C:407:LEU:HD23	3:C:802[B]:HEM:HBB1	1.86	0.57
1:A:36:HIS:CD2	1:A:36:HIS:H	2.23	0.56
1:A:607:LEU:HD11	1:A:632:LEU:HB3	1.88	0.56
4:A:1097:HOH:O	1:C:449[B]:HIS:HD2	1.89	0.55
3:B:802[B]:HEM:HBC1	1:C:114:ILE:HD12	1.88	0.55
1:C:407:LEU:CD2	3:C:802[B]:HEM:HBB1	2.37	0.55
1:C:725:ASP:HB2	1:C:728:PHE:CB	2.36	0.55
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.88	0.55
1:C:583:LYS:HD2	4:C:1217:HOH:O	2.05	0.55
1:D:61:ARG:NH1	1:D:66:ASN:HA	2.22	0.54
1:C:411:ARG:HG2	3:C:802[B]:HEM:C2C	2.42	0.54
1:C:629:HIS:HD2	4:C:1212:HOH:O	1.92	0.53
1:D:201:ASN:ND2	3:D:802[B]:HEM:HMB1	2.24	0.53
3:A:802[B]:HEM:HBC2	3:A:802[B]:HEM:CMC	2.39	0.53
1:A:392:HIS:ND1	1:A:415:TYR:HB3	2.07	0.53
1:C:359:LEU:H	1:C:507:HIS:CD2	2.27	0.53
1:C:725:ASP:CB	1:C:726:GLY:HA3	2.39	0.53
1:C:725:ASP:CB	1:C:726:GLY:CA	2.83	0.52
1:A:725:ASP:H	1:A:728:PHE:HB3	1.73	0.52
1:B:206:PHE:CD2	3:B:802[B]:HEM:HAB	2.45	0.52
1:C:610:GLU:O	1:C:610:GLU:HG3	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:636:ARG:HA	4:B:1506:HOH:O	2.11	0.51
1:A:201:ASN:CG	3:A:802[B]:HEM:HMB2	2.31	0.51
1:B:128:HIS:HA	1:B:168:THR:O	2.11	0.51
1:C:725:ASP:HB3	1:C:726:GLY:HA3	1.87	0.50
1:B:37:ARG:NH1	4:B:1520:HOH:O	2.31	0.50
1:B:29:LEU:N	4:B:1464:HOH:O	2.26	0.50
2:C:801[A]:HDD:HBD2	4:C:1095:HOH:O	2.11	0.49
1:C:28:SER:HA	4:C:1635:HOH:O	2.11	0.49
1:C:631:LYS:HG3	1:C:633:LEU:HD13	1.94	0.49
1:D:201:ASN:ND2	3:D:802[B]:HEM:CMB	2.75	0.49
1:C:274:ILE:HD12	3:C:802[B]:HEM:HMB1	1.94	0.49
1:A:716:GLU:HG2	4:A:1304:HOH:O	2.12	0.48
1:C:610:GLU:HB3	1:C:671:ASN:HB2	1.95	0.48
1:A:448:MET:O	1:A:449[A]:HIS:HB2	2.13	0.48
2:D:801[A]:HDD:HBD2	4:D:1133:HOH:O	2.13	0.48
1:B:411:ARG:HG2	3:B:802[B]:HEM:C2C	2.48	0.48
1:C:521:ARG:HH11	1:C:521:ARG:HB2	1.77	0.48
1:D:201:ASN:CG	3:D:802[B]:HEM:CMB	2.82	0.48
1:C:392:HIS:CG	1:C:415:TYR:CB	2.85	0.47
1:C:521:ARG:CG	1:C:521:ARG:NH1	2.20	0.47
1:C:725:ASP:HB2	1:C:728:PHE:HB2	1.96	0.47
1:C:201:ASN:CG	3:C:802[B]:HEM:CMB	2.79	0.47
1:D:703:LYS:CE	4:D:1568:HOH:O	2.56	0.47
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.97	0.47
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.30	0.47
1:D:128:HIS:HA	1:D:168:THR:O	2.14	0.47
3:B:802[B]:HEM:HBC2	3:B:802[B]:HEM:CMC	2.45	0.47
1:A:578:ASP:HB2	4:A:1657:HOH:O	2.15	0.47
3:D:802[B]:HEM:HMC2	3:D:802[B]:HEM:CBC	2.37	0.46
1:C:201:ASN:ND2	3:C:802[B]:HEM:HMB1	2.30	0.46
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.51	0.46
1:B:267:ARG:HD2	4:B:1134:HOH:O	2.15	0.46
1:B:359:LEU:H	1:B:507:HIS:CD2	2.33	0.46
1:B:344:GLU:H	1:B:344:GLU:CD	2.18	0.46
1:D:612:ARG:HD3	4:D:1559:HOH:O	2.15	0.46
2:A:801[A]:HDD:HBD2	4:A:997:HOH:O	2.15	0.46
1:A:201:ASN:CG	3:A:802[B]:HEM:CMB	2.84	0.46
1:D:128:HIS:CE1	1:D:169:VAL:HG22	2.51	0.46
1:A:128:HIS:HA	1:A:168:THR:O	2.16	0.45
1:C:725:ASP:OD1	1:C:726:GLY:HA3	2.15	0.45
2:D:801[A]:HDD:HMB1	2:D:801[A]:HDD:HBB1	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ARG:HG2	3:A:802[B]:HEM:C2C	2.51	0.45
1:C:593:ILE:HA	1:C:594:PRO:HD2	1.80	0.45
1:A:692:LEU:HB2	1:A:740:ARG:HB3	1.98	0.45
1:B:525:ASP:OD2	4:B:945:HOH:O	2.21	0.45
1:D:535:VAL:O	1:D:537:PRO:HD3	2.17	0.45
1:D:392:HIS:CG	1:D:415:TYR:CB	2.82	0.45
1:B:713:GLN:NE2	1:B:713:GLN:H	2.15	0.45
1:A:460:TYR:CE2	1:B:238:THR:HB	2.52	0.45
1:B:133:ALA:HA	1:B:164:VAL:O	2.17	0.44
3:C:802[B]:HEM:CMC	3:C:802[B]:HEM:CBC	2.83	0.44
1:D:252:ASN:HD22	1:D:252:ASN:HA	1.67	0.44
1:B:552:LEU:HD22	1:B:556:GLN:HG3	1.98	0.44
1:C:411:ARG:HD2	3:C:802[B]:HEM:HBB2	2.00	0.44
1:A:349:PHE:CD1	1:A:349:PHE:N	2.86	0.44
1:B:634:TYR:O	1:B:653:THR:HA	2.17	0.44
2:C:801[A]:HDD:HMB1	2:C:801[A]:HDD:HBB1	1.99	0.44
1:C:460:TYR:CE2	1:D:238:THR:HB	2.53	0.44
1:C:552:LEU:HD21	1:C:571:LEU:CD1	2.45	0.44
1:A:114:ILE:HD12	2:D:801[A]:HDD:HBC2	1.99	0.44
1:B:583:LYS:H	1:B:583:LYS:HG2	0.96	0.44
1:C:404:ASN:O	1:C:405:ASP:C	2.55	0.43
1:C:725:ASP:HB2	1:C:728:PHE:HB3	1.98	0.43
1:D:184:GLY:HA3	2:D:801[A]:HDD:HMA2	2.00	0.43
1:A:459:ASN:HD22	1:A:459:ASN:H	1.66	0.43
1:B:696:ALA:HB1	1:B:728:PHE:CZ	2.53	0.43
2:B:801[A]:HDD:HMB1	2:B:801[A]:HDD:CBB	2.44	0.43
1:A:369:ARG:NH2	1:A:369:ARG:HG3	2.34	0.43
1:A:612:ARG:NH1	1:A:669:OCS:OD3	2.51	0.43
1:A:634:TYR:O	1:A:653:THR:HA	2.18	0.43
2:A:801[A]:HDD:HMB1	2:A:801[A]:HDD:CBB	2.33	0.43
1:B:459:ASN:H	1:B:459:ASN:HD22	1.67	0.43
1:C:76:GLU:O	1:C:77:ASN:HB2	2.18	0.43
1:D:634:TYR:O	1:D:653:THR:HA	2.19	0.43
1:A:319:ARG:HD3	1:D:227:TRP:O	2.18	0.43
1:B:552:LEU:HA	4:B:1563:HOH:O	2.18	0.43
1:B:610:GLU:HB3	1:B:671:ASN:HB2	2.01	0.43
1:C:252:ASN:HD22	1:C:252:ASN:HA	1.67	0.43
1:C:535:VAL:O	1:C:537:PRO:HD3	2.18	0.43
1:B:364:LEU:HD11	1:B:580:ASN:HB2	2.01	0.43
1:D:361:PRO:HD2	1:D:364:LEU:HD12	1.99	0.43
1:C:201:ASN:ND2	3:C:802[B]:HEM:HMB2	2.28	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ILE:HD12	2:A:801[A]:HDD:HMB1	2.01	0.42
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.34	0.42
1:C:415:TYR:O	1:C:419:GLN:HG2	2.18	0.42
1:C:128:HIS:HA	1:C:168:THR:O	2.19	0.42
1:C:459:ASN:H	1:C:459:ASN:HD22	1.66	0.42
1:D:205:ILE:H	1:D:205:ILE:HD13	1.84	0.42
1:D:38:PRO:HG2	1:D:51:ALA:HB2	2.00	0.42
1:D:708:ILE:HG13	1:D:710:ILE:HG12	2.02	0.42
1:B:558:VAL:HG12	1:B:562:LEU:HD22	2.02	0.42
1:D:574:THR:HG23	4:D:1299:HOH:O	2.20	0.42
1:B:648:LEU:HA	1:B:649:PRO:HD2	1.67	0.42
1:C:38:PRO:HG2	1:C:51:ALA:HB2	2.01	0.42
1:C:634:TYR:CG	1:C:635:SER:N	2.88	0.42
4:B:1430:HOH:O	1:D:449:HIS:HD2	2.01	0.42
1:D:461:GLU:HA	1:D:462:PRO:C	2.40	0.42
1:C:577:PRO:HG2	4:C:1493:HOH:O	2.18	0.42
1:B:624:LYS:HD3	4:B:1513:HOH:O	2.20	0.41
1:C:488:ARG:NH1	4:C:1460:HOH:O	2.17	0.41
1:A:252:ASN:HD22	1:A:252:ASN:HA	1.70	0.41
1:A:335:GLU:OE1	1:A:369:ARG:HG2	2.20	0.41
3:A:802[B]:HEM:HBC2	3:A:802[B]:HEM:HMC2	2.02	0.41
1:B:51:ALA:HB1	1:B:52:PRO:HD2	2.02	0.41
1:D:37:ARG:HD2	4:D:1424:HOH:O	2.20	0.41
1:A:207:PHE:O	1:A:249:THR:HA	2.21	0.41
1:C:583:LYS:O	1:C:584:LYS:HB3	2.20	0.41
2:B:801[A]:HDD:HBD2	4:B:1043:HOH:O	2.20	0.41
1:A:369:ARG:HG3	1:A:369:ARG:HH21	1.86	0.41
1:B:91:ASP:OD1	1:D:461:GLU:OE1	2.38	0.41
1:B:521:ARG:NH2	1:B:745:ILE:HD13	2.36	0.41
1:D:207:PHE:O	1:D:249:THR:HA	2.20	0.41
1:D:552:LEU:HD22	1:D:552:LEU:HA	1.67	0.41
1:B:751:ILE:HD13	1:B:751:ILE:HG21	1.78	0.41
1:C:133:ALA:HA	1:C:164:VAL:O	2.21	0.41
1:C:238:THR:HB	1:D:460:TYR:CE2	2.56	0.41
1:C:137:TYR:HB2	1:C:159[A]:ILE:HD12	2.03	0.40
3:A:802[B]:HEM:HMC2	3:A:802[B]:HEM:CBC	2.51	0.40
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.57	0.40
1:D:359:LEU:H	1:D:507:HIS:HD2	1.67	0.40
1:A:488:ARG:NH2	4:A:1592:HOH:O	2.54	0.40
1:A:333:GLU:OE1	1:A:372:LYS:HE3	2.21	0.40
1:B:562:LEU:HA	1:C:637:MET:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:686:MET:HB3	1:B:751:ILE:HD11	2.03	0.40
1:C:65:LEU:HD21	1:C:135:HIS:CG	2.57	0.40
1:D:459:ASN:HD22	1:D:459:ASN:H	1.69	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	726/753 (96%)	708 (98%)	15 (2%)	3 (0%)	30	17
1	B	723/753 (96%)	705 (98%)	17 (2%)	1 (0%)	48	32
1	C	725/753 (96%)	708 (98%)	15 (2%)	2 (0%)	37	23
1	D	725/753 (96%)	714 (98%)	10 (1%)	1 (0%)	48	32
All	All	2899/3012 (96%)	2835 (98%)	57 (2%)	7 (0%)	44	29

