



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 07:05 PM EDT

PDB ID : 9CA3 / pdb_00009ca3
Title : Crystal structure of MarE C280S in complex with cyanide bound heme and its native substrate, beta-methyl-L-tryptophan
Authors : Shin, I.; Liu, A.
Deposited on : 2024-06-16
Resolution : 1.89 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

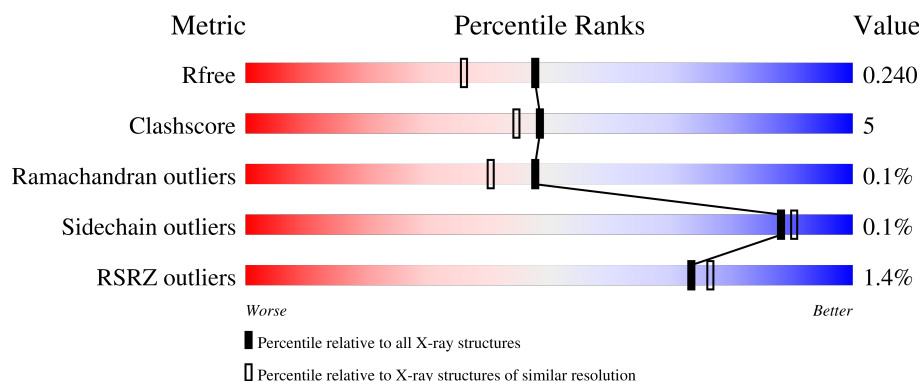
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.89 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	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	286	 2% 81% 8% 11%
1	B	286	 81% 9% 9%
1	C	286	 81% 9% 9%
1	D	286	 2% 80% 10% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8998 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.

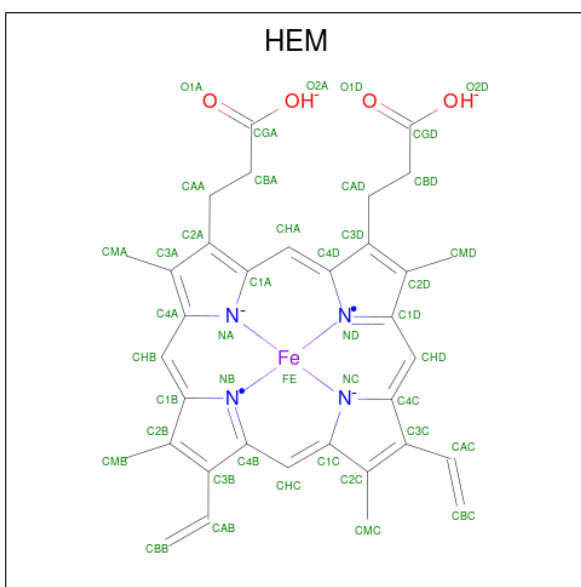
- Molecule 1 is a protein called Tryptophan 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2026	1272	372	376	6			
1	B	260	Total	C	N	O	S	0	0	0
			2069	1297	379	388	5			
1	C	260	Total	C	N	O	S	0	1	0
			2078	1301	382	390	5			
1	D	258	Total	C	N	O	S	0	1	0
			2061	1292	377	386	6			

There are 12 discrepancies between the modelled and reference sequences:

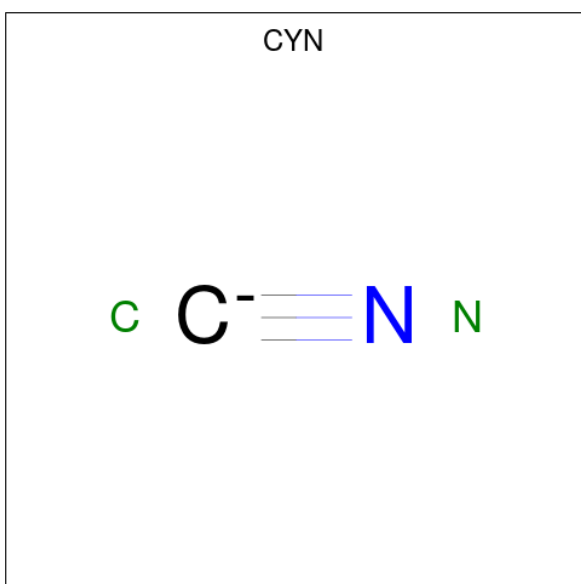
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP X2D878
A	0	HIS	-	expression tag	UNP X2D878
A	280	SER	CYS	engineered mutation	UNP X2D878
B	-1	GLY	-	expression tag	UNP X2D878
B	0	HIS	-	expression tag	UNP X2D878
B	280	SER	CYS	engineered mutation	UNP X2D878
C	-1	GLY	-	expression tag	UNP X2D878
C	0	HIS	-	expression tag	UNP X2D878
C	280	SER	CYS	engineered mutation	UNP X2D878
D	-1	GLY	-	expression tag	UNP X2D878
D	0	HIS	-	expression tag	UNP X2D878
D	280	SER	CYS	engineered mutation	UNP X2D878

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



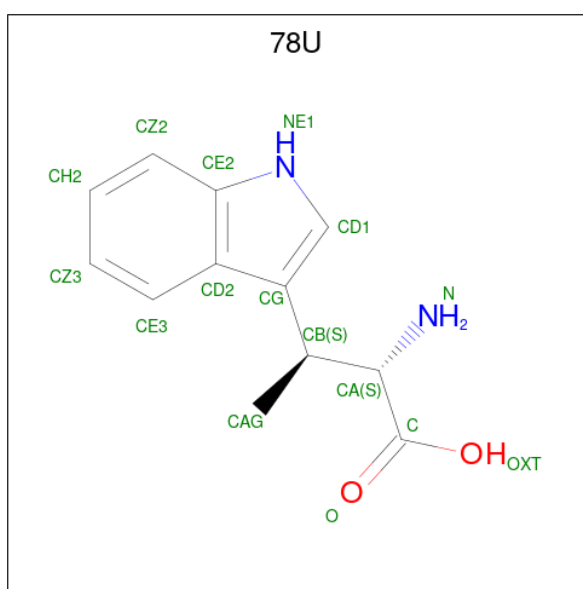
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is CYANIDE ION (CCD ID: CYN) (formula: CN) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is (betaS)-beta-methyl-L-tryptophan (CCD ID: 78U) (formula: C₁₂H₁₄N₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 16 12 2 2	0	0
4	B	1	Total C N O 16 12 2 2	0	0
4	C	1	Total C N O 16 12 2 2	0	0
4	D	1	Total C N O 16 12 2 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	100	Total O 100 100	0	0

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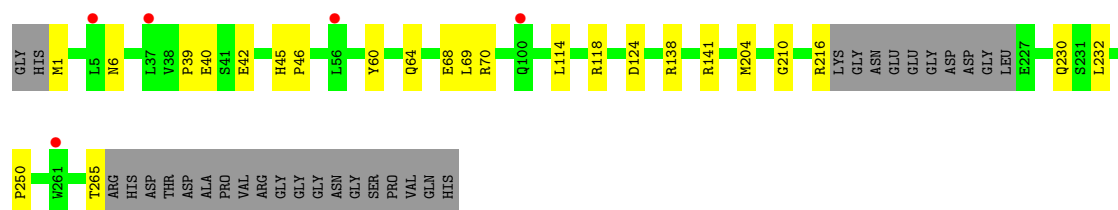
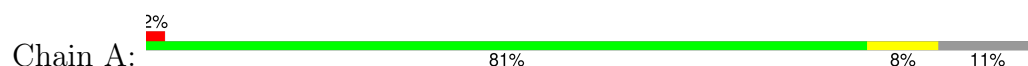
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	143	Total 143	O 143	0	0
5	C	166	Total 166	O 166	0	0
5	D	111	Total 111	O 111	0	0

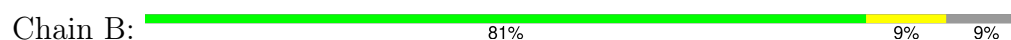
3 Residue-property plots [i](#)

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.

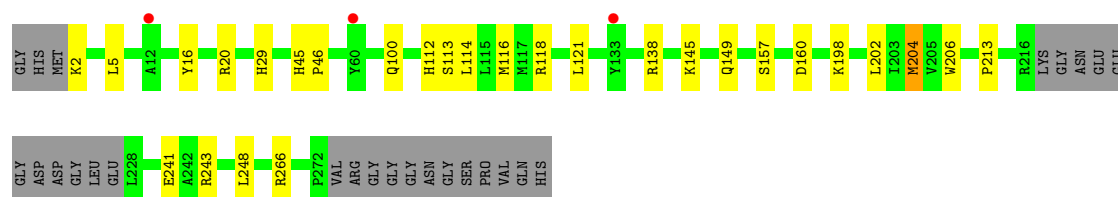
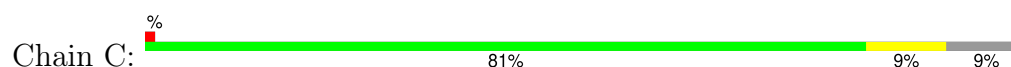
- Molecule 1: Tryptophan 2,3-dioxygenase



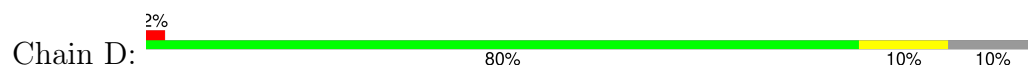
- Molecule 1: Tryptophan 2,3-dioxygenase

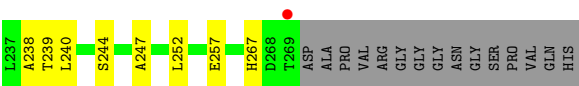


- Molecule 1: Tryptophan 2,3-dioxygenase



- Molecule 1: Tryptophan 2,3-dioxygenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.03Å 112.96Å 83.34Å 90.00° 111.25° 90.00°	Depositor
Resolution (Å)	43.24 – 1.89 43.24 – 1.89	Depositor EDS
% Data completeness (in resolution range)	95.8 (43.24-1.89) 88.6 (43.24-1.89)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.75 (at 1.88Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.193 , 0.241 0.193 , 0.240	Depositor DCC
R_{free} test set	1992 reflections (2.12%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 27.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8998	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.58% 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: HEM, 78U, CYN

