



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:52 PM UTC

PDB ID : 8JS6 / pdb_00008js6
Title : Dimeric PAS domains of oxygen sensor FixL in complex with cyanide-bound ferric heme
Authors : Kamaya, M.; Koteishi, H.; Sawai, H.; Sugimoto, H.; Shiro, Y.
Deposited on : 2023-06-19
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

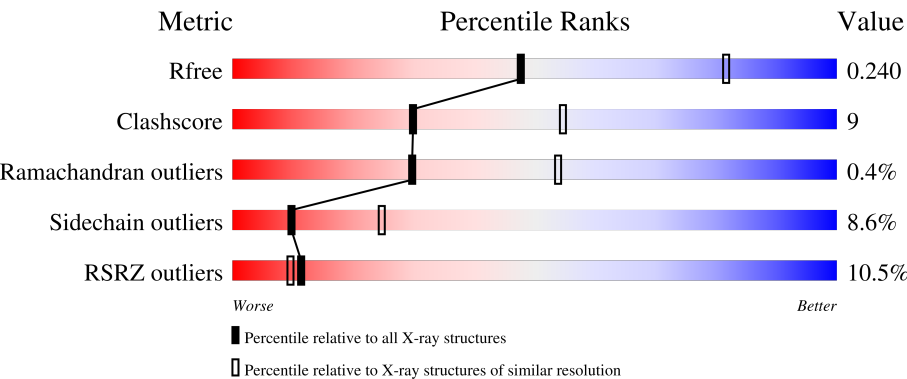
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	273	8% 68% 21% • 7%
1	B	273	10% 71% 19% • 7%
1	C	273	9% 70% 19% • 8%
1	D	273	7% 73% 15% • 7%
1	E	273	8% 72% 18% • 8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	273	13% 71% 17% • 8%
1	G	273	10% 68% 21% • 9%
1	H	273	8% 69% 20% • 9%
1	I	273	11% 69% 20% • 8%
1	J	273	13% 67% 23% • 8%

2 Entry composition

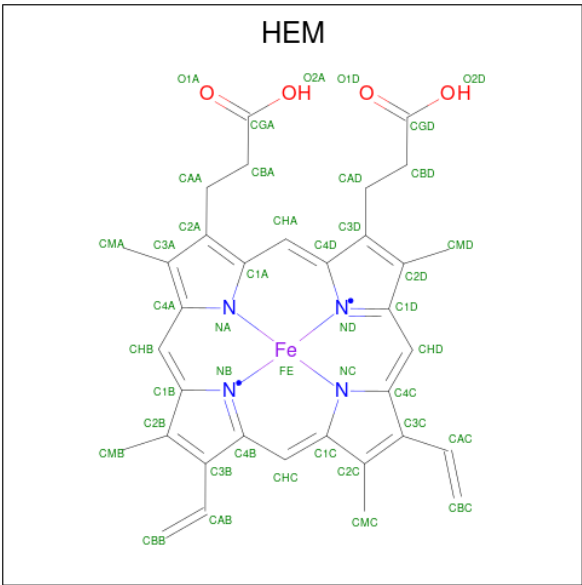
There are 5 unique types of molecules in this entry. The entry contains 20477 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Sensor protein FixL.

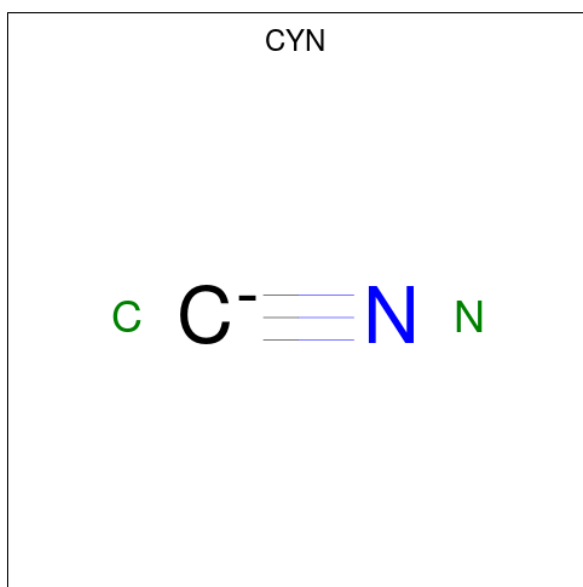
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	253	Total	C	N	O	S	0	3	0
			2021	1260	373	384	4			
1	B	253	Total	C	N	O	S	0	0	0
			1998	1245	365	384	4			
1	C	251	Total	C	N	O	S	0	0	0
			1983	1234	363	382	4			
1	D	253	Total	C	N	O	S	0	1	0
			2005	1250	367	384	4			
1	E	251	Total	C	N	O	S	0	0	0
			1981	1234	363	380	4			
1	F	251	Total	C	N	O	S	0	0	0
			1981	1234	363	380	4			
1	G	249	Total	C	N	O	S	0	0	0
			1966	1223	361	378	4			
1	H	249	Total	C	N	O	S	0	1	0
			1972	1228	362	378	4			
1	I	251	Total	C	N	O	S	0	0	0
			1980	1234	363	379	4			
1	J	251	Total	C	N	O	S	0	1	0
			1987	1239	364	380	4			

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



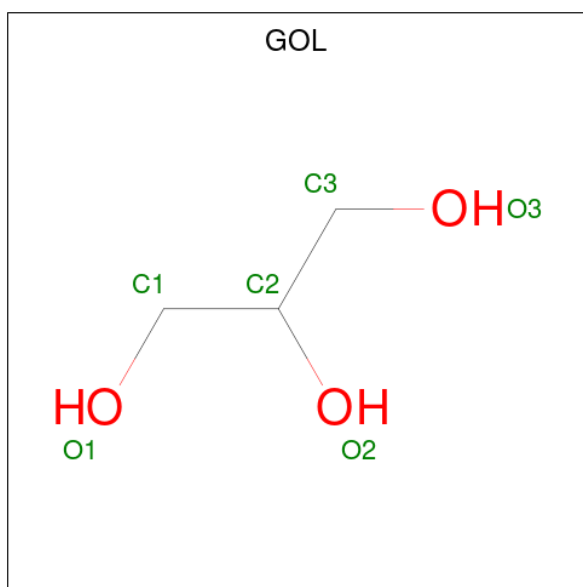
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	G	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	H	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	I	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	J	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	0	0
			2	1	1		
3	B	1	Total	C	N	0	0
			2	1	1		
3	C	1	Total	C	N	0	0
			2	1	1		
3	D	1	Total	C	N	0	0
			2	1	1		
3	E	1	Total	C	N	0	0
			2	1	1		
3	F	1	Total	C	N	0	0
			2	1	1		
3	G	1	Total	C	N	0	0
			2	1	1		
3	H	1	Total	C	N	0	0
			2	1	1		
3	I	1	Total	C	N	0	0
			2	1	1		
3	J	1	Total	C	N	0	0
			2	1	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	D	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	E	1	Total	C	O	0	0
			6	3	3		
4	F	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	G	1	Total	C	O	0	0
			6	3	3		
4	H	1	Total	C	O	0	0
			6	3	3		
4	I	1	Total	C	O	0	0
			6	3	3		
4	J	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	J	1	Total	C	O	0	0
			6	3	3		

