



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:00 AM UTC

PDB ID : 9JN6 / pdb_00009jn6
Title : Crystal structure of KtzT-C197A in complex with HEME and product
Authors : Li, Y.L.; Yang, Y.Y.; Huang, J.-W.; Chen, C.-C.; Guo, R.-T.
Deposited on : 2024-09-22
Resolution : 1.72 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

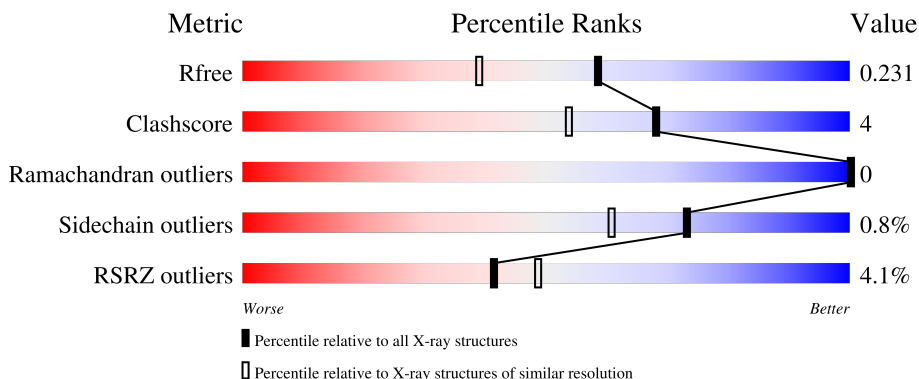
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

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	218	5% 91% 7%
1	B	218	5% 92% 6%
1	C	218	3% 91% 6%
1	D	218	3% 91% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7493 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 FMN-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	213	Total	C	N	O	S	0	0	0
			1610	1018	302	285	5			
1	C	212	Total	C	N	O	S	0	0	0
			1606	1016	301	284	5			
1	D	213	Total	C	N	O	S	0	0	0
			1610	1018	302	285	5			
1	A	214	Total	C	N	O	S	0	0	0
			1617	1022	303	287	5			

There are 24 discrepancies between the modelled and reference sequences:

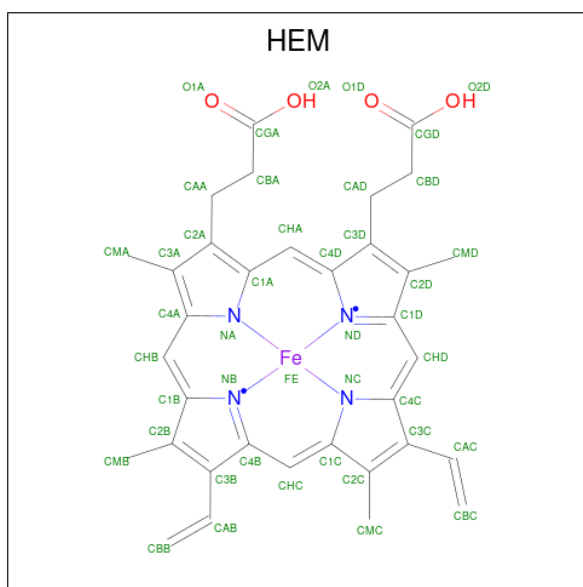
Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	ALA	-	expression tag	UNP A8CF72
B	-3	GLY	-	expression tag	UNP A8CF72
B	-2	ALA	-	expression tag	UNP A8CF72
B	-1	GLY	-	expression tag	UNP A8CF72
B	0	ALA	-	expression tag	UNP A8CF72
B	197	ALA	CYS	engineered mutation	UNP A8CF72
C	-4	ALA	-	expression tag	UNP A8CF72
C	-3	GLY	-	expression tag	UNP A8CF72
C	-2	ALA	-	expression tag	UNP A8CF72
C	-1	GLY	-	expression tag	UNP A8CF72
C	0	ALA	-	expression tag	UNP A8CF72
C	197	ALA	CYS	engineered mutation	UNP A8CF72
D	-4	ALA	-	expression tag	UNP A8CF72
D	-3	GLY	-	expression tag	UNP A8CF72
D	-2	ALA	-	expression tag	UNP A8CF72
D	-1	GLY	-	expression tag	UNP A8CF72
D	0	ALA	-	expression tag	UNP A8CF72
D	197	ALA	CYS	engineered mutation	UNP A8CF72
A	-4	ALA	-	expression tag	UNP A8CF72
A	-3	GLY	-	expression tag	UNP A8CF72
A	-2	ALA	-	expression tag	UNP A8CF72

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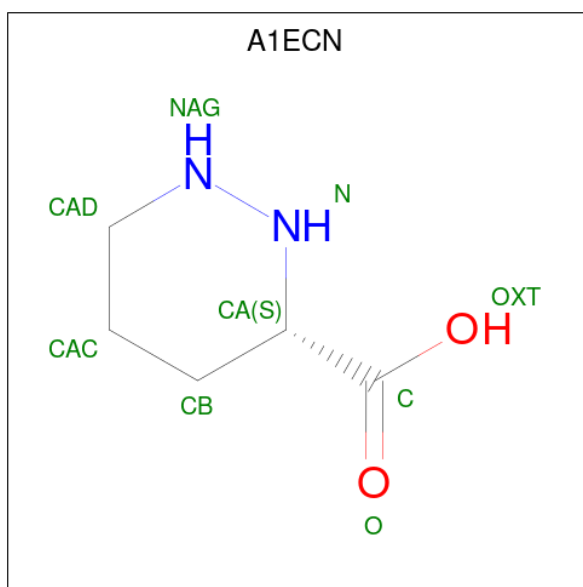
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP A8CF72
A	0	ALA	-	expression tag	UNP A8CF72
A	197	ALA	CYS	engineered mutation	UNP A8CF72

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 3 is (3 {S})-1,2-diazinane-3-carboxylic acid (CCD ID: A1ECN) (formula: $C_5H_{10}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			9	5	2	2		
3	D	1	Total	C	N	O	0	0
			9	5	2	2		
3	A	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	214	Total	O	0	0
			214	214		
4	C	231	Total	O	0	0
			231	231		
4	D	190	Total	O	0	0
			190	190		
4	A	216	Total	O	0	0
			216	216		

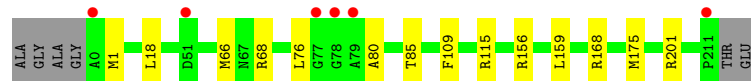
3 Residue-property plots [i](#)

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: FMN-binding protein



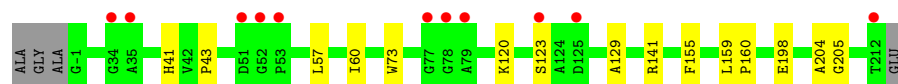
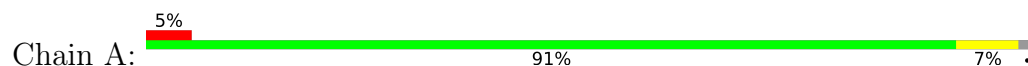
- Molecule 1: FMN-binding protein



- Molecule 1: FMN-binding protein



- Molecule 1: FMN-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.88Å 101.61Å 111.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.24 – 1.72 29.24 – 1.72	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.24-1.72) 99.3 (29.24-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 1.72Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.187 , 0.222 (Not available) , 0.231	Depositor DCC
R_{free} test set	1999 reflections (1.81%)	wwPDB-VP
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.419	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7493	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0935e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1ECN, 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	1.14	2/1661 (0.1%)	1.27	3/2268 (0.1%)
1	B	1.14	2/1654 (0.1%)	1.29	0/2258
1	C	1.14	2/1650 (0.1%)	1.25	1/2253 (0.0%)
1	D	1.08	0/1654	1.25	2/2258 (0.1%)
All	All	1.13	6/6619 (0.1%)	1.26	6/9037 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	65	HIS	CE1-NE2	9.10	1.41	1.32
1	B	136	ALA	C-O	6.59	1.31	1.24
1	A	205	GLY	C-O	6.14	1.30	1.23
1	C	115	ARG	C-O	5.38	1.30	1.23
1	C	85	THR	C-O	5.14	1.30	1.24
1	A	129	ALA	CA-CB	-5.08	1.45	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	PHE	CA-CB-CG	6.10	119.90	113.80
1	A	204	ALA	CA-C-N	6.04	126.81	119.99
1	A	204	ALA	C-N-CA	6.04	126.81	119.99
1	D	66	MET	CG-SD-CE	-5.74	88.27	100.90
1	C	68	ARG	CG-CD-NE	-5.46	99.98	112.00
1	D	158	ILE	O-C-N	5.39	127.37	122.14

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	1617	0	1595	8	0
1	B	1610	0	1588	10	0
1	C	1606	0	1585	13	0
1	D	1610	0	1588	10	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	1	0
3	A	9	0	0	0	0
3	B	9	0	0	0	0
3	D	9	0	0	1	0
4	A	216	0	0	4	0
4	B	214	0	0	6	1
4	C	231	0	0	6	1
4	D	190	0	0	1	0
All	All	7493	0	6476	47	1

