



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:54 pm BST

PDB ID : 6PYY
Title : Crystal Structure of human Tryptophan 2,3-dioxygenase in complex with PF-06840003 in Active Site and Exo site
Authors : Pham, K.N.; Lewis-Ballester, A.; Yeh, S.R.
Deposited on : 2019-07-31
Resolution : 2.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

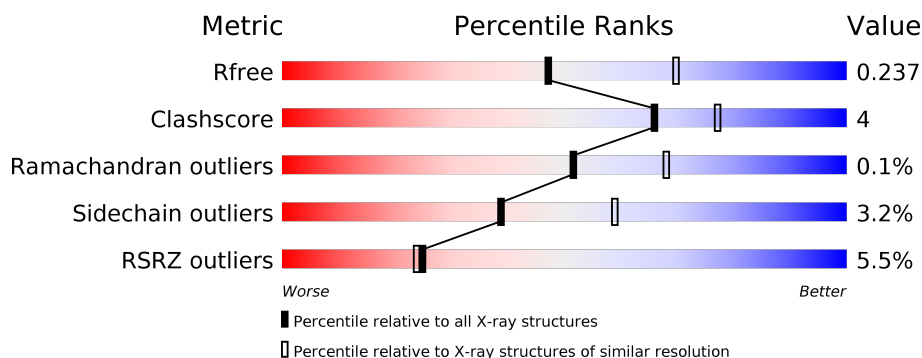
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 on 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	380	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>12%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	380	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>7%</div> <div>10%</div> </div> </div>
1	C	380	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>9%</div> <div>•</div> <div>13%</div> </div> </div>
1	D	380	<div> <div>6%</div> <div> <div></div> <div>82%</div> <div>8%</div> <div>•</div> <div>9%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12156 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	351	Total	C	N	O	S	0	0	0
			2936	1882	516	527	11			
1	B	342	Total	C	N	O	S	0	0	0
			2846	1827	494	514	11			
1	C	332	Total	C	N	O	S	0	0	0
			2749	1770	481	487	11			
1	D	347	Total	C	N	O	S	0	0	0
			2905	1865	513	516	11			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	MET	-	initiating methionine	UNP P48775
A	390	GLU	-	expression tag	UNP P48775
A	391	HIS	-	expression tag	UNP P48775
A	392	HIS	-	expression tag	UNP P48775
A	393	HIS	-	expression tag	UNP P48775
A	394	HIS	-	expression tag	UNP P48775
A	395	HIS	-	expression tag	UNP P48775
A	396	HIS	-	expression tag	UNP P48775
B	17	MET	-	initiating methionine	UNP P48775
B	390	GLU	-	expression tag	UNP P48775
B	391	HIS	-	expression tag	UNP P48775
B	392	HIS	-	expression tag	UNP P48775
B	393	HIS	-	expression tag	UNP P48775
B	394	HIS	-	expression tag	UNP P48775
B	395	HIS	-	expression tag	UNP P48775
B	396	HIS	-	expression tag	UNP P48775
C	17	MET	-	initiating methionine	UNP P48775
C	390	GLU	-	expression tag	UNP P48775
C	391	HIS	-	expression tag	UNP P48775
C	392	HIS	-	expression tag	UNP P48775
C	393	HIS	-	expression tag	UNP P48775

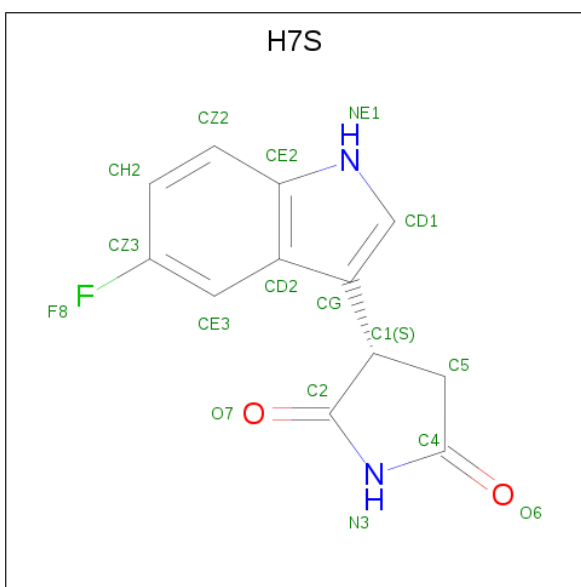
Continued on next page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	394	HIS	-	expression tag	UNP P48775
C	395	HIS	-	expression tag	UNP P48775
C	396	HIS	-	expression tag	UNP P48775
D	17	MET	-	initiating methionine	UNP P48775
D	390	GLU	-	expression tag	UNP P48775
D	391	HIS	-	expression tag	UNP P48775
D	392	HIS	-	expression tag	UNP P48775
D	393	HIS	-	expression tag	UNP P48775
D	394	HIS	-	expression tag	UNP P48775
D	395	HIS	-	expression tag	UNP P48775
D	396	HIS	-	expression tag	UNP P48775

- # HEM

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

- WORLDWIDE
PDB
PROTEIN DATA BANK



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			17	12	1	2	2		
3	A	1	Total	C	F	N	O	0	0
			17	12	1	2	2		
3	B	1	Total	C	F	N	O	0	0
			17	12	1	2	2		
3	B	1	Total	C	F	N	O	0	0
			17	12	1	2	2		
3	C	1	Total	C	F	N	O	0	0
			17	12	1	2	2		
3	C	1	Total	C	F	N	O	0	0
			17	12	1	2	2		
3	D	1	Total	C	F	N	O	0	0
			17	12	1	2	2		
3	D	1	Total	C	F	N	O	0	0
			17	12	1	2	2		

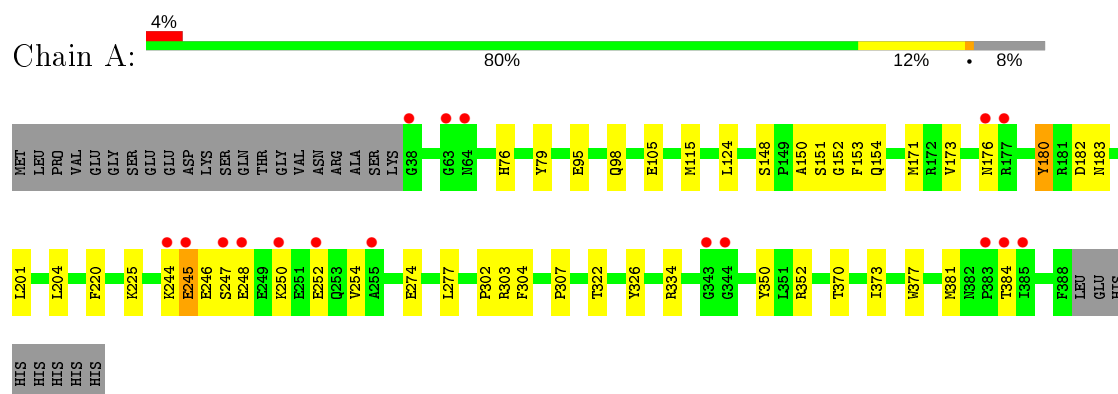
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	114	Total	O	0	0
			114	114		
4	B	111	Total	O	0	0
			111	111		
4	C	80	Total	O	0	0
			80	80		
4	D	107	Total	O	0	0
			107	107		

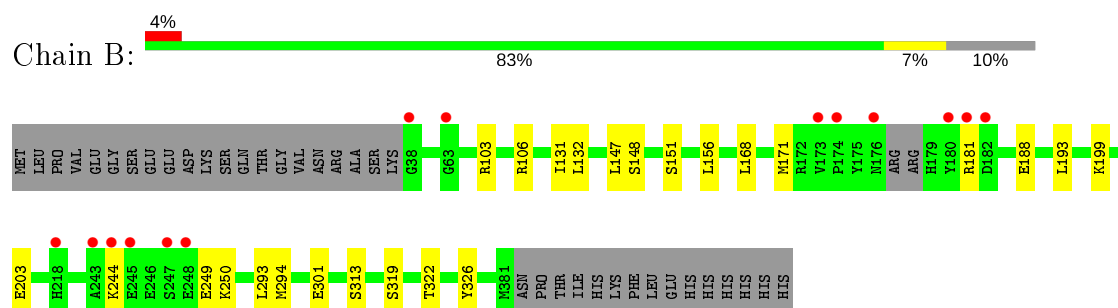
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

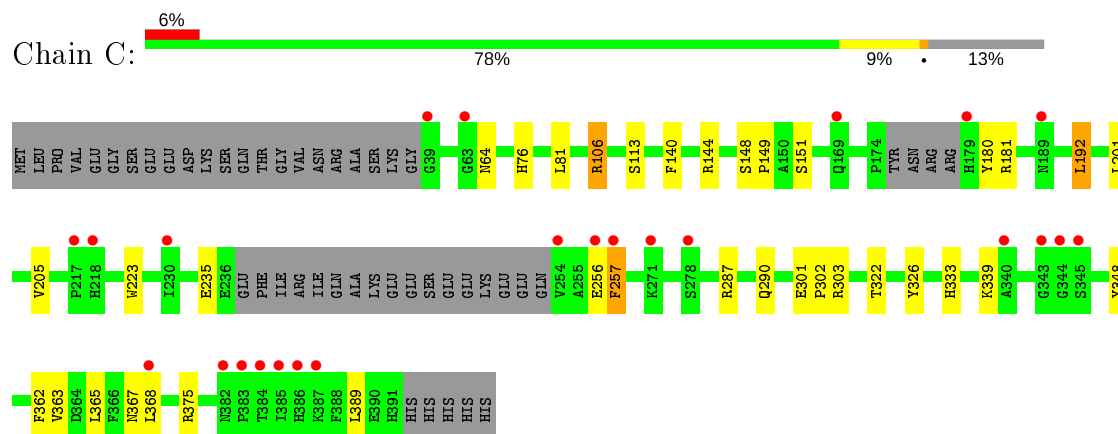
• Molecule 1: Tryptophan 2,3-dioxygenase



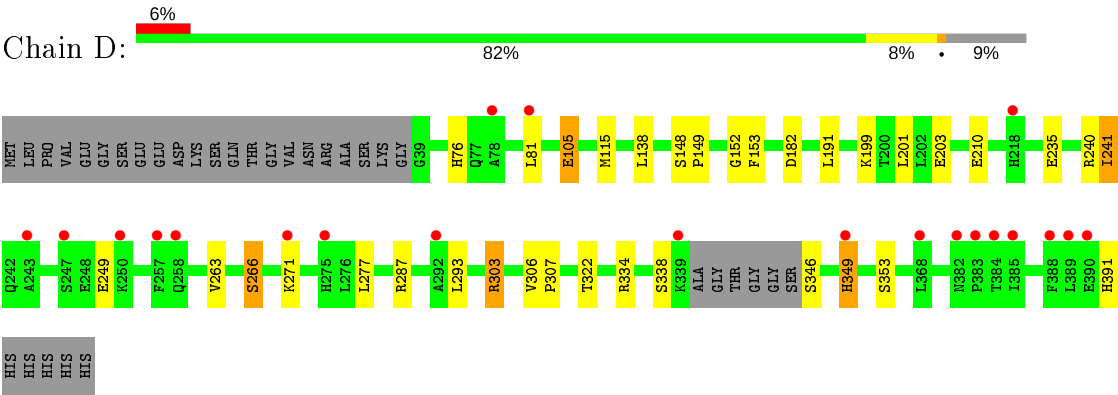
• Molecule 1: Tryptophan 2,3-dioxygenase



• Molecule 1: Tryptophan 2,3-dioxygenase



● Molecule 1: Tryptophan 2,3-dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	144.19Å 154.04Å 87.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 2.40 29.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.90-2.40) 99.9 (29.90-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.191 , 0.237 0.196 , 0.237	Depositor DCC
R_{free} test set	3776 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12156	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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, H7S

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	0.72	0/3005	0.81	0/4048
1	B	0.70	0/2910	0.81	0/3918
1	C	0.71	0/2814	0.81	0/3794
1	D	0.71	0/2973	0.81	0/4007
All	All	0.71	0/11702	0.81	0/15767

There are no bond length outliers.

There are no bond angle outliers.