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	0.35	0/2072	0.54	0/2814
1	B	0.42	0/2117	0.61	2/2878 (0.1%)
1	C	0.43	0/2129	0.65	2/2893 (0.1%)
1	D	0.40	0/2111	0.60	0/2867
All	All	0.40	0/8429	0.60	4/11452 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	204	MET	CA-CB-CG	6.63	127.36	114.10
1	B	123	GLU	CA-C-N	-5.40	111.22	121.54
1	B	123	GLU	C-N-CA	-5.40	111.22	121.54
1	C	204	MET	CG-SD-CE	-5.01	89.87	100.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2026	0	1974	23	0
1	B	2069	0	2007	26	0
1	C	2078	0	2015	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2061	0	2001	23	0
2	A	43	0	30	3	0
2	B	43	0	30	3	0
2	C	43	0	30	3	0
2	D	43	0	30	2	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	16	0	0	0	0
4	B	16	0	0	0	0
4	C	16	0	0	0	0
4	D	16	0	0	0	0
5	A	100	0	0	0	0
5	B	143	0	0	4	0
5	C	166	0	0	8	0
5	D	111	0	0	3	0
All	All	8998	0	8117	91	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 (91) 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:266:ARG:NH2	1:C:121:LEU:O	1.92	1.02
1:B:121:LEU:O	1:C:266:ARG:NH2	1.99	0.95
1:C:2:LYS:NZ	5:C:401:HOH:O	2.14	0.80
1:B:141:ARG:NH1	1:B:251:GLU:OE2	2.15	0.74
1:D:118:ARG:NH2	5:D:402:HOH:O	2.23	0.70
1:C:202:LEU:HD21	1:C:241:GLU:HG3	1.74	0.68
1:C:204:MET:HE1	2:C:301:HEM:C1C	2.29	0.67
1:D:204:MET:HE1	2:D:301:HEM:C1C	2.33	0.62
1:A:70:ARG:NH2	1:B:40:GLU:OE2	2.31	0.62
1:C:29:HIS:HE1	5:C:546:HOH:O	1.83	0.59
1:C:118:ARG:HA	1:C:121:LEU:HD12	1.85	0.58
1:A:230:GLN:HG3	1:D:267:HIS:CE1	2.39	0.57
1:A:204:MET:HE1	2:A:301:HEM:C1C	2.39	0.57
1:D:238:ALA:O	5:D:401:HOH:O	2.18	0.56
1:B:45:HIS:ND1	1:B:46:PRO:HD2	2.20	0.56
1:B:245:GLN:OE1	5:B:401:HOH:O	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:MET:HE1	2:B:301:HEM:C1C	2.41	0.55
1:C:204:MET:HE1	2:C:301:HEM:C2C	2.42	0.55
1:A:124:ASP:N	1:A:232:LEU:O	2.36	0.54
2:B:301:HEM:CMC	2:B:301:HEM:HBC2	2.39	0.53
1:C:248:LEU:O	5:C:403:HOH:O	2.19	0.52
2:B:301:HEM:HBC2	2:B:301:HEM:HMC1	1.91	0.52
1:A:45:HIS:ND1	1:A:46:PRO:HD2	2.26	0.51
1:D:144:TRP:HZ3	1:D:252:LEU:HD21	1.75	0.51
1:D:164:GLN:HE22	1:D:177:SER:HB2	1.76	0.51
1:C:243:ARG:NH2	2:C:301:HEM:O2A	2.31	0.50
1:D:40:GLU:HG2	5:D:455:HOH:O	2.11	0.49
1:A:114:LEU:HD11	2:A:301:HEM:HBC1	1.93	0.49
1:C:198:LYS:NZ	5:C:404:HOH:O	2.44	0.49
1:B:100:GLN:NE2	5:B:406:HOH:O	2.46	0.49
1:D:236:SER:O	1:D:239:THR:HG22	2.12	0.49
1:B:141:ARG:NE	1:B:141:ARG:HA	2.28	0.48
1:A:118:ARG:NH2	1:A:230:GLN:O	2.45	0.48
1:D:145:LYS:HA	1:D:145:LYS:HD2	1.59	0.48
1:A:1:MET:HE3	1:A:1:MET:HB2	1.81	0.48
1:C:114:LEU:C	1:C:114:LEU:HD13	2.40	0.47
1:A:60:TYR:CE2	1:B:60:TYR:HE2	2.31	0.47
1:D:137[A]:ARG:NH2	1:D:247:ALA:O	2.47	0.47
1:B:45:HIS:CE1	1:B:113:SER:HB3	2.50	0.47
1:A:60:TYR:HE2	1:B:60:TYR:CE2	2.33	0.47
1:D:2:LYS:HE2	1:D:17:ASP:CG	2.41	0.46
1:A:45:HIS:CG	1:A:46:PRO:HD2	2.50	0.46
1:A:60:TYR:CE2	1:B:60:TYR:CE2	3.03	0.46
1:A:39:PRO:HB2	1:A:42:GLU:HG3	1.99	0.45
1:D:267:HIS:CG	1:D:267:HIS:O	2.69	0.45
1:B:138:ARG:HH11	1:B:138:ARG:HG3	1.81	0.45
1:B:123:GLU:O	1:B:232:LEU:O	2.34	0.45
1:A:70:ARG:NH1	1:B:6:ASN:HD21	2.15	0.45
1:B:45:HIS:CE1	1:B:46:PRO:HD2	2.53	0.44
1:C:29:HIS:HD2	5:C:445:HOH:O	1.99	0.44
1:C:16:TYR:OH	5:C:402:HOH:O	2.17	0.44
1:A:216:ARG:HH11	1:A:216:ARG:HG3	1.82	0.44
1:B:206:TRP:CE2	1:B:213:PRO:HD3	2.53	0.44
1:A:64:GLN:O	1:A:68:GLU:HG2	2.18	0.43
1:D:2:LYS:HE2	1:D:17:ASP:OD2	2.17	0.43
1:C:45:HIS:ND1	1:C:46:PRO:HD2	2.33	0.43
1:D:183:VAL:O	1:D:187:MET:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:GLN:OE1	1:D:100:GLN:OE1	2.37	0.43
1:D:45:HIS:CG	1:D:46:PRO:HD2	2.53	0.43
1:D:240:LEU:HD13	2:D:301:HEM:HAD2	2.01	0.43
1:D:45:HIS:ND1	1:D:46:PRO:HD2	2.33	0.43
2:A:301:HEM:HMC1	2:A:301:HEM:HBC2	1.99	0.43
1:B:266:ARG:HB2	5:B:473:HOH:O	2.18	0.43
1:C:206:TRP:CE2	1:C:213:PRO:HD3	2.54	0.43
1:C:145:LYS:O	1:C:149:GLN:HG2	2.19	0.42
1:C:112:HIS:CE1	1:C:116:MET:HE3	2.54	0.42
1:A:6:ASN:HB3	1:A:40:GLU:OE2	2.19	0.42
1:B:118:ARG:NH2	1:B:230:GLN:O	2.50	0.42
1:C:45:HIS:CE1	1:C:113:SER:HB3	2.54	0.42
1:A:40:GLU:HG2	5:B:451:HOH:O	2.19	0.42
1:C:45:HIS:CG	1:C:46:PRO:HD2	2.54	0.42
1:C:45:HIS:CE1	1:C:46:PRO:HD2	2.54	0.41
1:C:266:ARG:HB2	5:C:516:HOH:O	2.20	0.41
1:B:45:HIS:CG	1:B:46:PRO:HD2	2.56	0.41
1:B:202:LEU:HD21	1:B:241:GLU:HG3	2.03	0.41
1:A:141:ARG:NH2	1:A:250:PRO:HD2	2.36	0.41
1:C:2:LYS:HB3	1:C:20:ARG:HG2	2.03	0.41
1:C:20:ARG:NH2	1:D:129:ASP:OD1	2.50	0.41
1:C:5:LEU:HD23	1:C:5:LEU:HA	1.90	0.41
1:B:145:LYS:HD3	1:B:145:LYS:HA	1.86	0.41
1:D:169:TYR:CZ	1:D:171:GLY:HA3	2.56	0.41
1:C:157:SER:O	1:C:160[A]:ASP:HB2	2.21	0.41
1:A:265:THR:HG23	1:D:119:ASN:ND2	2.36	0.40
1:C:138:ARG:HD2	5:C:415:HOH:O	2.19	0.40
1:A:69:LEU:HD23	1:A:69:LEU:HA	1.94	0.40
1:A:138:ARG:HG3	1:A:138:ARG:HH11	1.87	0.40
1:A:210:GLY:HA3	1:D:257:GLU:HG3	2.03	0.40
1:B:114:LEU:C	1:B:114:LEU:HD13	2.46	0.40
1:B:157:SER:O	1:B:160:ASP:HB2	2.22	0.40
1:B:252:LEU:HA	1:B:252:LEU:HD23	1.80	0.40
1:D:198:LYS:HD3	1:D:244:SER:HA	2.02	0.40

There are no symmetry-related clashes.

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	251/286 (88%)	249 (99%)	2 (1%)	0	100	100
1	B	256/286 (90%)	253 (99%)	3 (1%)	0	100	100
1	C	257/286 (90%)	257 (100%)	0	0	100	100
1	D	255/286 (89%)	246 (96%)	8 (3%)	1 (0%)	30	22
All	All	1019/1144 (89%)	1005 (99%)	13 (1%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	10	PRO

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	211/235 (90%)	211 (100%)	0	100	100
1	B	217/235 (92%)	216 (100%)	1 (0%)	81	84
1	C	218/235 (93%)	218 (100%)	0	100	100
1	D	216/235 (92%)	216 (100%)	0	100	100
All	All	862/940 (92%)	861 (100%)	1 (0%)	88	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	139	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	100	GLN
1	A	245	GLN
1	B	6	ASN
1	B	100	GLN
1	B	199	GLN
1	C	149	GLN
1	C	199	GLN
1	D	164	GLN
1	D	199	GLN

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](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	D	301	1	50,50,50	1.47	9 (18%)	67,82,82	1.44	11 (16%)
3	CYN	B	302	-	1,1,1	0.17	0	-		
3	CYN	C	302	-	1,1,1	0.23	0	-		
2	HEM	C	301	1	50,50,50	1.39	9 (18%)	67,82,82	1.32	6 (8%)
4	78U	A	303	-	16,17,17	1.45	2 (12%)	21,24,24	4.69	5 (23%)
4	78U	D	303	-	16,17,17	1.53	2 (12%)	21,24,24	4.48	6 (28%)
3	CYN	D	302	-	1,1,1	0.25	0	-		
2	HEM	B	301	1	50,50,50	1.38	7 (14%)	67,82,82	1.48	9 (13%)
4	78U	B	303	-	16,17,17	1.58	2 (12%)	21,24,24	4.31	7 (33%)
4	78U	C	303	-	16,17,17	1.62	4 (25%)	21,24,24	4.24	8 (38%)
3	CYN	A	302	-	1,1,1	0.21	0	-		
2	HEM	A	301	1	50,50,50	1.38	7 (14%)	67,82,82	1.26	6 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	D	301	1	-	6/14/54/54	-
2	HEM	C	301	1	-	1/14/54/54	-
4	78U	A	303	-	-	2/12/12/12	0/2/2/2
4	78U	D	303	-	-	3/12/12/12	0/2/2/2
2	HEM	B	301	1	-	0/14/54/54	-
4	78U	B	303	-	-	2/12/12/12	0/2/2/2
4	78U	C	303	-	-	1/12/12/12	0/2/2/2
2	HEM	A	301	1	-	0/14/54/54	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	301	HEM	FE-NB	4.51	2.08	1.94
4	C	303	78U	CD2-CG	-4.07	1.36	1.44
4	B	303	78U	CD2-CG	-4.06	1.36	1.44
2	C	301	HEM	FE-ND	4.01	2.07	1.94
2	D	301	HEM	FE-NC	3.97	2.08	1.95
4	D	303	78U	CD2-CG	-3.92	1.36	1.44
4	A	303	78U	CD2-CG	-3.78	1.37	1.44
2	A	301	HEM	FE-NB	3.68	2.06	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	303	78U	CD2-CE2	-3.57	1.37	1.41
2	A	301	HEM	FE-NC	3.52	2.06	1.95
2	B	301	HEM	CMC-C2C	3.50	1.57	1.50
4	C	303	78U	CD2-CE2	-3.19	1.37	1.41
4	B	303	78U	CD2-CE2	-3.13	1.37	1.41
2	A	301	HEM	CAB-C3B	3.10	1.55	1.47
2	C	301	HEM	CMC-C2C	3.06	1.57	1.50
4	A	303	78U	CD2-CE2	-2.97	1.37	1.41
2	C	301	HEM	CAC-C3C	2.96	1.55	1.47
2	B	301	HEM	CAB-C3B	2.82	1.54	1.47
2	D	301	HEM	FE-ND	2.79	2.03	1.94
2	C	301	HEM	CAB-C3B	2.74	1.54	1.47
2	D	301	HEM	CAB-C3B	2.65	1.54	1.47
2	B	301	HEM	CAC-C3C	2.63	1.54	1.47
2	A	301	HEM	CMC-C2C	2.60	1.56	1.50
2	D	301	HEM	CAC-C3C	2.57	1.54	1.47
2	B	301	HEM	FE-NC	2.53	2.03	1.95
2	A	301	HEM	CAC-C3C	2.48	1.54	1.47
2	B	301	HEM	FE-NA	2.47	2.03	1.95
2	D	301	HEM	CMC-C2C	2.43	1.55	1.50
2	C	301	HEM	CMD-C2D	2.42	1.55	1.50
2	A	301	HEM	FE-NA	2.35	2.02	1.95
2	B	301	HEM	CMD-C2D	2.32	1.55	1.50
2	D	301	HEM	C1B-NB	-2.28	1.36	1.40
2	B	301	HEM	C3B-C2B	-2.25	1.32	1.37
2	C	301	HEM	CMB-C2B	2.20	1.55	1.50
2	C	301	HEM	FE-NC	2.20	2.02	1.95
2	C	301	HEM	C2A-C3A	-2.09	1.33	1.38
4	C	303	78U	CB-CA	-2.08	1.52	1.55
2	D	301	HEM	C2A-C3A	-2.06	1.33	1.38
2	C	301	HEM	C1B-NB	-2.04	1.36	1.40
4	C	303	78U	CD1-CG	2.03	1.39	1.36
2	A	301	HEM	CMB-C2B	2.02	1.54	1.50
2	D	301	HEM	CMB-C2B	2.00	1.54	1.50