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	710	ILE
1	A	75	SER
1	A	709	LYS
1	B	75	SER
1	C	75	SER
1	C	724	ALA
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	612/634 (96%)	595 (97%)	17 (3%)	38	21
1	B	609/634 (96%)	579 (95%)	30 (5%)	21	7
1	C	611/634 (96%)	578 (95%)	33 (5%)	18	6
1	D	611/634 (96%)	584 (96%)	27 (4%)	24	9
All	All	2443/2536 (96%)	2336 (96%)	107 (4%)	25	9

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	GLU
1	A	73[A]	LYS
1	A	73[B]	LYS
1	A	185	PHE
1	A	205	ILE
1	A	227	TRP
1	A	252	ASN
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	565	GLU
1	A	709	LYS
1	A	713	GLN
1	A	716	GLU
1	A	732	LEU
1	A	747	LYS
1	B	73	LYS
1	B	155	ASP
1	B	185	PHE
1	B	191	THR
1	B	195	ILE
1	B	205	ILE
1	B	213	LYS
1	B	227	TRP
1	B	237	ASP
1	B	252	ASN
1	B	379	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	565	GLU
1	B	566	LEU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	595	ASP
1	B	612	ARG
1	B	616	LEU
1	B	633	LEU
1	B	703	LYS
1	B	707	THR
1	B	713	GLN
1	B	732	LEU
1	B	750	LYS
1	B	751	ILE
1	C	37	ARG
1	C	61	ARG
1	C	159[A]	ILE
1	C	159[B]	ILE
1	C	185	PHE
1	C	198	LEU
1	C	205	ILE
1	C	227	TRP
1	C	237	ASP
1	C	252	ASN
1	C	375	LEU
1	C	377	ARG
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	531	LEU
1	C	571	LEU
1	C	584	LYS
1	C	606	LEU
1	C	612	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	616	LEU
1	C	633	LEU
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU
1	C	709	LYS
1	C	725	ASP
1	C	730	ASP
1	C	733	LEU
1	C	750	LYS
1	D	48	GLN
1	D	49	PRO
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	344	GLU
1	D	369	ARG
1	D	440	TYR
1	D	459	ASN
1	D	521	ARG
1	D	552	LEU
1	D	554	LEU
1	D	574	THR
1	D	582	LEU
1	D	584	LYS
1	D	612	ARG
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 (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	A	713	GLN
1	B	157	ASN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	B	713	GLN
1	C	252	ASN
1	C	368	GLN
1	C	459	ASN
1	C	507	HIS
1	C	556	GLN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	252	ASN
1	D	449	HIS
1	D	459	ASN
1	D	507	HIS
1	D	556	GLN
1	D	629	HIS
1	D	671	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OCS	D	669	1	6,8,9	2.10	2 (33%)	7,11,13	2.49	3 (42%)
1	OCS	A	669	1	6,8,9	1.78	1 (16%)	7,11,13	1.55	1 (14%)
1	OCS	C	669	1	6,8,9	1.69	1 (16%)	7,11,13	2.06	3 (42%)
1	OCS	B	669	1	6,8,9	2.17	1 (16%)	7,11,13	2.47	3 (42%)

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

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

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	669	OCS	OD2-SG	4.74	1.65	1.47
1	A	669	OCS	OD2-SG	4.16	1.62	1.47
1	D	669	OCS	OD2-SG	4.14	1.62	1.47
1	C	669	OCS	OD2-SG	3.87	1.61	1.47
1	D	669	OCS	CB-CA	2.35	1.55	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	669	OCS	OD1-SG-CB	5.38	114.79	106.76
1	B	669	OCS	OD1-SG-CB	5.18	114.49	106.76
1	C	669	OCS	OD2-SG-CB	3.21	112.17	105.97
1	A	669	OCS	OD3-SG-CB	-2.84	102.51	106.76
1	C	669	OCS	OD2-SG-OD3	-2.69	104.68	111.40
1	C	669	OCS	OD1-SG-CB	-2.50	103.03	106.76
1	D	669	OCS	OD3-SG-OD1	-2.42	105.97	113.82
1	B	669	OCS	OD3-SG-CB	-2.37	103.21	106.76
1	D	669	OCS	OD2-SG-OD3	2.32	117.21	111.40
1	B	669	OCS	OD2-SG-CB	-2.03	102.05	105.97

There are no chirality outliers.

All (8) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	669	OCS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	HEM	A	802[B]	1	42,50,50	2.29	15 (35%)	46,82,82	3.15	20 (43%)
2	HDD	A	801[A]	1	41,52,52	1.57	9 (21%)	34,89,89	3.55	17 (50%)
3	HEM	D	802[B]	1	42,50,50	2.47	16 (38%)	46,82,82	2.97	18 (39%)
2	HDD	B	801[A]	1,4	41,52,52	1.51	7 (17%)	34,89,89	2.98	18 (52%)
2	HDD	C	801[A]	1	41,52,52	1.63	9 (21%)	34,89,89	3.07	16 (47%)
3	HEM	C	802[B]	1	42,50,50	2.29	15 (35%)	46,82,82	3.40	21 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HDD	D	801[A]	1	41,52,52	1.97	8 (19%)	34,89,89	2.87	14 (41%)
3	HEM	B	802[B]	1	42,50,50	2.42	17 (40%)	46,82,82	2.70	20 (43%)

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
3	HEM	A	802[B]	1	-	4/12/54/54	-
2	HDD	A	801[A]	1	-	2/5/89/89	0/1/9/9
3	HEM	D	802[B]	1	-	4/12/54/54	-
2	HDD	B	801[A]	1,4	-	2/5/89/89	0/1/9/9
2	HDD	C	801[A]	1	-	2/5/89/89	0/1/9/9
3	HEM	C	802[B]	1	-	4/12/54/54	-
2	HDD	D	801[A]	1	-	2/5/89/89	0/1/9/9
3	HEM	B	802[B]	1	-	4/12/54/54	-