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

All (47) 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:C:159:LEU:HD21	4:C:409:HOH:O	1.18	1.25
1:B:40:THR:HG23	4:B:401:HOH:O	1.58	1.04
1:C:159:LEU:CD2	4:C:409:HOH:O	1.89	0.92
1:A:41:HIS:CD2	4:A:462:HOH:O	2.27	0.87
1:A:41:HIS:HD2	4:A:462:HOH:O	1.59	0.84
1:C:168:ARG:NH1	4:C:401:HOH:O	2.11	0.82
1:B:40:THR:CG2	4:B:401:HOH:O	2.22	0.81
1:C:156:ARG:HD2	4:C:404:HOH:O	1.82	0.79
1:B:41:HIS:HD2	4:B:528:HOH:O	1.64	0.79
1:B:41:HIS:CD2	4:B:528:HOH:O	2.38	0.76
1:D:1:MET:HE3	4:A:462:HOH:O	1.85	0.76
1:D:132:ARG:HD3	1:D:152:LEU:HD22	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:301:HEM:HHC	2:A:301:HEM:HBB2	1.73	0.68
1:D:191:ARG:HD2	1:D:208:ASP:OD2	1.97	0.64
1:D:132:ARG:HD3	1:D:152:LEU:CD2	2.31	0.59
1:A:141:ARG:HD3	4:A:565:HOH:O	2.02	0.59
1:C:159:LEU:CG	4:C:409:HOH:O	2.38	0.59
1:C:156:ARG:NH1	4:C:404:HOH:O	2.33	0.58
1:D:90:ASN:O	4:D:401:HOH:O	2.18	0.56
1:C:76:LEU:O	1:C:80:ALA:HB2	2.08	0.53
1:A:57:LEU:O	1:A:60:ILE:HG12	2.11	0.50
2:C:301:HEM:HBB2	2:C:301:HEM:HHC	1.93	0.49
1:B:40:THR:CB	4:B:401:HOH:O	2.47	0.48
3:D:302:A1ECN:N	2:A:301:HEM:ND	2.61	0.48
2:A:301:HEM:HBC2	2:A:301:HEM:HHD	1.95	0.48
1:B:79:ALA:HB1	1:B:117:GLU:CD	2.39	0.48
1:C:18:LEU:C	1:C:18:LEU:HD23	2.38	0.47
1:C:18:LEU:HD23	1:C:18:LEU:O	2.15	0.47
1:B:121:VAL:CG1	1:B:126:ASP:HB2	2.44	0.47
1:D:188:ARG:HG2	1:D:191:ARG:HH22	1.78	0.47
1:D:46:VAL:HG13	1:D:60:ILE:HD12	1.97	0.46
1:B:66:MET:HA	2:B:301:HEM:HBA1	1.96	0.46
1:D:195:GLY:O	1:D:201:ARG:HD3	2.17	0.45
2:D:301:HEM:HBB2	2:D:301:HEM:HHC	1.98	0.45
1:A:73:TRP:CZ2	1:A:120:LYS:HD3	2.53	0.44
2:B:301:HEM:HHC	2:B:301:HEM:HBB2	1.98	0.44
1:B:57:LEU:O	1:B:60:ILE:HG12	2.19	0.43
1:A:159:LEU:N	1:A:160:PRO:CD	2.81	0.43
1:B:18:LEU:C	1:B:18:LEU:HD23	2.44	0.43
4:B:528:HOH:O	1:C:1:MET:HE3	2.19	0.42
1:C:66:MET:HA	2:C:301:HEM:HBA1	2.02	0.42
1:D:57:LEU:O	1:D:60:ILE:HG12	2.19	0.42
1:D:188:ARG:HG2	1:D:191:ARG:NH2	2.34	0.42
1:C:109:PHE:CE2	1:C:175:MET:HG2	2.56	0.41
1:C:109:PHE:CZ	1:C:175:MET:HG2	2.56	0.40
1:A:43:PRO:HG3	2:A:301:HEM:CHB	2.51	0.40
1:A:198:GLU:HA	1:A:198:GLU:OE1	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:442:HOH:O	4:C:583:HOH:O[3_445]	2.14	0.06

5.3 Torsion angles

5.3.1 Protein backbone

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	212/218 (97%)	207 (98%)	5 (2%)	0	100	100
1	B	211/218 (97%)	203 (96%)	8 (4%)	0	100	100
1	C	210/218 (96%)	205 (98%)	5 (2%)	0	100	100
1	D	211/218 (97%)	204 (97%)	7 (3%)	0	100	100
All	All	844/872 (97%)	819 (97%)	25 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	159/160 (99%)	158 (99%)	1 (1%)	78	68
1	B	158/160 (99%)	157 (99%)	1 (1%)	78	68
1	C	158/160 (99%)	157 (99%)	1 (1%)	78	68
1	D	158/160 (99%)	156 (99%)	2 (1%)	61	43
All	All	633/640 (99%)	628 (99%)	5 (1%)	73	61

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	123	SER
1	C	201	ARG

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Mol	Chain	Res	Type
1	D	201	ARG
1	D	209	ARG
1	A	123	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	183	GLN
1	D	38	HIS
1	D	192	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	A1ECN	A	302	2	9,9,9	1.58	2 (22%)	8,11,11	2.33	3 (37%)
2	HEM	A	301	1,3	50,50,50	1.58	8 (16%)	67,82,82	1.95	20 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	B	301	1	50,50,50	1.54	10 (20%)	67,82,82	1.89	15 (22%)
3	A1ECN	D	302	2	9,9,9	1.90	3 (33%)	8,11,11	2.38	3 (37%)
2	HEM	D	301	1,3	50,50,50	1.63	9 (18%)	67,82,82	1.69	15 (22%)
3	A1ECN	B	302	2	9,9,9	2.06	4 (44%)	8,11,11	3.09	2 (25%)
2	HEM	C	301	1,3	50,50,50	1.75	12 (24%)	67,82,82	1.79	12 (17%)

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	A1ECN	A	302	2	-	0/3/12/12	0/1/1/1
2	HEM	A	301	1,3	-	6/14/54/54	-
2	HEM	B	301	1	-	5/14/54/54	-
3	A1ECN	D	302	2	-	0/3/12/12	0/1/1/1
2	HEM	D	301	1,3	-	5/14/54/54	-
3	A1ECN	B	302	2	-	0/3/12/12	0/1/1/1
2	HEM	C	301	1,3	-	2/14/54/54	-

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	HEM	FE-NB	5.20	2.10	1.94
2	B	301	HEM	FE-NB	4.82	2.09	1.94
2	D	301	HEM	FE-NB	4.70	2.09	1.94
2	A	301	HEM	FE-NB	4.65	2.09	1.94
2	D	301	HEM	FE-NC	4.16	2.08	1.95
2	B	301	HEM	FE-NC	3.98	2.08	1.95
3	B	302	A1ECN	CB-CA	-3.85	1.46	1.53
2	A	301	HEM	C1D-ND	-3.84	1.31	1.38
2	D	301	HEM	C1B-NB	-3.67	1.33	1.40
3	D	302	A1ECN	CAD-NAG	3.62	1.51	1.47
2	C	301	HEM	C4D-ND	-3.57	1.34	1.40
2	D	301	HEM	C1C-C2C	-3.54	1.38	1.45
2	A	301	HEM	FE-NC	3.23	2.05	1.95
2	A	301	HEM	C3B-C4B	3.21	1.51	1.44
2	B	301	HEM	C4D-C3D	3.18	1.50	1.45
2	C	301	HEM	C1B-NB	-3.17	1.34	1.40
2	C	301	HEM	C1C-C2C	-3.12	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	HEM	CHA-C4D	2.97	1.44	1.38
3	A	302	A1ECN	CAD-NAG	2.95	1.50	1.47
2	C	301	HEM	FE-NC	2.94	2.04	1.95
2	B	301	HEM	C1B-NB	-2.92	1.35	1.40
2	C	301	HEM	C3B-C4B	2.90	1.50	1.44
2	A	301	HEM	CBA-CGA	2.77	1.57	1.50
2	C	301	HEM	CHC-C1C	2.77	1.43	1.38
2	A	301	HEM	C1B-NB	-2.72	1.35	1.40
3	B	302	A1ECN	CA-C	2.69	1.59	1.52
3	D	302	A1ECN	NAG-N	-2.67	1.39	1.43
2	D	301	HEM	O2A-CGA	-2.62	1.22	1.30
2	A	301	HEM	C1C-NC	-2.53	1.34	1.39
2	D	301	HEM	C3C-C4C	-2.53	1.41	1.46
2	C	301	HEM	C4D-C3D	2.47	1.49	1.45
2	C	301	HEM	CMA-C3A	2.44	1.55	1.50
2	D	301	HEM	C4D-ND	-2.44	1.36	1.40
3	B	302	A1ECN	CAC-CB	2.39	1.59	1.53
2	A	301	HEM	CMA-C3A	2.36	1.55	1.50
2	B	301	HEM	FE-NA	2.32	2.02	1.95
2	C	301	HEM	C2A-C3A	-2.30	1.32	1.38
2	B	301	HEM	O1A-CGA	2.25	1.29	1.22
2	B	301	HEM	C1C-C2C	-2.13	1.41	1.45
2	B	301	HEM	CHA-C4D	2.11	1.42	1.38
2	D	301	HEM	C1C-NC	-2.09	1.35	1.39
3	B	302	A1ECN	OXT-C	-2.09	1.24	1.30
3	D	302	A1ECN	O-C	2.08	1.28	1.22
2	C	301	HEM	C4B-NB	-2.07	1.34	1.38
2	B	301	HEM	C3D-C2D	-2.05	1.32	1.36
3	A	302	A1ECN	CB-CA	-2.04	1.49	1.53
2	D	301	HEM	C3B-C4B	2.03	1.48	1.44
2	B	301	HEM	C3C-C2C	2.00	1.41	1.37