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	303	78U	CB-CG-CD1	-15.60	100.46	127.81
4	D	303	78U	CB-CG-CD1	-14.59	102.23	127.81
4	B	303	78U	CB-CG-CD1	-13.93	103.38	127.81
4	A	303	78U	CD2-CG-CB	13.57	151.64	125.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	303	78U	CB-CG-CD1	-13.13	104.79	127.81
4	D	303	78U	CD2-CG-CB	12.60	149.77	125.51
4	B	303	78U	CD2-CG-CB	12.20	149.01	125.51
4	C	303	78U	CD2-CG-CB	11.72	148.08	125.51
2	B	301	HEM	CHC-C4B-NB	4.91	129.71	124.42
2	A	301	HEM	CHC-C4B-NB	4.15	128.89	124.42
4	C	303	78U	CZ2-CE2-CD2	-4.03	118.29	122.19
2	C	301	HEM	CHC-C4B-NB	3.92	128.65	124.42
2	D	301	HEM	CHC-C4B-NB	3.77	128.48	124.42
2	B	301	HEM	CBA-CAA-C2A	-3.51	102.83	112.53
2	C	301	HEM	CBA-CAA-C2A	-3.33	103.33	112.53
2	B	301	HEM	C4C-C3C-C2C	3.23	109.61	106.81
2	D	301	HEM	CBA-CAA-C2A	-3.01	104.21	112.53
4	C	303	78U	CE2-NE1-CD1	-3.00	106.41	109.08
4	D	303	78U	CG-CD1-NE1	-2.95	107.92	110.31
2	D	301	HEM	C4D-ND-C1D	2.95	108.70	105.21
4	A	303	78U	CG-CD1-NE1	-2.94	107.93	110.31
4	D	303	78U	CZ2-CE2-CD2	-2.87	119.41	122.19
4	B	303	78U	CZ2-CE2-CD2	-2.77	119.50	122.19
2	C	301	HEM	C1B-NB-C4B	2.70	108.40	105.21
4	C	303	78U	CB-CA-C	2.66	114.72	110.63
2	D	301	HEM	C2A-C1A-NA	-2.64	107.23	110.15
2	B	301	HEM	C4A-CHB-C1B	-2.60	120.14	126.25
4	C	303	78U	CE2-CD2-CG	2.54	109.35	106.98
2	D	301	HEM	C1B-NB-C4B	2.50	108.17	105.21
2	B	301	HEM	C4A-C3A-C2A	2.46	109.63	106.82
4	B	303	78U	CE2-NE1-CD1	-2.45	106.89	109.08
4	A	303	78U	CZ2-CE2-CD2	-2.38	119.88	122.19
4	D	303	78U	OXT-C-CA	2.38	122.35	114.15
2	C	301	HEM	CBD-CAD-C3D	-2.36	106.01	112.53
2	A	301	HEM	C1B-NB-C4B	2.35	107.99	105.21
4	D	303	78U	CD2-CG-CD1	2.29	108.00	106.25
2	A	301	HEM	C4D-ND-C1D	2.27	107.90	105.21
2	D	301	HEM	CHD-C4C-NC	2.23	126.88	124.45
2	D	301	HEM	C3D-C4D-ND	-2.23	107.73	110.17
4	B	303	78U	OXT-C-CA	2.20	121.75	114.15
4	B	303	78U	CG-CD1-NE1	-2.20	108.52	110.31
2	C	301	HEM	C4C-C3C-C2C	2.17	108.69	106.81
2	D	301	HEM	O1A-CGA-CBA	-2.16	116.25	123.09
2	D	301	HEM	C2D-C1D-ND	-2.15	107.41	109.90
4	A	303	78U	CD2-CG-CD1	2.15	107.90	106.25
2	B	301	HEM	CHA-C4D-ND	2.14	127.01	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	HEM	C4D-ND-C1D	2.13	107.73	105.21
2	A	301	HEM	C3B-C2B-C1B	2.13	108.01	106.41
2	D	301	HEM	C4C-C3C-C2C	2.12	108.65	106.81
2	D	301	HEM	CAD-C3D-C4D	2.10	128.36	124.70
2	B	301	HEM	CMB-C2B-C1B	-2.09	121.77	125.03
4	C	303	78U	CE3-CD2-CG	-2.09	130.11	133.68
2	A	301	HEM	C4C-C3C-C2C	2.09	108.62	106.81
4	C	303	78U	CAG-CB-CA	2.08	114.29	111.12
4	B	303	78U	CE2-CD2-CG	2.05	108.89	106.98
2	A	301	HEM	CBA-CAA-C2A	-2.03	106.92	112.53
2	B	301	HEM	C4D-ND-C1D	2.01	107.58	105.21
2	B	301	HEM	C1B-NB-C4B	2.00	107.58	105.21

There are no chirality outliers.

All (15) torsion outliers are listed below:

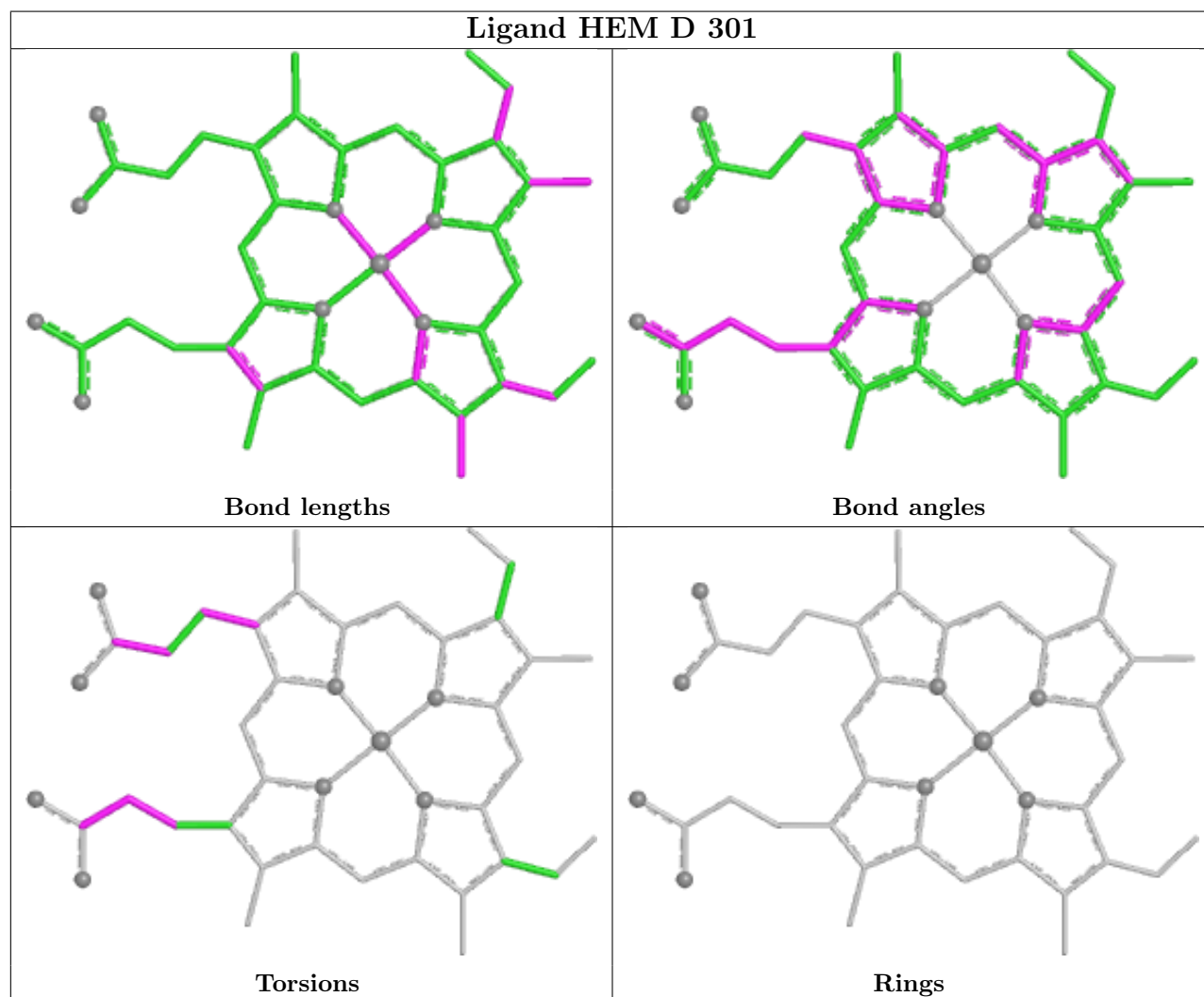
Mol	Chain	Res	Type	Atoms
2	C	301	HEM	C2A-CAA-CBA-CGA
2	D	301	HEM	C2A-CAA-CBA-CGA
2	D	301	HEM	C4D-C3D-CAD-CBD
2	D	301	HEM	C2D-C3D-CAD-CBD
4	A	303	78U	OXT-C-CA-N
4	C	303	78U	OXT-C-CA-N
4	B	303	78U	CAG-CB-CG-CD1
4	D	303	78U	CAG-CB-CG-CD1
2	D	301	HEM	CAD-CBD-CGD-O2D
2	D	301	HEM	CAD-CBD-CGD-O1D
4	A	303	78U	O-C-CA-N
4	D	303	78U	C-CA-CB-CAG
4	B	303	78U	CA-CB-CG-CD2
4	D	303	78U	CA-CB-CG-CD2
2	D	301	HEM	CAA-CBA-CGA-O2A

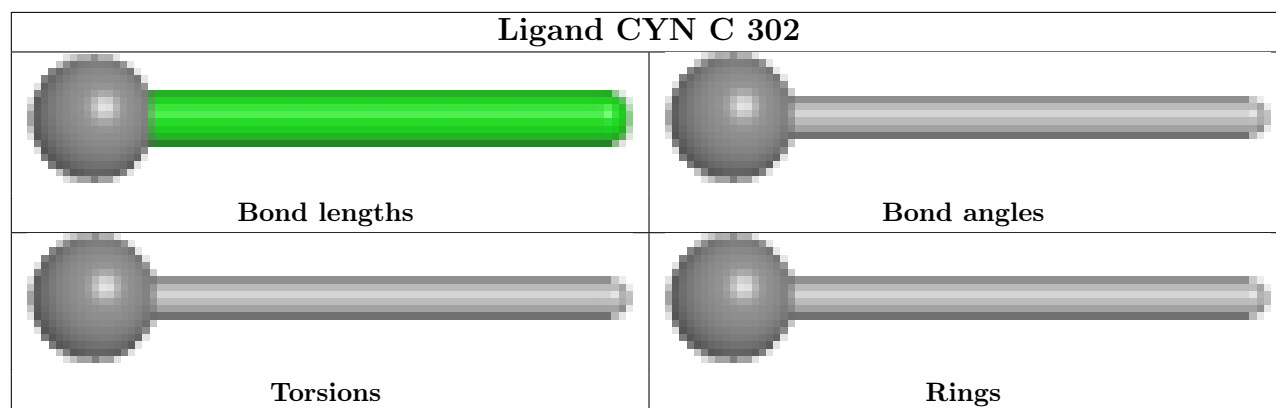
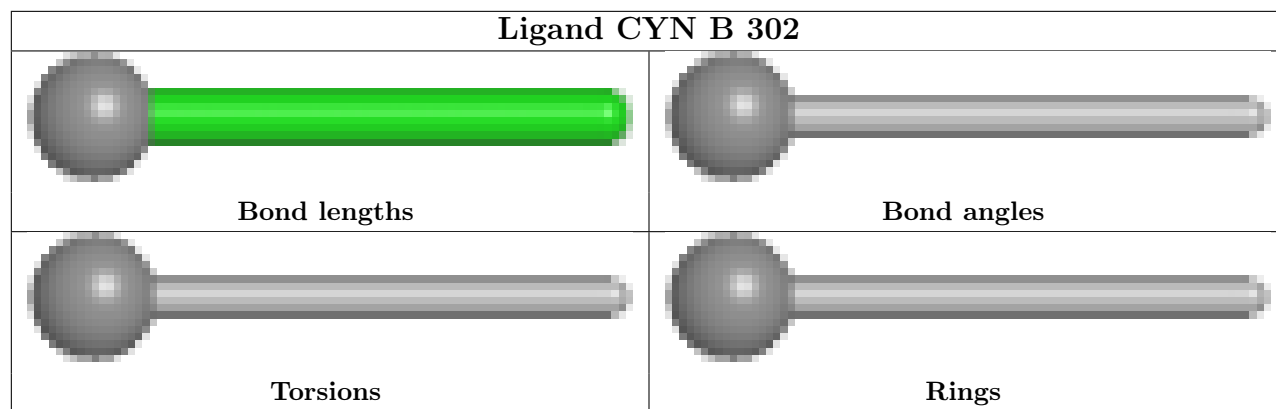
There are no ring outliers.