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802[B]	HEM	C1A-NA	6.10	1.48	1.36
3	B	802[B]	HEM	C4A-NA	5.81	1.48	1.36
2	D	801[A]	HDD	O1D-CGD	5.59	1.44	1.35
3	A	802[B]	HEM	C1A-NA	5.59	1.47	1.36
3	B	802[B]	HEM	C1A-NA	5.59	1.47	1.36
3	D	802[B]	HEM	C4A-NA	5.39	1.47	1.36
3	C	802[B]	HEM	C1A-NA	5.36	1.47	1.36
3	B	802[B]	HEM	C3C-C4C	5.24	1.49	1.41
3	C	802[B]	HEM	C4A-NA	5.05	1.46	1.36
3	A	802[B]	HEM	C4A-NA	5.01	1.46	1.36
3	A	802[B]	HEM	CHA-C4D	4.96	1.46	1.34
3	C	802[B]	HEM	CHA-C4D	4.88	1.46	1.34
3	D	802[B]	HEM	C3B-C2B	4.84	1.47	1.37
2	D	801[A]	HDD	C3B-C2B	4.83	1.46	1.40
3	A	802[B]	HEM	C3C-C4C	4.82	1.48	1.41
3	C	802[B]	HEM	C3C-C4C	4.82	1.48	1.41
2	D	801[A]	HDD	C3C-C2C	4.68	1.46	1.40
3	D	802[B]	HEM	C3C-C4C	4.62	1.48	1.41
3	D	802[B]	HEM	C3C-C2C	4.40	1.46	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	802[B]	HEM	CHA-C4D	4.37	1.45	1.34
3	B	802[B]	HEM	CHA-C4D	4.36	1.45	1.34
3	D	802[B]	HEM	C2C-C1C	4.19	1.51	1.42
3	B	802[B]	HEM	CHB-C1B	4.18	1.44	1.34
2	A	801[A]	HDD	C3B-C2B	4.07	1.45	1.40
3	D	802[B]	HEM	C3D-C2D	4.00	1.45	1.36
2	C	801[A]	HDD	O1D-CGD	3.96	1.41	1.35
3	C	802[B]	HEM	C3D-C2D	3.93	1.45	1.36
3	B	802[B]	HEM	C3C-C2C	3.92	1.45	1.40
3	B	802[B]	HEM	C3D-C2D	3.79	1.44	1.36
3	C	802[B]	HEM	CHB-C1B	3.78	1.43	1.34
2	C	801[A]	HDD	C3C-C2C	3.74	1.45	1.40
2	A	801[A]	HDD	O1D-CGD	3.56	1.41	1.35
3	D	802[B]	HEM	CHB-C1B	3.54	1.43	1.34
3	A	802[B]	HEM	C3D-C2D	3.54	1.44	1.36
2	D	801[A]	HDD	C2B-C1B	3.50	1.50	1.42
3	A	802[B]	HEM	C1B-NB	-3.45	1.34	1.40
3	C	802[B]	HEM	C3C-C2C	3.44	1.45	1.40
3	B	802[B]	HEM	C3B-C2B	3.41	1.44	1.37
3	A	802[B]	HEM	C3B-C2B	3.40	1.44	1.37
2	C	801[A]	HDD	O1D-C3D	3.39	1.52	1.46
3	A	802[B]	HEM	CHB-C1B	3.37	1.42	1.34
2	B	801[A]	HDD	C3C-C2C	3.28	1.44	1.40
2	B	801[A]	HDD	C3B-C4B	3.21	1.46	1.41
3	C	802[B]	HEM	C3B-C2B	3.19	1.43	1.37
2	D	801[A]	HDD	C3B-C4B	3.19	1.46	1.41
3	B	802[B]	HEM	C1B-NB	-3.15	1.34	1.40
3	A	802[B]	HEM	C3C-C2C	2.96	1.44	1.40
3	B	802[B]	HEM	C2A-C3A	2.93	1.46	1.37
3	C	802[B]	HEM	C2A-C3A	2.80	1.46	1.37
3	A	802[B]	HEM	C2C-C1C	2.80	1.48	1.42
2	C	801[A]	HDD	C3B-C4B	2.77	1.45	1.41
2	A	801[A]	HDD	C2B-C1B	2.76	1.48	1.42
2	A	801[A]	HDD	C4C-NC	-2.74	1.30	1.36
2	A	801[A]	HDD	C1A-CHA	2.72	1.48	1.41
3	B	802[B]	HEM	C2C-C1C	2.71	1.48	1.42
3	C	802[B]	HEM	FE-ND	2.70	2.13	1.98
2	B	801[A]	HDD	C1A-CHA	2.69	1.48	1.41
3	D	802[B]	HEM	C2A-C3A	2.67	1.45	1.37
2	D	801[A]	HDD	OND-C2D	2.63	1.47	1.42
3	A	802[B]	HEM	CHD-C1D	2.63	1.48	1.40
3	D	802[B]	HEM	CHD-C1D	2.62	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802[B]	HEM	FE-NB	2.62	2.12	1.98
3	C	802[B]	HEM	CHD-C1D	2.61	1.48	1.40
2	C	801[A]	HDD	C1C-CHC	2.54	1.48	1.41
3	A	802[B]	HEM	C4D-ND	-2.54	1.35	1.40
3	D	802[B]	HEM	FE-NB	2.52	2.12	1.98
2	B	801[A]	HDD	C3B-C2B	2.45	1.43	1.40
3	D	802[B]	HEM	CHC-C4B	2.44	1.47	1.40
3	D	802[B]	HEM	C1B-NB	-2.43	1.36	1.40
3	A	802[B]	HEM	C2A-C3A	2.41	1.44	1.37
3	D	802[B]	HEM	C4D-ND	-2.40	1.36	1.40
2	B	801[A]	HDD	O1D-CGD	2.40	1.39	1.35
2	C	801[A]	HDD	C2A-C3A	2.40	1.44	1.37
3	B	802[B]	HEM	C4D-ND	-2.35	1.36	1.40
2	C	801[A]	HDD	C3B-C2B	2.34	1.43	1.40
2	D	801[A]	HDD	C2A-C3A	2.30	1.44	1.37
3	D	802[B]	HEM	FE-ND	2.29	2.10	1.98
3	A	802[B]	HEM	FE-NB	2.29	2.10	1.98
2	A	801[A]	HDD	C4C-CHD	2.26	1.47	1.41
2	A	801[A]	HDD	C2A-C3A	2.23	1.44	1.37
3	B	802[B]	HEM	CHC-C4B	2.22	1.47	1.40
3	A	802[B]	HEM	FE-ND	2.22	2.10	1.98
3	C	802[B]	HEM	FE-NB	2.22	2.10	1.98
2	A	801[A]	HDD	CMC-C2C	2.21	1.56	1.51
3	C	802[B]	HEM	C4D-ND	-2.20	1.36	1.40
2	D	801[A]	HDD	C1D-ND	2.16	1.41	1.37
2	B	801[A]	HDD	O1D-C3D	2.15	1.50	1.46
3	B	802[B]	HEM	FE-ND	2.13	2.09	1.98
2	A	801[A]	HDD	C3B-C4B	2.12	1.44	1.41
3	B	802[B]	HEM	CHD-C1D	2.10	1.46	1.40
2	C	801[A]	HDD	C4A-NA	-2.09	1.32	1.36
2	B	801[A]	HDD	C3D-C2D	-2.07	1.50	1.55
3	C	802[B]	HEM	C4B-NB	-2.06	1.34	1.38
3	B	802[B]	HEM	C1A-CHA	2.05	1.46	1.41
2	C	801[A]	HDD	C4C-NC	-2.05	1.32	1.36
3	C	802[B]	HEM	C2C-C1C	2.03	1.47	1.42

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801[A]	HDD	C3D-O1D-CGD	10.10	120.56	111.14
3	C	802[B]	HEM	C3B-C2B-C1B	-10.02	98.88	106.41
3	A	802[B]	HEM	C3B-C2B-C1B	-9.97	98.92	106.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801[A]	HDD	O1D-CGD-O2D	9.85	129.11	120.81
3	A	802[B]	HEM	C2B-C1B-NB	9.64	120.92	109.84
2	A	801[A]	HDD	O1D-CGD-O2D	9.31	128.66	120.81
3	D	802[B]	HEM	C3B-C2B-C1B	-9.02	99.64	106.41
2	B	801[A]	HDD	O1D-CGD-O2D	8.53	127.99	120.81
3	D	802[B]	HEM	C2B-C1B-NB	8.21	119.28	109.84
3	C	802[B]	HEM	C3B-C4B-NB	7.57	114.91	109.47
3	C	802[B]	HEM	C2B-C1B-NB	7.50	118.46	109.84
3	B	802[B]	HEM	C3B-C2B-C1B	-7.23	100.98	106.41
3	C	802[B]	HEM	C3D-C4D-ND	7.22	118.09	110.17
2	D	801[A]	HDD	O1D-CGD-O2D	6.89	126.61	120.81
2	A	801[A]	HDD	O1D-CGD-CBD	-6.78	103.99	110.17
3	B	802[B]	HEM	C2B-C1B-NB	6.77	117.63	109.84
2	D	801[A]	HDD	C4A-C3A-C2A	-6.56	102.44	107.00
2	D	801[A]	HDD	CBD-CAD-C3D	6.26	112.91	103.98
2	C	801[A]	HDD	C4A-C3A-C2A	-6.25	102.65	107.00
3	C	802[B]	HEM	C2D-C1D-ND	5.98	116.81	109.90
3	A	802[B]	HEM	C3B-C4B-NB	5.90	113.71	109.47
2	C	801[A]	HDD	OND-C2D-CMD	-5.65	98.53	109.45
2	B	801[A]	HDD	C4A-C3A-C2A	-5.53	103.15	107.00
3	B	802[B]	HEM	C2D-C1D-ND	5.46	116.21	109.90
3	D	802[B]	HEM	C2D-C1D-ND	5.31	116.04	109.90
3	D	802[B]	HEM	C3B-C4B-NB	5.30	113.27	109.47
3	D	802[B]	HEM	CAA-CBA-CGA	-5.21	99.81	113.83
2	D	801[A]	HDD	C3D-O1D-CGD	5.18	115.97	111.14
2	A	801[A]	HDD	OND-C2D-CMD	-5.10	99.58	109.45
3	B	802[B]	HEM	C3B-C4B-NB	5.09	113.12	109.47
2	B	801[A]	HDD	O1D-CGD-CBD	-4.85	105.75	110.17
3	A	802[B]	HEM	C3D-C4D-ND	4.80	115.43	110.17
3	D	802[B]	HEM	C3D-C4D-ND	4.67	115.30	110.17
3	C	802[B]	HEM	C4D-ND-C1D	-4.60	99.76	105.21
2	B	801[A]	HDD	CAA-CBA-CGA	-4.54	101.61	113.83
3	B	802[B]	HEM	C3D-C4D-ND	4.50	115.11	110.17
3	A	802[B]	HEM	C1B-NB-C4B	-4.49	99.89	105.21
3	A	802[B]	HEM	C2D-C1D-ND	4.48	115.08	109.90
2	A	801[A]	HDD	C4A-C3A-C2A	-4.47	103.89	107.00
3	C	802[B]	HEM	CHA-C4D-C3D	-4.37	117.17	125.23
2	B	801[A]	HDD	CBA-CAA-C2A	-4.30	105.31	112.54
2	A	801[A]	HDD	CBD-CAD-C3D	4.19	109.95	103.98
3	B	802[B]	HEM	C1D-C2D-C3D	-4.17	102.59	106.98
3	C	802[B]	HEM	C2C-C3C-C4C	4.13	109.78	106.90
3	C	802[B]	HEM	C1D-C2D-C3D	-4.10	102.67	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801[A]	HDD	CAA-CBA-CGA	-4.10	102.80	113.83
2	C	801[A]	HDD	C2D-C1D-CHD	-4.09	117.91	124.27
3	D	802[B]	HEM	CHB-C1B-C2B	-4.07	115.42	126.94
2	D	801[A]	HDD	C2D-C1D-CHD	-4.04	117.99	124.27
2	B	801[A]	HDD	C2D-C1D-CHD	-4.03	118.00	124.27
2	D	801[A]	HDD	OND-C2D-CMD	-4.02	101.67	109.45
3	D	802[B]	HEM	C1D-C2D-C3D	-4.02	102.75	106.98
3	C	802[B]	HEM	C1B-NB-C4B	-3.99	100.48	105.21
2	D	801[A]	HDD	C3C-C4C-NC	3.95	114.32	109.21
3	B	802[B]	HEM	CHD-C1D-C2D	-3.95	118.79	125.03
2	B	801[A]	HDD	CMB-C2B-C3B	3.90	132.49	124.68
3	C	802[B]	HEM	CBB-CAB-C3B	-3.89	108.08	127.53
3	A	802[B]	HEM	CHB-C1B-C2B	-3.87	115.99	126.94
2	B	801[A]	HDD	CMC-C2C-C3C	3.78	132.24	124.68
3	C	802[B]	HEM	CMD-C2D-C1D	3.73	130.87	125.03
3	A	802[B]	HEM	CBB-CAB-C3B	-3.69	109.10	127.53
3	D	802[B]	HEM	C4A-C3A-C2A	-3.68	104.43	107.00
2	C	801[A]	HDD	C3D-O1D-CGD	3.66	114.55	111.14
2	C	801[A]	HDD	CMB-C2B-C3B	3.65	131.97	124.68
2	B	801[A]	HDD	OND-C2D-CMD	-3.63	102.44	109.45
3	C	802[B]	HEM	CAA-CBA-CGA	-3.58	104.18	113.83
2	A	801[A]	HDD	O1D-C3D-CAD	-3.57	96.46	103.06
3	D	802[B]	HEM	CBD-CAD-C3D	-3.55	102.71	112.53
3	B	802[B]	HEM	CBD-CAD-C3D	-3.53	102.79	112.53
2	C	801[A]	HDD	C4C-CHD-C1D	-3.51	123.35	130.04
3	A	802[B]	HEM	C1D-C2D-C3D	-3.50	103.30	106.98
3	C	802[B]	HEM	CMB-C2B-C1B	3.44	130.41	125.03
2	C	801[A]	HDD	C3C-C4C-NC	3.41	113.62	109.21
2	A	801[A]	HDD	CMC-C2C-C1C	3.38	133.41	128.46
3	C	802[B]	HEM	CHC-C4B-C3B	-3.37	119.40	124.57
2	C	801[A]	HDD	CAA-CBA-CGA	-3.33	104.85	113.83
3	B	802[B]	HEM	CBB-CAB-C3B	-3.33	110.90	127.53
2	A	801[A]	HDD	CBA-CAA-C2A	-3.31	106.97	112.54
3	A	802[B]	HEM	C2C-C3C-C4C	3.31	109.21	106.90
2	A	801[A]	HDD	C4C-CHD-C1D	-3.27	123.80	130.04
2	C	801[A]	HDD	O1D-CGD-CBD	-3.24	107.21	110.17
3	A	802[B]	HEM	CHA-C4D-C3D	-3.23	119.27	125.23
2	A	801[A]	HDD	C2D-C1D-CHD	-3.17	119.33	124.27
2	A	801[A]	HDD	C1A-CHA-C4D	-3.17	123.99	130.04
3	A	802[B]	HEM	CAA-CBA-CGA	-3.17	105.30	113.83
3	A	802[B]	HEM	C4B-CHC-C1C	-3.12	118.44	122.56
2	B	801[A]	HDD	C1A-CHA-C4D	-3.12	124.08	130.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801[A]	HDD	C2B-C3B-C4B	3.12	109.08	106.90
3	C	802[B]	HEM	C4D-C3D-C2D	-3.11	102.36	106.89
2	B	801[A]	HDD	C3D-O1D-CGD	3.10	114.04	111.14
3	A	802[B]	HEM	CMD-C2D-C1D	3.09	129.86	125.03
3	D	802[B]	HEM	CHD-C1D-C2D	-3.07	120.18	125.03
3	B	802[B]	HEM	CHB-C1B-C2B	-3.06	118.26	126.94
2	D	801[A]	HDD	CMA-C3A-C2A	3.06	130.71	124.94
3	A	802[B]	HEM	CBD-CAD-C3D	-3.02	104.18	112.53
2	B	801[A]	HDD	C3C-C4C-NC	3.00	113.08	109.21
2	C	801[A]	HDD	CBD-CAD-C3D	2.98	108.24	103.98
3	D	802[B]	HEM	C1B-NB-C4B	-2.93	101.74	105.21
2	D	801[A]	HDD	CAA-CBA-CGA	-2.87	106.09	113.83
3	B	802[B]	HEM	CMC-C2C-C3C	2.84	130.36	124.68
3	D	802[B]	HEM	CMD-C2D-C1D	2.79	129.39	125.03
3	A	802[B]	HEM	O2D-CGD-CBD	2.74	122.67	114.00
3	C	802[B]	HEM	CHB-C1B-NB	-2.74	120.98	124.37
3	D	802[B]	HEM	C4D-ND-C1D	-2.71	101.99	105.21
2	B	801[A]	HDD	C4C-CHD-C1D	-2.71	124.87	130.04
3	C	802[B]	HEM	C4B-CHC-C1C	-2.70	119.00	122.56
3	C	802[B]	HEM	CHD-C1D-C2D	-2.70	120.77	125.03
3	D	802[B]	HEM	C3C-C4C-NC	2.68	116.00	110.94
3	B	802[B]	HEM	C4D-ND-C1D	-2.63	102.09	105.21
2	D	801[A]	HDD	C4B-CHC-C1C	2.60	131.28	123.67
3	D	802[B]	HEM	CBA-CAA-C2A	2.58	116.88	112.54
3	A	802[B]	HEM	C4D-ND-C1D	-2.57	102.17	105.21
2	D	801[A]	HDD	C4C-CHD-C1D	-2.56	125.16	130.04
3	C	802[B]	HEM	CBD-CAD-C3D	-2.56	105.46	112.53
2	C	801[A]	HDD	C1A-CHA-C4D	-2.54	125.20	130.04
3	B	802[B]	HEM	CHA-C4D-C3D	-2.53	120.57	125.23
2	D	801[A]	HDD	O1D-CGD-CBD	-2.49	107.90	110.17
2	C	801[A]	HDD	CBA-CAA-C2A	-2.40	108.50	112.54
2	A	801[A]	HDD	CMD-C2D-C3D	2.36	121.33	115.11
3	B	802[B]	HEM	C1B-NB-C4B	-2.33	102.44	105.21
2	C	801[A]	HDD	O2A-CGA-CBA	2.33	121.35	114.00
3	B	802[B]	HEM	C4C-CHD-C1D	-2.32	119.49	122.56
2	A	801[A]	HDD	C3C-C4C-NC	2.31	112.20	109.21
3	D	802[B]	HEM	CMB-C2B-C3B	2.31	134.03	128.43
3	D	802[B]	HEM	C4D-C3D-C2D	-2.30	103.55	106.89
2	A	801[A]	HDD	C3D-C4D-CHA	-2.30	117.47	124.14
2	B	801[A]	HDD	CMA-C3A-C2A	2.29	129.27	124.94
3	C	802[B]	HEM	CHB-C1B-C2B	-2.29	120.45	126.94
3	A	802[B]	HEM	CHD-C1D-C2D	-2.26	121.47	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801[A]	HDD	CHA-C4D-ND	2.24	127.38	124.28
2	D	801[A]	HDD	O1D-C3D-CAD	-2.22	98.95	103.06
3	B	802[B]	HEM	O2D-CGD-CBD	2.22	121.00	114.00
2	B	801[A]	HDD	C2B-C3B-C4B	2.19	108.42	106.90
3	B	802[B]	HEM	CHC-C4B-C3B	-2.18	121.22	124.57
2	D	801[A]	HDD	CMB-C2B-C3B	2.18	129.04	124.68
3	B	802[B]	HEM	O1D-CGD-CBD	-2.16	116.26	123.09
3	B	802[B]	HEM	CMD-C2D-C3D	2.12	131.89	126.15
2	B	801[A]	HDD	CMD-C2D-C1D	2.11	116.26	112.68
3	B	802[B]	HEM	C4D-C3D-C2D	-2.11	103.81	106.89
3	A	802[B]	HEM	O1D-CGD-CBD	-2.11	116.40	123.09
2	A	801[A]	HDD	CMA-C3A-C2A	2.08	128.86	124.94
3	A	802[B]	HEM	C4D-C3D-C2D	-2.07	103.88	106.89
2	C	801[A]	HDD	CMC-C2C-C3C	2.02	128.72	124.68
2	B	801[A]	HDD	OND-C2D-C3D	-2.01	105.74	110.46