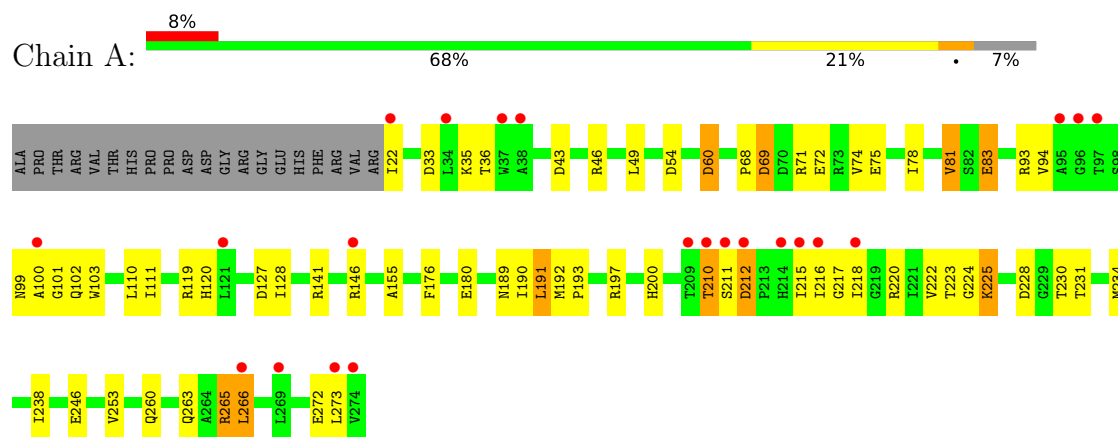
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	O	0	0
			10	10		
5	B	8	Total	O	0	0
			8	8		
5	C	5	Total	O	0	0
			5	5		
5	D	16	Total	O	0	0
			16	16		
5	E	3	Total	O	0	0
			3	3		
5	F	7	Total	O	0	0
			7	7		
5	G	5	Total	O	0	0
			5	5		
5	H	3	Total	O	0	0
			3	3		
5	I	3	Total	O	0	0
			3	3		
5	J	3	Total	O	0	0
			3	3		

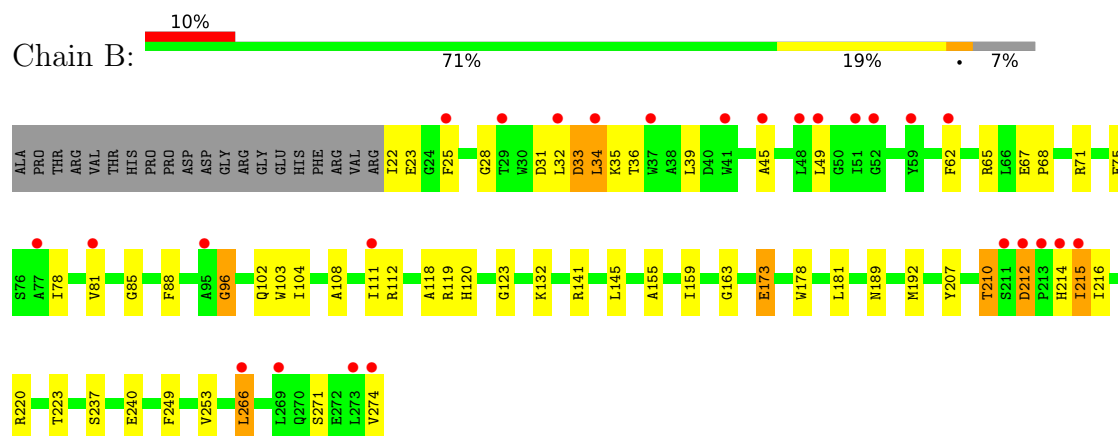
3 Residue-property plots [i](#)

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.

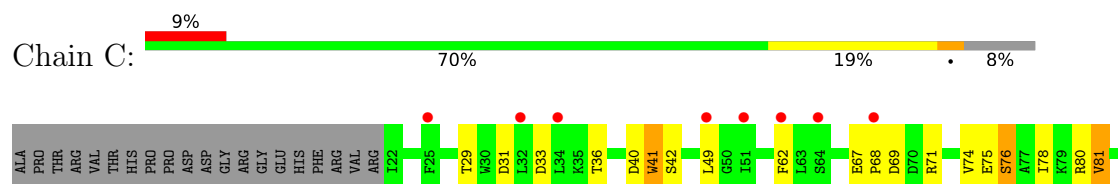
• Molecule 1: Sensor protein FixL

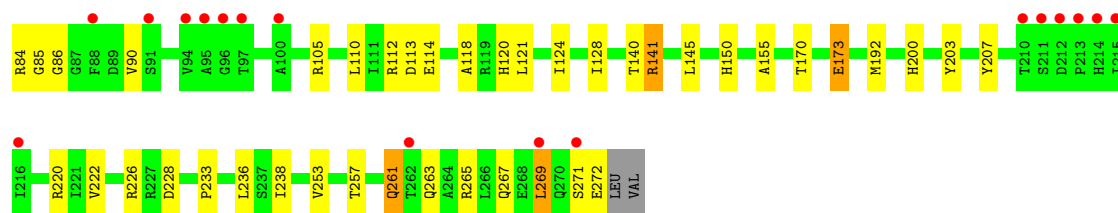


• Molecule 1: Sensor protein FixL

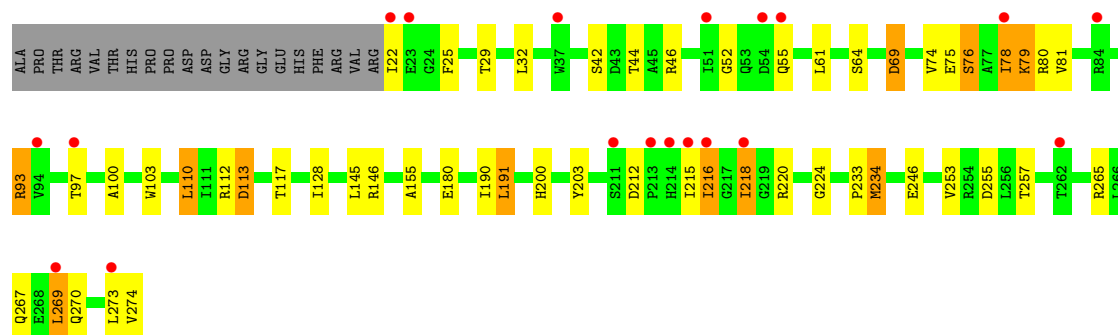
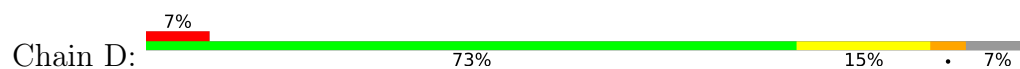