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	2936	0	2899	29	0
1	B	2846	0	2808	18	0
1	C	2749	0	2709	26	0
1	D	2905	0	2858	20	0
2	A	43	0	30	6	0
2	B	43	0	30	3	0
2	C	43	0	30	4	0
2	D	43	0	30	5	0
3	A	34	0	0	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	34	0	0	2	0
3	C	34	0	0	1	0
3	D	34	0	0	1	0
4	A	114	0	0	2	0
4	B	111	0	0	1	0
4	C	80	0	0	0	0
4	D	107	0	0	2	0
All	All	12156	0	11394	92	0

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

All (92) 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)
2:B:401:HEM:HHH	2:B:401:HEM:HBC2	1.74	0.70
2:A:401:HEM:HMB2	2:A:401:HEM:HBB2	1.75	0.69
1:A:150:ALA:HA	1:A:154:GLN:HE22	1.60	0.66
1:D:303:ARG:HH22	3:D:403:H7S:C5	2.13	0.61
1:D:346:SER:OG	1:D:349:HIS:HB2	2.00	0.60
1:C:181:ARG:HD3	1:C:192:LEU:HD12	1.84	0.60
2:A:401:HEM:HBC2	2:A:401:HEM:HHH	1.83	0.60
2:C:401:HEM:HMB1	2:C:401:HEM:HBB2	1.84	0.59
1:A:245:GLU:O	1:A:247:SER:N	2.36	0.57
2:C:401:HEM:HHH	2:C:401:HEM:HBC2	1.87	0.56
1:B:151:SER:HB2	3:B:402:H7S:O7	2.06	0.55
1:C:223:TRP:CG	1:C:290:GLN:NE2	2.75	0.55
2:B:401:HEM:HBB2	2:B:401:HEM:HHH	1.89	0.54
1:C:223:TRP:CD1	1:C:290:GLN:NE2	2.76	0.54
1:A:326:TYR:OH	1:C:322:THR:CG2	2.56	0.54
1:C:180:TYR:CE1	1:C:192:LEU:HD11	2.43	0.53
1:D:263:VAL:O	1:D:266:SER:HB2	2.09	0.52
1:A:176:ASN:ND2	1:A:350:TYR:OH	2.45	0.50
2:D:401:HEM:HBC2	2:D:401:HEM:HHH	1.93	0.50
1:A:151:SER:HB2	3:A:402:H7S:O7	2.10	0.50
1:A:334:ARG:HD2	4:A:559:HOH:O	2.11	0.50
1:C:151:SER:HB2	3:C:402:H7S:O7	2.11	0.50
1:D:263:VAL:O	1:D:266:SER:CB	2.60	0.49
1:A:115:MET:HE2	1:A:201:LEU:HD21	1.95	0.49
2:C:401:HEM:CMB	2:C:401:HEM:HBB2	2.43	0.49
1:C:140:PHE:CE2	1:C:144:ARG:HD3	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:365:LEU:HA	1:C:368:LEU:HD12	1.94	0.49
1:B:326:TYR:OH	1:D:322:THR:HG22	2.12	0.49
1:C:76:HIS:NE2	2:C:401:HEM:C2C	2.80	0.49
1:A:150:ALA:HA	1:A:154:GLN:NE2	2.27	0.49
1:B:301:GLU:OE1	1:C:106:ARG:NH1	2.46	0.48
1:A:76:HIS:NE2	2:A:401:HEM:C2C	2.81	0.48
2:A:401:HEM:CMB	2:A:401:HEM:HBB2	2.43	0.48
1:C:362:PHE:HB3	1:C:365:LEU:HD12	1.96	0.48
1:B:168:LEU:HD12	1:B:171:MET:HE3	1.95	0.48
1:D:210:GLU:HG2	1:D:287:ARG:HG2	1.96	0.47
1:B:181:ARG:NH1	1:B:193:LEU:HD11	2.29	0.47
1:D:306:VAL:N	1:D:307:PRO:CD	2.78	0.47
2:D:401:HEM:HBB2	2:D:401:HEM:HMB1	1.97	0.47
1:A:105:GLU:OE2	3:A:403:H7S:O6	2.33	0.47
1:C:181:ARG:CD	1:C:192:LEU:HD12	2.44	0.46
1:A:248:GLU:O	1:A:252:GLU:HG2	2.15	0.46
1:A:152:GLY:HA3	2:A:401:HEM:C1D	2.50	0.46
1:C:363:VAL:HG22	1:C:367:ASN:ND2	2.30	0.46
1:B:106:ARG:HB3	1:B:106:ARG:CZ	2.46	0.45
1:A:326:TYR:OH	1:C:322:THR:HG22	2.16	0.45
1:B:326:TYR:OH	1:D:322:THR:CG2	2.65	0.45
2:D:401:HEM:CMB	2:D:401:HEM:HBB2	2.47	0.45
1:A:277:LEU:HD12	1:A:277:LEU:HA	1.89	0.45
1:A:304:PHE:C	1:A:307:PRO:HD2	2.37	0.45
1:B:156:LEU:HD22	1:B:188:GLU:HG2	1.99	0.44
1:A:373:ILE:HD12	1:A:377:TRP:HB2	2.00	0.44
1:D:334:ARG:HD2	4:D:578:HOH:O	2.19	0.43
1:C:180:TYR:HE1	1:C:192:LEU:HD11	1.83	0.43
1:C:81:LEU:HD12	1:D:81:LEU:HD12	2.00	0.43
1:A:303:ARG:HG3	1:D:391:HIS:CB	2.49	0.43
1:C:257:PHE:CD1	1:C:257:PHE:C	2.91	0.43
1:C:333:HIS:HB2	1:C:348:TYR:CE1	2.53	0.43
1:C:148:SER:HA	1:C:149:PRO:HA	1.70	0.42
1:A:182:ASP:OD1	1:A:183:ASN:N	2.52	0.42
1:B:319:SER:O	1:B:322:THR:HG22	2.20	0.42
1:B:244:LYS:HB2	1:B:250:LYS:HD2	2.00	0.42
1:B:132:LEU:CD2	2:B:401:HEM:HBB2	2.49	0.42
1:B:181:ARG:CZ	1:B:193:LEU:HD11	2.50	0.42
1:B:199:LYS:HA	1:B:203:GLU:OE1	2.20	0.42
1:C:303:ARG:HD3	1:C:389:LEU:HA	2.01	0.42
1:A:176:ASN:O	1:A:180:TYR:HB3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:ILE:HD13	1:D:241:ILE:HA	1.89	0.42
1:A:244:LYS:HB2	1:A:250:LYS:HD2	2.01	0.41
1:A:322:THR:HG21	1:C:326:TYR:OH	2.20	0.41
1:D:235:GLU:HA	4:D:592:HOH:O	2.20	0.41
1:A:124:LEU:HD22	1:B:131:ILE:CD1	2.50	0.41
1:B:168:LEU:HB2	1:B:171:MET:HG3	2.02	0.41
1:D:76:HIS:NE2	2:D:401:HEM:C2C	2.89	0.41
1:C:301:GLU:O	1:C:302:PRO:C	2.59	0.41
1:A:98:GLN:HG3	1:A:204:LEU:HD21	2.03	0.41
1:B:199:LYS:HE2	4:B:605:HOH:O	2.20	0.41
1:D:199:LYS:HA	1:D:203:GLU:OE2	2.20	0.41
1:D:293:LEU:HD12	1:D:293:LEU:HA	1.91	0.41
1:D:115:MET:HE2	1:D:201:LEU:HD21	2.01	0.41
1:A:171:MET:HG3	4:A:579:HOH:O	2.21	0.40
1:C:201:LEU:O	1:C:205:VAL:HG23	2.21	0.40
1:C:287:ARG:O	1:C:290:GLN:HB2	2.21	0.40
1:D:191:LEU:HD12	1:D:191:LEU:HA	1.95	0.40
1:A:302:PRO:HG3	1:D:105:GLU:HG3	2.03	0.40
1:A:79:TYR:CD2	2:A:401:HEM:HAC	2.56	0.40
1:B:103:ARG:HA	3:B:403:H7S:N3	2.37	0.40
1:A:326:TYR:OH	1:C:322:THR:HG21	2.21	0.40
1:A:220:PHE:O	1:A:225:LYS:NZ	2.48	0.40
1:D:152:GLY:HA3	2:D:401:HEM:C1D	2.57	0.40
1:A:370:THR:HA	1:C:339:LYS:HG3	2.04	0.40
1:B:294:MET:HE2	1:B:294:MET:HB2	1.96	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	349/380 (92%)	338 (97%)	10 (3%)	1 (0%)	41 55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	338/380 (89%)	328 (97%)	10 (3%)	0	100	100
1	C	326/380 (86%)	302 (93%)	24 (7%)	0	100	100
1	D	343/380 (90%)	334 (97%)	9 (3%)	0	100	100
All	All	1356/1520 (89%)	1302 (96%)	53 (4%)	1 (0%)	51	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	GLU

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	318/348 (91%)	307 (96%)	11 (4%)	36	55
1	B	307/348 (88%)	302 (98%)	5 (2%)	62	79
1	C	296/348 (85%)	288 (97%)	8 (3%)	44	65
1	D	313/348 (90%)	297 (95%)	16 (5%)	24	39
All	All	1234/1392 (89%)	1194 (97%)	40 (3%)	39	59

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	GLU
1	A	148	SER
1	A	153	PHE
1	A	173	VAL
1	A	180	TYR
1	A	245	GLU
1	A	254	VAL
1	A	274	GLU
1	A	352	ARG
1	A	381	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	384	THR
1	B	147	LEU
1	B	148	SER
1	B	249	GLU
1	B	293	LEU
1	B	313	SER
1	C	64	ASN
1	C	106	ARG
1	C	113	SER
1	C	192	LEU
1	C	235	GLU
1	C	256	GLU
1	C	257	PHE
1	C	375	ARG
1	D	105	GLU
1	D	138	LEU
1	D	148	SER
1	D	149	PRO
1	D	153	PHE
1	D	182	ASP
1	D	240	ARG
1	D	241	ILE
1	D	249	GLU
1	D	266	SER
1	D	271	LYS
1	D	277	LEU
1	D	303	ARG
1	D	338	SER
1	D	349	HIS
1	D	353	SER

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

Mol	Chain	Res	Type
1	A	170	ASN
1	A	386	HIS
1	D	44	ASN

5.3.3 RNA ⓘ

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 carbohydrates 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	$\# Z > 2$
3	H7S	C	402	-	17,19,19	2.24	5 (29%)	19,28,28	2.18	7 (36%)
3	H7S	C	403	-	17,19,19	2.50	5 (29%)	19,28,28	1.45	3 (15%)
3	H7S	D	402	-	17,19,19	1.91	3 (17%)	19,28,28	2.38	9 (47%)
2	HEM	D	401	1	27,50,50	0.83	0	17,82,82	1.95	4 (23%)
3	H7S	A	403	-	17,19,19	2.75	6 (35%)	19,28,28	2.16	3 (15%)
2	HEM	B	401	1	27,50,50	1.07	2 (7%)	17,82,82	2.20	5 (29%)
2	HEM	A	401	1	27,50,50	0.96	2 (7%)	17,82,82	1.88	4 (23%)
3	H7S	B	403	-	17,19,19	2.31	7 (41%)	19,28,28	2.21	4 (21%)
3	H7S	D	403	-	17,19,19	2.41	4 (23%)	19,28,28	1.48	3 (15%)
3	H7S	B	402	-	17,19,19	2.04	6 (35%)	19,28,28	2.29	8 (42%)
2	HEM	C	401	1	27,50,50	0.98	1 (3%)	17,82,82	2.13	3 (17%)
3	H7S	A	402	-	17,19,19	2.19	6 (35%)	19,28,28	1.90	5 (26%)

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	H7S	C	402	-	-	0/0/16/16	0/3/3/3
3	H7S	C	403	-	-	0/0/16/16	0/3/3/3
3	H7S	D	402	-	-	0/0/16/16	0/3/3/3
2	HEM	D	401	1	-	0/6/54/54	-
3	H7S	A	403	-	-	0/0/16/16	0/3/3/3
2	HEM	B	401	1	-	0/6/54/54	-
2	HEM	A	401	1	-	0/6/54/54	-
3	H7S	B	403	-	-	0/0/16/16	0/3/3/3
3	H7S	D	403	-	-	0/0/16/16	0/3/3/3
3	H7S	B	402	-	-	0/0/16/16	0/3/3/3
2	HEM	C	401	1	-	0/6/54/54	-
3	H7S	A	402	-	-	0/0/16/16	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	403	H7S	CG-CD2	7.85	1.49	1.40
3	A	403	H7S	CG-CD2	7.72	1.49	1.40
3	C	403	H7S	CG-CD2	7.17	1.48	1.40
3	C	402	H7S	CG-CD2	6.19	1.47	1.40
3	B	403	H7S	CG-CD2	5.56	1.47	1.40
3	D	402	H7S	CG-CD2	5.47	1.46	1.40
3	A	402	H7S	CG-CD2	5.18	1.46	1.40
3	B	402	H7S	CG-CD2	4.70	1.46	1.40
3	C	403	H7S	C2-N3	-4.41	1.31	1.37
3	A	403	H7S	C2-N3	-4.30	1.32	1.37
3	A	402	H7S	C4-N3	-4.26	1.31	1.37
3	C	402	H7S	C4-N3	-3.93	1.31	1.37
3	B	403	H7S	C2-N3	-3.90	1.32	1.37
2	B	401	HEM	C3B-C2B	-3.90	1.35	1.40
3	B	402	H7S	C4-N3	-3.70	1.31	1.37
3	A	403	H7S	C4-N3	-3.62	1.32	1.37
3	B	403	H7S	C5-C1	-3.50	1.50	1.54
3	C	403	H7S	C4-N3	-3.49	1.32	1.37
3	A	402	H7S	C2-N3	-3.34	1.33	1.37
3	A	403	H7S	C5-C1	-3.29	1.51	1.54
3	B	402	H7S	C2-N3	-3.14	1.33	1.37
3	C	402	H7S	C2-N3	-2.97	1.33	1.37
3	A	403	H7S	CE3-CD2	-2.88	1.36	1.42
3	D	403	H7S	C4-N3	-2.83	1.33	1.37
3	B	403	H7S	CZ2-CE2	-2.81	1.37	1.41
3	B	403	H7S	CE3-CD2	-2.73	1.36	1.42
3	D	403	H7S	C5-C1	-2.69	1.51	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	H7S	CE3-CD2	-2.58	1.37	1.42
3	D	402	H7S	C4-N3	-2.53	1.33	1.37
3	C	403	H7S	CZ2-CE2	-2.48	1.37	1.41
3	A	402	H7S	CE3-CZ3	2.39	1.40	1.36
3	D	403	H7S	C2-N3	-2.35	1.34	1.37
2	A	401	HEM	C3B-C2B	-2.31	1.37	1.40
3	C	403	H7S	CD2-CE2	2.27	1.48	1.42
2	C	401	HEM	C4D-C3D	2.23	1.47	1.42
3	A	402	H7S	CE3-CD2	-2.22	1.37	1.42
3	A	402	H7S	CD2-CE2	2.21	1.48	1.42
3	B	402	H7S	CD2-CE2	2.21	1.48	1.42
3	B	403	H7S	C4-N3	-2.20	1.34	1.37
2	B	401	HEM	C1A-NA	2.17	1.40	1.36
2	A	401	HEM	C4D-C3D	2.17	1.47	1.42
3	C	402	H7S	CE3-CD2	-2.15	1.37	1.42
3	A	403	H7S	CZ2-CE2	-2.09	1.38	1.41
3	B	403	H7S	CE2-NE1	-2.09	1.32	1.38
3	B	402	H7S	CE3-CD2	-2.02	1.38	1.42
3	C	402	H7S	C5-C4	2.02	1.53	1.51
3	B	402	H7S	CE3-CZ3	2.01	1.39	1.36