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	302	A1ECN	CAD-NAG-N	6.48	117.15	110.41
2	A	301	HEM	C3B-C4B-NB	-6.42	104.86	109.47
2	C	301	HEM	C3B-C4B-NB	-5.57	105.47	109.47
2	B	301	HEM	C3B-C4B-NB	-5.51	105.51	109.47
2	C	301	HEM	C1B-NB-C4B	5.24	111.42	105.21
3	B	302	A1ECN	CB-CAC-CAD	5.20	121.58	110.55
3	A	302	A1ECN	CAC-CAD-NAG	-4.80	107.48	112.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	HEM	C1B-NB-C4B	4.71	110.78	105.21
2	B	301	HEM	CHA-C4D-ND	4.67	130.15	124.37
2	B	301	HEM	C1B-NB-C4B	4.66	110.73	105.21
2	C	301	HEM	CHC-C4B-NB	4.53	129.30	124.42
2	D	301	HEM	C3B-C2B-C1B	4.43	109.74	106.41
2	B	301	HEM	CHD-C1D-ND	4.40	129.16	124.42
3	D	302	A1ECN	CAC-CAD-NAG	-4.15	108.21	112.84
2	B	301	HEM	CHD-C4C-NC	4.05	128.86	124.45
2	D	301	HEM	CHB-C1B-NB	3.96	129.27	124.37
3	D	302	A1ECN	CAC-CB-CA	-3.91	105.82	110.97
2	A	301	HEM	C1B-NB-C4B	3.81	109.72	105.21
2	C	301	HEM	CHD-C4C-NC	3.76	128.54	124.45
2	A	301	HEM	CAD-CBD-CGD	3.58	123.16	113.67
2	A	301	HEM	CAD-C3D-C4D	3.54	130.87	124.70
2	A	301	HEM	CHD-C1D-ND	3.42	128.10	124.42
2	C	301	HEM	C3C-C2C-C1C	3.30	110.17	107.05
2	C	301	HEM	CAC-C3C-C4C	3.30	132.70	124.82
2	B	301	HEM	CHC-C4B-NB	3.24	127.91	124.42
2	D	301	HEM	C4B-C3B-C2B	-3.19	104.35	107.28
2	A	301	HEM	CHB-C1B-NB	3.17	128.28	124.37
2	D	301	HEM	C3B-C4B-NB	-3.05	107.28	109.47
2	D	301	HEM	CAC-C3C-C4C	2.95	131.85	124.82
2	A	301	HEM	CHD-C1D-C2D	-2.94	120.39	125.03
3	D	302	A1ECN	C-CA-N	-2.94	103.82	109.08
2	B	301	HEM	CHD-C1D-C2D	-2.93	120.40	125.03
2	A	301	HEM	CHC-C4B-NB	2.91	127.55	124.42
2	A	301	HEM	CHA-C4D-ND	2.87	127.92	124.37
2	B	301	HEM	C3D-C4D-ND	-2.87	107.03	110.17
2	B	301	HEM	CMA-C3A-C4A	2.85	129.76	125.42
2	D	301	HEM	CHC-C4B-NB	2.84	127.48	124.42
2	B	301	HEM	C1A-CHA-C4D	-2.83	119.59	126.25
2	A	301	HEM	CHD-C4C-NC	2.80	127.50	124.45
2	B	301	HEM	C4C-CHD-C1D	-2.73	120.22	126.02
2	D	301	HEM	CAB-C3B-C2B	-2.72	119.60	128.43
2	D	301	HEM	CHD-C1D-C2D	-2.70	120.76	125.03
2	D	301	HEM	CAB-C3B-C4B	2.61	135.94	124.39
2	D	301	HEM	C1D-C2D-C3D	-2.60	104.25	106.98
2	A	301	HEM	CAB-C3B-C2B	-2.59	120.01	128.43
2	A	301	HEM	O2D-CGD-CBD	2.53	122.01	114.00
2	A	301	HEM	O2A-CGA-CBA	2.53	122.00	114.00
2	C	301	HEM	CHB-C1B-NB	2.52	127.49	124.37
2	C	301	HEM	C1C-CHC-C4B	-2.51	120.68	126.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	HEM	CHB-C1B-NB	2.50	127.46	124.37
2	A	301	HEM	CAC-C3C-C4C	2.48	130.75	124.82
2	D	301	HEM	CHA-C4D-ND	2.42	127.36	124.37
2	A	301	HEM	CAD-C3D-C2D	-2.38	123.41	127.87
2	A	301	HEM	C4C-NC-C1C	2.37	109.69	105.82
3	A	302	A1ECN	O-C-CA	-2.37	114.60	122.26
2	D	301	HEM	C2D-C1D-ND	2.36	112.63	109.90
2	C	301	HEM	C4A-NA-C1A	-2.36	101.97	105.82
3	A	302	A1ECN	CAC-CB-CA	-2.35	107.87	110.97
2	C	301	HEM	C4C-C3C-C2C	-2.31	104.81	106.81
2	C	301	HEM	CHC-C1C-NC	2.27	126.93	124.45
2	B	301	HEM	O2D-CGD-CBD	2.27	121.17	114.00
2	A	301	HEM	CHA-C1A-NA	2.17	127.80	123.86
2	B	301	HEM	C4C-C3C-C2C	-2.17	104.93	106.81
2	C	301	HEM	CAA-C2A-C1A	2.16	129.15	124.94
2	A	301	HEM	CHB-C1B-C2B	-2.12	120.93	126.95
2	D	301	HEM	CMD-C2D-C1D	2.10	128.31	125.03
2	D	301	HEM	CMB-C2B-C3B	-2.04	123.50	128.43
2	B	301	HEM	CAC-C3C-C4C	2.02	129.65	124.82
2	A	301	HEM	C3C-C2C-C1C	2.02	108.95	107.05
2	A	301	HEM	O1D-CGD-CBD	-2.01	116.71	123.09

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	HEM	C3D-CAD-CBD-CGD
2	D	301	HEM	C4B-C3B-CAB-CBB
2	A	301	HEM	C4B-C3B-CAB-CBB
2	A	301	HEM	CAD-CBD-CGD-O1D
2	D	301	HEM	CAD-CBD-CGD-O1D
2	A	301	HEM	CAD-CBD-CGD-O2D
2	D	301	HEM	CAA-CBA-CGA-O1A
2	A	301	HEM	CAA-CBA-CGA-O2A
2	D	301	HEM	CAA-CBA-CGA-O2A
2	A	301	HEM	CAA-CBA-CGA-O1A
2	B	301	HEM	CAD-CBD-CGD-O2D
2	D	301	HEM	CAD-CBD-CGD-O2D
2	B	301	HEM	C3D-CAD-CBD-CGD
2	C	301	HEM	CAA-CBA-CGA-O2A
2	C	301	HEM	CAA-CBA-CGA-O1A
2	B	301	HEM	CAA-CBA-CGA-O1A