• Molecule 1: Sensor protein FixL

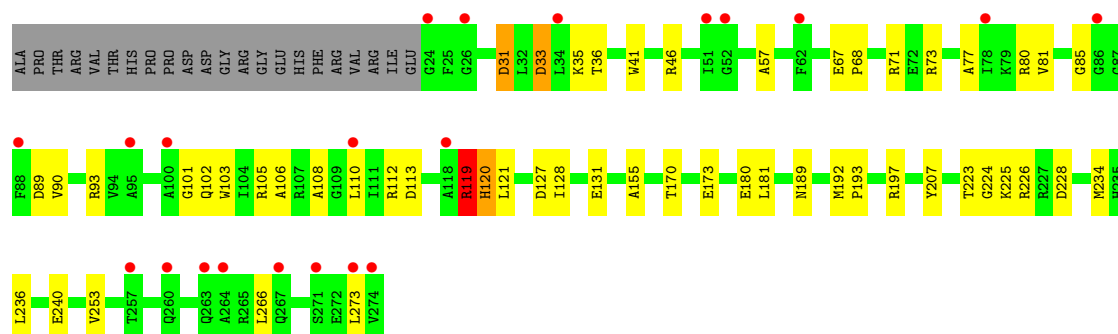




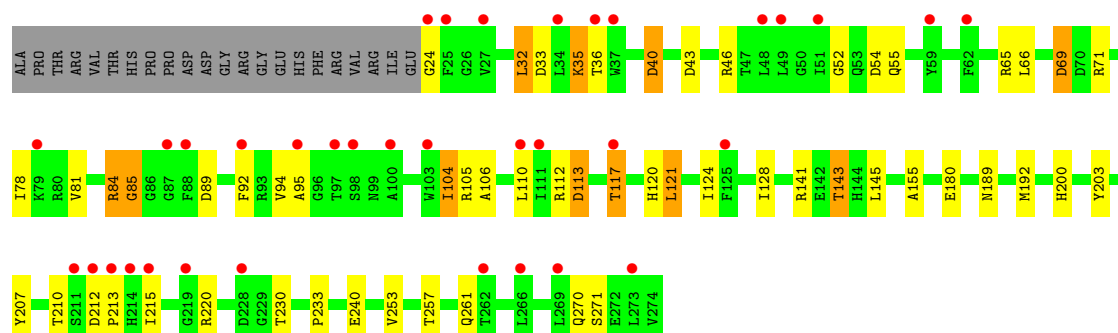
• Molecule 1: Sensor protein FixL



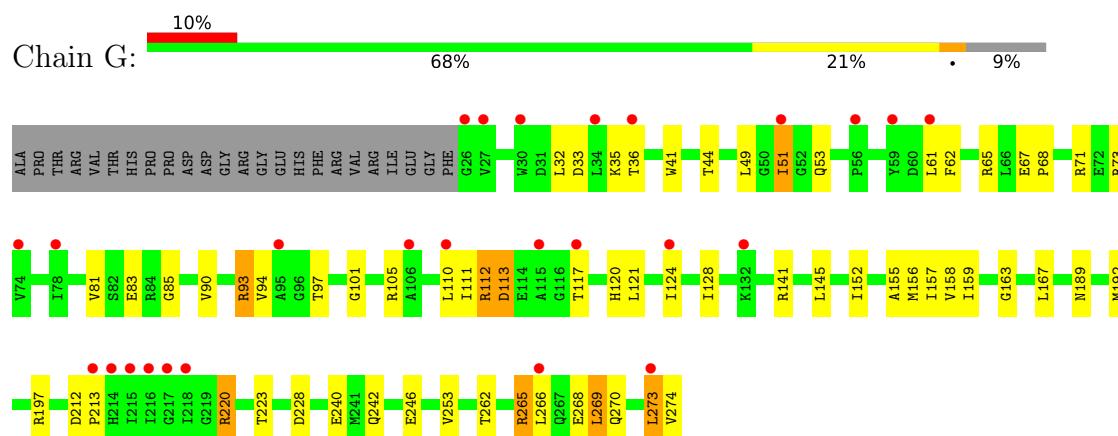
• Molecule 1: Sensor protein FixL



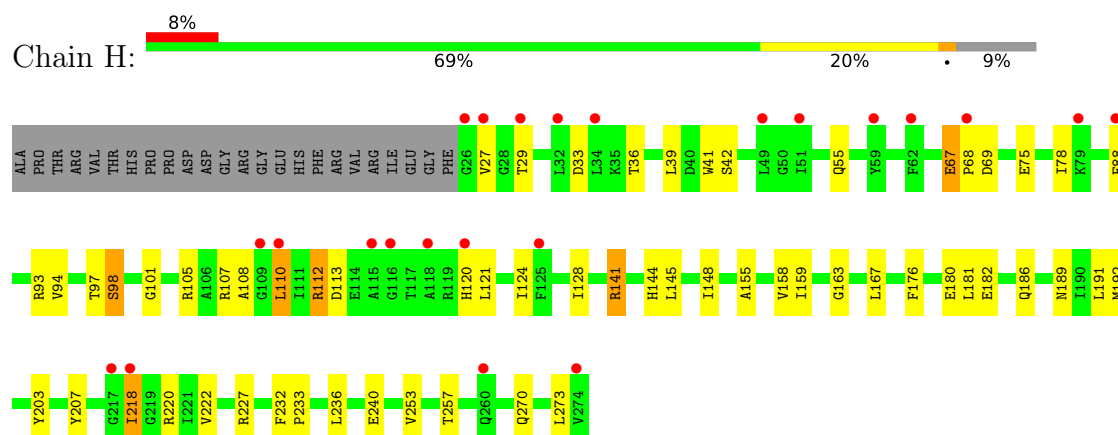
• Molecule 1: Sensor protein FixL



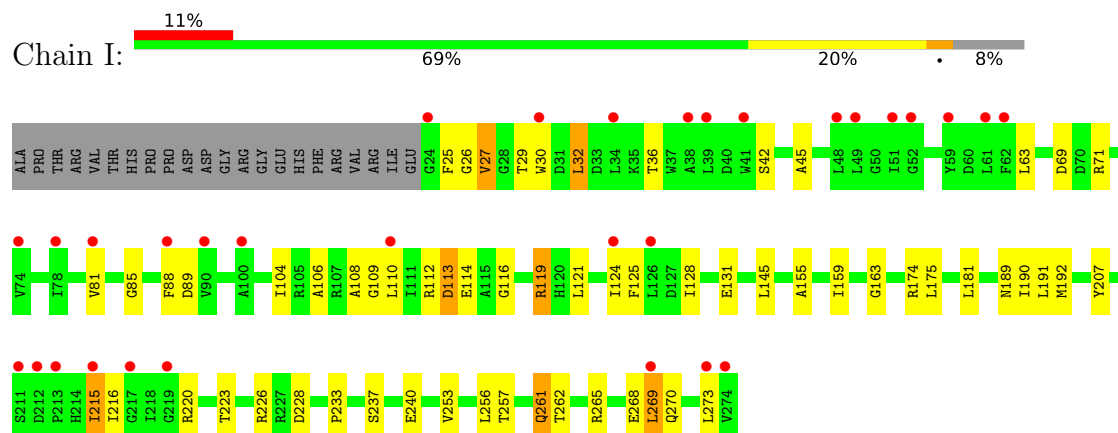
- Molecule 1: Sensor protein FixL



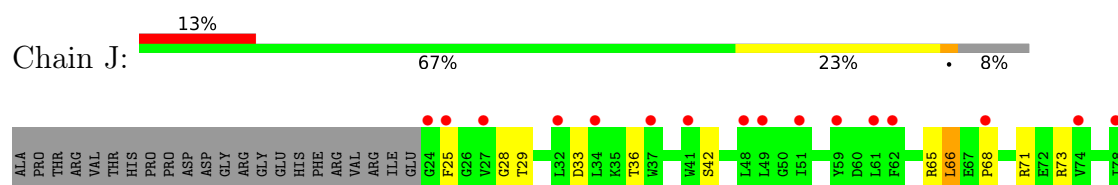
- Molecule 1: Sensor protein FixL

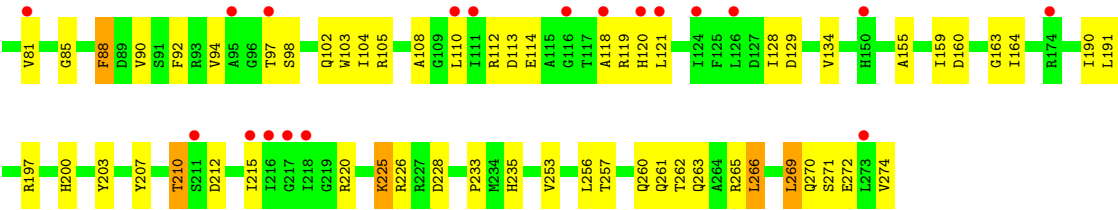


- Molecule 1: Sensor protein FixL



- Molecule 1: Sensor protein FixL





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	187.83Å 198.73Å 266.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.68 – 2.70 49.68 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.68-2.70) 94.4 (49.68-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.219 , 0.247 (Not available) , 0.240	Depositor DCC
R_{free} test set	6822 reflections (2.69%)	wwPDB-VP
Wilson B-factor (Å ²)	74.9	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 92.1	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	0.95	EDS
Total number of atoms	20477	wwPDB-VP
Average B, all atoms (Å ²)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.96% 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, CYN, GOL

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	0.39	1/2070 (0.0%)	0.62	1/2797 (0.0%)
1	B	0.31	0/2037	0.57	1/2754 (0.0%)
1	C	0.30	0/2022	0.55	0/2733