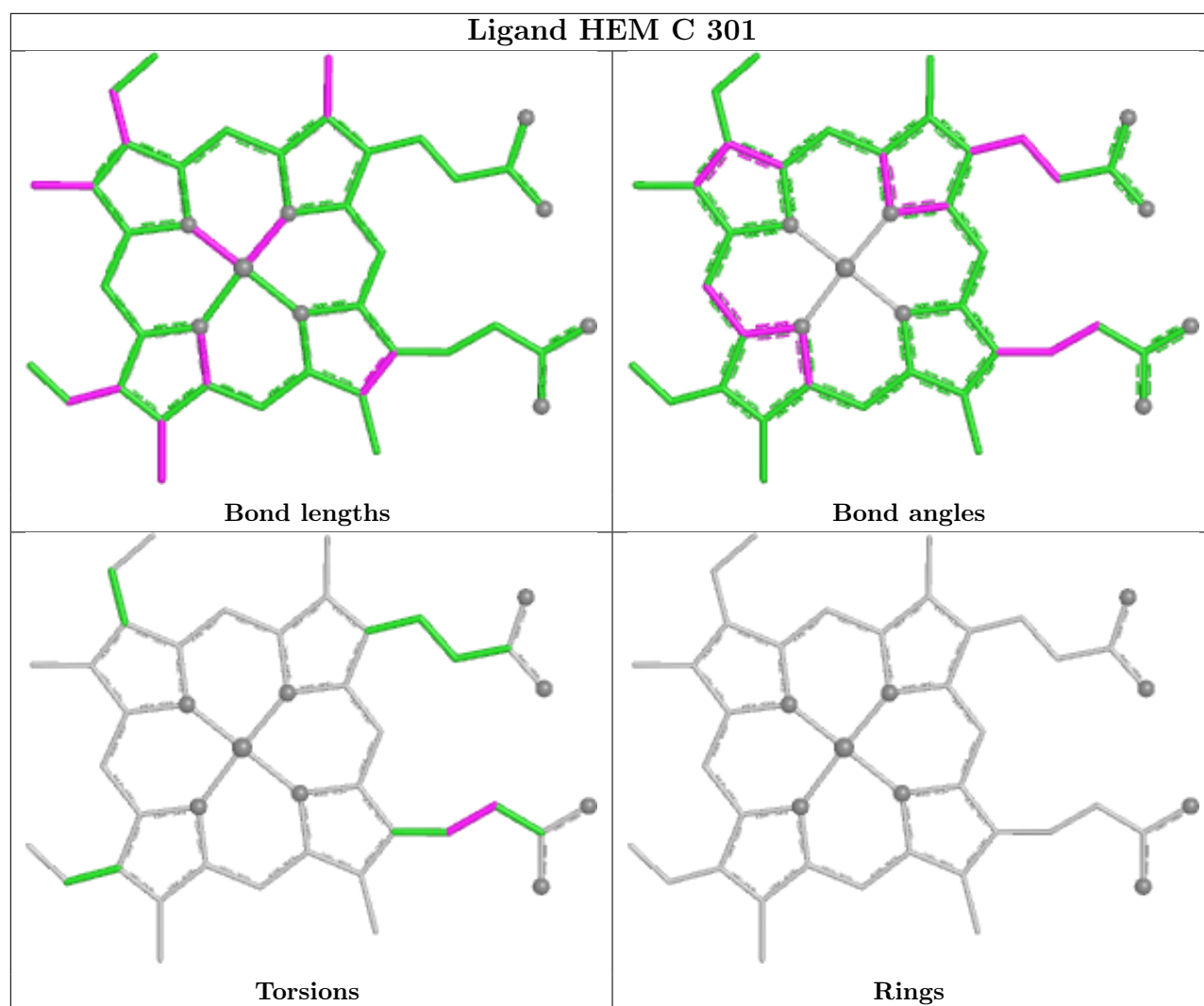
4 monomers are involved in 11 short contacts:

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

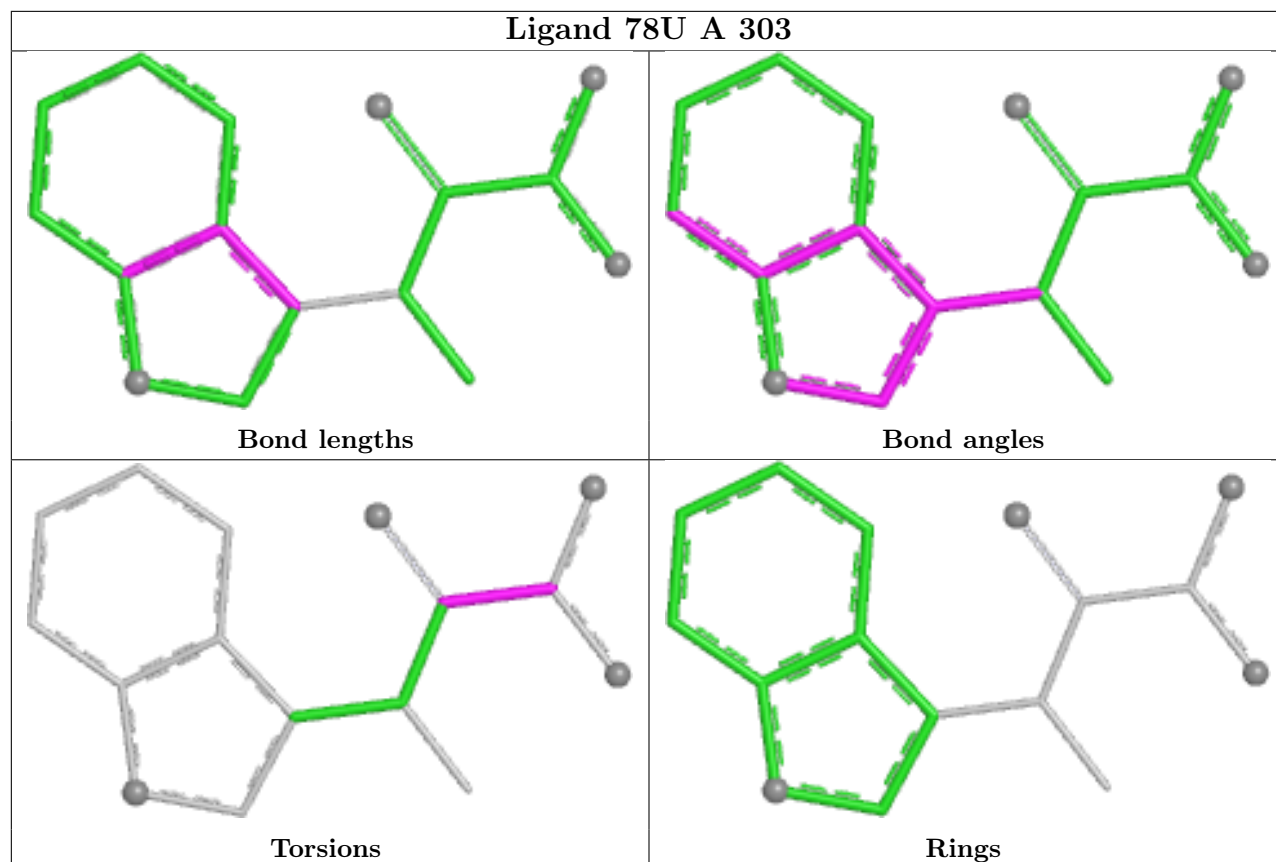
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