There are no chirality outliers.

All (24) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

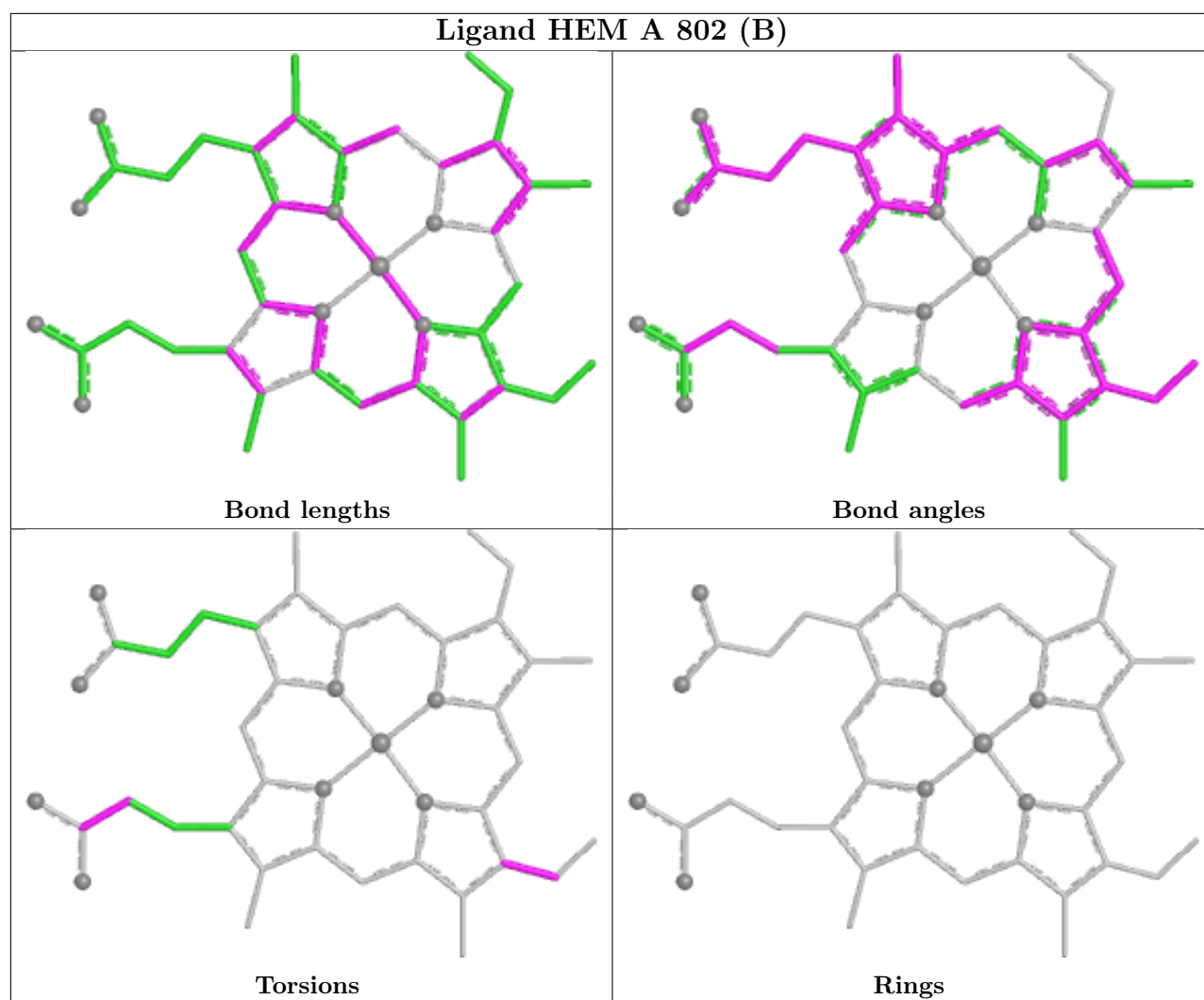
Mol	Chain	Res	Type	Atoms
2	C	801[A]	HDD	CAA-CBA-CGA-O2A
2	B	801[A]	HDD	CAA-CBA-CGA-O2A

There are no ring outliers.