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	H7S	C1-C5-C4	-7.91	99.06	105.58
2	C	401	HEM	CBD-CAD-C3D	-7.46	98.74	112.48
3	A	403	H7S	C1-C5-C4	-6.68	100.08	105.58
2	B	401	HEM	CBD-CAD-C3D	-6.16	101.13	112.48
2	D	401	HEM	CBD-CAD-C3D	-5.36	102.60	112.48
2	A	401	HEM	CBD-CAD-C3D	-5.12	103.04	112.48
3	B	402	H7S	CG-CD2-CE2	-4.78	101.85	106.83
3	C	403	H7S	CG-CD2-CE2	-4.70	101.94	106.83
3	C	402	H7S	CG-CD2-CE2	-4.50	102.15	106.83
3	B	402	H7S	C5-C1-C2	-4.42	101.48	103.64
3	C	402	H7S	C5-C1-C2	-4.35	101.51	103.64
3	A	402	H7S	CG-CD2-CE2	-4.32	102.33	106.83
3	D	402	H7S	C5-C1-C2	-4.08	101.64	103.64
3	D	402	H7S	CG-CD2-CE2	-4.07	102.60	106.83
3	A	403	H7S	C5-C1-C2	-4.04	101.66	103.64
3	D	403	H7S	CG-CD2-CE2	-4.04	102.63	106.83
3	A	402	H7S	C1-C5-C4	-3.99	102.29	105.58
3	D	402	H7S	O6-C4-C5	-3.78	121.41	126.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	403	H7S	CG-CD2-CE2	-3.51	103.18	106.83
3	D	402	H7S	CE3-CD2-CE2	3.45	122.98	118.26
3	C	402	H7S	C1-C5-C4	-3.37	102.80	105.58
3	B	402	H7S	C1-C5-C4	-3.36	102.81	105.58
3	B	402	H7S	CZ2-CH2-CZ3	3.34	122.57	118.74
2	D	401	HEM	CBA-CAA-C2A	-3.30	106.39	112.49
2	B	401	HEM	C1D-C2D-C3D	-3.28	104.72	107.00
3	C	402	H7S	CZ3-CE3-CD2	-3.27	116.24	118.80
2	A	401	HEM	CAD-CBD-CGD	3.26	118.14	112.67
3	D	402	H7S	O6-C4-N3	3.25	129.37	125.00
3	D	402	H7S	CZ3-CE3-CD2	-3.21	116.28	118.80
2	B	401	HEM	CAD-CBD-CGD	3.21	118.06	112.67
2	D	401	HEM	CAD-CBD-CGD	3.03	117.75	112.67
3	D	402	H7S	CG-C1-C2	3.01	119.94	112.14
3	A	402	H7S	C5-C1-C2	-2.96	102.19	103.64
3	A	402	H7S	CE3-CD2-CE2	2.96	122.30	118.26
3	D	403	H7S	O7-C2-N3	2.91	128.46	124.94
3	B	402	H7S	CZ3-CE3-CD2	-2.79	116.62	118.80
3	B	402	H7S	CE3-CD2-CE2	2.76	122.03	118.26
3	B	403	H7S	C5-C1-CG	-2.73	109.47	115.14
3	C	402	H7S	CE3-CD2-CE2	2.72	121.98	118.26
3	B	403	H7S	CG-CD2-CE2	-2.70	104.02	106.83
2	A	401	HEM	C3C-C4C-NC	-2.56	106.12	110.94
3	B	402	H7S	C5-C1-CG	2.55	120.46	115.14
3	B	403	H7S	O6-C4-C5	-2.44	123.18	126.39
3	A	402	H7S	CZ3-CE3-CD2	-2.43	116.89	118.80
2	C	401	HEM	CAD-CBD-CGD	2.39	116.69	112.67
2	C	401	HEM	CBA-CAA-C2A	-2.37	108.11	112.49
3	C	402	H7S	CZ2-CH2-CZ3	2.36	121.44	118.74
3	D	403	H7S	C1-C5-C4	-2.35	103.64	105.58
2	A	401	HEM	CMA-C3A-C4A	-2.35	124.86	128.46
3	D	402	H7S	C5-C1-CG	-2.31	110.34	115.14
3	C	402	H7S	C5-C1-CG	2.29	119.92	115.14
2	B	401	HEM	C3B-C4B-NB	-2.28	106.27	109.21
3	B	402	H7S	CH2-CZ2-CE2	-2.25	118.01	120.84
3	C	403	H7S	C1-C5-C4	-2.20	103.77	105.58
2	B	401	HEM	CMA-C3A-C4A	-2.10	125.23	128.46
3	C	403	H7S	CZ2-CH2-CZ3	2.08	121.12	118.74
2	D	401	HEM	CMA-C3A-C4A	-2.03	125.34	128.46
3	D	402	H7S	O7-C2-N3	2.01	127.38	124.94

There are no chirality outliers.

There are no torsion outliers.

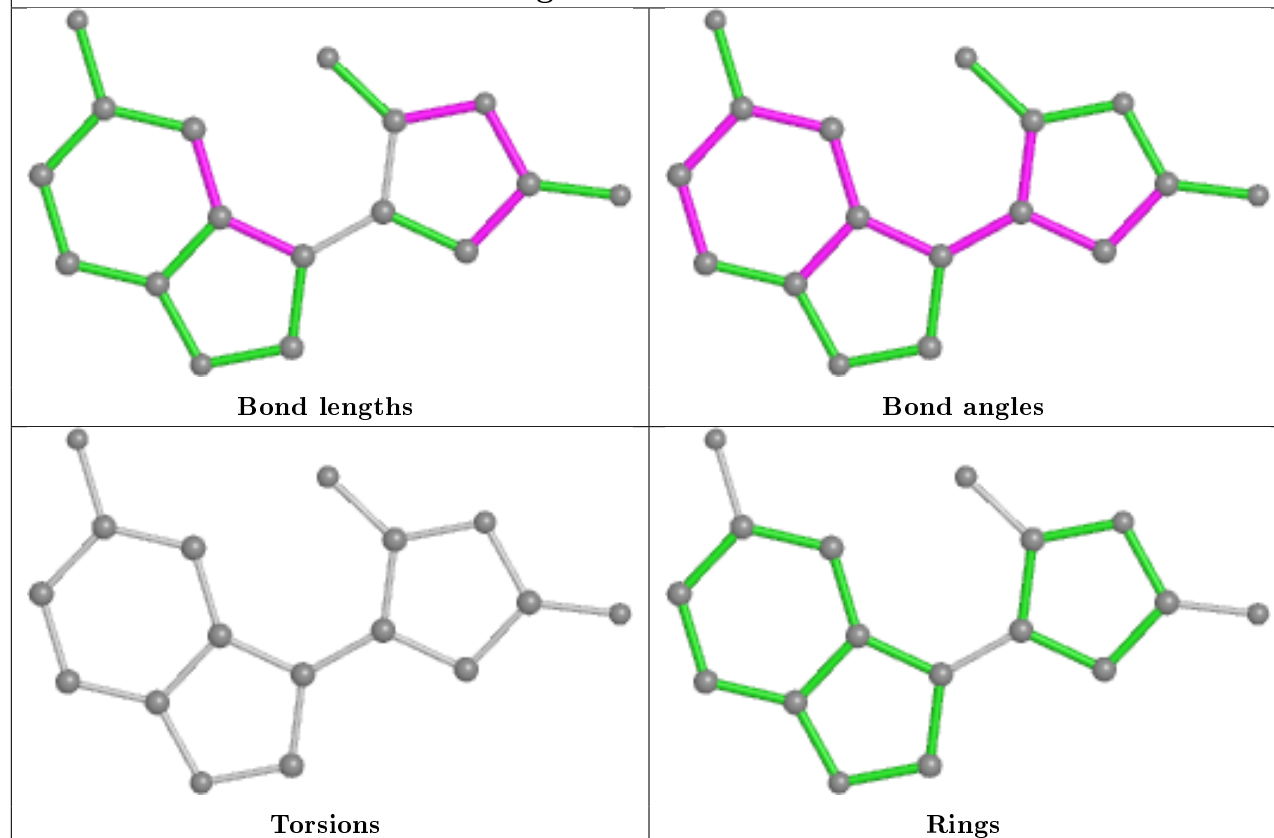
There are no ring outliers.

10 monomers are involved in 24 short contacts:

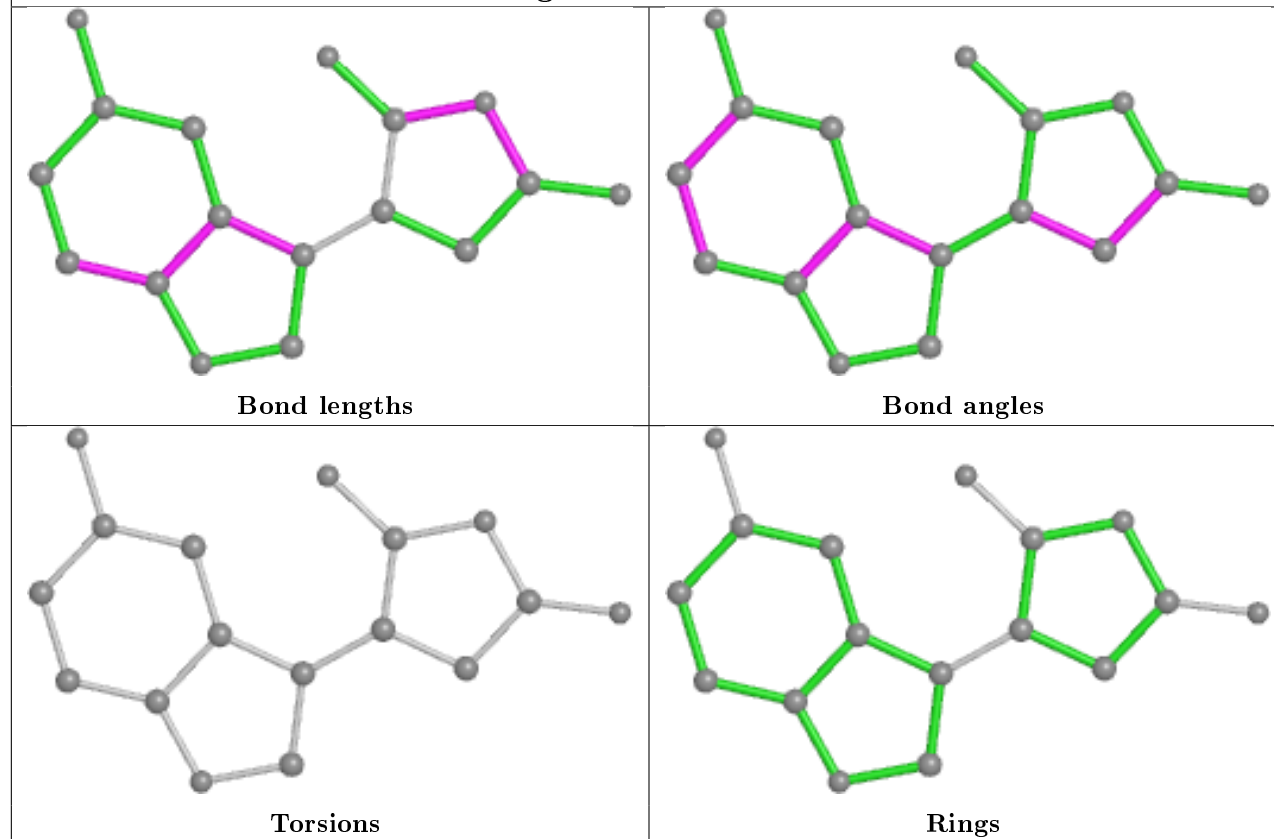
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	H7S	1	0
2	D	401	HEM	5	0
3	A	403	H7S	1	0
2	B	401	HEM	3	0
2	A	401	HEM	6	0
3	B	403	H7S	1	0
3	D	403	H7S	1	0
3	B	402	H7S	1	0
2	C	401	HEM	4	0
3	A	402	H7S	1	0