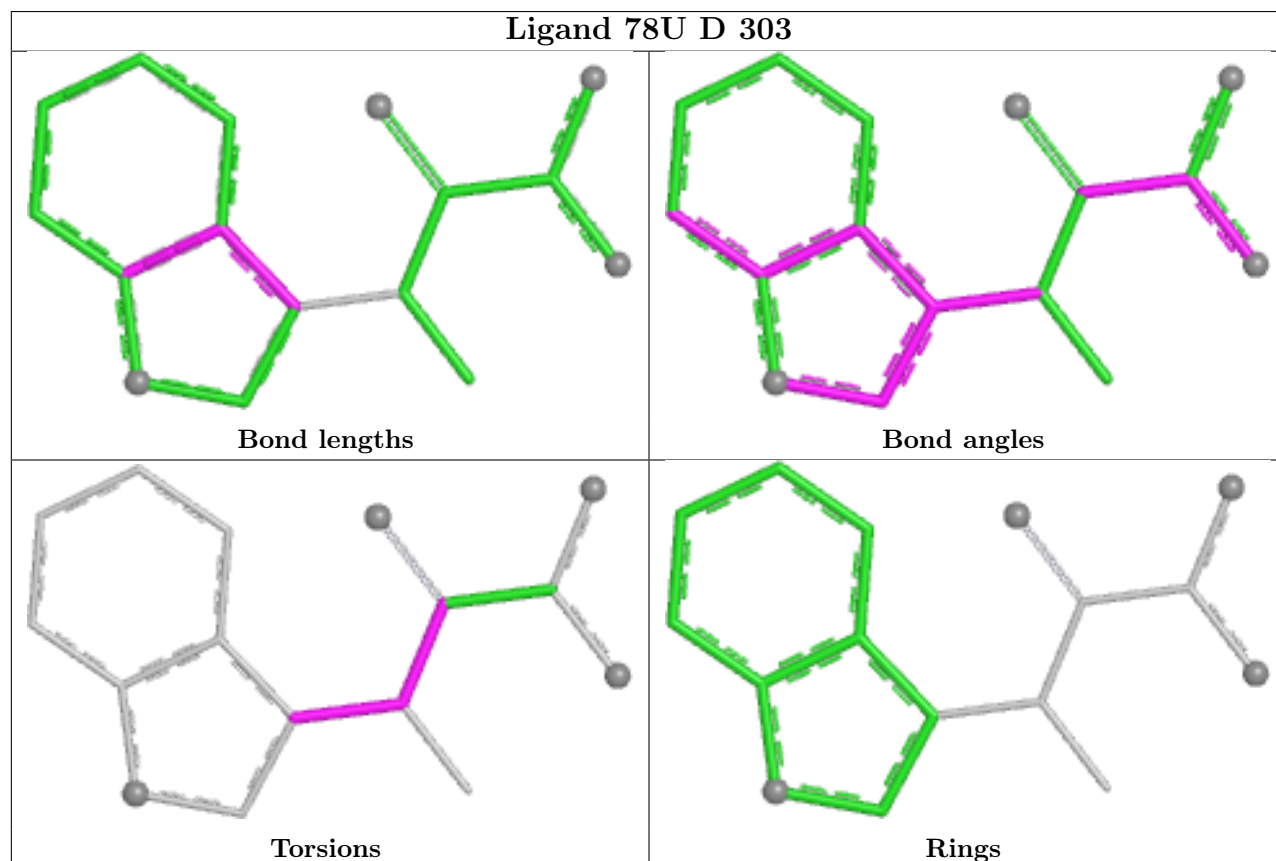


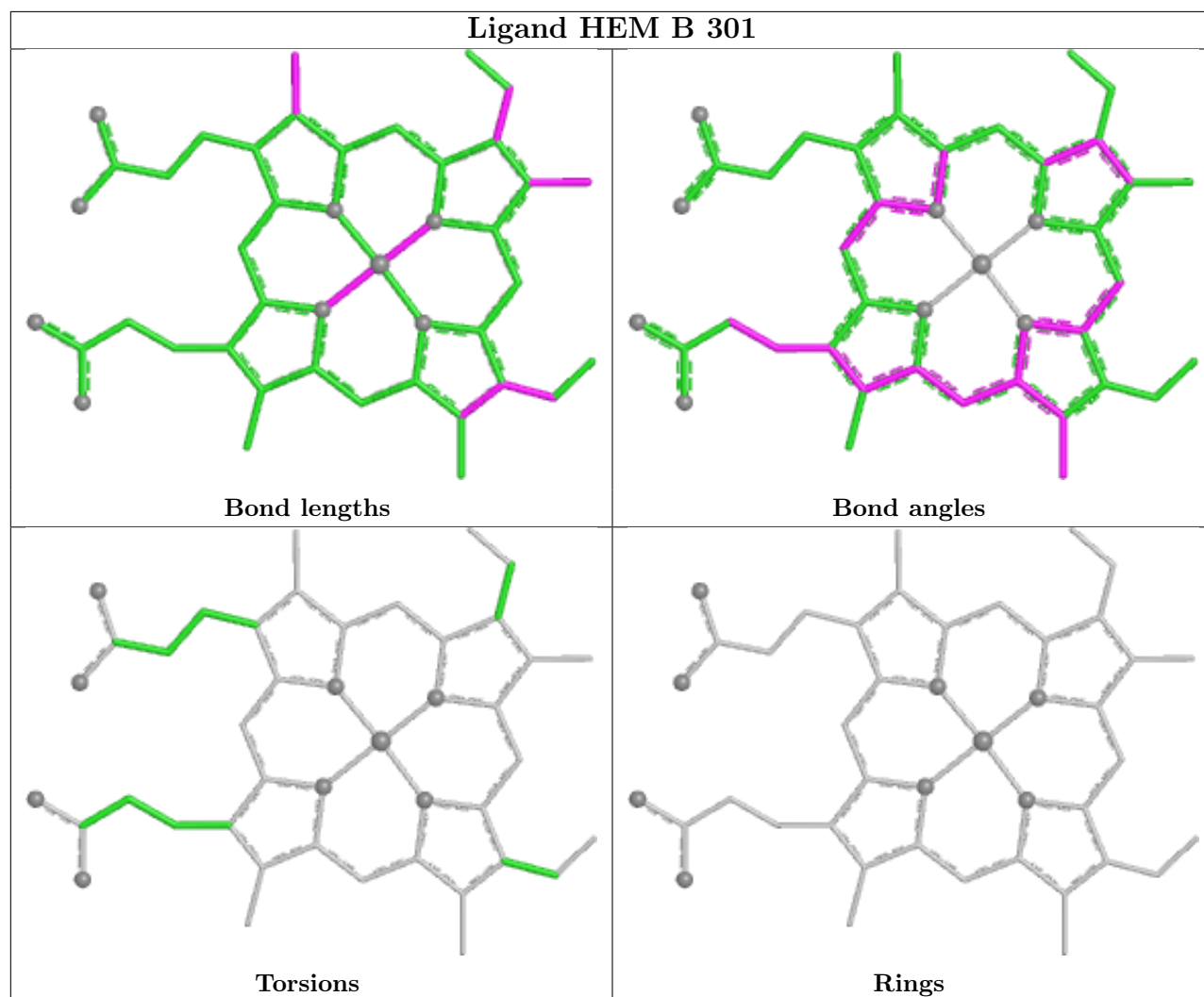
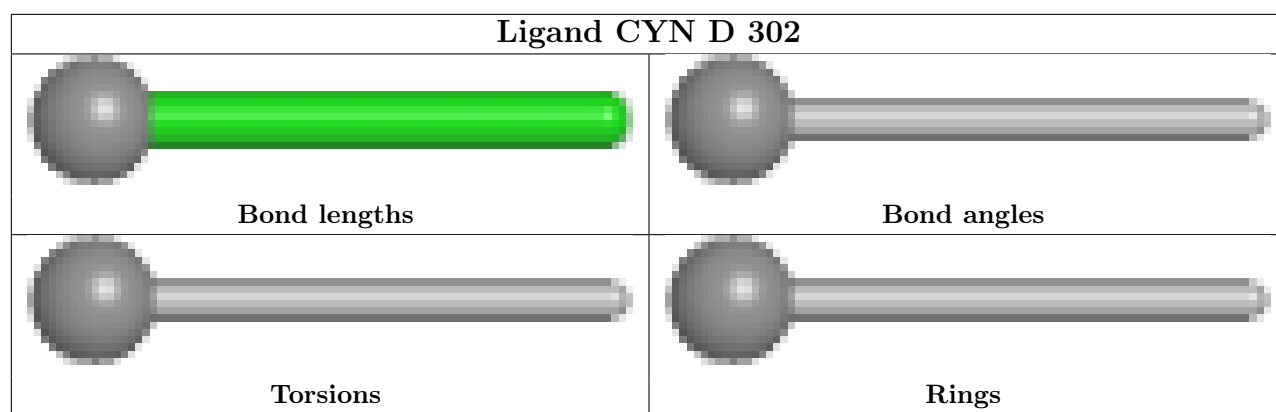