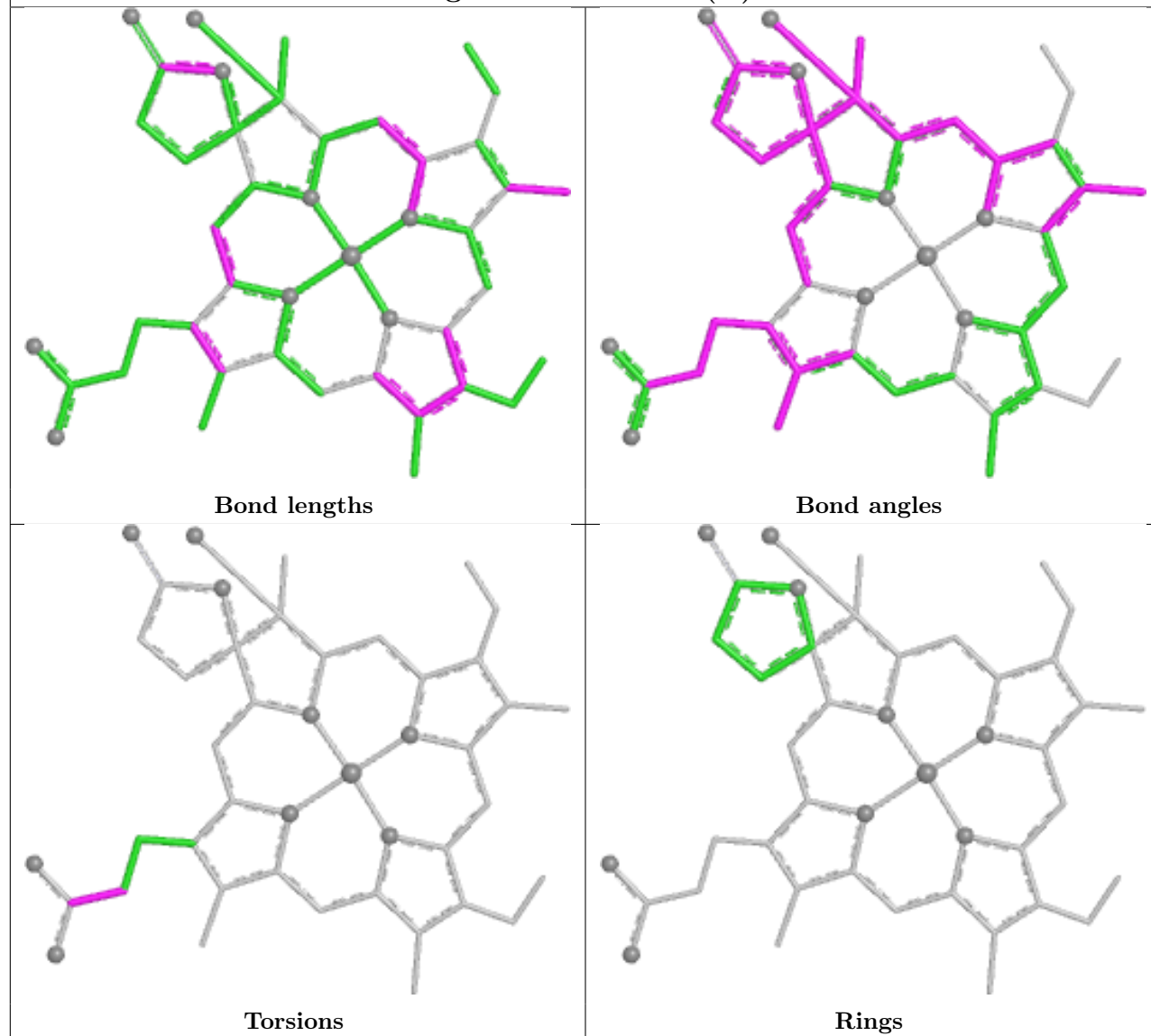
8 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802[B]	HEM	8	0
2	A	801[A]	HDD	4	0
3	D	802[B]	HEM	9	0
2	B	801[A]	HDD	3	0
2	C	801[A]	HDD	2	0
3	C	802[B]	HEM	15	0
2	D	801[A]	HDD	4	0
3	B	802[B]	HEM	6	0

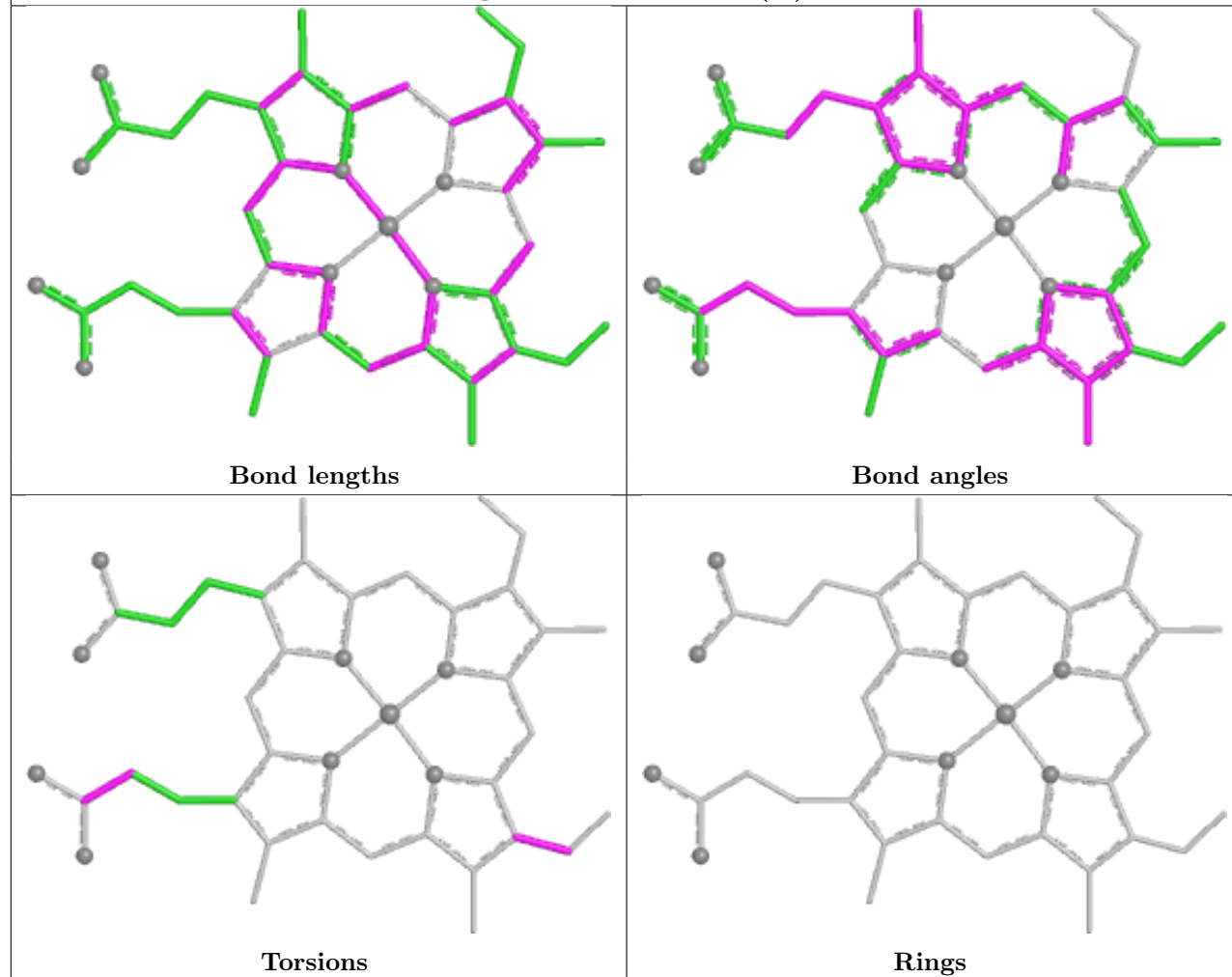
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



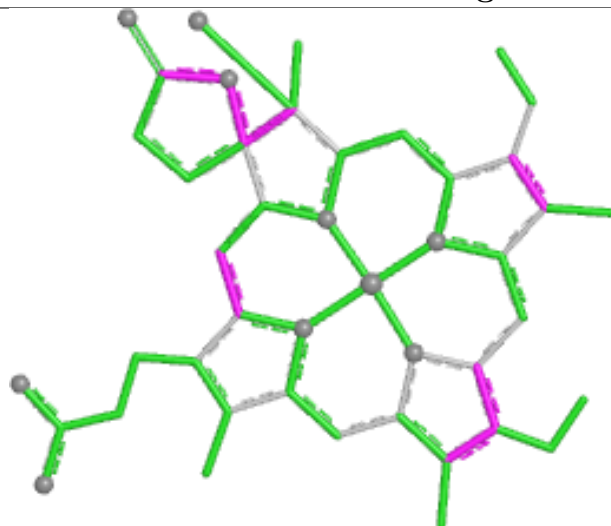
Ligand HDD A 801 (A)



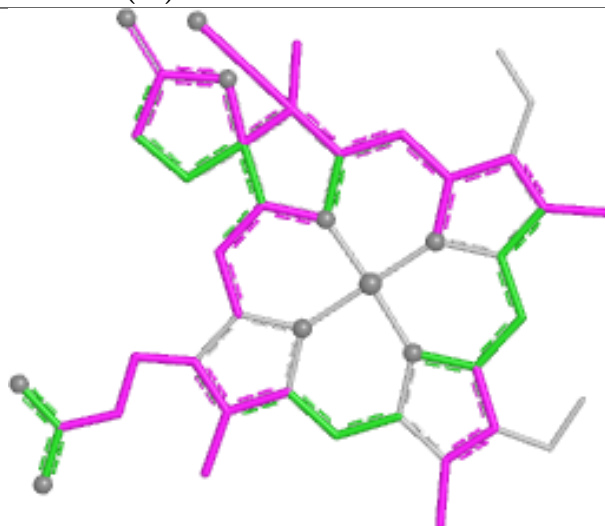
Ligand HEM D 802 (B)



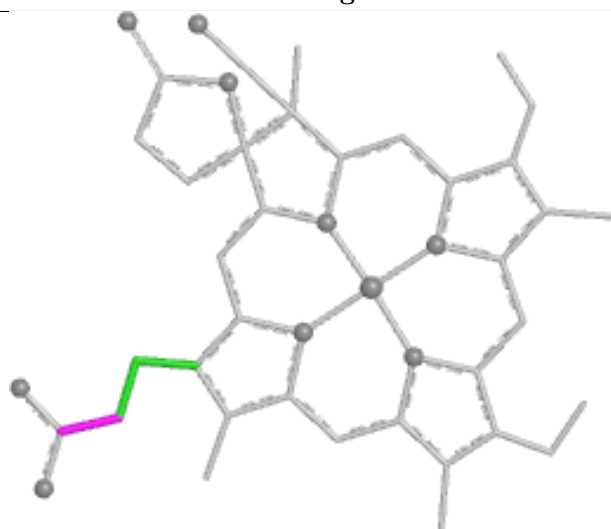
Ligand HDD B 801 (A)