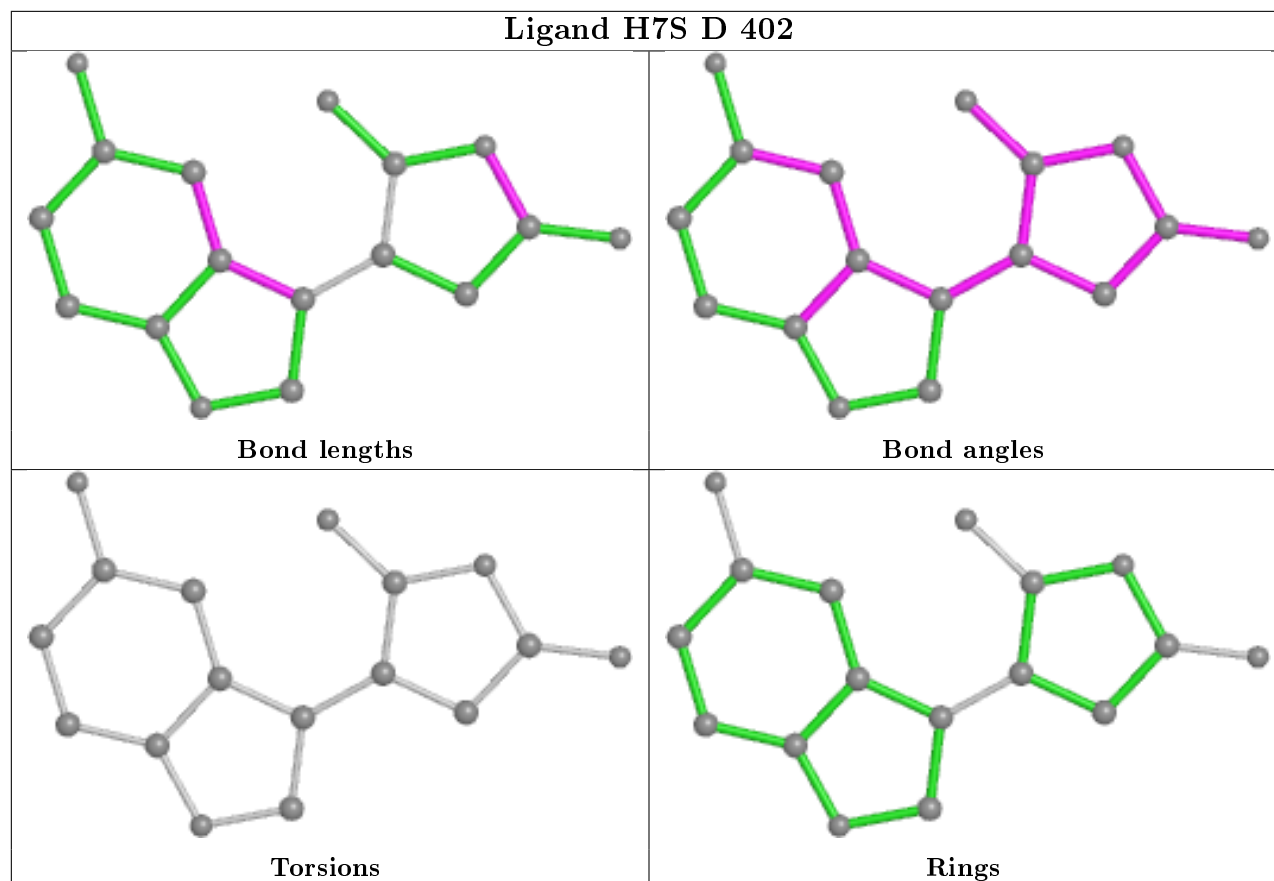
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