1	D	0.37	0/2048	0.63	0/2769
1	E	0.30	0/2020	0.60	0/2731
1	F	0.30	0/2020	0.57	0/2731
1	G	0.29	0/2004	0.56	2/2710 (0.1%)
1	H	0.29	0/2013	0.58	0/2722
1	I	0.30	0/2019	0.56	0/2730
1	J	0.29	0/2029	0.59	0/2743
All	All	0.32	1/20282 (0.0%)	0.58	4/27420 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	ASP	CA-CB	-5.40	1.49	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	215	ILE	N-CA-C	-6.76	106.19	112.96
1	A	100	ALA	N-CA-C	-6.17	107.59	114.62
1	G	35	LYS	CA-C-N	5.55	132.15	121.54
1	G	35	LYS	C-N-CA	5.55	132.15	121.54

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	2021	0	1981	40	0
1	B	1998	0	1948	37	0
1	C	1983	0	1928	36	0
1	D	2005	0	1955	28	0
1	E	1981	0	1931	34	0
1	F	1981	0	1931	28	0
1	G	1966	0	1919	31	0
1	H	1972	0	1924	32	0
1	I	1980	0	1928	38	0
1	J	1987	0	1936	48	0
2	A	43	0	30	0	0
2	B	43	0	30	3	0
2	C	43	0	30	5	0
2	D	43	0	30	3	0
2	E	43	0	30	2	0
2	F	43	0	30	3	0
2	G	43	0	30	2	0
2	H	43	0	30	2	0
2	I	43	0	30	2	0
2	J	43	0	30	3	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
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
4	A	12	0	16	4	0
4	B	6	0	7	1	0
4	C	6	0	8	0	0
4	D	12	0	15	3	0
4	E	12	0	16	1	0
4	F	6	0	8	2	0
4	G	12	0	16	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	6	0	7	0	0
4	I	6	0	8	0	0
4	J	12	0	16	1	0
5	A	10	0	0	0	0
5	B	8	0	0	0	0
5	C	5	0	0	0	0
5	D	16	0	0	0	0
5	E	3	0	0	0	0
5	F	7	0	0	0	0
5	G	5	0	0	0	0
5	H	3	0	0	0	0
5	I	3	0	0	0	0
5	J	3	0	0	0	0
All	All	20477	0	19798	343	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 9.