Ligand 78U A 303

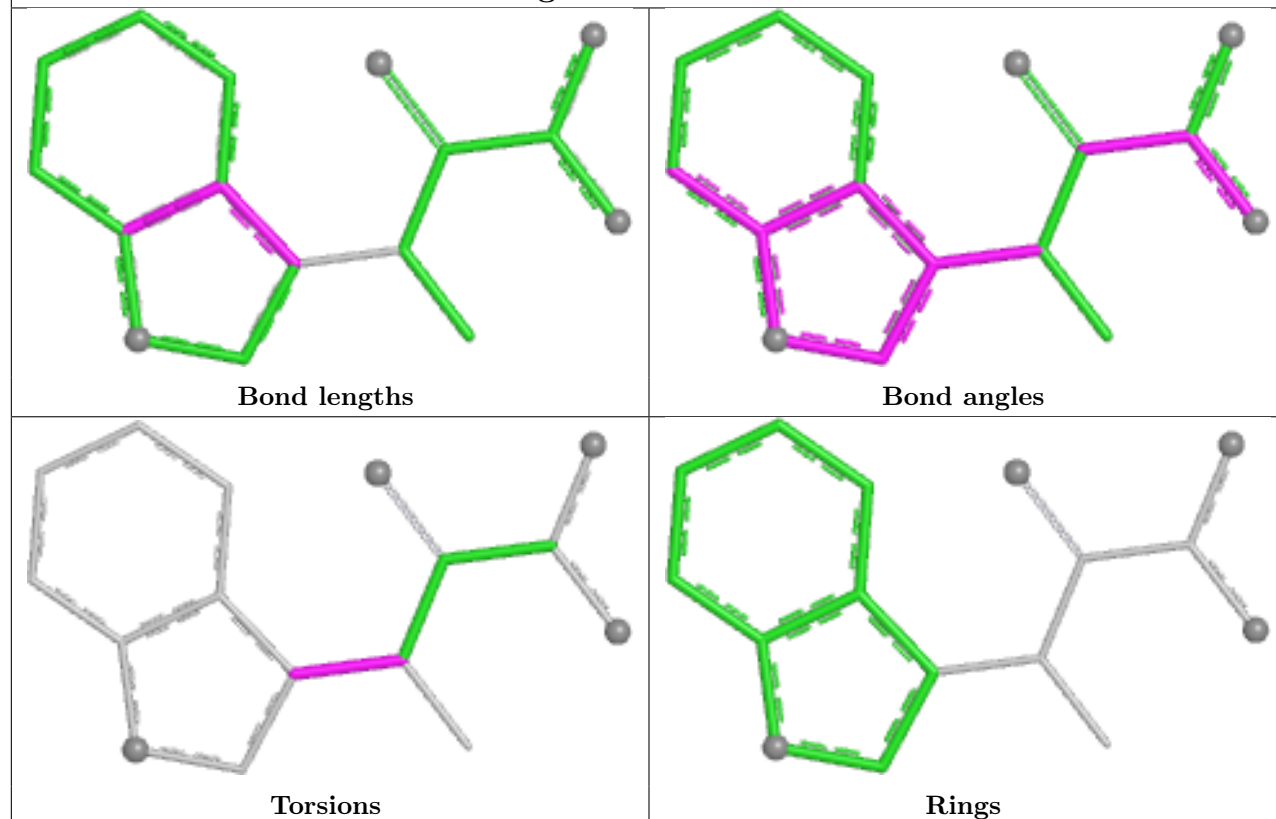


Ligand 78U D 303

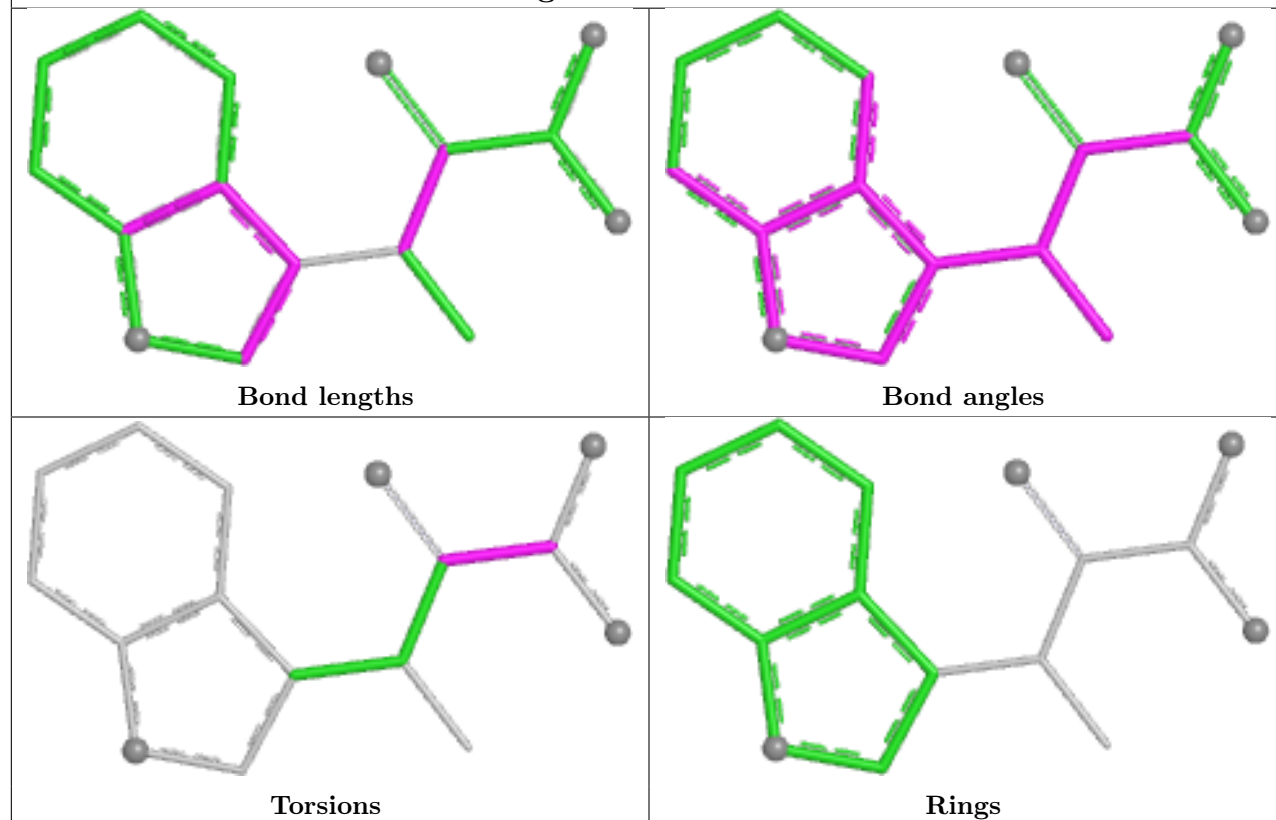


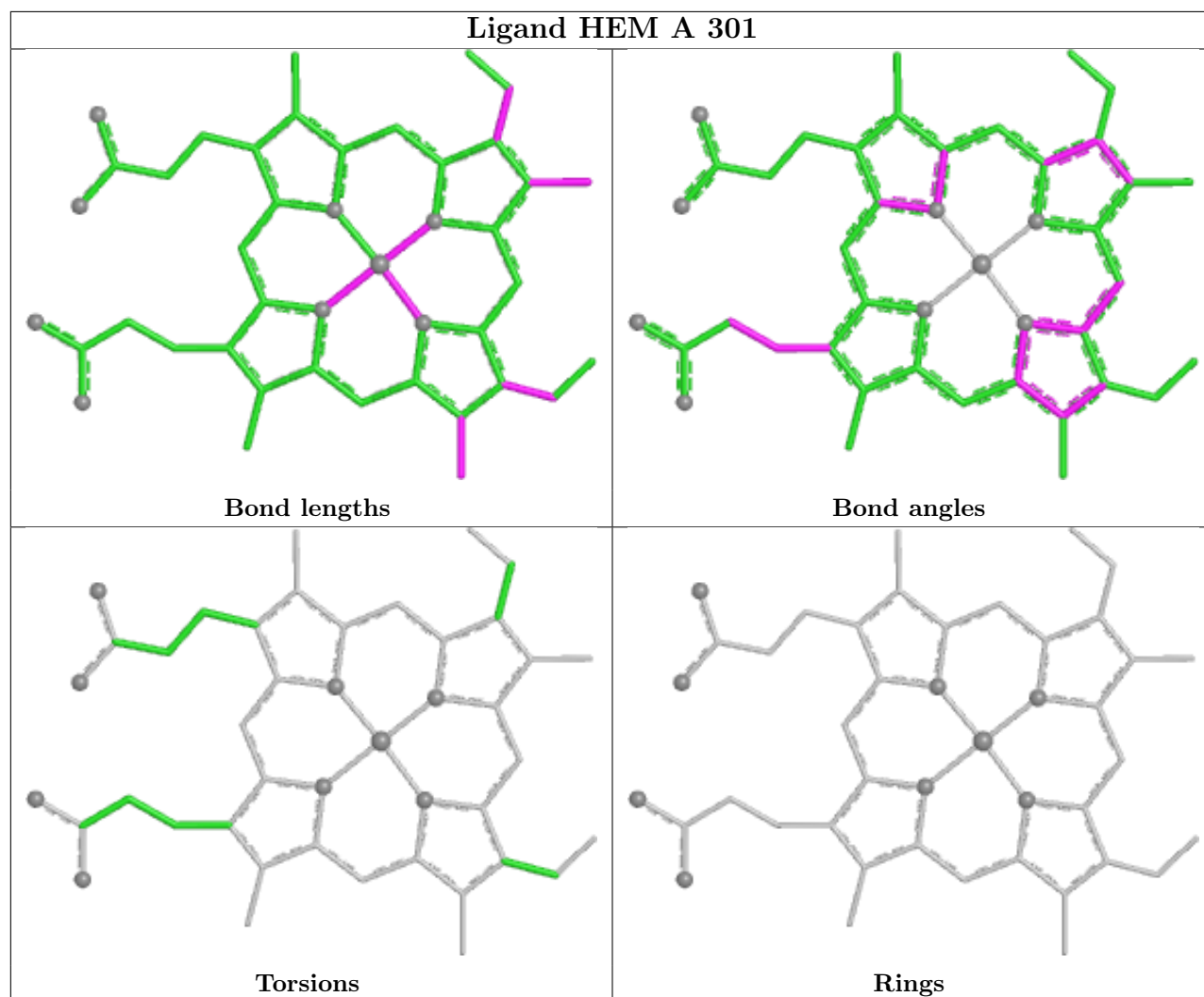
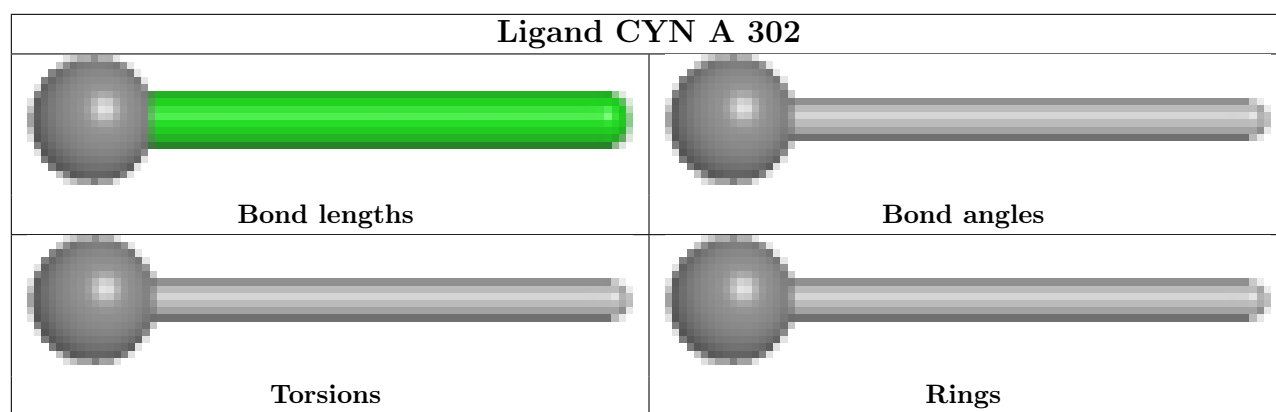


Ligand 78U B 303



Ligand 78U C 303





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	255/286 (89%)	0.20	5 (1%) 65 69	29, 40, 59, 68	0
1	B	260/286 (90%)	0.09	1 (0%) 88 90	28, 36, 57, 67	0
1	C	260/286 (90%)	0.02	3 (1%) 76 79	20, 33, 48, 58	1 (0%)
1	D	258/286 (90%)	0.22	5 (1%) 66 70	23, 38, 58, 78	1 (0%)
All	All	1033/1144 (90%)	0.13	14 (1%) 73 76	20, 37, 56, 78	2 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	234	GLY	5.6
1	D	233	GLY	5.0
1	C	12	ALA	3.4
1	C	133	TYR	3.0
1	A	5	LEU	2.8
1	A	100	GLN	2.6
1	A	261	TRP	2.5
1	B	2	LYS	2.3
1	C	60	TYR	2.2
1	D	269	THR	2.2
1	A	56	LEU	2.2
1	D	235	ARG	2.2
1	A	37	LEU	2.1
1	D	137[A]	ARG	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

There are no oligosaccharides in this entry.

6.4 Ligands

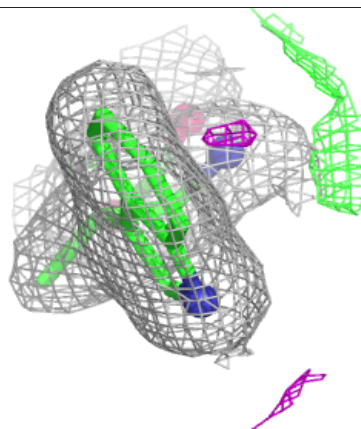
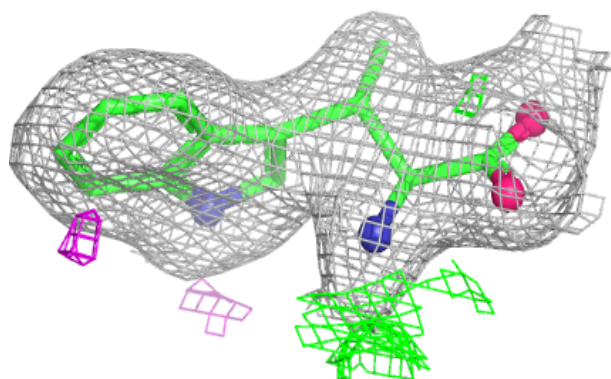
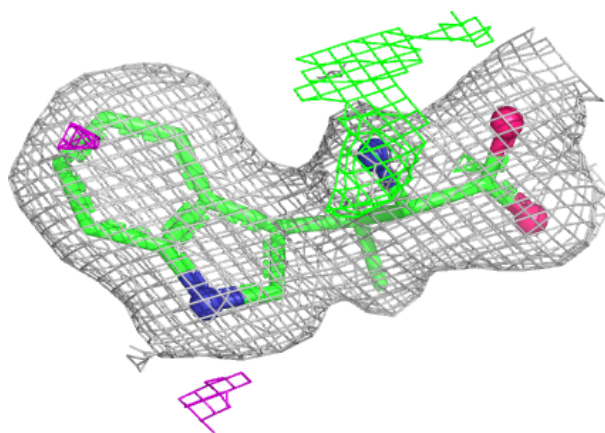
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	78U	C	303	16/16	0.92	0.08	32,33,36,36	0
4	78U	A	303	16/16	0.93	0.08	40,47,52,54	0
4	78U	D	303	16/16	0.93	0.07	34,37,42,47	0
3	CYN	C	302	2/2	0.94	0.14	28,28,28,33	0
4	78U	B	303	16/16	0.94	0.07	31,35,37,37	0
2	HEM	A	301	43/43	0.96	0.08	37,42,57,59	0
3	CYN	D	302	2/2	0.96	0.07	29,29,29,32	0
3	CYN	A	302	2/2	0.96	0.07	39,39,39,40	0
2	HEM	B	301	43/43	0.97	0.08	26,31,43,48	0
3	CYN	B	302	2/2	0.97	0.06	30,30,30,31	0
2	HEM	C	301	43/43	0.97	0.08	24,29,44,45	0
2	HEM	D	301	43/43	0.97	0.08	27,33,51,56	0

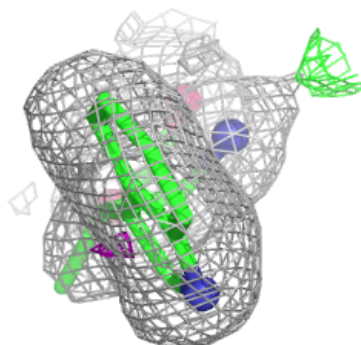
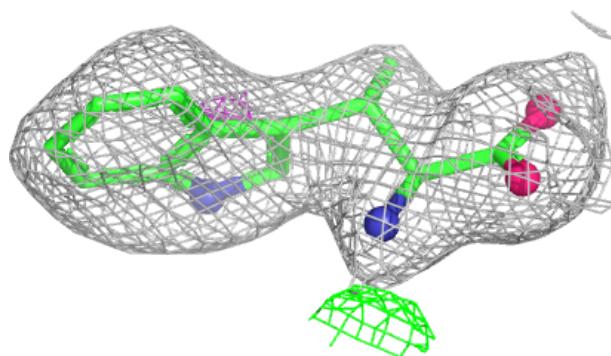
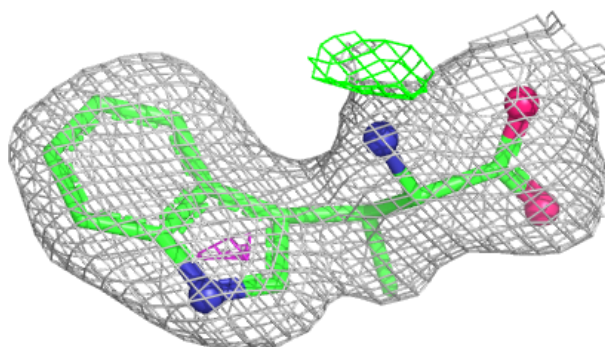
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 78U C 303:

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

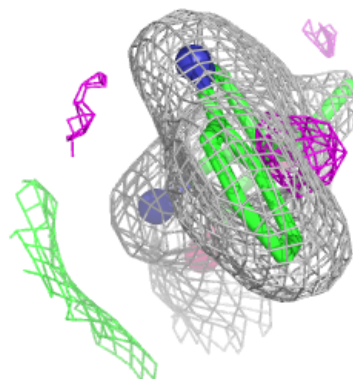
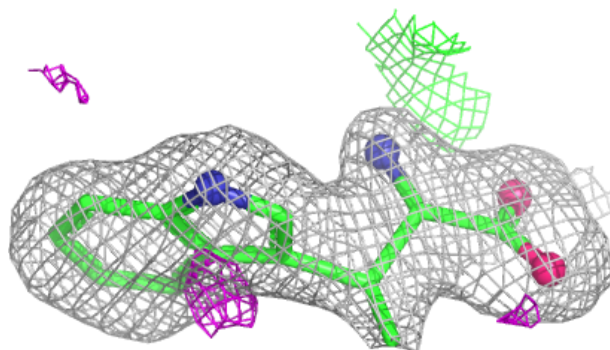
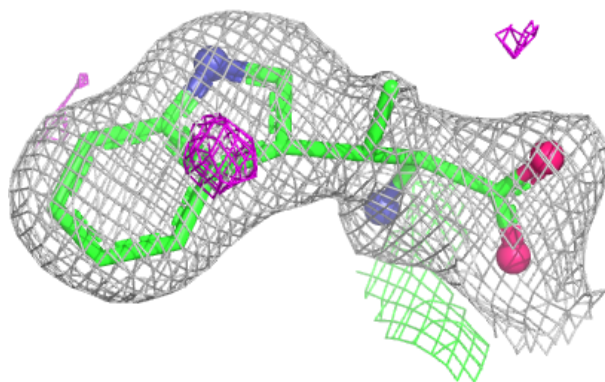
**Electron density around 78U A 303:**

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



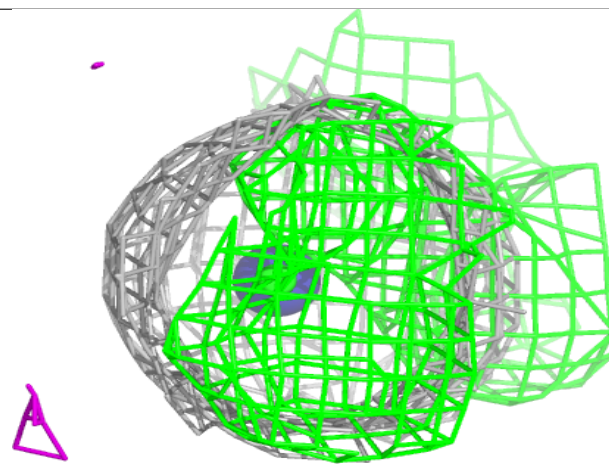
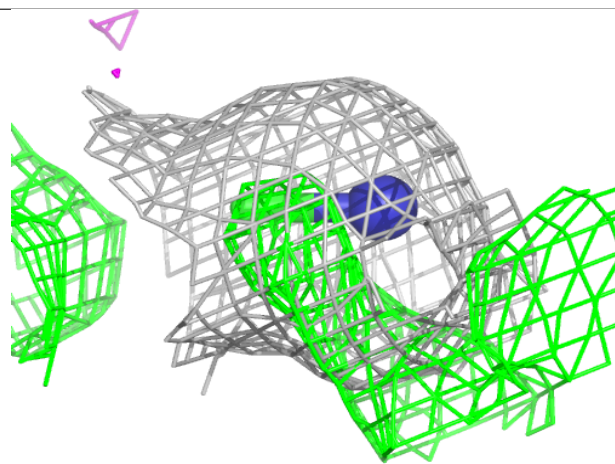
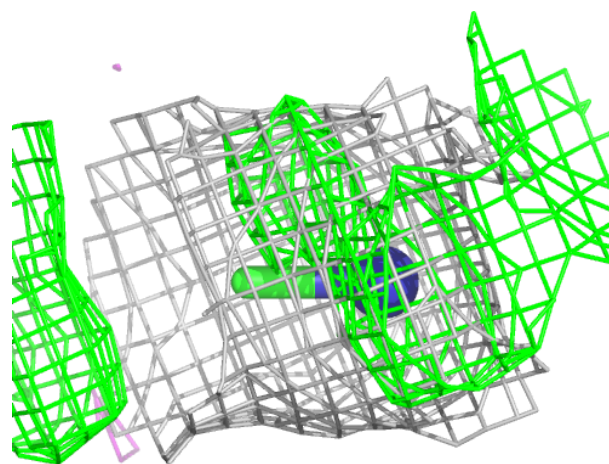
Electron density around 78U D 303:

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



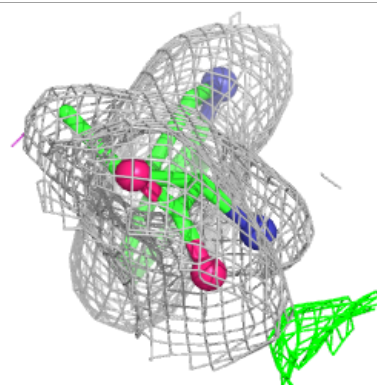
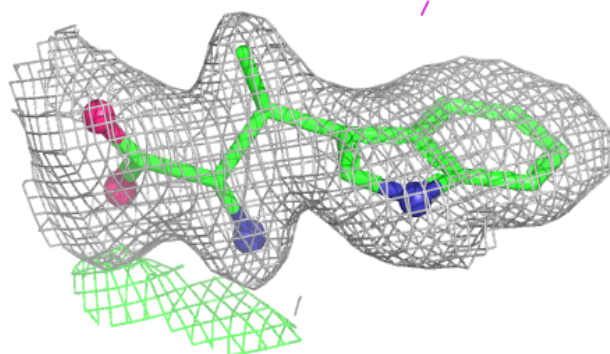
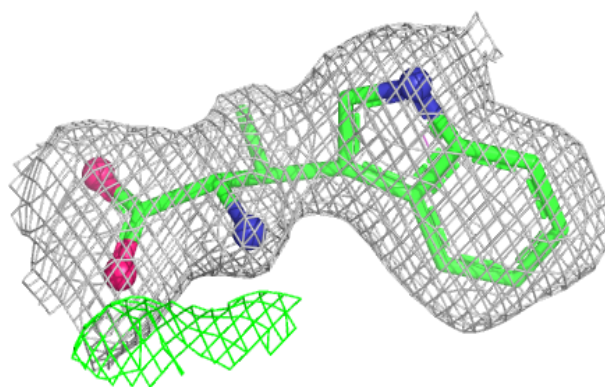
Electron density around CYN C 302:

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

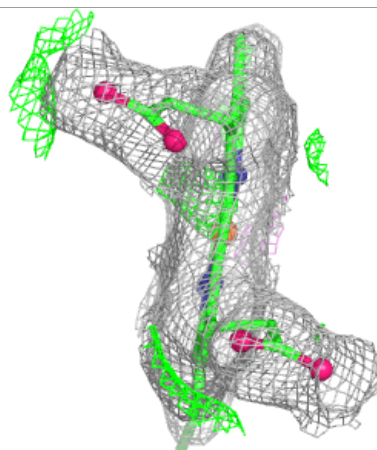
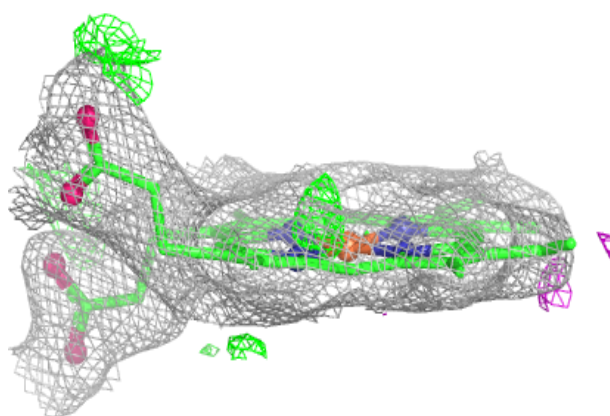
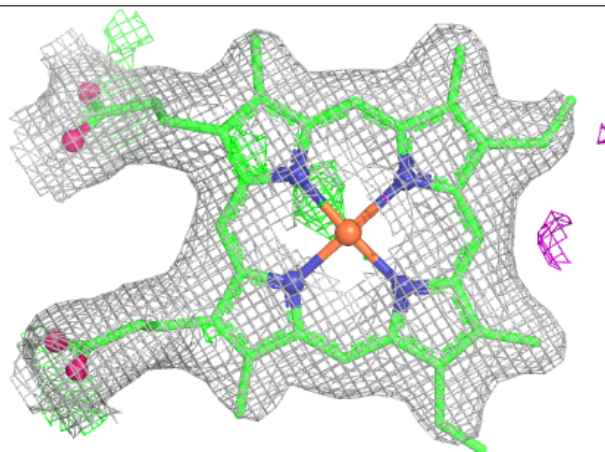


Electron density around 78U B 303:

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

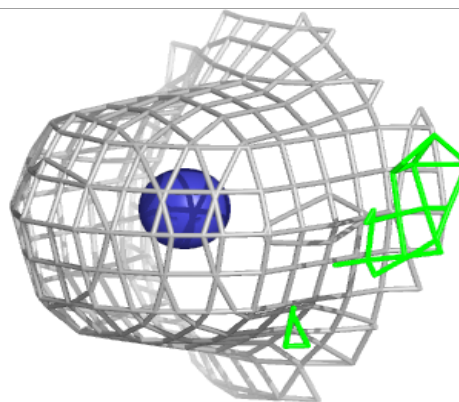
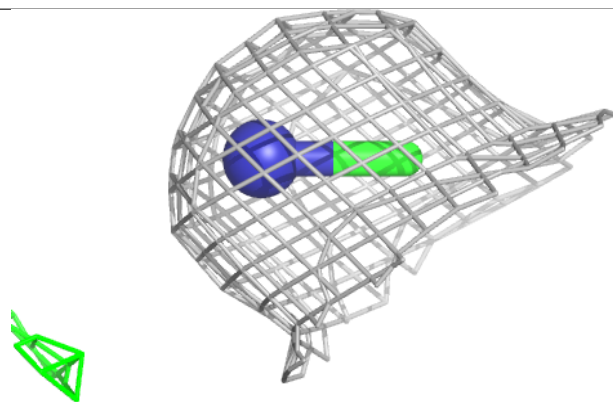
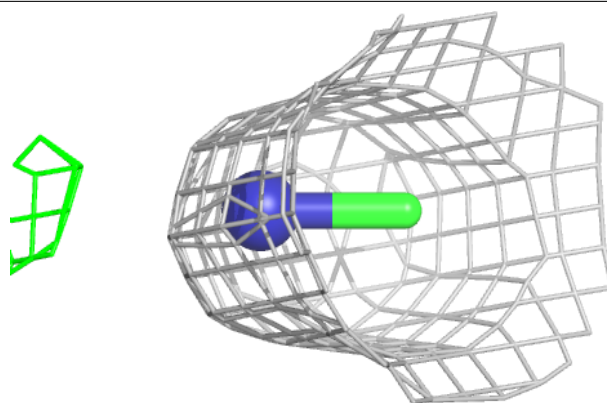
**Electron density around HEM A 301:**