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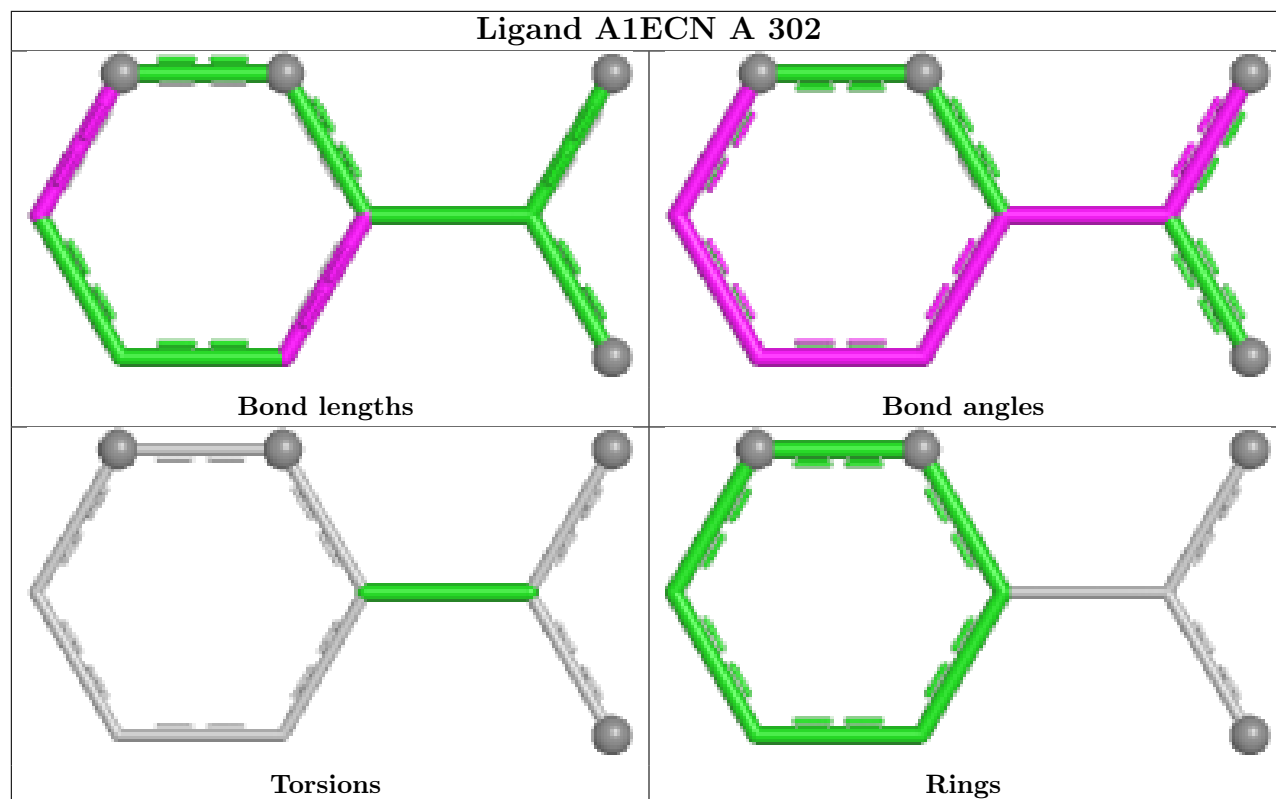
Mol	Chain	Res	Type	Atoms
2	B	301	HEM	CAA-CBA-CGA-O2A
2	B	301	HEM	CAD-CBD-CGD-O1D

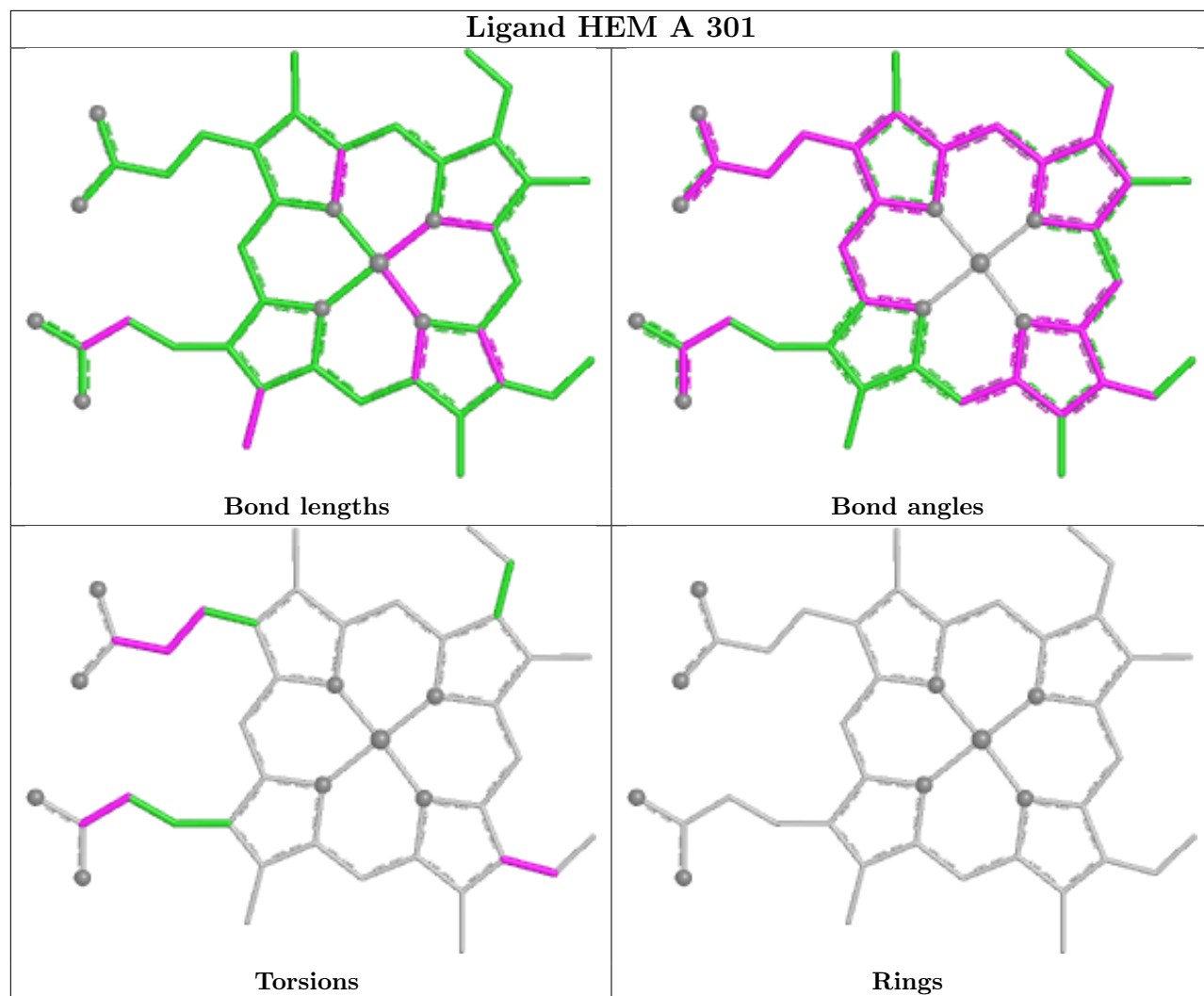
There are no ring outliers.

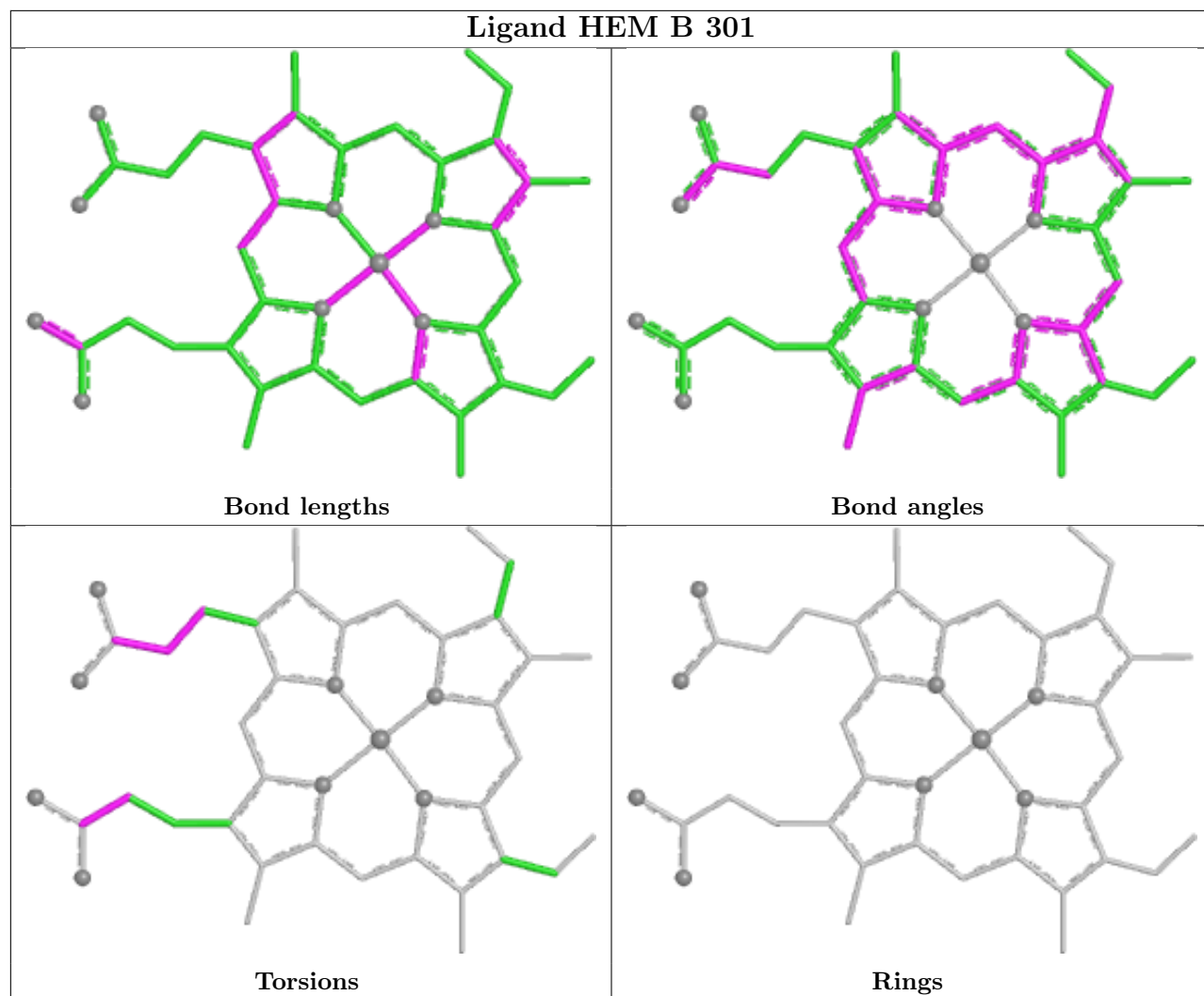
5 monomers are involved in 9 short contacts:

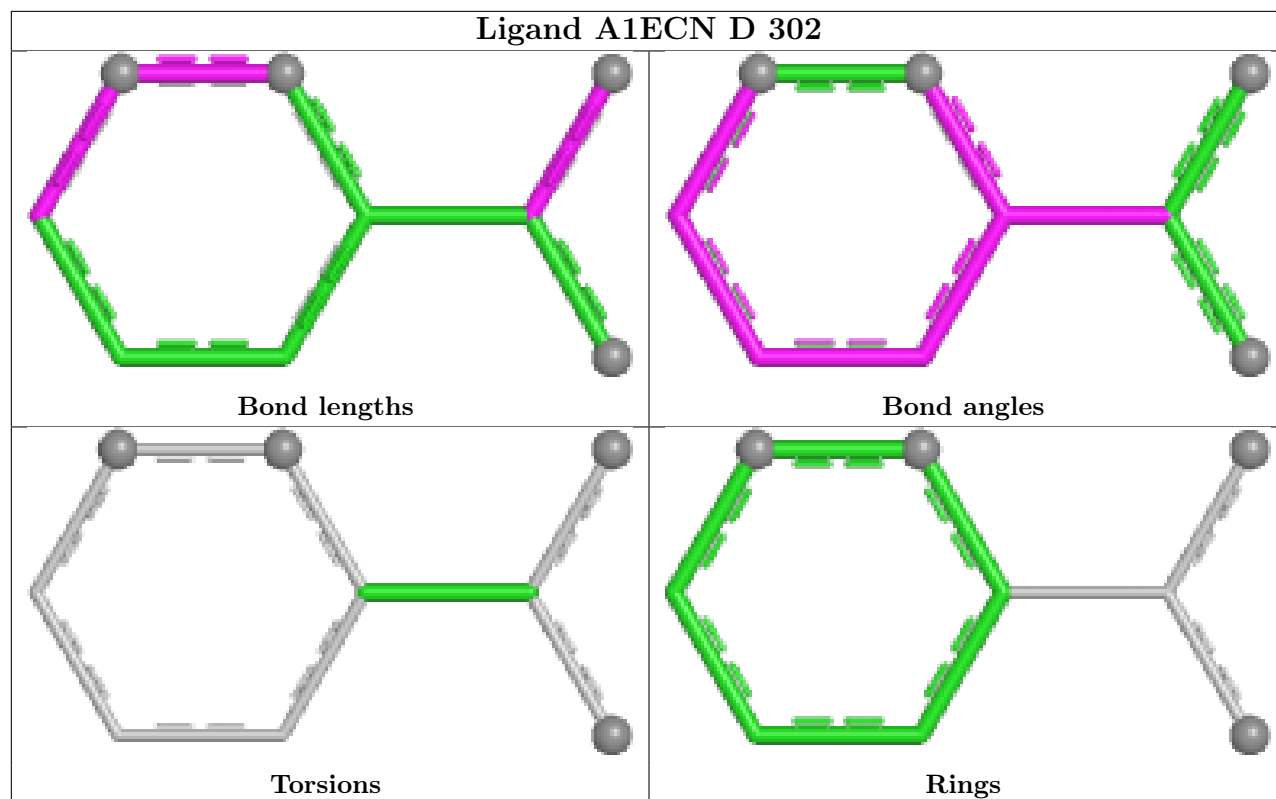
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	HEM	4	0
2	B	301	HEM	2	0
3	D	302	A1ECN	1	0
2	D	301	HEM	1	0
2	C	301	HEM	2	0

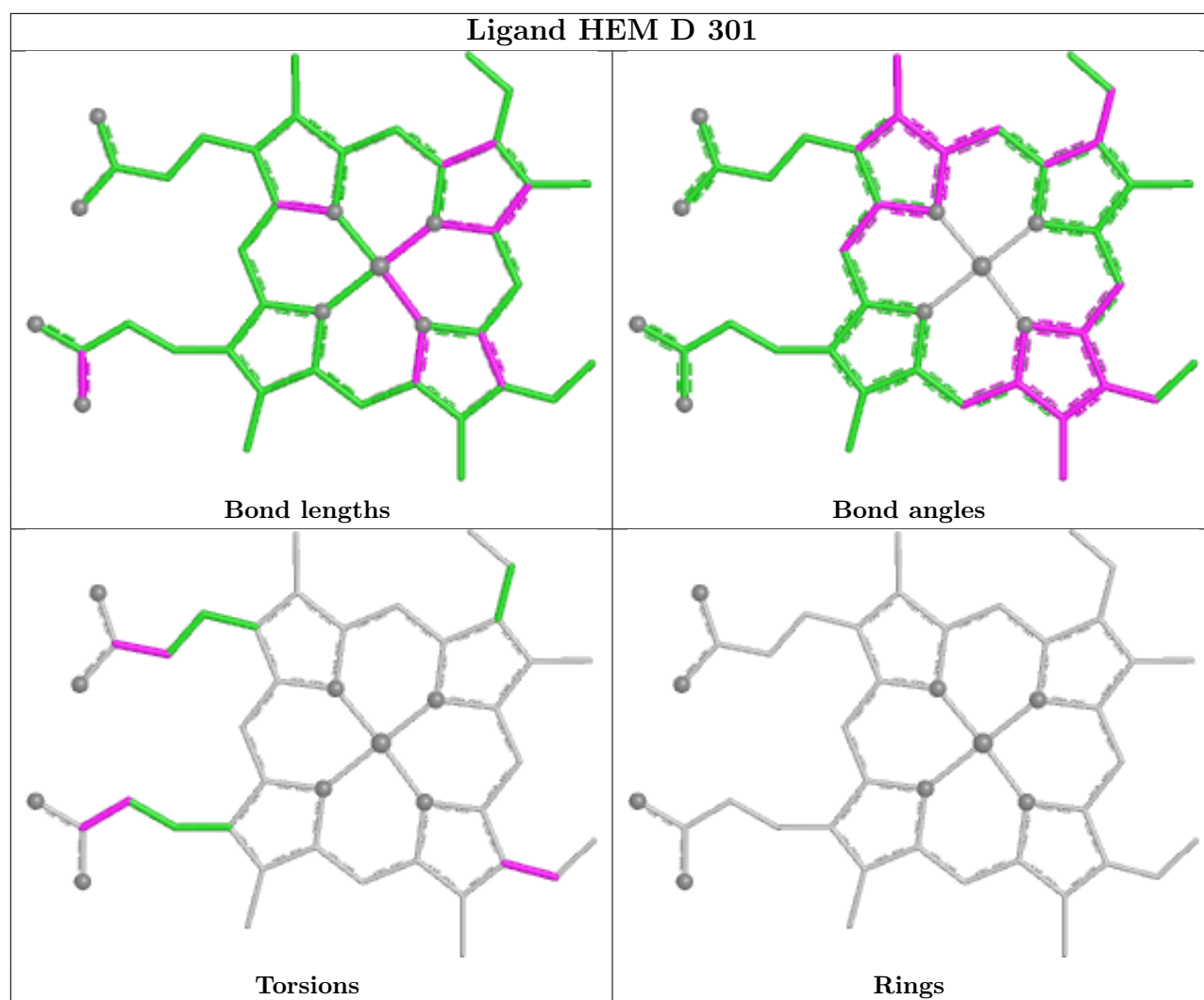
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