All (343) 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:A:189:ASN:HA	1:A:192:MET:HE2	1.58	0.83
1:A:210:THR:HG22	1:A:212:ASP:H	1.46	0.81
1:J:29:THR:HG22	1:J:42:SER:HB2	1.65	0.77
1:A:192:MET:HE1	1:A:200:HIS:HB2	1.64	0.76
1:C:269:LEU:HG	1:D:269:LEU:HD13	1.69	0.74
1:D:69:ASP:N	1:D:69:ASP:OD1	2.20	0.73
1:E:224:GLY:HA3	1:E:234:MET:HE3	1.71	0.73
1:D:233:PRO:HD2	1:D:257:THR:HG22	1.69	0.72
1:G:51:ILE:HG23	1:G:53:GLN:H	1.55	0.72
1:G:81:VAL:HA	1:G:85:GLY:HA3	1.72	0.71
1:G:93:ARG:HE	1:G:101:GLY:HA3	1.56	0.70
2:H:302:HEM:HBB2	2:H:302:HEM:HHC	1.74	0.69
1:B:34:LEU:HD12	1:B:35:LYS:HG3	1.74	0.69
1:D:218:ILE:HG22	1:H:218:ILE:HG13	1.73	0.69
1:J:155:ALA:HB3	1:J:253:VAL:HB	1.75	0.69
1:A:224:GLY:HA3	1:A:234:MET:HE3	1.74	0.69
1:G:155:ALA:HB3	1:G:253:VAL:HB	1.75	0.69
1:A:192:MET:HE3	1:A:197:ARG:HA	1.74	0.68
1:B:141:ARG:NH1	4:B:301:GOL:O2	2.25	0.68
1:H:105:ARG:HE	1:H:107:ARG:HD2	1.56	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ARG:HE	1:C:118:ALA:HB2	1.58	0.68
1:H:155:ALA:HB3	1:H:253:VAL:HB	1.75	0.68
1:E:155:ALA:HB3	1:E:253:VAL:HB	1.75	0.67
1:A:33:ASP:OD2	1:A:119:ARG:NH1	2.27	0.67
2:B:302:HEM:HHC	2:B:302:HEM:HBB2	1.78	0.66
1:B:81:VAL:HA	1:B:85:GLY:HA3	1.76	0.66
1:C:155:ALA:HB3	1:C:253:VAL:HB	1.78	0.66
1:C:81:VAL:HG11	1:C:121:LEU:HD13	1.78	0.65
1:F:66:LEU:HB2	1:F:71:ARG:HB3	1.77	0.65
1:J:73:ARG:HH11	1:J:90:VAL:HG23	1.62	0.64
2:E:601:HEM:HHC	2:E:601:HEM:HBB2	1.79	0.64
1:G:220:ARG:NH2	2:G:601:HEM:O2D	2.31	0.64
2:F:302:HEM:HBB2	2:F:302:HEM:HHC	1.80	0.64
2:G:601:HEM:HHC	2:G:601:HEM:HBB2	1.80	0.64
1:E:180:GLU:HG3	1:E:181:LEU:HD12	1.80	0.63
1:D:155:ALA:HB3	1:D:253:VAL:HB	1.79	0.63
2:C:601:HEM:HHC	2:C:601:HEM:HBB2	1.81	0.63
1:E:31:ASP:OD1	1:E:31:ASP:N	2.31	0.63
1:H:33:ASP:HB3	1:H:120:HIS:HB3	1.80	0.63
1:A:102:GLN:NE2	1:A:127:ASP:OD1	2.32	0.63
1:I:81:VAL:HA	1:I:85:GLY:HA3	1.79	0.62
1:B:271:SER:HA	1:B:274:VAL:HG12	1.82	0.61
1:H:141:ARG:HE	1:H:141:ARG:HA	1.65	0.61
1:F:40:ASP:OD1	1:F:40:ASP:N	2.35	0.60
1:H:98:SER:O	1:H:98:SER:OG	2.20	0.60
1:A:111:ILE:HD11	1:B:22:ILE:HG13	1.82	0.60
1:A:69:ASP:OD1	1:A:69:ASP:N	2.35	0.60
1:C:141:ARG:NH1	4:D:302:GOL:O3	2.35	0.59
1:J:68:PRO:HA	1:J:71:ARG:HG2	1.81	0.59
1:A:225:LYS:HB3	1:A:231:THR:HG22	1.85	0.59
1:D:220:ARG:NH2	2:D:303:HEM:O1D	2.35	0.59
1:A:22:ILE:HA	1:B:111:ILE:HG13	1.86	0.58
1:G:273:LEU:HD13	1:H:273:LEU:HD11	1.85	0.58
1:G:240:GLU:OE1	1:G:242:GLN:NE2	2.37	0.58
1:F:141:ARG:NH2	4:F:301:GOL:O2	2.35	0.58
1:B:189:ASN:HA	1:B:192:MET:HE3	1.85	0.58
1:F:213:PRO:HB3	1:I:174:ARG:HH21	1.69	0.57
1:J:112:ARG:HE	1:J:118:ALA:HB2	1.69	0.57
1:D:46:ARG:NH2	1:D:55:GLN:O	2.38	0.57
1:A:180:GLU:OE2	1:D:146:ARG:NH2	2.38	0.57
1:A:266:LEU:HG	1:B:266:LEU:HD23	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ARG:NH1	1:B:96:GLY:O	2.38	0.56
2:C:601:HEM:HBD1	2:C:601:HEM:HHA	1.86	0.56
1:F:155:ALA:HB3	1:F:253:VAL:HB	1.86	0.56
1:H:159:ILE:HD12	1:H:163:GLY:HA2	1.87	0.56
1:C:74:VAL:HG22	1:C:90:VAL:HG21	1.86	0.56
1:I:220:ARG:NH1	2:I:601:HEM:HAA1	2.20	0.56
1:A:54:ASP:N	1:A:54:ASP:OD1	2.34	0.56
1:I:269:LEU:HD22	1:J:269:LEU:HB2	1.87	0.56
1:I:269:LEU:HB2	1:J:269:LEU:HD23	1.88	0.55
1:J:159:ILE:HD12	1:J:163:GLY:HA2	1.88	0.55
1:B:207:TYR:HE1	1:B:215:ILE:HG23	1.72	0.55
1:G:145:LEU:HB2	4:G:603:GOL:H2	1.88	0.55
1:J:33:ASP:HA	1:J:120:HIS:HA	1.87	0.55
1:A:260:GLN:HA	1:A:263:GLN:HG2	1.89	0.55
1:G:33:ASP:HB3	1:G:120:HIS:ND1	2.21	0.55
1:H:88:PHE:O	1:H:107:ARG:HA	2.06	0.55
1:J:88:PHE:CD2	1:J:108:ALA:HB3	2.42	0.55
1:I:155:ALA:HB3	1:I:253:VAL:HB	1.89	0.55
1:G:269:LEU:HG	1:H:270:GLN:CD	2.32	0.54
1:I:128:ILE:HB	1:I:131:GLU:HB2	1.88	0.54
1:E:81:VAL:HG11	1:E:121:LEU:HD11	1.87	0.54
1:G:159:ILE:HD12	1:G:163:GLY:HA2	1.89	0.54
1:F:33:ASP:HA	1:F:120:HIS:HA	1.89	0.54
1:J:88:PHE:HD2	1:J:108:ALA:HB3	1.70	0.54
1:E:81:VAL:HA	1:E:85:GLY:HA3	1.89	0.54
1:G:41:TRP:HZ3	1:G:62:PHE:HB2	1.72	0.54