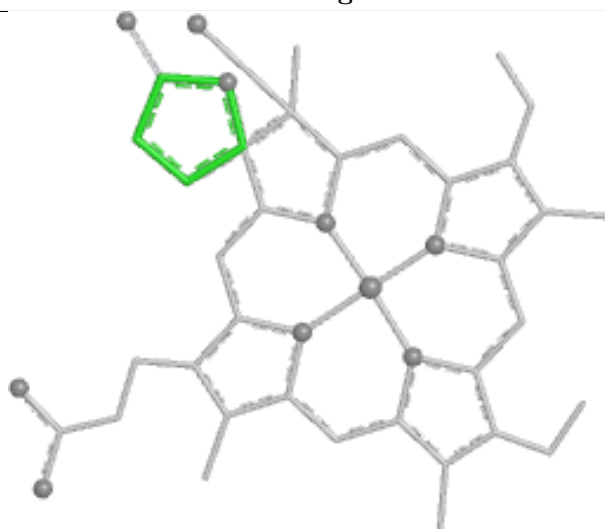
Bond lengths



Bond angles

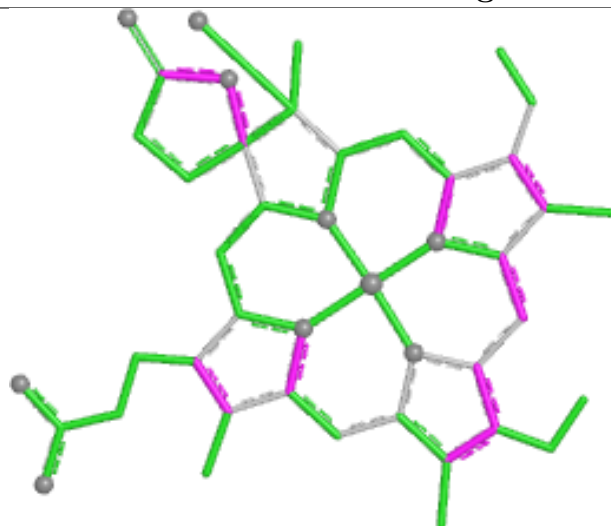


Torsions

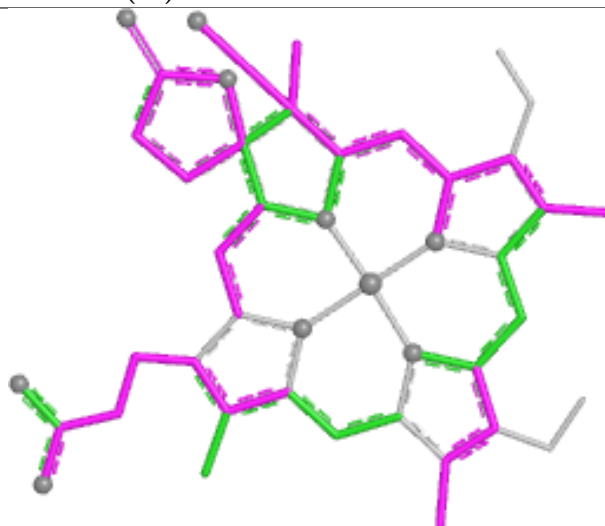


Rings

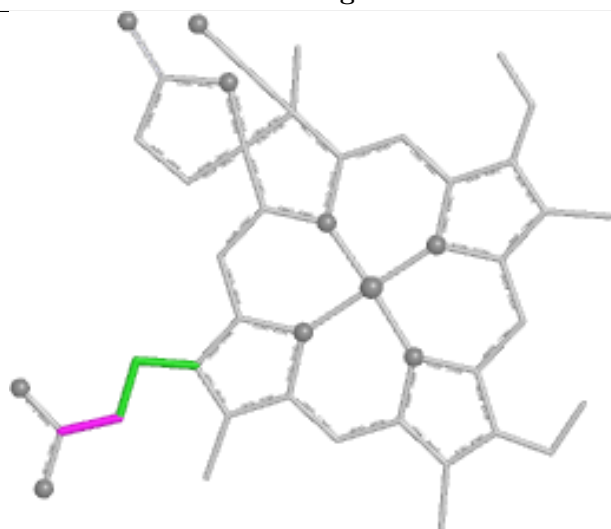
Ligand HDD C 801 (A)



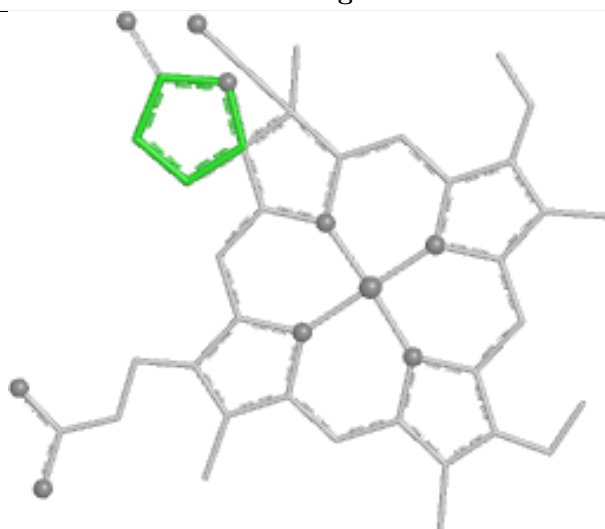
Bond lengths



Bond angles

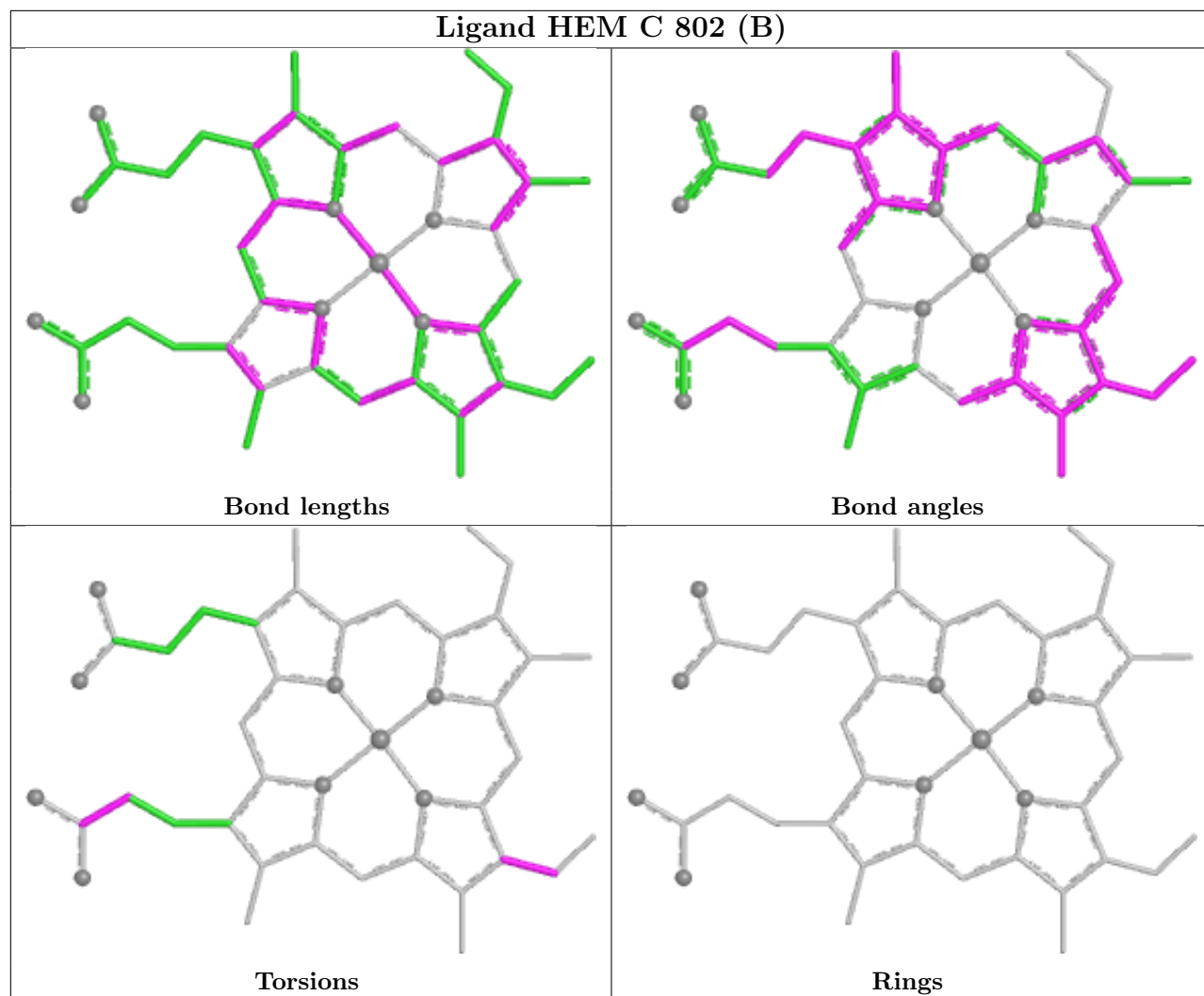


Torsions

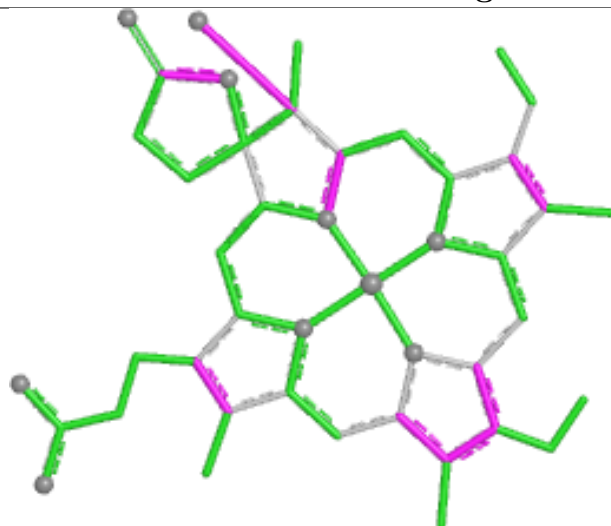


Rings

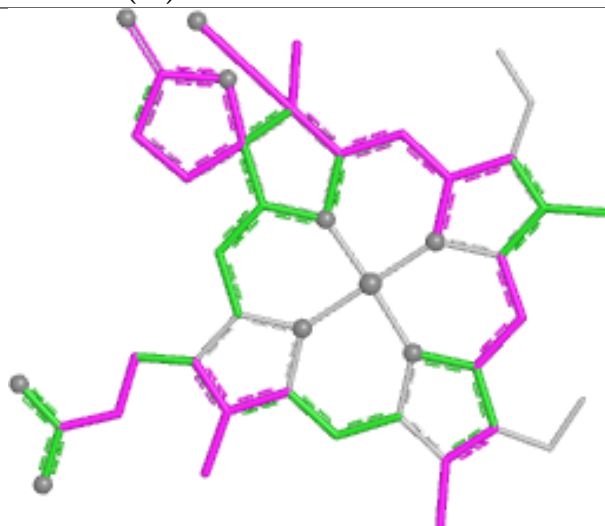
Ligand HEM C 802 (B)



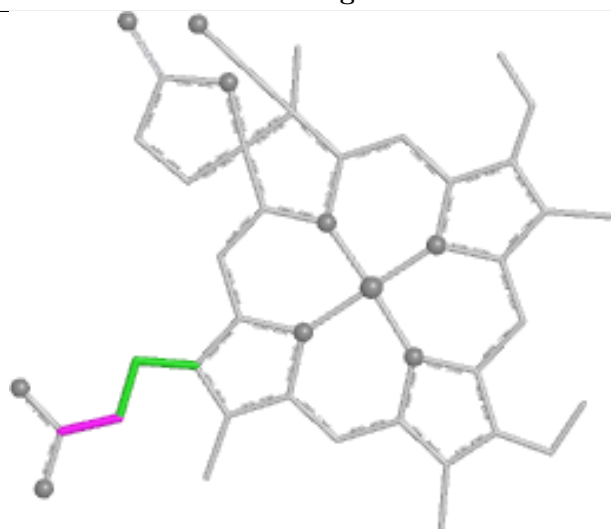
Ligand HDD D 801 (A)