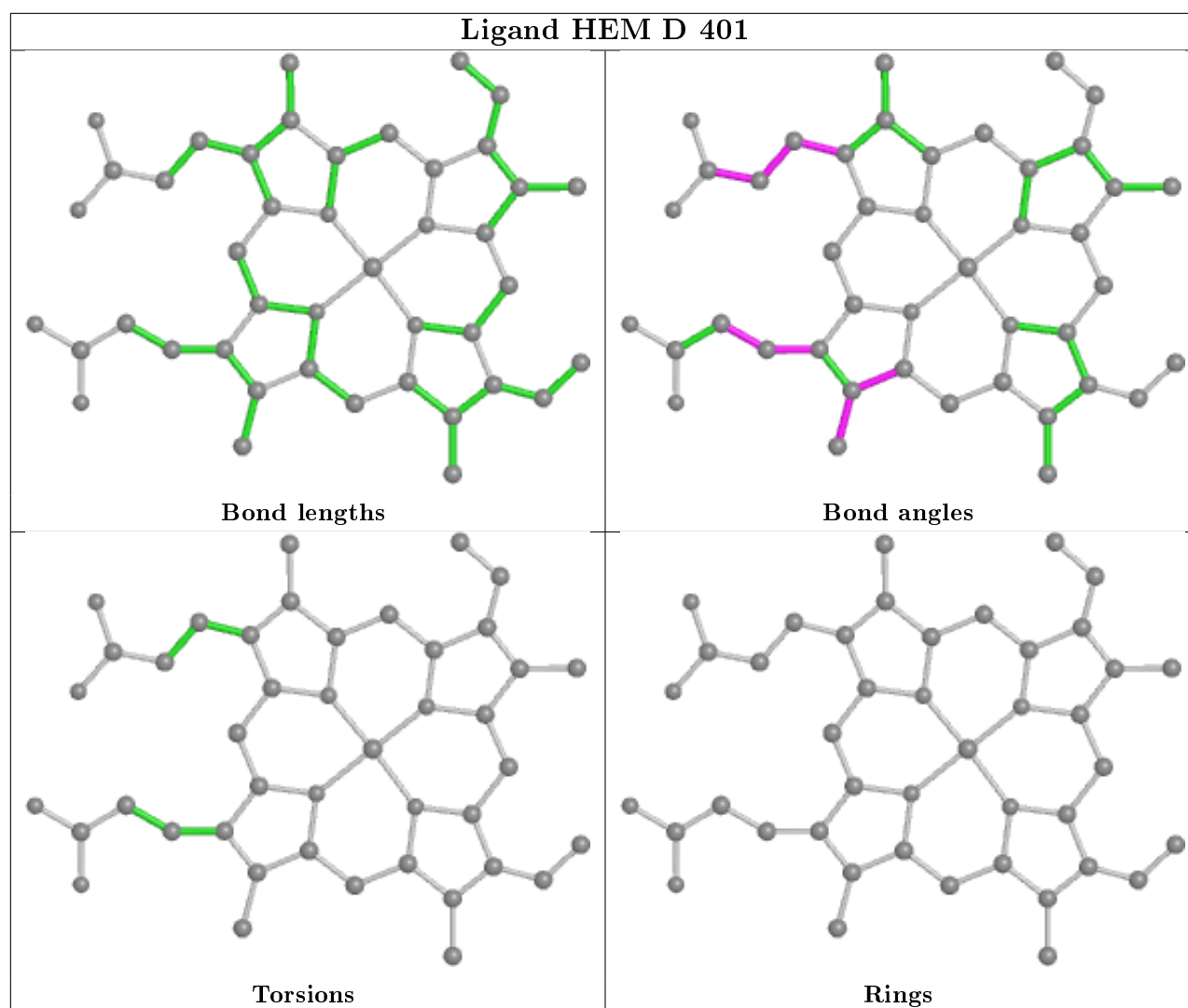
Ligand H7S C 402

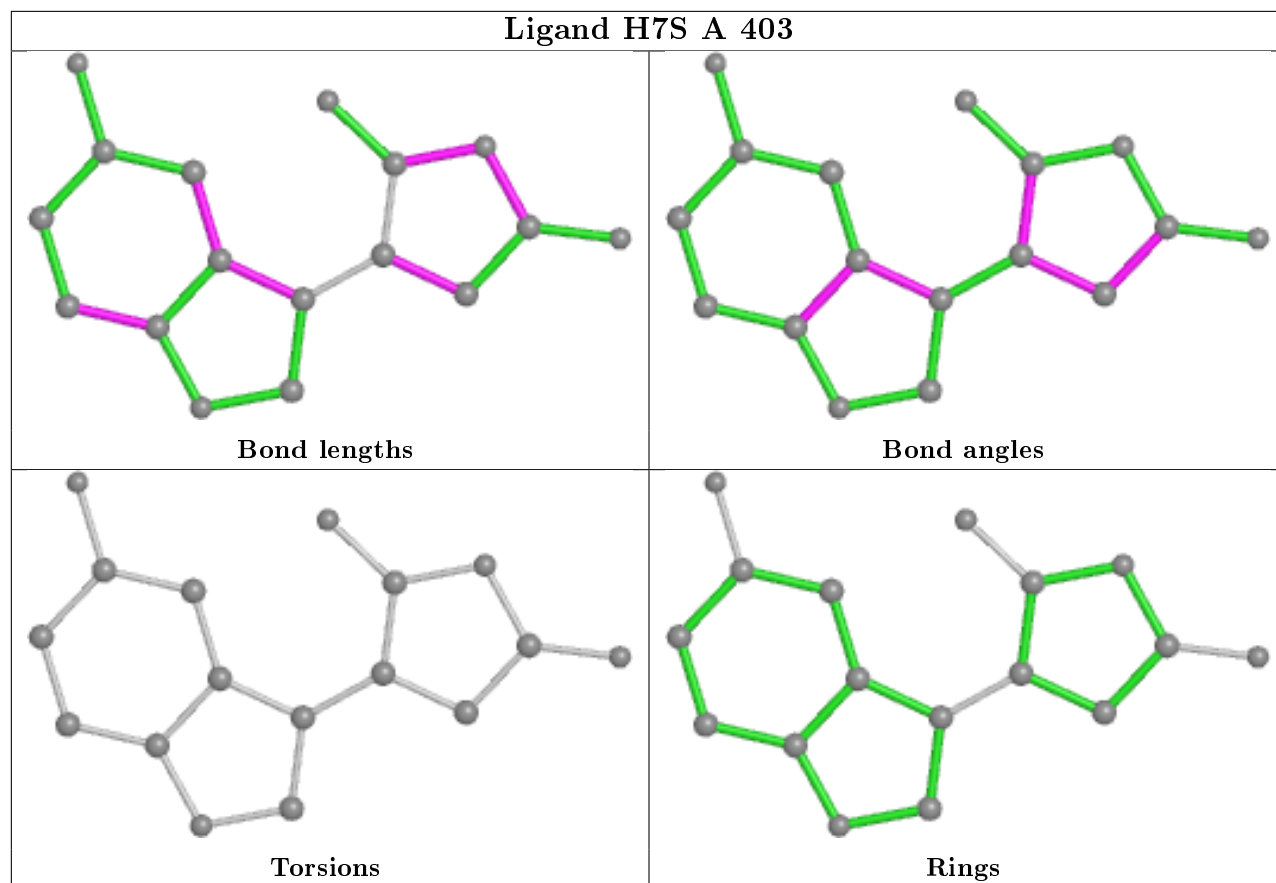


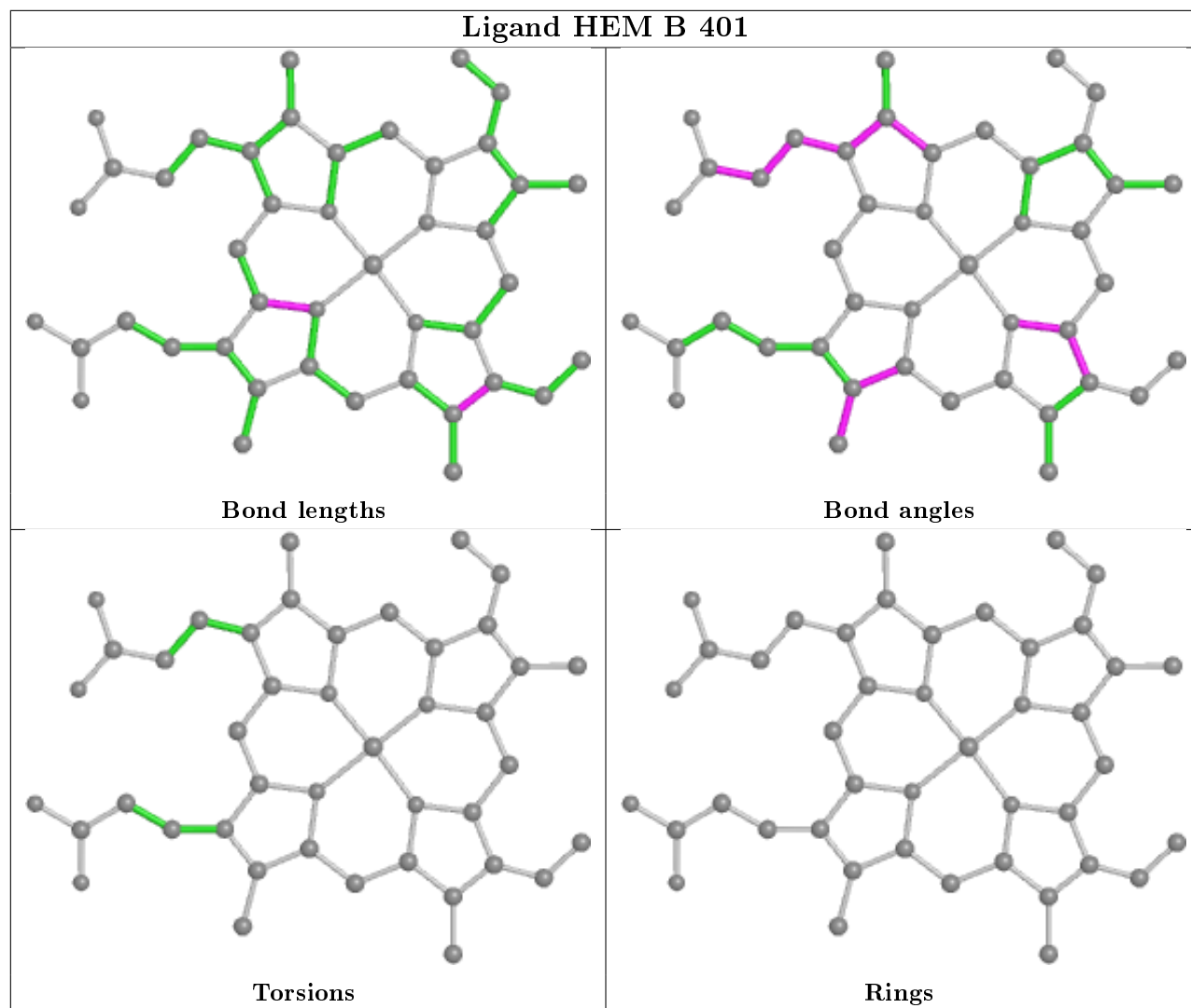
Ligand H7S C 403

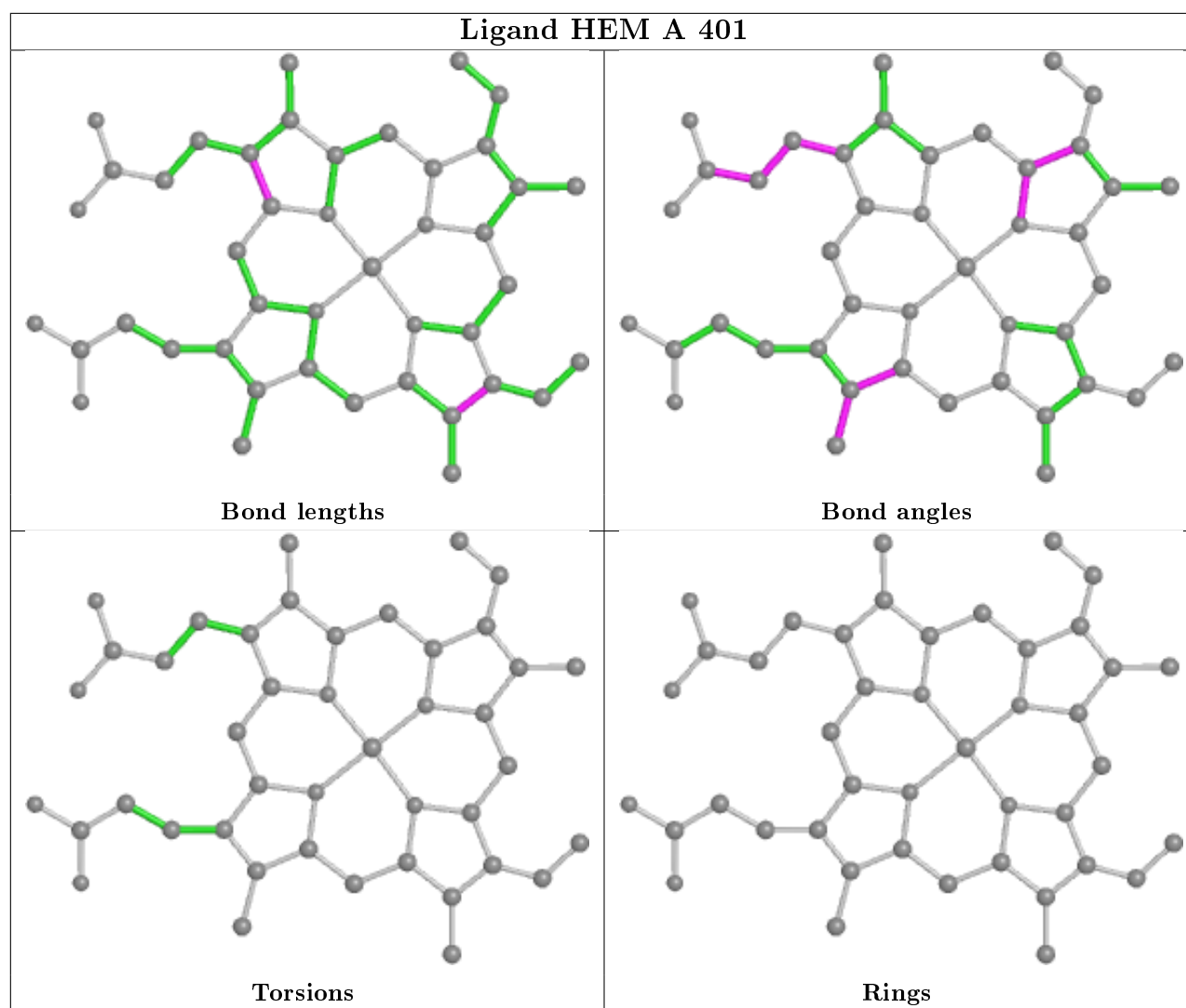




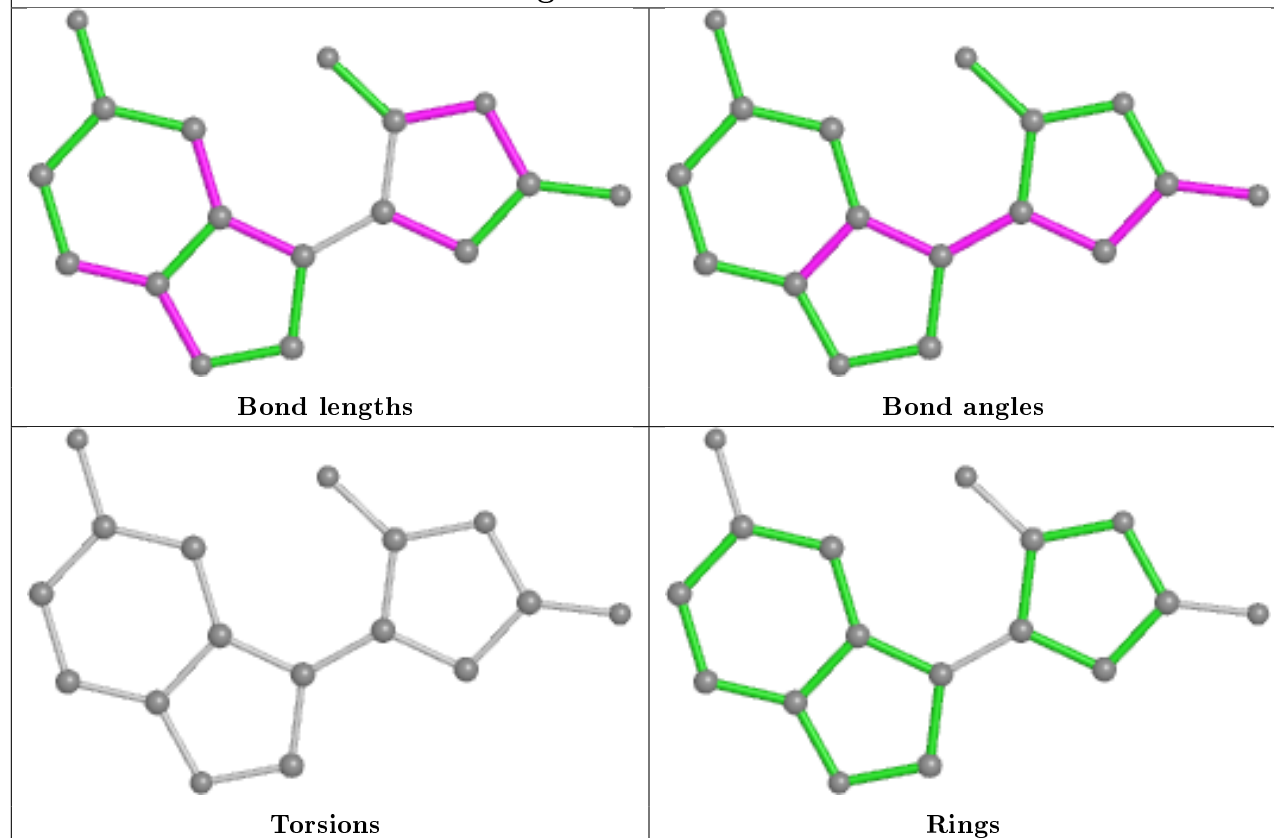




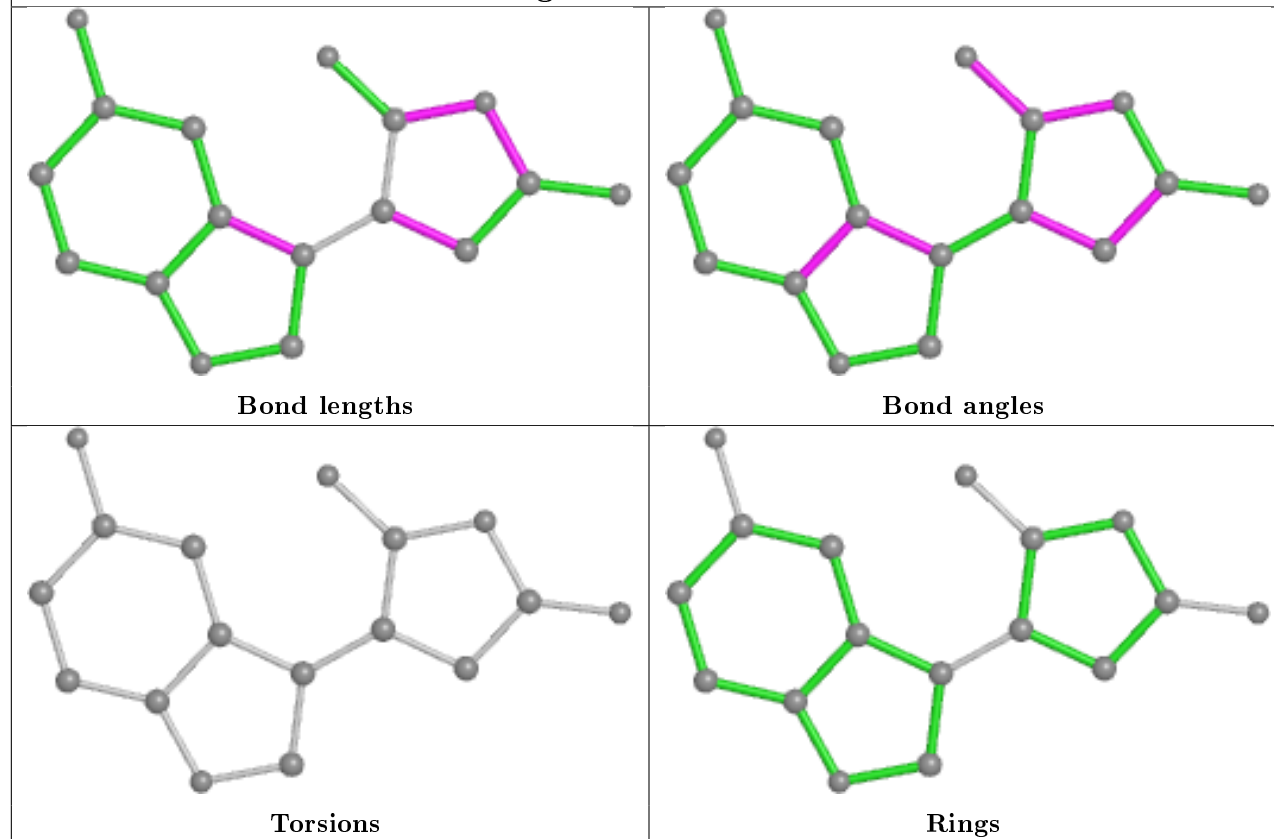


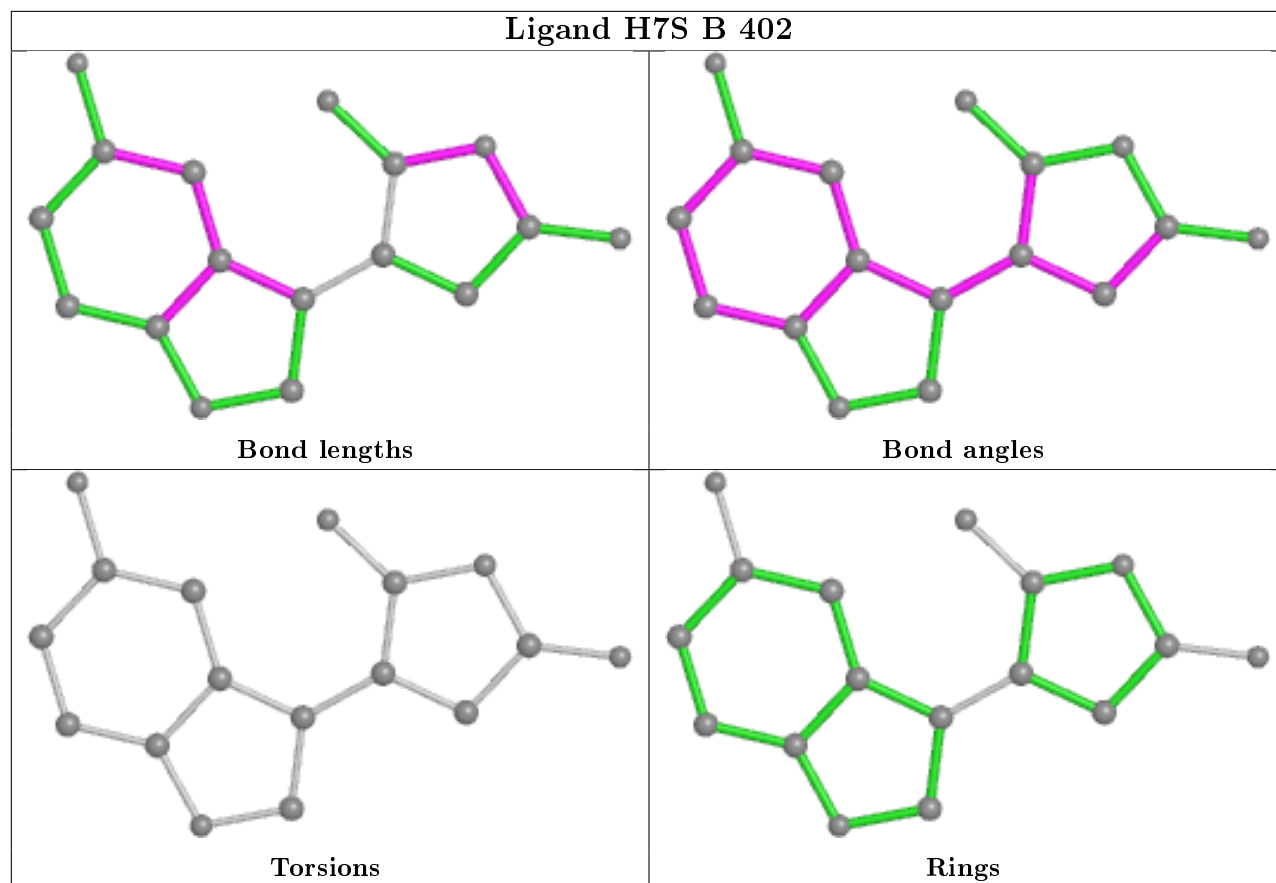


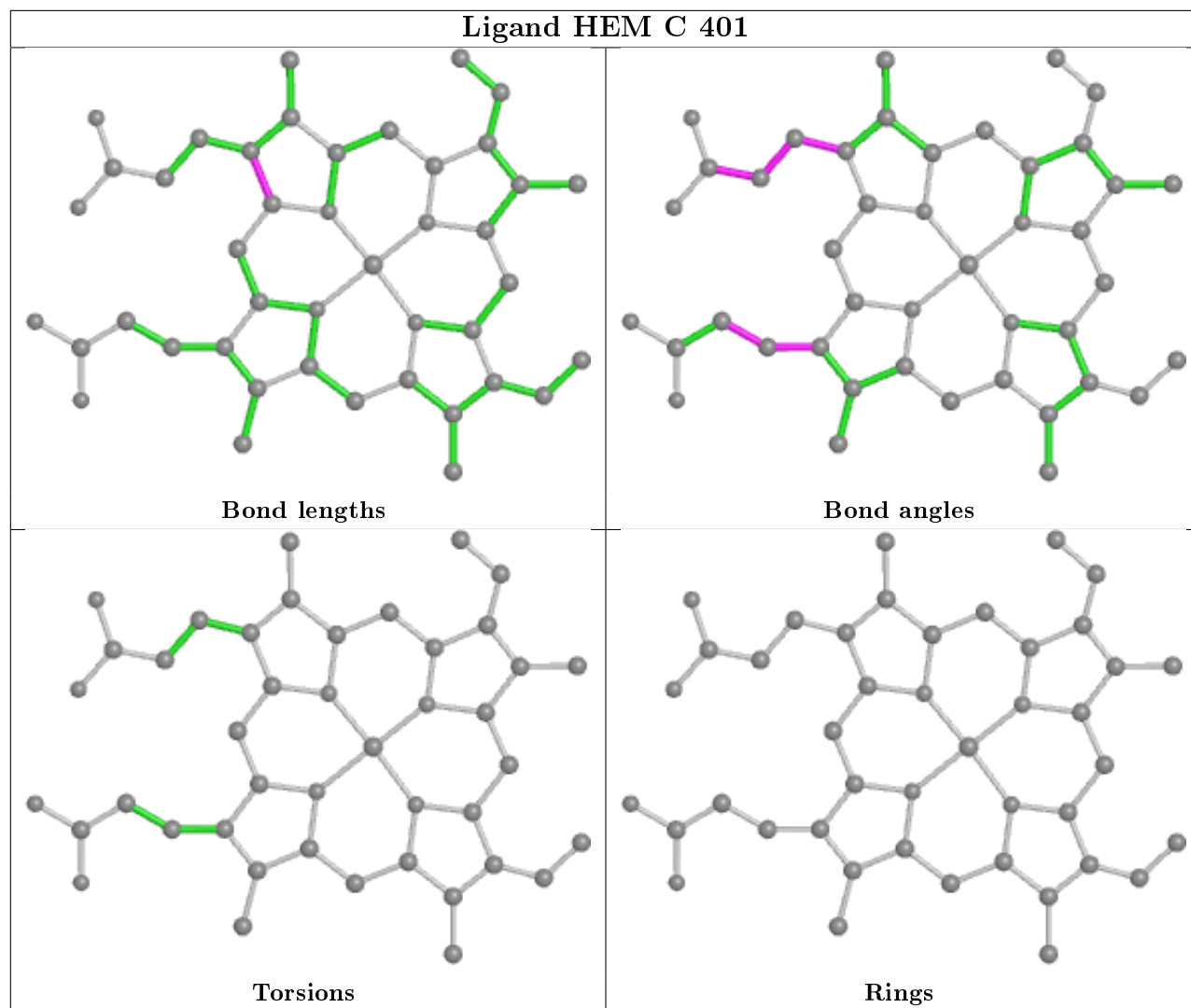
Ligand H7S B 403

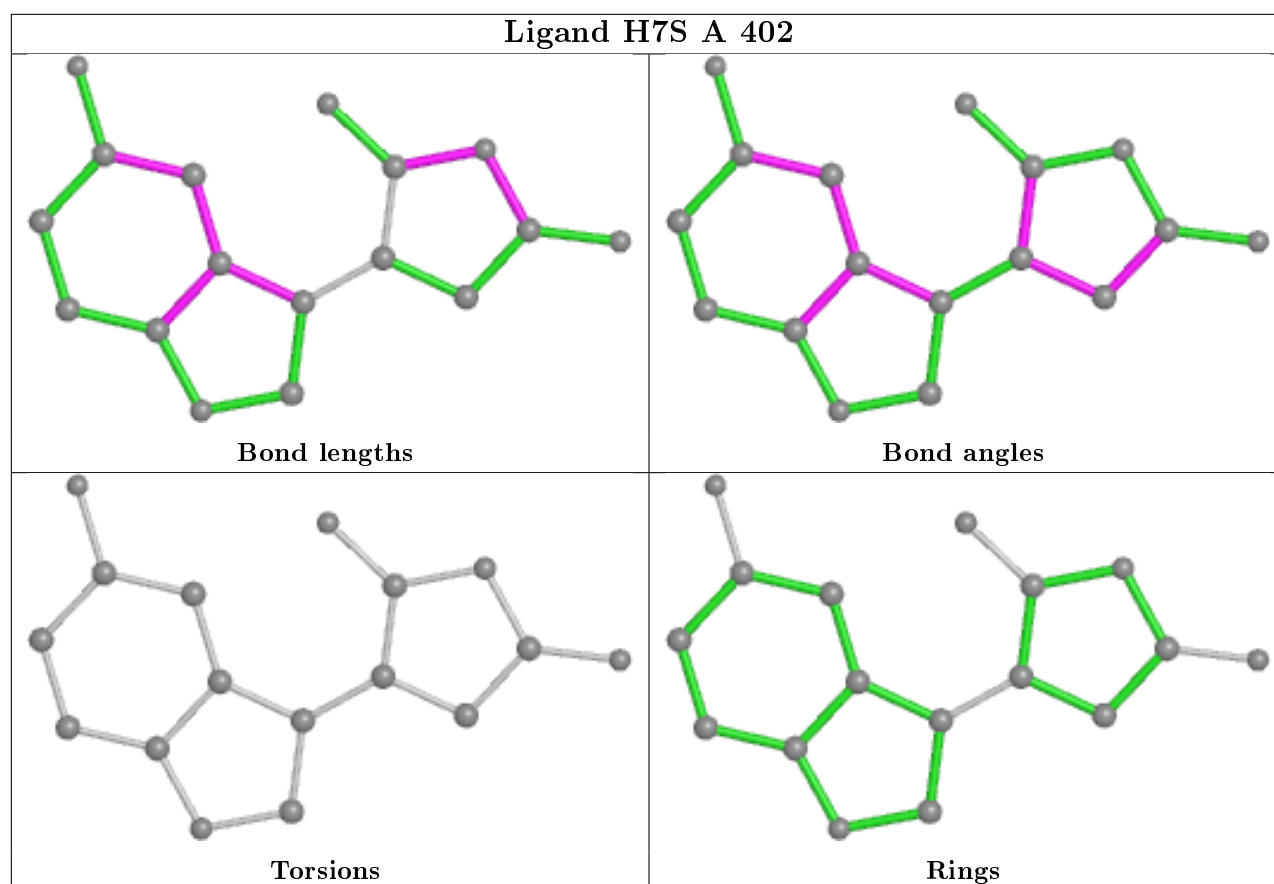


Ligand H7S D 403









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	351/380 (92%)	0.02	17 (4%) 30 29	32, 50, 102, 125	0
1	B	342/380 (90%)	-0.10	14 (4%) 37 36	29, 48, 95, 140	0
1	C	332/380 (87%)	0.09	24 (7%) 15 14	33, 58, 106, 161	0
1	D	347/380 (91%)	-0.02	21 (6%) 21 20	30, 52, 106, 145	0
All	All	1372/1520 (90%)	-0.00	76 (5%) 25 24	29, 52, 104, 161	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	218	HIS	6.1
1	D	384	THR	5.6
1	C	344	GLY	5.6
1	D	385	ILE	5.4
1	B	173	VAL	4.8
1	D	388	PHE	4.8
1	D	389	LEU	4.1
1	B	248	GLU	4.1
1	B	243	ALA	4.0
1	B	182	ASP	4.0
1	C	217	PRO	3.9
1	A	250	LYS	3.9
1	D	383	PRO	3.8
1	C	257	PHE	3.8
1	B	174	PRO	3.8
1	D	218	HIS	3.8
1	B	247	SER	3.7
1	B	38	GLY	3.6
1	C	340	ALA	3.5
1	B	244	LYS	3.4
1	C	179	HIS	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	39	GLY	3.3
1	A	255	ALA	3.3
1	C	385	ILE	3.2
1	A	252	GLU	3.2
1	C	383	PRO	3.2
1	B	245	GLU	3.1
1	C	382	ASN	3.0