1:A:111:ILE:HB	1:A:120:HIS:HB2	1.90	0.54
1:C:29:THR:HG22	1:C:42:SER:HB2	1.89	0.54
1:J:88:PHE:HE1	1:J:90:VAL:HG12	1.73	0.54
1:F:65:ARG:O	1:F:95:ALA:N	2.32	0.54
1:F:233:PRO:HD2	1:F:257:THR:HG22	1.90	0.53
1:I:131:GLU:OE1	1:I:131:GLU:N	2.40	0.53
1:A:155:ALA:HB3	1:A:253:VAL:HB	1.89	0.53
1:B:155:ALA:HB3	1:B:253:VAL:HB	1.91	0.53
1:E:73:ARG:HH11	1:E:90:VAL:HG13	1.73	0.53
1:J:226:ARG:HB2	1:J:228:ASP:HB3	1.90	0.53
1:I:190:ILE:HG13	1:I:191:LEU:HD12	1.89	0.53
1:F:43:ASP:HA	1:F:46:ARG:HD2	1.92	0.52
1:I:63:LEU:HD22	1:I:71:ARG:HB2	1.91	0.52
1:E:68:PRO:HA	1:E:71:ARG:HG2	1.92	0.52
1:H:233:PRO:HD2	1:H:257:THR:HG22	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:29:THR:HG22	1:I:42:SER:HB2	1.92	0.52
1:E:33:ASP:OD1	1:E:33:ASP:N	2.42	0.52
1:E:113:ASP:H	1:E:119:ARG:HG2	1.73	0.52
1:G:113:ASP:HB2	1:G:117:THR:H	1.73	0.52
1:H:203:TYR:HB3	2:H:302:HEM:HAA1	1.91	0.52
1:G:270:GLN:O	1:G:274:VAL:HG23	2.09	0.52
1:H:145:LEU:HD21	1:H:167:LEU:HD21	1.90	0.51
1:E:89:ASP:HA	1:E:106:ALA:O	2.10	0.51
1:J:200:HIS:HA	1:J:203:TYR:CD2	2.46	0.51
1:B:33:ASP:HB3	1:B:120:HIS:ND1	2.26	0.51
1:C:261:GLN:O	1:C:265:ARG:HG3	2.10	0.51
1:E:33:ASP:HA	1:E:120:HIS:HB3	1.91	0.51
1:H:182:GLU:O	1:H:186:GLN:NE2	2.43	0.51
1:D:52:GLY:HA2	1:D:55:GLN:HB2	1.93	0.51
1:H:189:ASN:HA	1:H:192:MET:HE3	1.92	0.51
1:C:76:SER:O	1:C:80:ARG:HG3	2.11	0.51
1:F:89:ASP:HA	1:F:106:ALA:O	2.10	0.51
1:B:68:PRO:HA	1:B:71:ARG:HG2	1.92	0.51
1:F:200:HIS:HA	1:F:203:TYR:CD2	2.46	0.51
1:I:207:TYR:HE2	1:I:215:ILE:HG23	1.76	0.50
1:E:108:ALA:HB1	1:E:121:LEU:HD22	1.93	0.50
1:E:226:ARG:HB2	1:E:228:ASP:HB3	1.92	0.50
1:D:113:ASP:HB2	1:D:117:THR:H	1.75	0.50
1:D:190:ILE:HG13	1:D:191:LEU:HD13	1.93	0.50
1:J:25:PHE:HE2	1:J:28:GLY:N	2.09	0.50
1:I:273:LEU:HD21	1:J:272:GLU:HB3	1.93	0.50
1:C:105:ARG:HB2	1:C:128:ILE:HD13	1.94	0.50
1:F:113:ASP:HB2	1:F:117:THR:H	1.76	0.50
1:C:192:MET:HE1	1:C:200:HIS:CD2	2.47	0.49
1:G:65:ARG:HB3	1:G:94:VAL:HG13	1.94	0.49
1:I:30:TRP:CZ3	1:I:32:LEU:HB3	2.47	0.49
1:I:112:ARG:HB3	1:I:116:GLY:HA2	1.94	0.49
4:E:603:GOL:H32	1:F:145:LEU:HD13	1.94	0.49
1:I:88:PHE:CE2	1:I:108:ALA:HB3	2.48	0.49
1:A:60:ASP:N	1:A:60:ASP:OD1	2.46	0.49
1:E:113:ASP:HB2	1:E:119:ARG:HH11	1.77	0.49
1:H:207:TYR:OH	1:H:240:GLU:OE1	2.24	0.49
1:H:94:VAL:O	1:H:101:GLY:HA2	2.12	0.49
1:A:103:TRP:HB3	1:A:128:ILE:HG13	1.95	0.49
1:A:215:ILE:HG13	1:A:217:GLY:H	1.77	0.49
1:H:93:ARG:NE	1:H:101:GLY:HA3	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:39:LEU:HD22	1:H:41:TRP:HE3	1.78	0.49
1:C:49:LEU:HD21	1:C:62:PHE:HD1	1.76	0.49
1:C:145:LEU:HD13	4:D:302:GOL:H11	1.95	0.49
1:J:190:ILE:HG13	1:J:191:LEU:HD12	1.95	0.49
1:A:192:MET:HE1	1:A:200:HIS:CB	2.40	0.48
1:F:69:ASP:OD1	1:F:69:ASP:N	2.30	0.48
1:E:170:THR:HA	1:E:173:GLU:HG2	1.95	0.48
1:J:92:PHE:CZ	1:J:104:ILE:HD11	2.47	0.48
1:J:220:ARG:NH1	2:J:303:HEM:HBA1	2.28	0.48
4:A:603:GOL:O1	1:B:141:ARG:NH2	2.44	0.48
1:D:145:LEU:HD13	4:D:302:GOL:H32	1.95	0.48
1:D:270:GLN:O	1:D:274:VAL:HG13	2.12	0.48
1:J:197:ARG:HH12	1:J:225:LYS:HD3	1.77	0.48
1:D:81:VAL:HG22	1:D:110:LEU:HD23	1.95	0.48
1:B:28:GLY:HA3	1:B:45:ALA:HB2	1.96	0.48
1:C:150:HIS:ND1	1:C:170:THR:HG21	2.28	0.48
1:J:269:LEU:O	1:J:269:LEU:HD22	2.13	0.48
1:F:32:LEU:O	1:F:121:LEU:N	2.46	0.48
1:G:49:LEU:HD21	1:G:62:PHE:HD1	1.78	0.48
1:J:269:LEU:HD13	1:J:270:GLN:N	2.29	0.48
1:I:189:ASN:HA	1:I:192:MET:HE3	1.96	0.48
1:J:113:ASP:OD1	1:J:114:GLU:N	2.47	0.48
1:B:119:ARG:HB3	1:B:120:HIS:CD2	2.49	0.47
1:J:210:THR:HG21	1:J:215:ILE:HD12	1.95	0.47
1:A:75:GLU:O	1:A:78:ILE:HG13	2.13	0.47
1:E:193:PRO:HG3	1:E:223:THR:HG22	1.96	0.47
1:I:262:THR:HG23	1:J:266:LEU:HD21	1.97	0.47
1:J:220:ARG:NH2	2:J:303:HEM:O2D	2.47	0.47
1:A:193:PRO:HG3	1:A:223:THR:HG22	1.97	0.47
1:B:108:ALA:HA	1:B:123:GLY:HA3	1.96	0.47
1:I:29:THR:H	1:I:42:SER:HB3	1.80	0.47
1:J:88:PHE:CE1	1:J:90:VAL:HG12	2.50	0.47
1:B:31:ASP:OD1	1:B:120:HIS:HB3	2.14	0.47