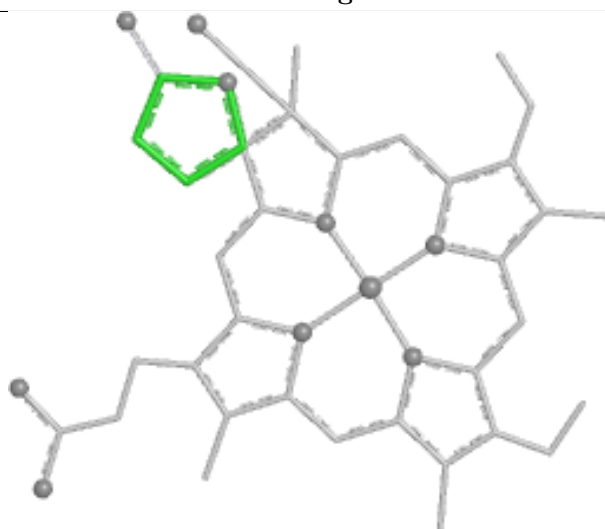
Bond lengths



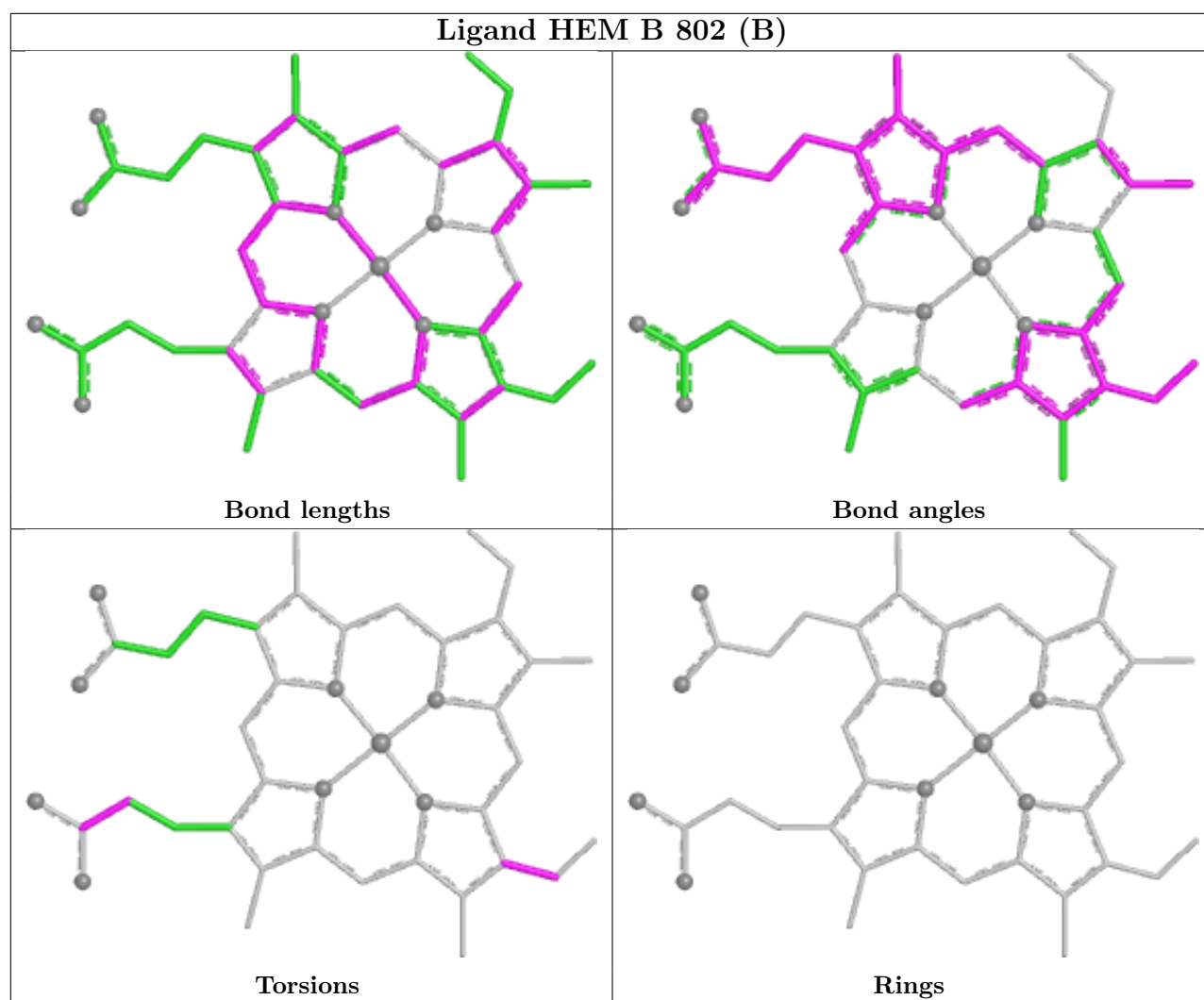
Bond angles



Torsions



Rings



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	725/753 (96%)	-0.67	5 (0%) 84 86	4, 11, 29, 60	4 (0%)
1	B	725/753 (96%)	-0.53	3 (0%) 89 90	5, 13, 36, 56	1 (0%)
1	C	725/753 (96%)	-0.56	5 (0%) 84 86	5, 12, 34, 56	3 (0%)
1	D	725/753 (96%)	-0.67	2 (0%) 90 91	4, 11, 28, 58	3 (0%)
All	All	2900/3012 (96%)	-0.61	15 (0%) 87 89	4, 11, 33, 60	11 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	726	GLY	3.6
1	A	711	ALA	3.3
1	C	725	ASP	3.1
1	A	710	ILE	3.0
1	A	712	ASP	2.9
1	C	595	ASP	2.7
1	B	726	GLY	2.7
1	B	583	LYS	2.5
1	A	713	GLN	2.5
1	C	596	GLY	2.3
1	D	595	ASP	2.3
1	B	568	ASP	2.2
1	D	28	SER	2.1
1	C	724	ALA	2.0
1	A	725	ASP	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	OCS	B	669	9/10	0.93	0.09	25,27,36,37	0
1	OCS	C	669	9/10	0.93	0.09	25,28,36,40	0
1	OCS	D	669	9/10	0.94	0.09	18,21,28,33	0
1	OCS	A	669	9/10	0.95	0.08	15,19,27,28	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

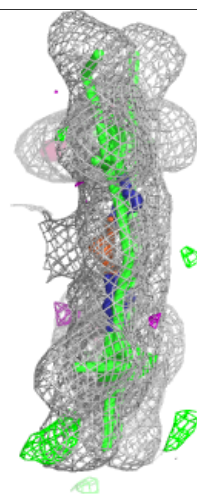
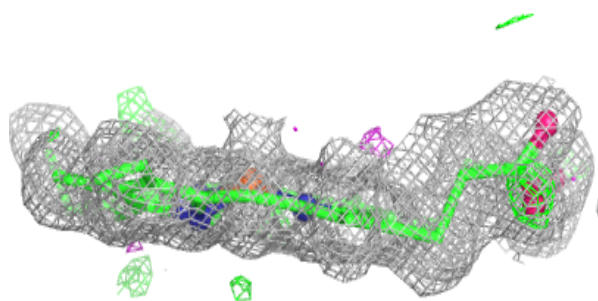
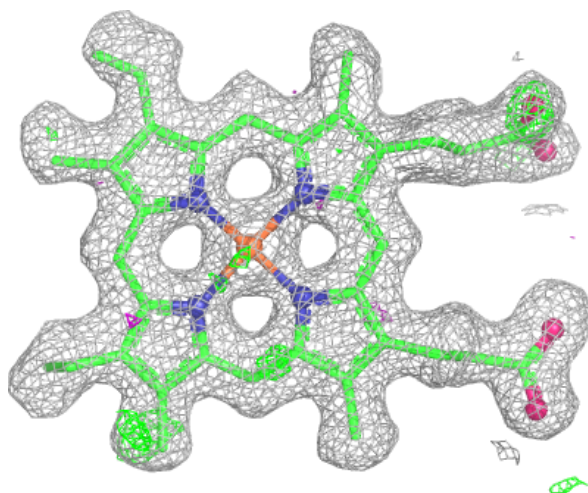
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	HEM	A	802[B]	43/43	0.97	0.06	3,4,5,5	43
3	HEM	B	802[B]	43/43	0.97	0.07	4,5,6,6	43
3	HEM	C	802[B]	43/43	0.98	0.06	3,5,5,5	43
3	HEM	D	802[B]	43/43	0.98	0.06	3,4,5,5	43
2	HDD	A	801[A]	44/44	0.99	0.05	4,6,9,11	44
2	HDD	B	801[A]	44/44	0.99	0.05	5,6,10,13	44
2	HDD	C	801[A]	44/44	0.99	0.05	5,6,9,11	44
2	HDD	D	801[A]	44/44	0.99	0.05	4,5,10,12	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.

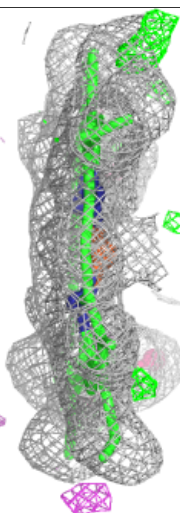
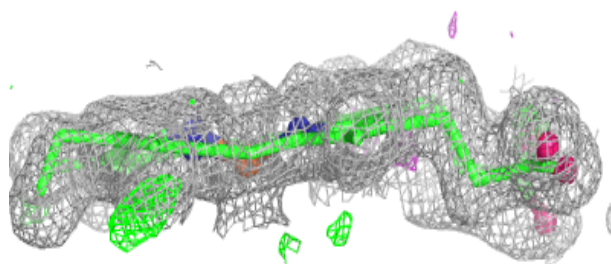
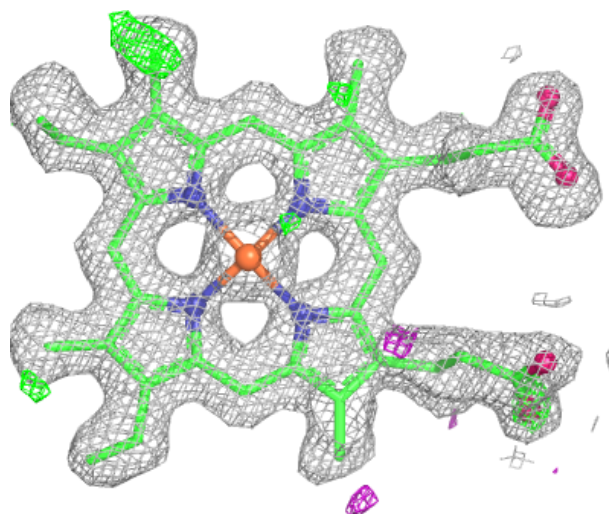
Electron density around HEM A 802 (B):

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



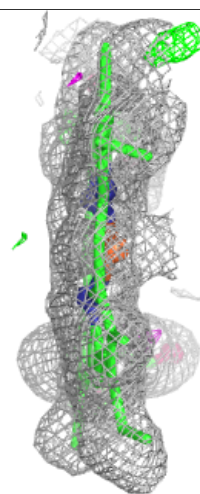
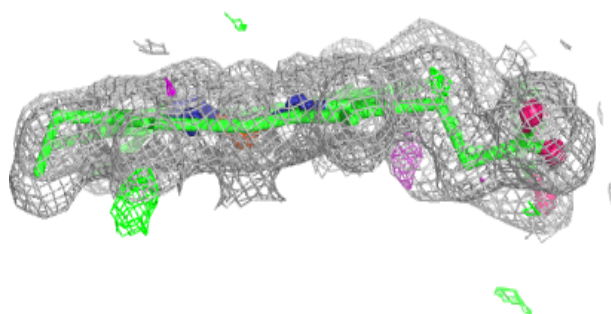
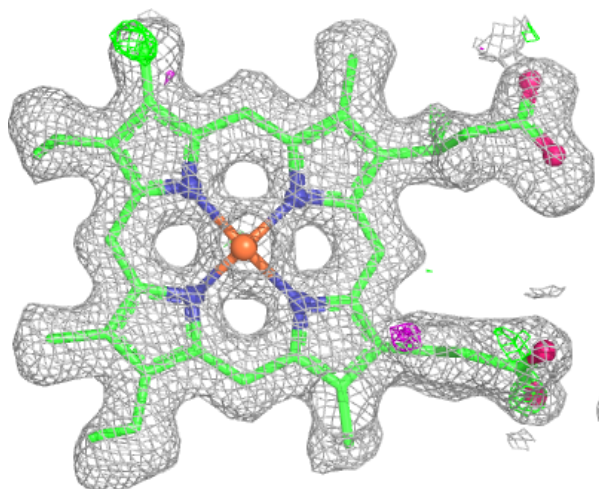
Electron density around HEM B 802 (B):