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

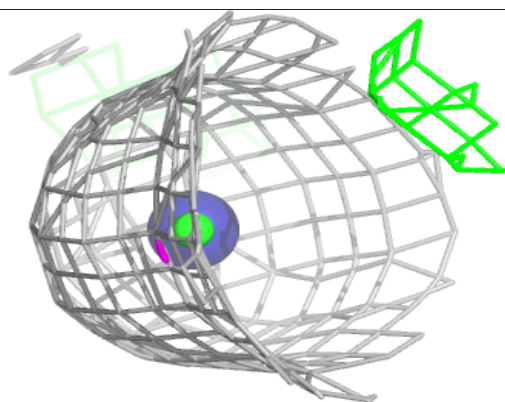
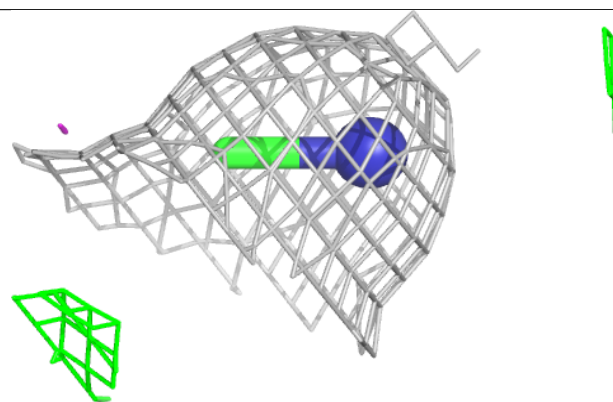
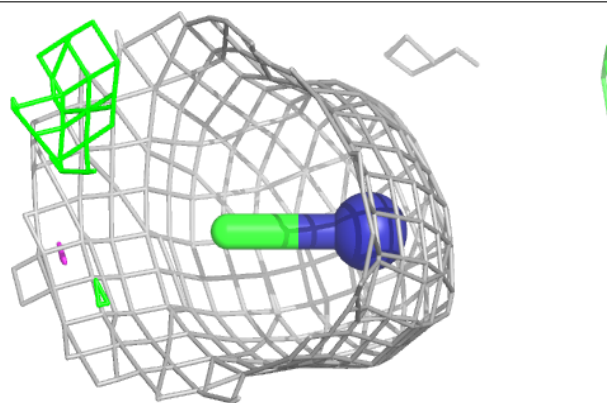


Electron density around CYN D 302:

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

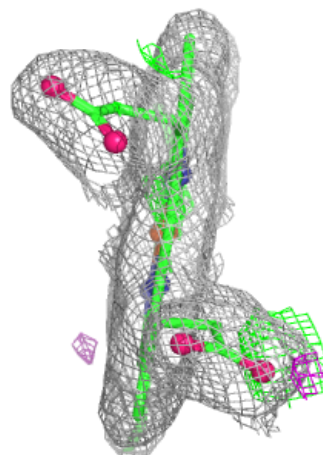
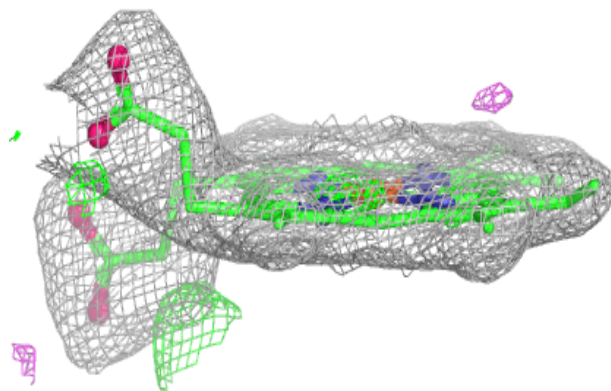
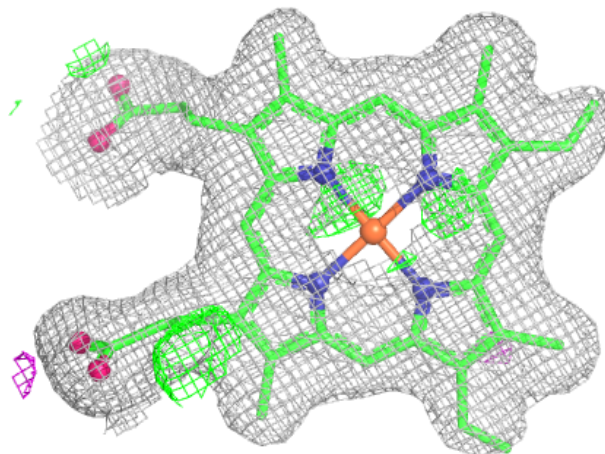
**Electron density around CYN A 302:**

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



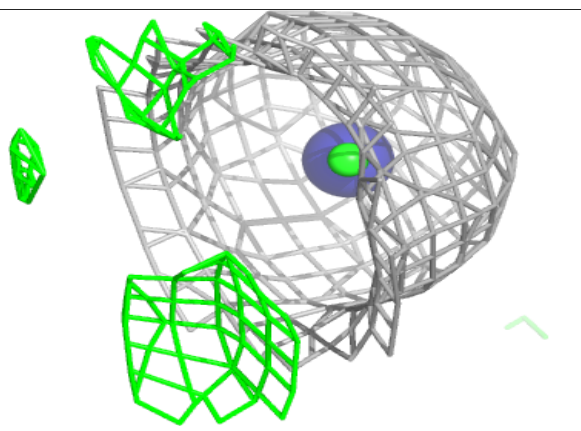
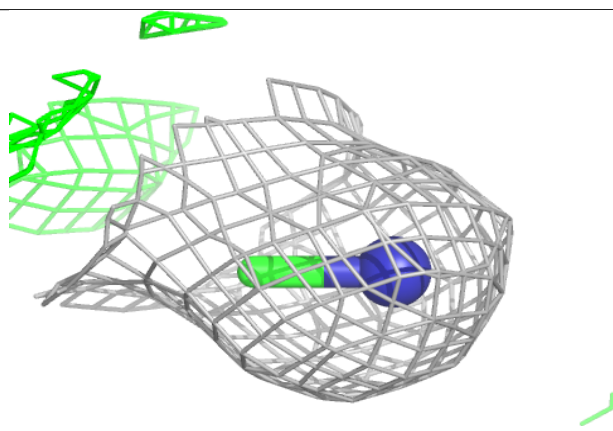
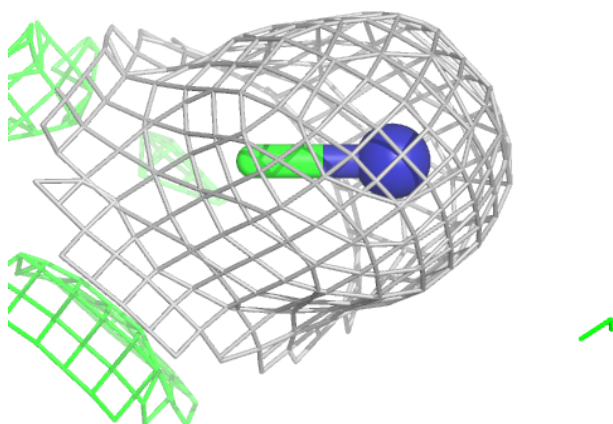
Electron density around HEM B 301:

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



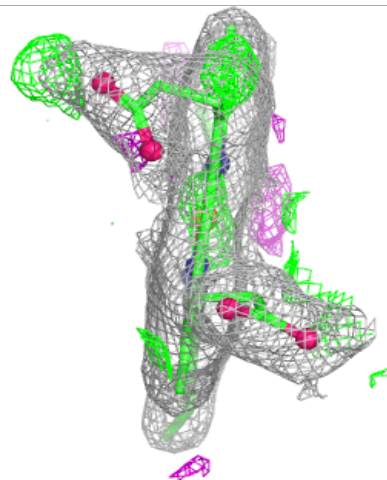
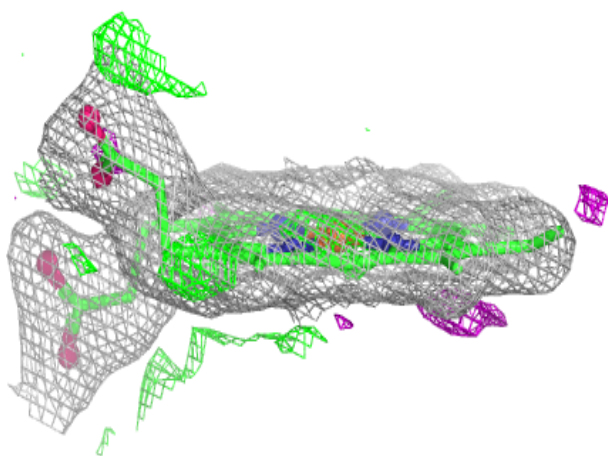
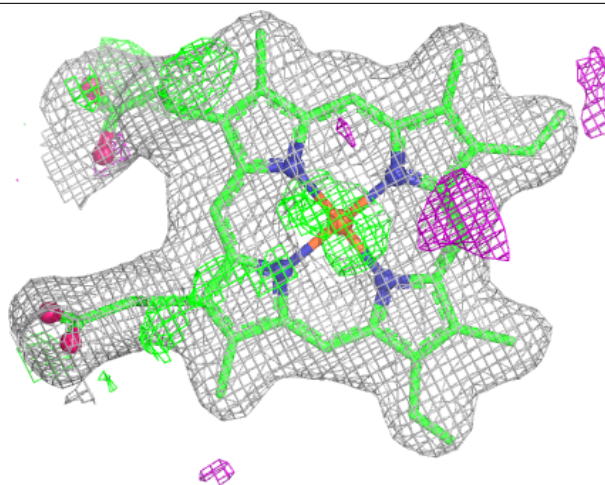
Electron density around CYN B 302:

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



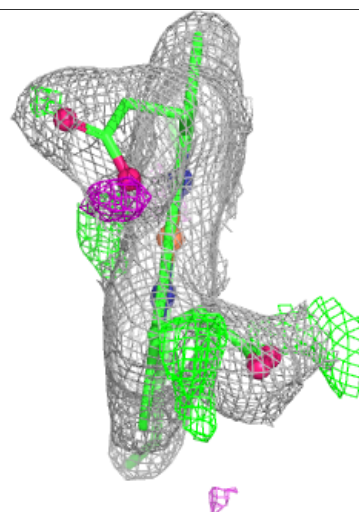
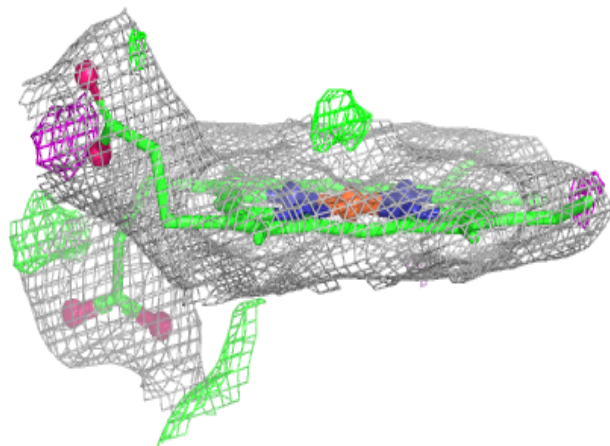
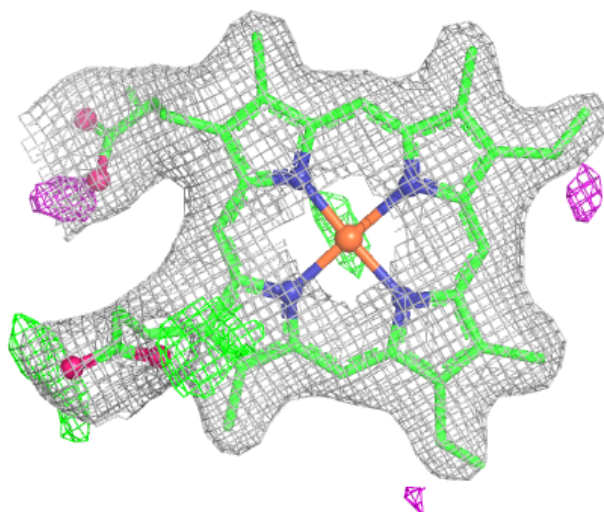
Electron density around HEM C 301:

$2mF_o-DF_c$ (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.