1:B:112:ARG:HA	1:B:118:ALA:HA	1.97	0.47
1:H:180:GLU:OE1	1:H:180:GLU:N	2.47	0.47
1:I:89:ASP:N	1:I:89:ASP:OD1	2.45	0.47
1:I:226:ARG:HB2	1:I:228:ASP:HB3	1.97	0.47
1:J:207:TYR:CD2	2:J:303:HEM:HBD1	2.50	0.47
1:J:233:PRO:HD2	1:J:257:THR:HG22	1.97	0.47
2:D:303:HEM:HHC	2:D:303:HEM:HBB2	1.97	0.47
1:G:105:ARG:HB2	1:G:128:ILE:HD13	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:108:ALA:HB1	1:H:121:LEU:HG	1.97	0.47
1:B:23:GLU:O	1:B:25:PHE:N	2.39	0.47
1:A:190:ILE:HG13	1:A:191:LEU:HD13	1.97	0.46
1:B:32:LEU:HD13	1:B:39:LEU:HD12	1.97	0.46
1:J:73:ARG:NH1	1:J:90:VAL:HG23	2.30	0.46
1:E:93:ARG:HH11	1:E:101:GLY:HA3	1.80	0.46
1:H:110:LEU:HD12	1:H:112:ARG:HG2	1.97	0.46
1:E:105:ARG:HB2	1:E:128:ILE:HD13	1.95	0.46
1:G:51:ILE:HG12	1:G:61:LEU:HD21	1.98	0.46
2:I:601:HEM:HMB2	2:I:601:HEM:HBB2	1.97	0.46
1:C:33:ASP:HA	1:C:120:HIS:HA	1.98	0.46
1:C:75:GLU:O	1:C:78:ILE:HG13	2.15	0.46
1:E:197:ARG:NH2	1:E:225:LYS:HE2	2.31	0.46
1:F:220:ARG:NH2	2:F:302:HEM:O2D	2.48	0.46
1:H:144:HIS:O	1:H:148:ILE:HG12	2.15	0.46
1:I:30:TRP:HZ3	1:I:32:LEU:HB3	1.80	0.46
1:F:81:VAL:HA	1:F:85:GLY:HA3	1.97	0.46
1:J:105:ARG:HB2	1:J:128:ILE:HD13	1.97	0.46
1:J:270:GLN:O	1:J:274:VAL:HG23	2.15	0.46
1:A:141:ARG:NH2	4:A:604:GOL:O1	2.47	0.46
1:J:81:VAL:HA	1:J:85:GLY:HA3	1.97	0.46
1:E:103:TRP:HB3	1:E:128:ILE:HG13	1.98	0.46
1:B:103:TRP:CD2	1:B:132:LYS:HD3	2.51	0.46
1:E:77:ALA:HA	1:E:80:ARG:HD2	1.98	0.46
1:H:69:ASP:OD1	1:H:69:ASP:N	2.44	0.46
1:J:210:THR:HG22	1:J:212:ASP:H	1.81	0.46
1:C:113:ASP:OD1	1:C:114:GLU:N	2.44	0.45
1:C:233:PRO:HD2	1:C:257:THR:HG22	1.98	0.45
1:C:29:THR:H	1:C:42:SER:HB3	1.81	0.45
1:E:189:ASN:HA	1:E:192:MET:HE3	1.98	0.45
1:I:145:LEU:HB2	4:J:302:GOL:H2	1.99	0.45
1:C:222:VAL:HB	2:C:601:HEM:HMB3	1.99	0.45
1:F:270:GLN:NE2	1:F:271:SER:HB2	2.32	0.45
1:G:73:ARG:HH11	1:G:90:VAL:HG23	1.81	0.45
1:J:197:ARG:NH1	1:J:225:LYS:HD3	2.31	0.45
1:A:265:ARG:HD2	1:B:266:LEU:HD11	1.99	0.45
1:D:200:HIS:HA	1:D:203:TYR:CD2	2.51	0.45
1:E:102:GLN:NE2	1:E:127:ASP:OD1	2.50	0.45
1:G:265:ARG:O	1:G:269:LEU:HD22	2.16	0.45
1:J:110:LEU:HD23	1:J:110:LEU:H	1.81	0.45
1:I:159:ILE:HD12	1:I:163:GLY:HA2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:235:HIS:HB2	1:J:256:LEU:HD11	1.99	0.45
1:A:228:ASP:HB3	1:A:230:THR:H	1.82	0.45
1:J:66:LEU:HD12	1:J:71:ARG:HA	1.98	0.45
1:D:255:ASP:OD1	1:D:257:THR:HG23	2.17	0.45
1:H:158:VAL:HB	1:H:167:LEU:HB2	1.99	0.45
1:I:45:ALA:HB1	1:I:125:PHE:HD2	1.82	0.45
1:A:176:PHE:CZ	1:A:234:MET:HE1	2.53	0.44
1:B:102:GLN:NE2	1:B:103:TRP:O	2.47	0.44
1:F:54:ASP:N	1:F:54:ASP:OD1	2.50	0.44
1:C:81:VAL:HG13	1:C:110:LEU:HD21	2.00	0.44
1:H:182:GLU:CD	1:H:227:ARG:HH22	2.26	0.44
1:J:263:GLN:HA	1:J:266:LEU:HD22	2.00	0.44
1:G:212:ASP:HA	1:G:213:PRO:HD3	1.78	0.44
1:J:103:TRP:N	1:J:129:ASP:OD1	2.44	0.44
1:B:220:ARG:NH1	2:B:302:HEM:O2D	2.41	0.44
1:D:224:GLY:HA3	1:D:234:MET:HE2	1.99	0.44
1:E:119:ARG:NE	1:E:119:ARG:HA	2.33	0.44
1:C:68:PRO:HA	1:C:71:ARG:HG2	2.00	0.44
1:G:68:PRO:HA	1:G:71:ARG:HG2	2.00	0.44
1:I:261:GLN:O	1:I:265:ARG:HG2	2.18	0.44
1:A:210:THR:HB	1:A:211:SER:H	1.65	0.43
1:I:25:PHE:HD1	1:I:27:VAL:H	1.64	0.43
1:I:109:GLY:HA3	1:J:25:PHE:C	2.43	0.43
1:B:181:LEU:HD22	1:F:143:THR:HG22	2.00	0.43
1:C:150:HIS:HA	1:C:170:THR:HG23	2.00	0.43
1:D:75:GLU:O	1:D:78:ILE:HG13	2.19	0.43
1:B:49:LEU:HD21	1:B:62:PHE:HD1	1.83	0.43
1:I:269:LEU:HD13	1:J:269:LEU:HD23	2.01	0.43
4:A:603:GOL:H32	1:B:145:LEU:HB2	2.01	0.43
1:F:189:ASN:HA	1:F:192:MET:HE3	2.00	0.43
1:C:200:HIS:HA	1:C:203:TYR:CD2	2.53	0.43
1:E:81:VAL:HG23	1:E:85:GLY:HA3	2.01	0.43
1:E:119:ARG:HB3	1:E:120:HIS:H	1.60	0.43
1:I:269:LEU:HD12	1:I:273:LEU:HD13	2.01	0.43
1:I:269:LEU:HG	1:I:270:GLN:N	2.31	0.43
1:C:207:TYR:HB2	2:C:601:HEM:HBD2	2.00	0.43
1:G:192:MET:HG3	1:G:197:ARG:HA	2.00	0.43
1:I:113:ASP:OD1	1:I:119:ARG:HB2	2.18	0.43
1:B:220:ARG:CZ	2:B:302:HEM:HBA1	2.49	0.43