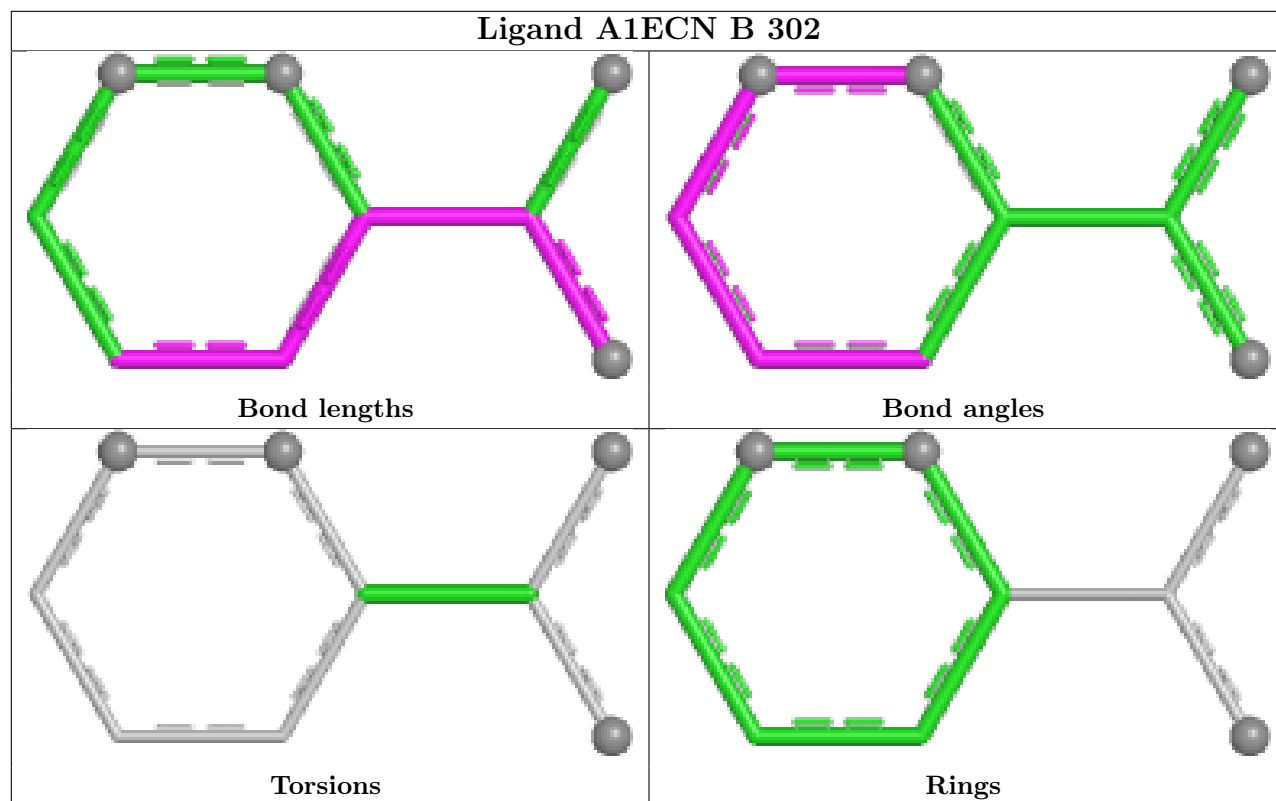


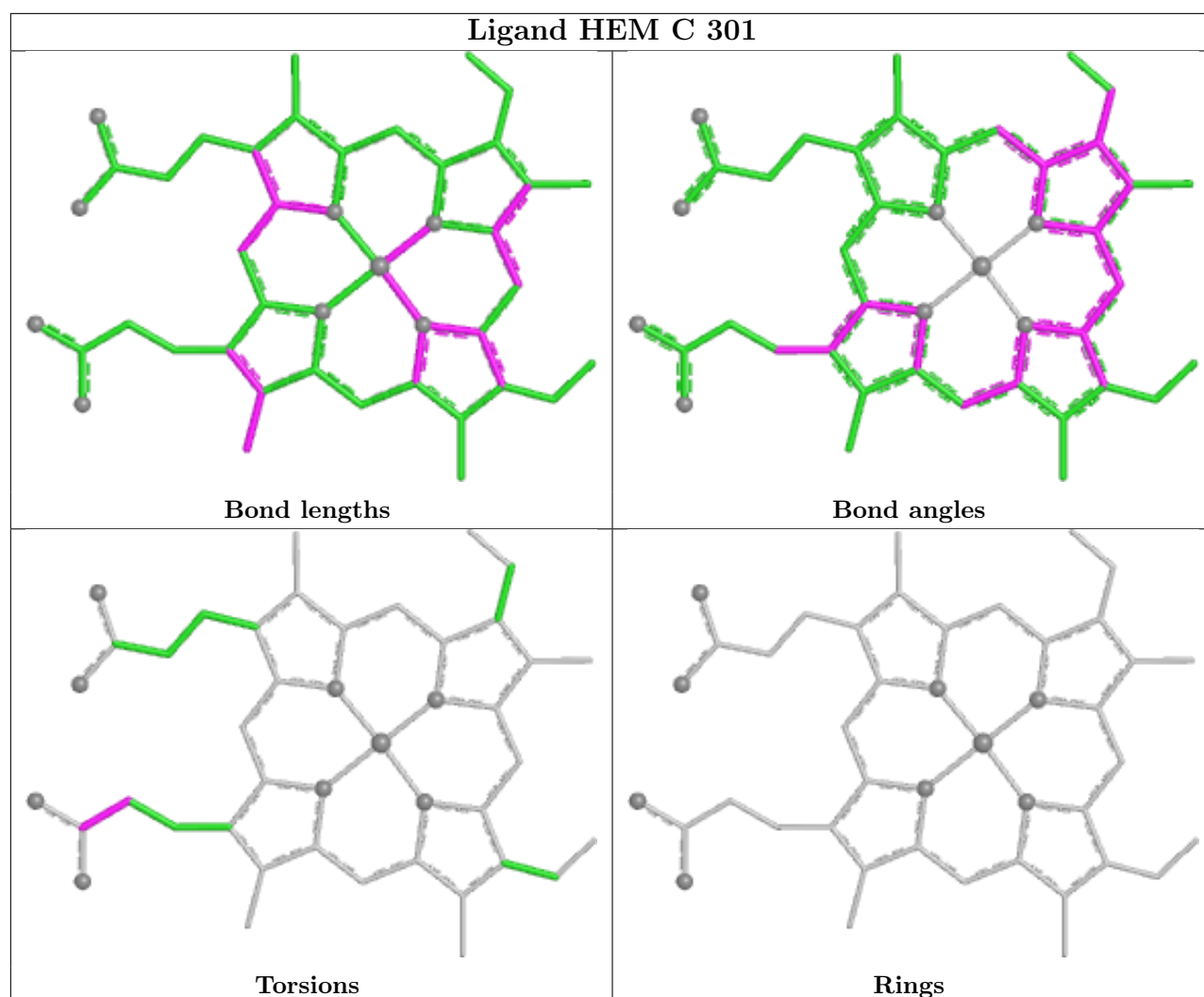












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	214/218 (98%)	0.35	11 (5%) 33 39	16, 23, 47, 72	0
1	B	213/218 (97%)	0.23	11 (5%) 33 38	15, 22, 43, 67	0
1	C	212/218 (97%)	0.22	6 (2%) 55 63	16, 23, 42, 61	0
1	D	213/218 (97%)	0.25	7 (3%) 49 58	17, 23, 45, 73	0
All	All	852/872 (97%)	0.27	35 (4%) 41 49	15, 23, 44, 73	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	212	THR	5.1
1	B	52	GLY	4.4
1	D	78	GLY	4.1
1	C	77	GLY	3.8
1	D	77	GLY	3.7
1	D	79	ALA	3.6
1	B	79	ALA	3.5
1	A	78	GLY	3.5
1	B	-1	GLY	3.4
1	B	78	GLY	3.2
1	A	52	GLY	3.2
1	C	78	GLY	3.2
1	B	51	ASP	2.9
1	A	51	ASP	2.8
1	A	79	ALA	2.8
1	D	-1	GLY	2.8
1	A	53	PRO	2.7
1	C	211	PRO	2.7
1	B	33	GLY	2.6
1	B	211	PRO	2.4
1	B	77	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	35	ALA	2.4
1	B	125	ASP	2.4
1	B	119	ARG	2.3
1	C	79	ALA	2.3
1	A	34	GLY	2.3
1	D	211	PRO	2.3
1	C	0	ALA	2.3
1	D	0	ALA	2.3
1	A	77	GLY	2.3
1	A	125	ASP	2.3
1	B	34	GLY	2.2
1	D	34	GLY	2.2
1	C	51	ASP	2.0
1	A	123	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

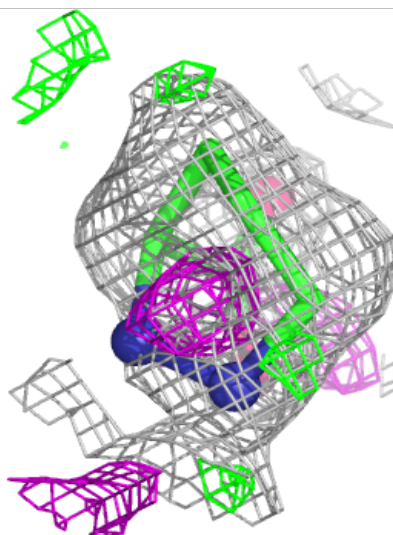
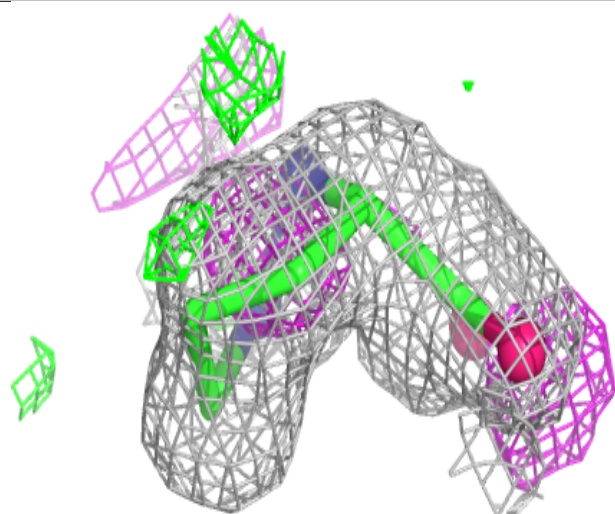
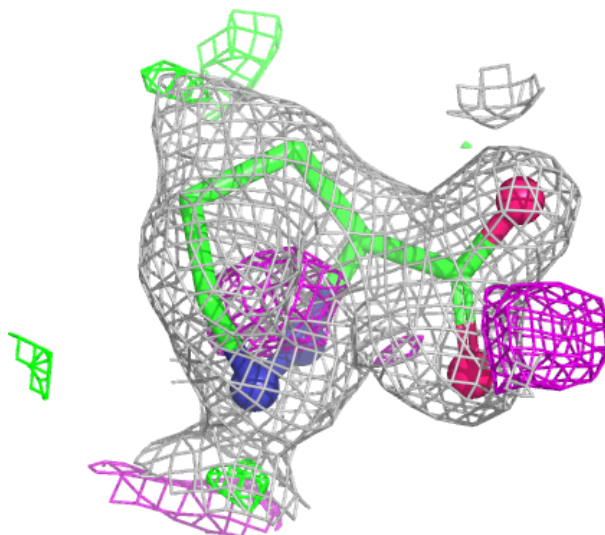
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	A1ECN	D	302	9/9	0.78	0.17	36,44,47,49	0
3	A1ECN	B	302	9/9	0.81	0.15	32,35,37,37	0
3	A1ECN	A	302	9/9	0.88	0.12	34,38,40,44	0
2	HEM	A	301	43/43	0.97	0.08	17,20,34,47	0
2	HEM	C	301	43/43	0.98	0.07	15,17,31,52	0
2	HEM	D	301	43/43	0.98	0.06	17,19,34,53	0
2	HEM	B	301	43/43	0.98	0.06	16,19,24,29	0