1	D	243	ALA	3.0
1	A	384	THR	3.0
1	B	176	ASN	3.0
1	C	368	LEU	2.9
1	C	278	SER	2.9
1	A	343	GLY	2.8
1	A	177	ARG	2.8
1	A	245	GLU	2.8
1	D	257	PHE	2.8
1	D	250	LYS	2.7
1	D	382	ASN	2.7
1	D	292	ALA	2.7
1	D	247	SER	2.7
1	A	38	GLY	2.7
1	C	345	SER	2.7
1	C	63	GLY	2.7
1	C	271	LYS	2.6
1	D	390	GLU	2.6
1	B	180	TYR	2.5
1	A	64	ASN	2.5
1	A	344	GLY	2.5
1	D	78	ALA	2.4
1	B	218	HIS	2.4
1	C	254	VAL	2.4
1	C	386	HIS	2.4
1	C	387	LYS	2.4
1	C	256	GLU	2.4
1	B	181	ARG	2.4
1	C	343	GLY	2.3
1	D	368	LEU	2.3
1	A	63	GLY	2.3
1	D	275	HIS	2.3
1	A	248	GLU	2.3
1	D	271	LYS	2.3
1	A	385	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	349	HIS	2.3
1	D	81	LEU	2.2
1	C	230	ILE	2.2
1	A	244	LYS	2.2
1	C	384	THR	2.2
1	D	339	LYS	2.1
1	A	176	ASN	2.1
1	B	63	GLY	2.1
1	C	169	GLN	2.1
1	A	247	SER	2.1
1	C	189	ASN	2.1
1	D	258	GLN	2.0
1	A	383	PRO	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 carbohydrates 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	H7S	D	403	17/17	0.86	0.20	58,70,112,116	0
3	H7S	A	403	17/17	0.88	0.18	48,53,79,84	0
3	H7S	C	402	17/17	0.91	0.19	61,73,85,86	0
3	H7S	C	403	17/17	0.91	0.19	61,67,97,105	0
3	H7S	B	403	17/17	0.92	0.19	48,60,89,96	0
3	H7S	D	402	17/17	0.93	0.15	58,63,71,72	0
3	H7S	A	402	17/17	0.93	0.15	60,70,80,84	0
3	H7S	B	402	17/17	0.95	0.13	51,58,71,75	0
2	HEM	C	401	43/43	0.96	0.12	45,52,58,64	0
2	HEM	A	401	43/43	0.96	0.14	40,47,53,60	0

Continued on next page...