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



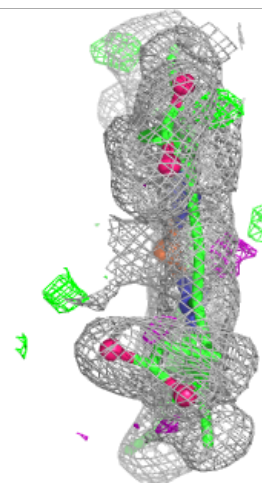
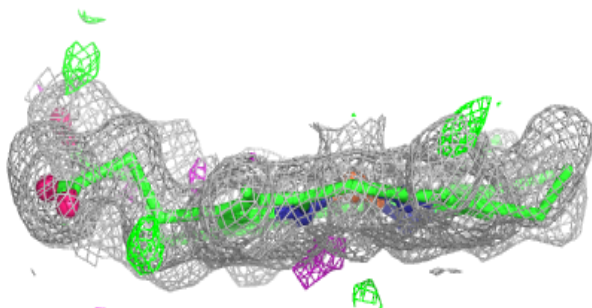
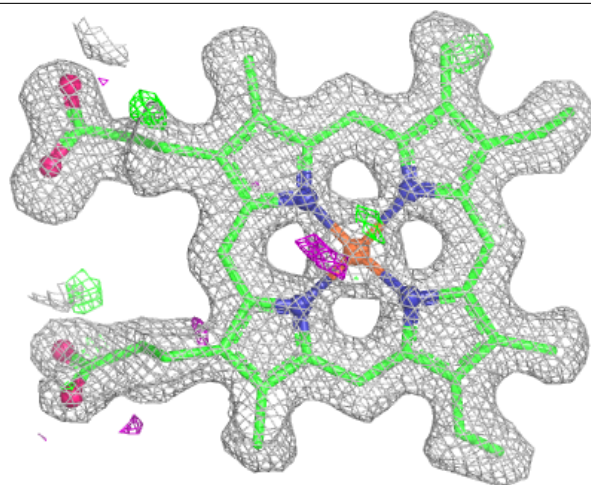
Electron density around HEM C 802 (B):

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



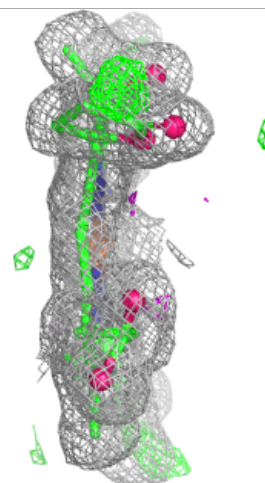
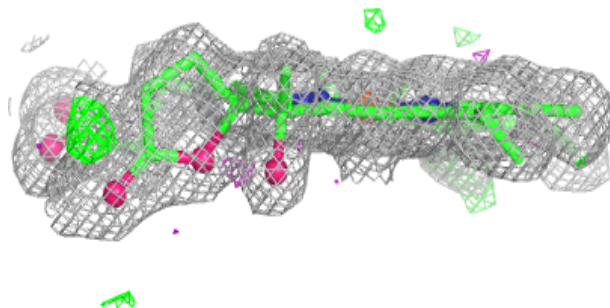
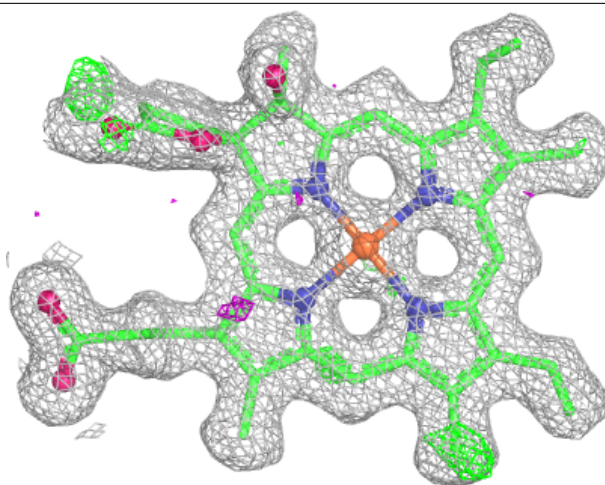
Electron density around HEM D 802 (B):

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



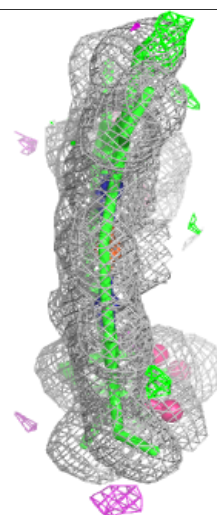
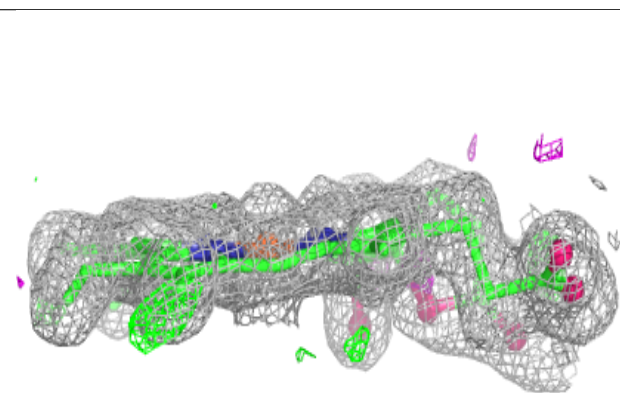
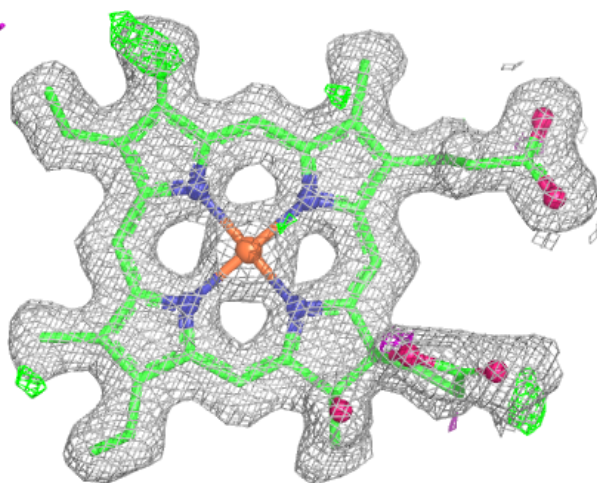
Electron density around HDD A 801 (A):

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



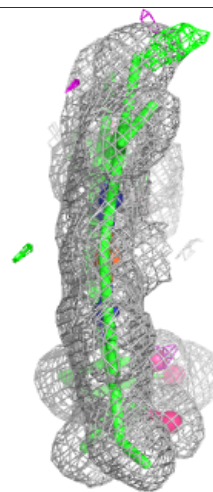
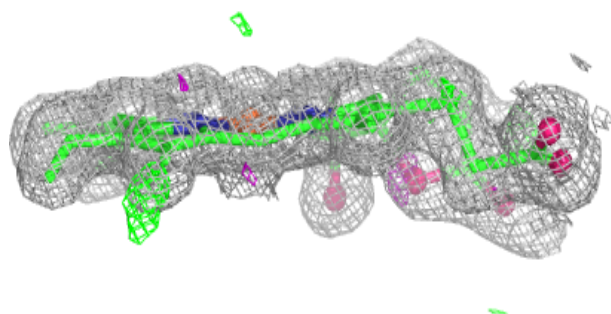
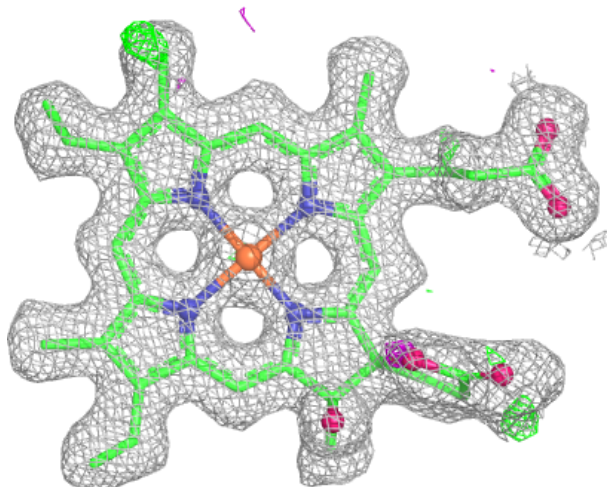
Electron density around HDD B 801 (A):

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



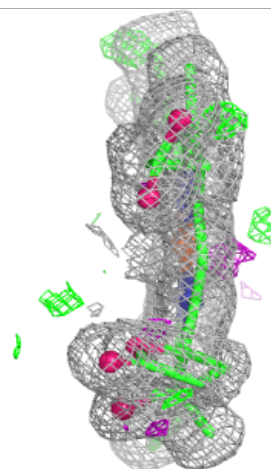
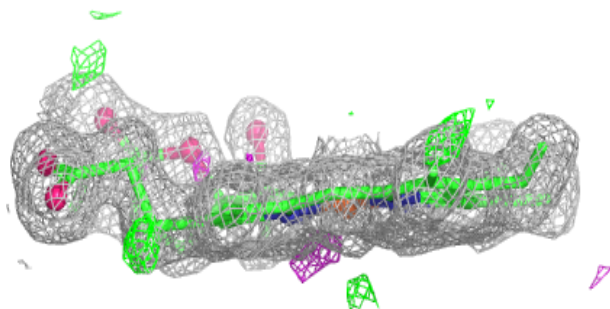
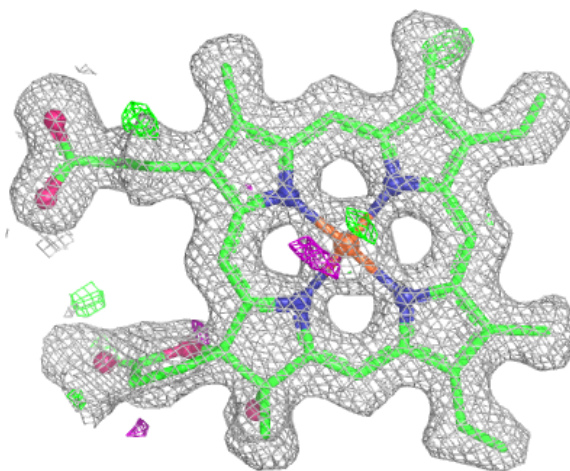
Electron density around HDD C 801 (A):

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.