The following is a graphical depiction of the model fit to experimental electron density of all

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

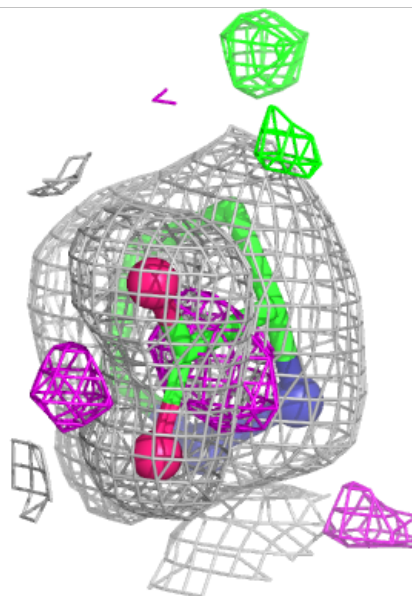
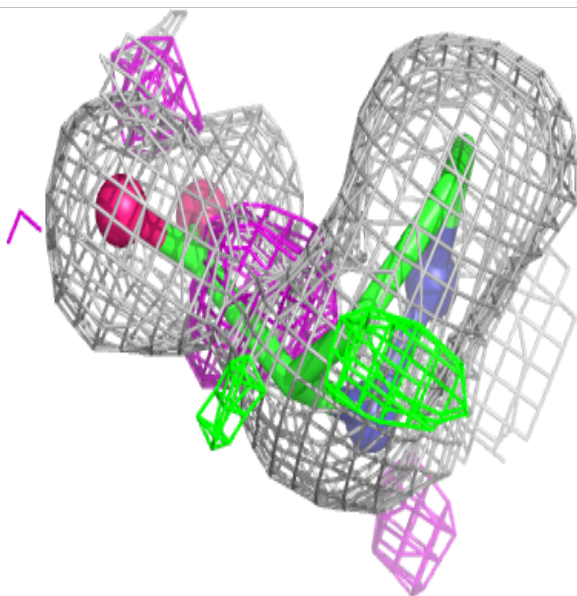
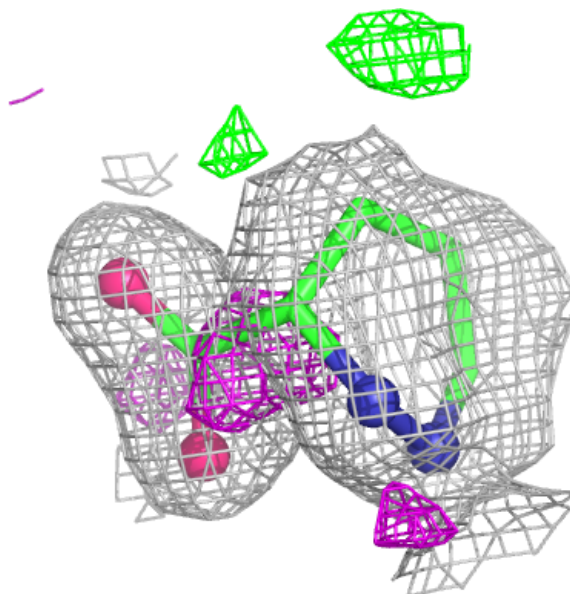
Electron density around A1ECN D 302:

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



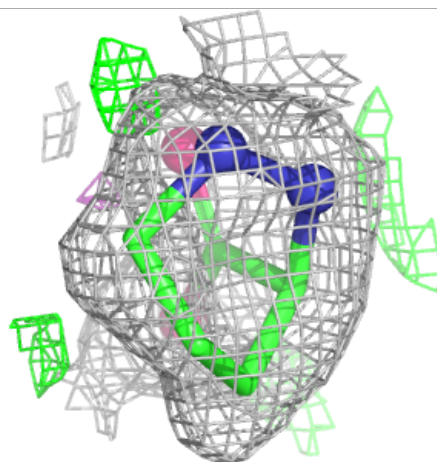
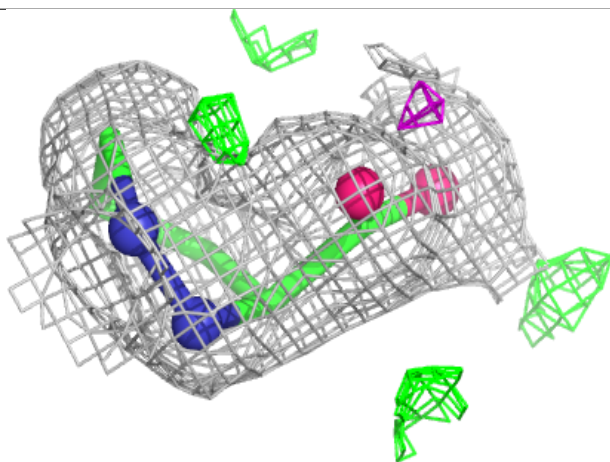
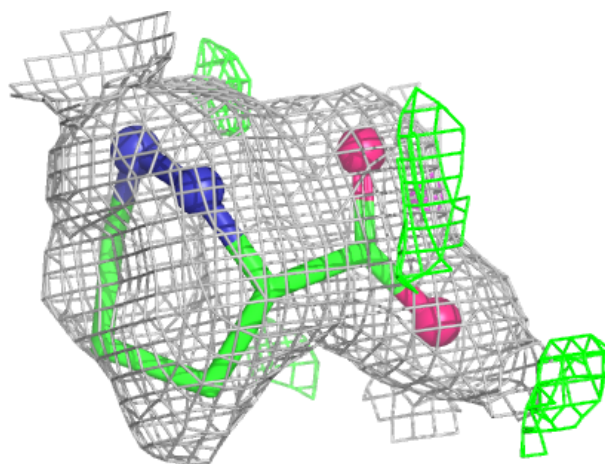
Electron density around A1ECN B 302:

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



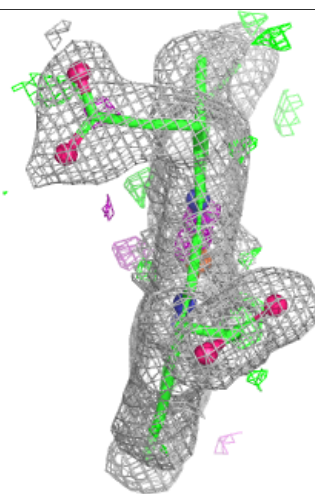
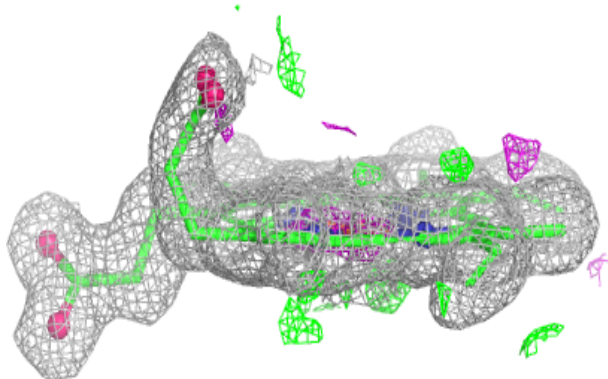
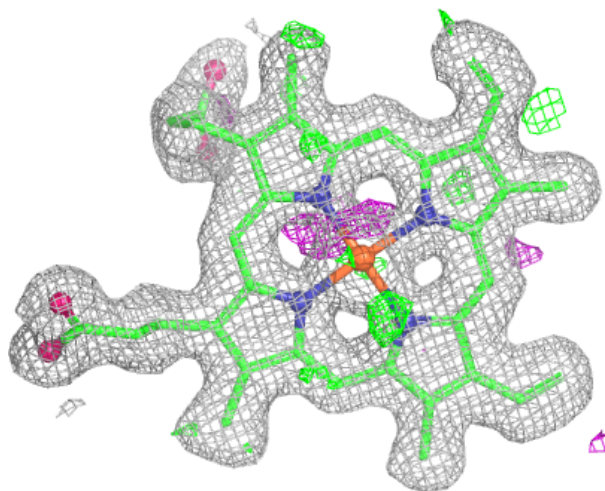
Electron density around A1ECN A 302:

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



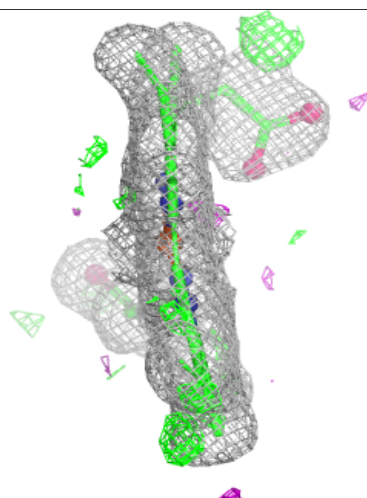
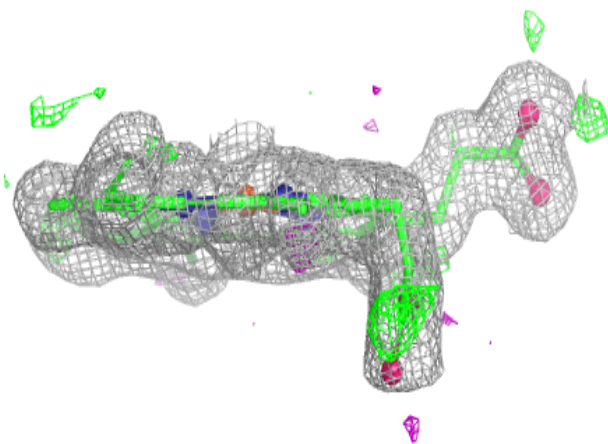
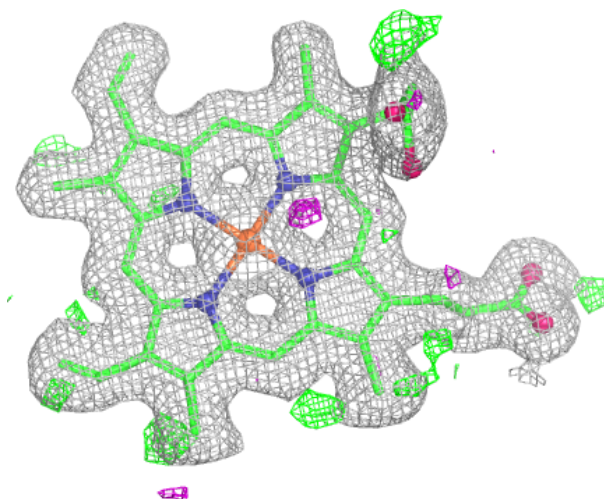
Electron density around HEM A 301:

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



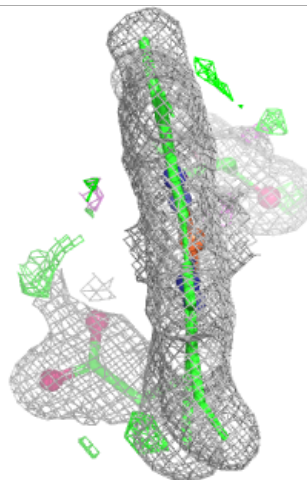
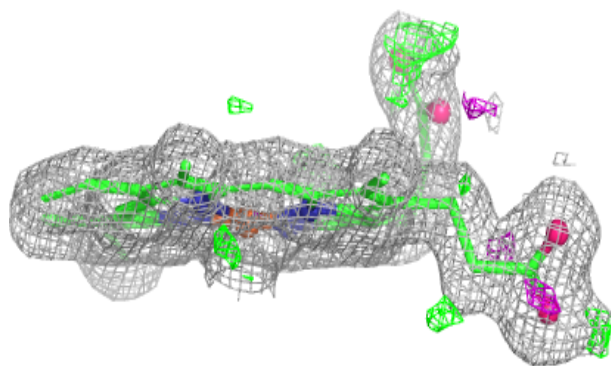
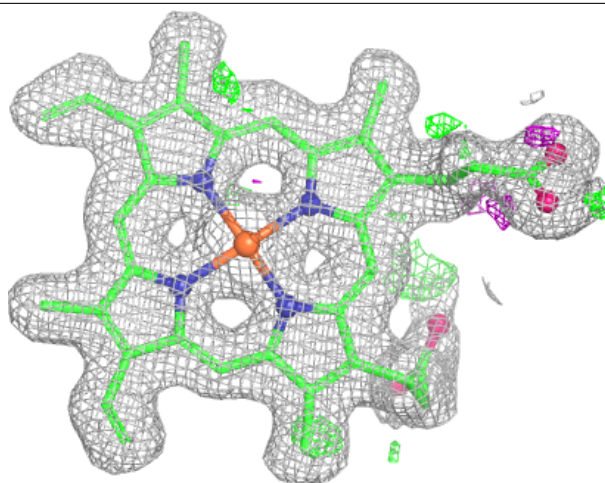
Electron density around HEM C 301:

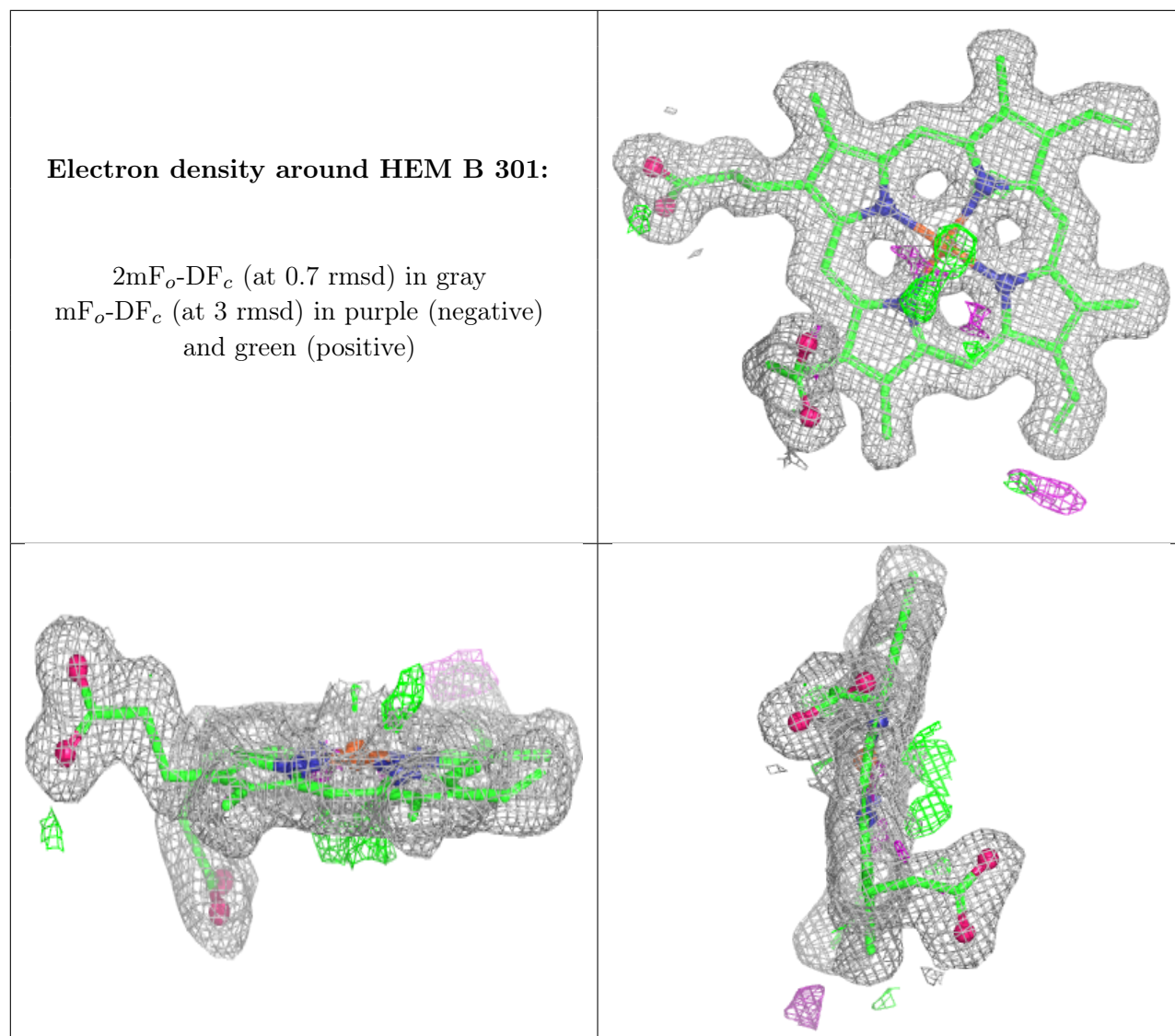
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM D 301:

$2mF_o-DF_c$ (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.