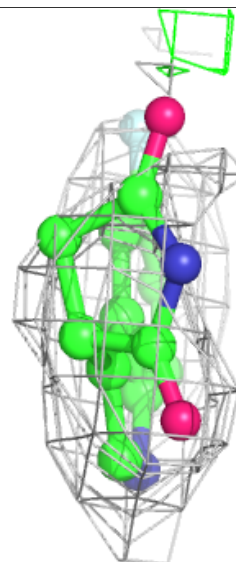
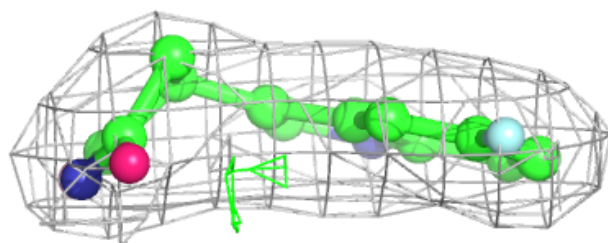
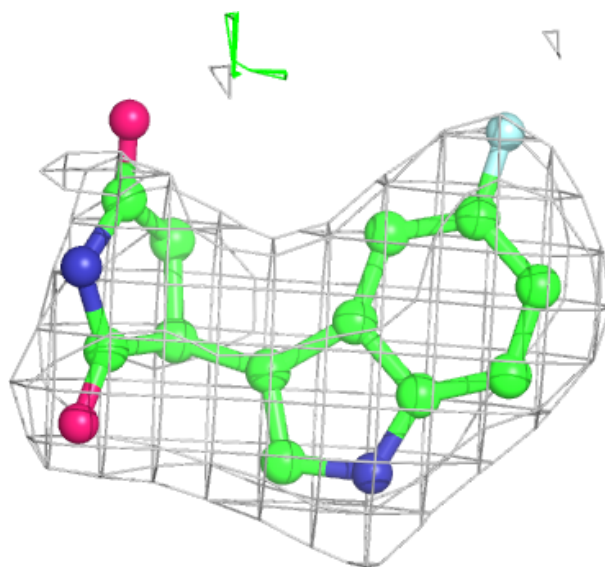
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HEM	D	401	43/43	0.97	0.11	37,42,56,71	0
2	HEM	B	401	43/43	0.97	0.12	37,43,51,55	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.

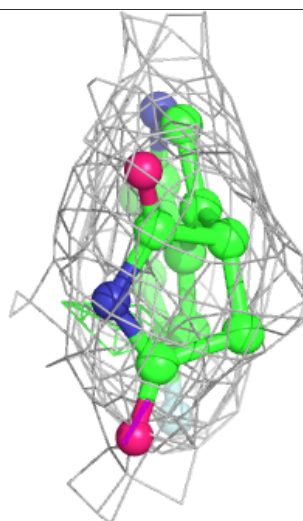
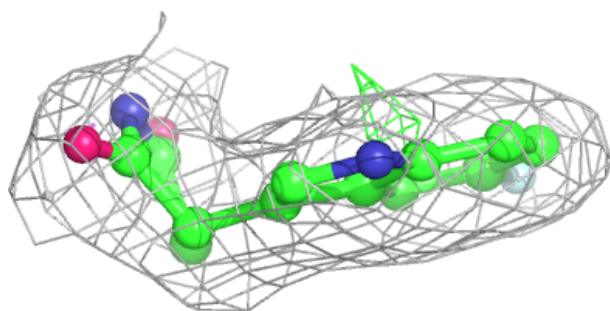
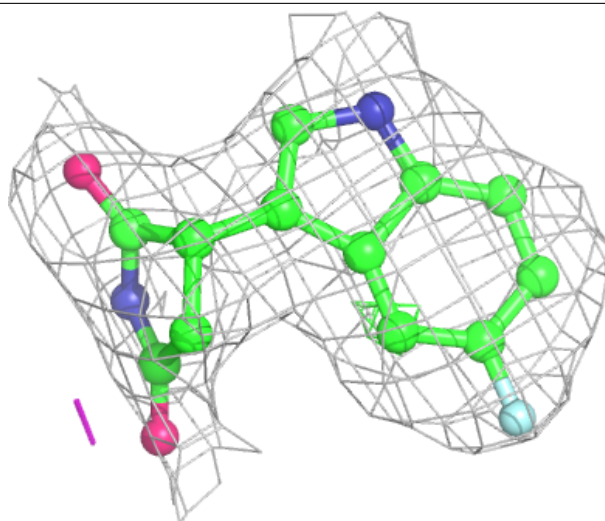
Electron density around H7S D 403:

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



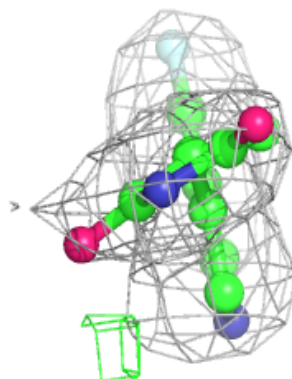
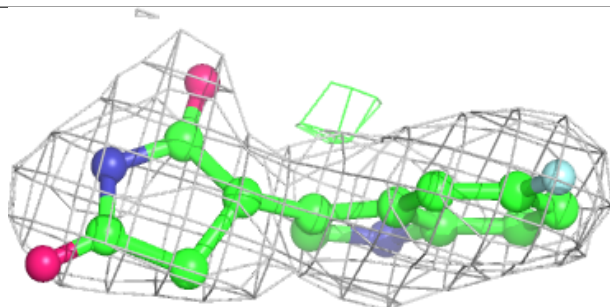
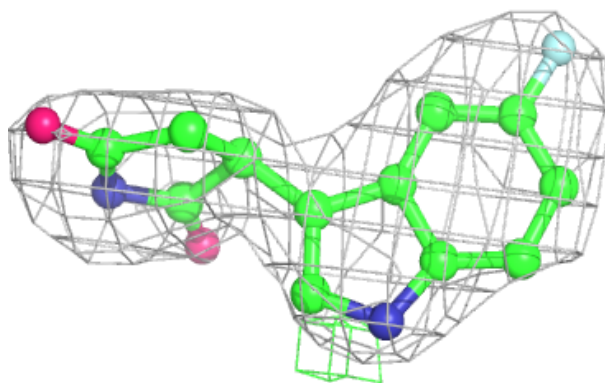
Electron density around H7S A 403:

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

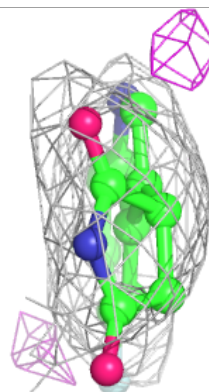
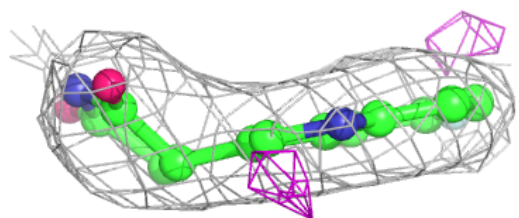
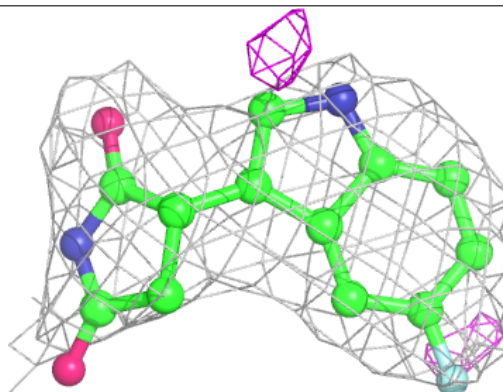


Electron density around H7S C 402:

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

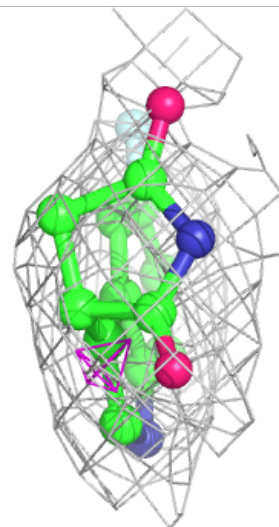
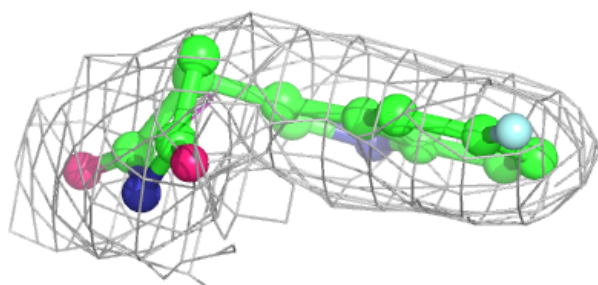
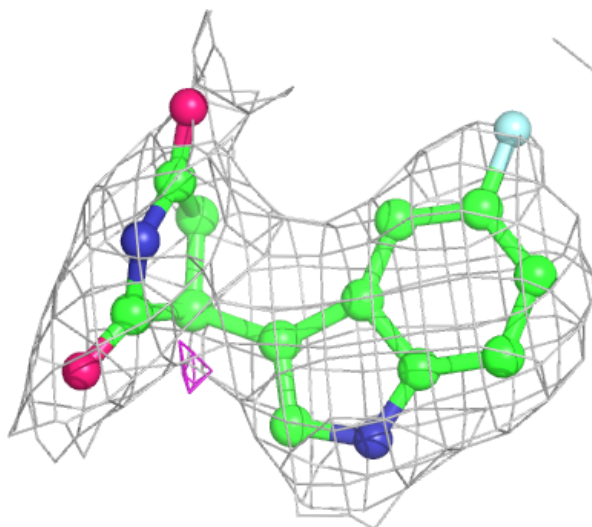
**Electron density around H7S C 403:**

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



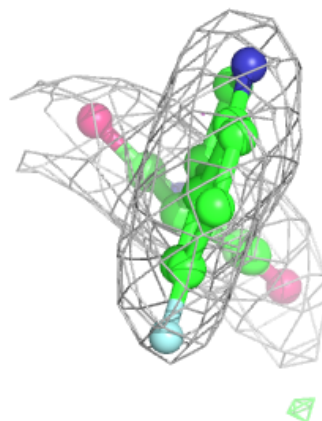
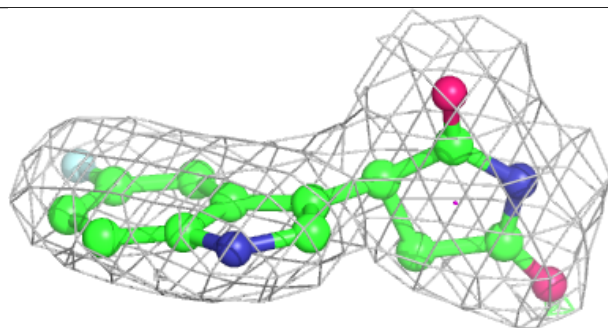
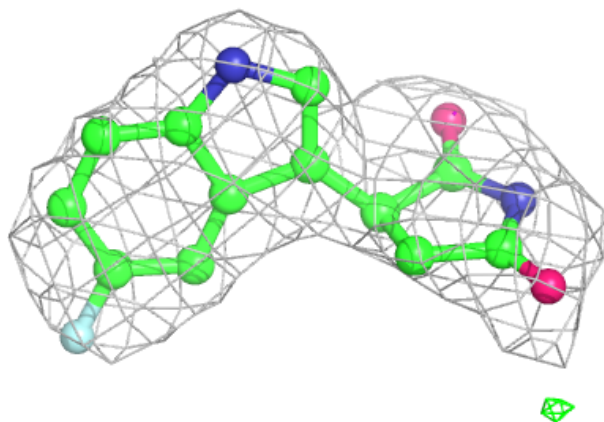
Electron density around H7S B 403:

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

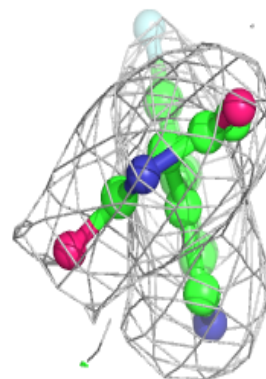
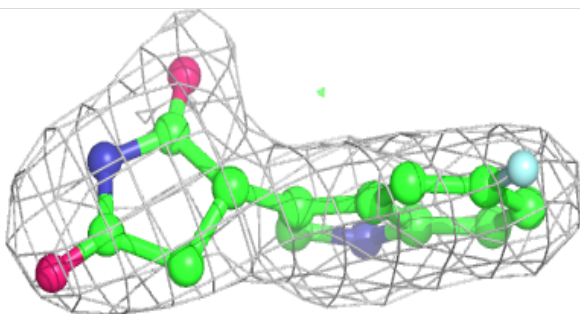
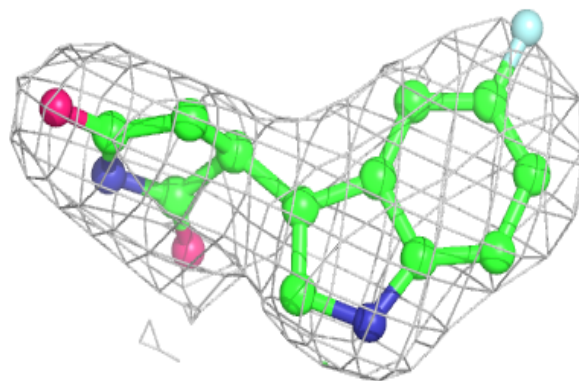


Electron density around H7S D 402:

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

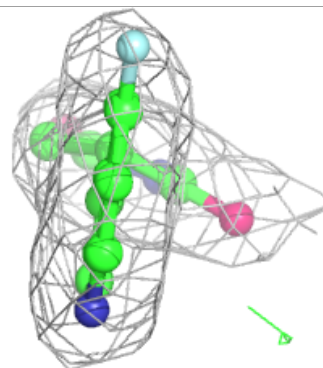
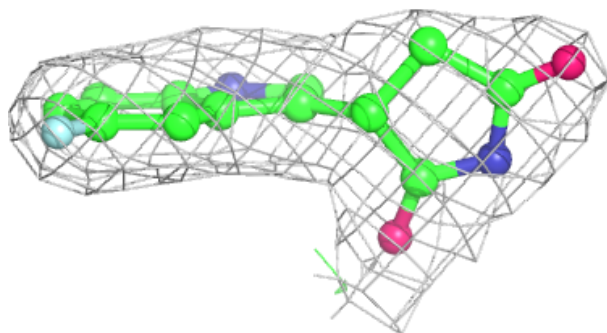
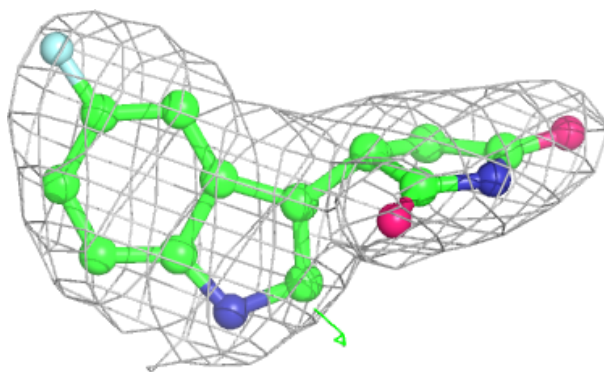
**Electron density around H7S A 402:**

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



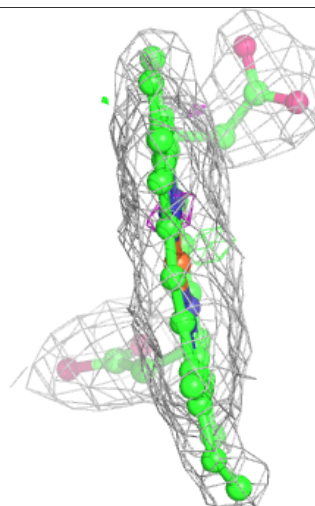
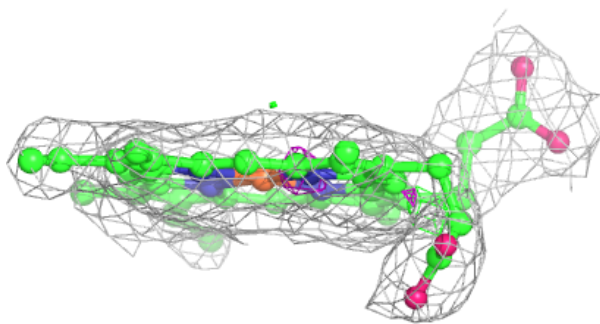
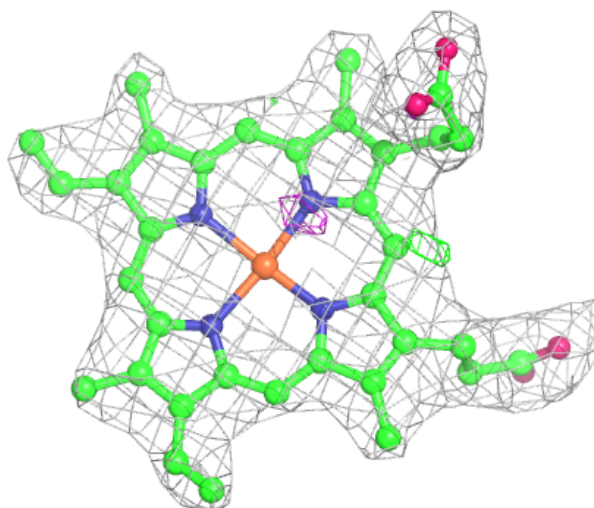
Electron density around H7S B 402:

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



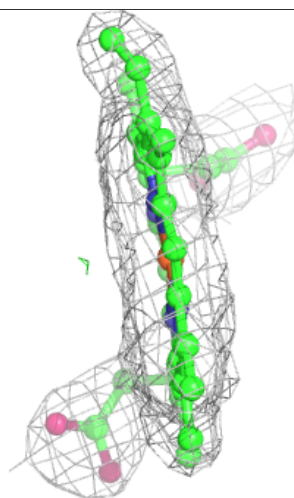
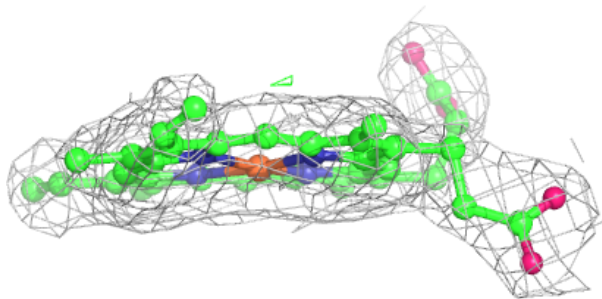
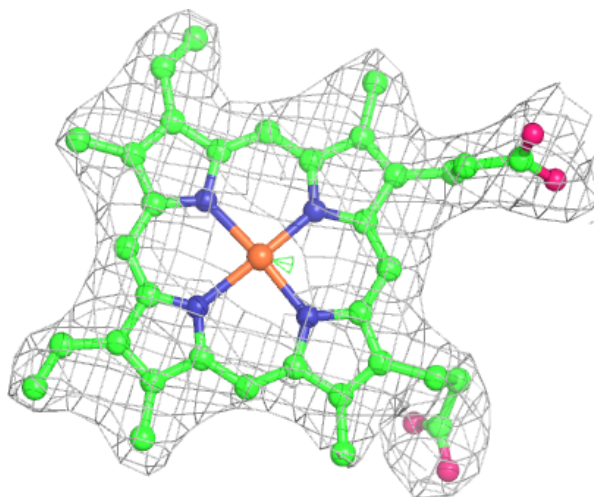
Electron density around HEM C 401:

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



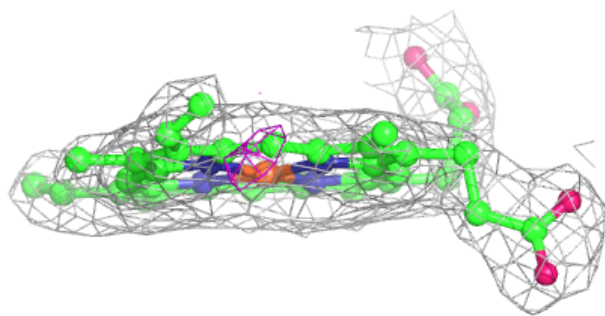
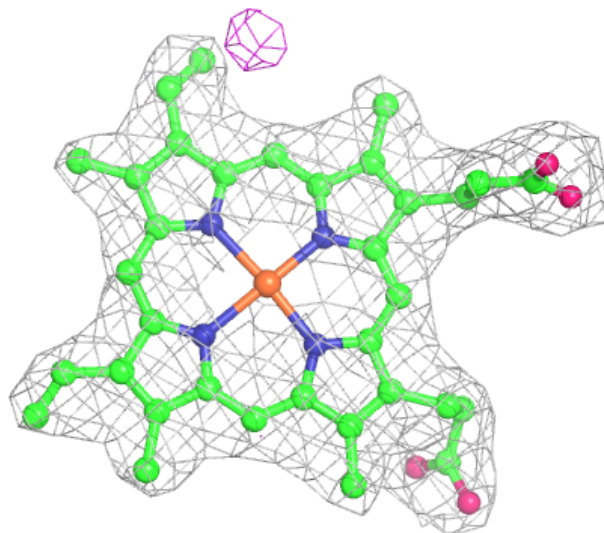
Electron density around HEM A 401:

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



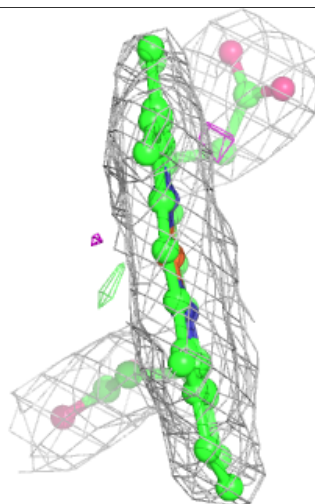
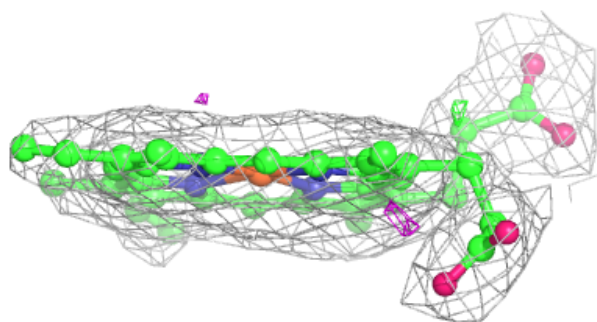
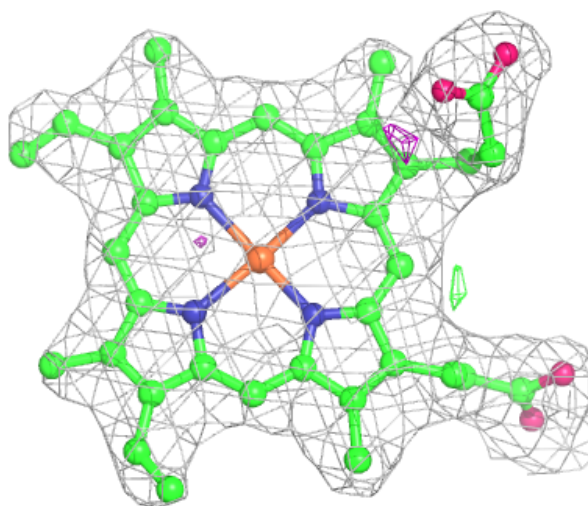
Electron density around HEM D 401:

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



Electron density around HEM B 401:

$2mF_o-DF_c$ (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.