1:C:85:GLY:HA2	1:C:110:LEU:HD12	2.00	0.43
1:H:29:THR:HG22	1:H:42:SER:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:25:PHE:HD1	1:I:26:GLY:N	2.16	0.43
1:A:43:ASP:O	1:A:46:ARG:HG3	2.19	0.42
1:A:146[A]:ARG:NE	1:D:180:GLU:OE2	2.52	0.42
4:A:603:GOL:H32	1:B:145:LEU:HD13	2.01	0.42
1:D:61:LEU:O	1:D:64:SER:OG	2.32	0.42
1:D:74:VAL:O	1:D:78:ILE:HG23	2.18	0.42
4:F:301:GOL:O3	4:F:301:GOL:O1	2.33	0.42
1:G:141:ARG:HE	4:G:603:GOL:HO3	1.63	0.42
1:J:65:ARG:HA	1:J:65:ARG:HD2	1.92	0.42
1:A:216:ILE:HG13	1:A:238:ILE:HB	2.01	0.42
1:D:93:ARG:HH11	1:D:100:ALA:HA	1.84	0.42
1:E:119:ARG:HG2	1:E:119:ARG:HH11	1.84	0.42
1:I:207:TYR:OH	1:I:240:GLU:OE1	2.29	0.42
2:E:601:HEM:HBC2	2:E:601:HEM:HMC2	2.01	0.42
1:F:35:LYS:HZ2	1:F:35:LYS:HG3	1.65	0.42
1:C:31:ASP:OD1	1:C:40:ASP:HB2	2.20	0.42
1:D:220:ARG:NH1	2:D:303:HEM:HBA1	2.34	0.42
1:A:93:ARG:HD3	1:A:101:GLY:HA3	2.01	0.42
1:A:74:VAL:O	1:A:78:ILE:HG23	2.20	0.42
1:B:173:GLU:HB3	1:B:178:TRP:O	2.19	0.42
1:C:269:LEU:HD13	1:C:269:LEU:HA	1.77	0.42
1:D:29:THR:HG22	1:D:42:SER:HB3	2.01	0.42
1:E:41:TRP:NE1	1:E:46:ARG:HG2	2.35	0.42
1:A:220:ARG:HG3	1:A:222:VAL:HG13	2.01	0.42
1:C:226:ARG:HB2	1:C:228:ASP:HB3	2.02	0.42
1:I:269:LEU:HB2	1:J:269:LEU:CD2	2.49	0.42
1:A:68:PRO:HA	1:A:71:ARG:HH11	1.84	0.42
1:C:236:LEU:HG	1:C:238:ILE:HD11	2.00	0.42
1:J:66:LEU:HD22	1:J:92:PHE:CE1	2.55	0.42
1:I:89:ASP:HA	1:I:106:ALA:O	2.20	0.42
1:J:160:ASP:CG	1:J:164:ILE:HG12	2.45	0.42
1:D:218:ILE:H	1:D:218:ILE:HG13	1.62	0.42
1:F:105:ARG:HB2	1:F:128:ILE:HD13	2.01	0.42
1:C:110:LEU:HD23	1:C:110:LEU:HA	1.85	0.41
1:E:207:TYR:OH	1:E:240:GLU:OE1	2.28	0.41
1:G:51:ILE:HD12	1:G:51:ILE:HA	1.77	0.41
1:G:158:VAL:HB	1:G:167:LEU:HB2	2.02	0.41
1:G:189:ASN:HA	1:G:192:MET:HE3	2.01	0.41
1:B:75:GLU:O	1:B:78:ILE:HG13	2.20	0.41
1:B:240:GLU:HG2	1:B:249:PHE:CE2	2.55	0.41
1:D:76:SER:HA	1:D:79:LYS:HD2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:ARG:O	1:D:269:LEU:HG	2.19	0.41
1:E:33:ASP:HA	1:E:120:HIS:HA	2.02	0.41
1:I:69:ASP:OD1	1:I:69:ASP:N	2.45	0.41
1:C:220:ARG:HG3	1:C:222:VAL:HG13	2.03	0.41
1:C:170:THR:HA	1:C:173:GLU:HG2	2.02	0.41
2:F:302:HEM:HMC2	2:F:302:HEM:HBC2	2.02	0.41
1:J:113:ASP:OD2	1:J:119:ARG:NH2	2.54	0.41
1:G:110:LEU:HD12	1:G:112:ARG:HD2	2.02	0.41
1:J:269:LEU:HD22	1:J:269:LEU:C	2.45	0.41
1:F:92:PHE:CZ	1:F:104:ILE:HD11	2.56	0.41
1:A:192:MET:CE	1:A:197:ARG:HA	2.49	0.41
1:B:88:PHE:HB3	1:B:108:ALA:HB3	2.03	0.41
1:H:232:PHE:HB2	1:H:257:THR:CG2	2.51	0.41
1:A:81:VAL:O	1:A:110:LEU:HD11	2.21	0.41
1:A:265:ARG:HG2	1:B:266:LEU:HD21	2.02	0.41
1:C:110:LEU:HD22	1:C:118:ALA:HB1	2.03	0.41
1:E:31:ASP:HA	1:E:121:LEU:O	2.21	0.40
1:E:41:TRP:CZ2	1:E:57:ALA:HA	2.57	0.40
1:H:67:GLU:HG2	1:H:68:PRO:HD2	2.03	0.40
1:H:75:GLU:O	1:H:78:ILE:HG12	2.21	0.40
1:I:233:PRO:HD2	1:I:257:THR:HG22	2.02	0.40
1:B:159:ILE:HD12	1:B:163:GLY:HA2	2.03	0.40
1:D:103:TRP:HB3	1:D:128:ILE:HG13	2.02	0.40
1:F:78:ILE:HA	1:F:81:VAL:HG12	2.02	0.40
1:G:33:ASP:HA	1:G:120:HIS:HA	2.03	0.40
1:C:41:TRP:HZ3	1:C:62:PHE:HB2	1.86	0.40
1:C:220:ARG:NH1	2:C:601:HEM:O2D	2.54	0.40
1:F:207:TYR:OH	1:F:240:GLU:OE1	2.36	0.40
1:A:33:ASP:CG	1:A:36:THR:HG22	2.47	0.40
1:E:110:LEU:HB2	1:F:24:GLY:N	2.37	0.40
1:F:52:GLY:HA2	1:F:55:GLN:HG2	2.03	0.40
1:G:152:ILE:HG21	1:G:156:MET:HE3	2.02	0.40
1:H:107:ARG:O	1:H:124:ILE:N	2.51	0.40
1:H:176:PHE:CE2	1:H:191:LEU:HB3	2.57	0.40
1:B:210:THR:HG22	1:B:212:ASP:H	1.87	0.40
1:G:262:THR:HG22	1:G:265:ARG:HH21	1.85	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	254/273 (93%)	242 (95%)	11 (4%)	1 (0%)	30	54
1	B	251/273 (92%)	238 (95%)	12 (5%)	1 (0%)	30	54
1	C	249/273 (91%)	232 (93%)	16 (6%)	1 (0%)	30	54
1	D	252/273 (92%)	238 (94%)	12 (5%)	2 (1%)	16	37
1	E	249/273 (91%)	232 (93%)	15 (6%)	2 (1%)	16	37
1	F	249/273 (91%)	234 (94%)	12 (5%)	3 (1%)	10	27
1	G	247/273 (90%)	235 (95%)	12 (5%)	0	100	100
1	H	248/273 (91%)	234 (94%)	14 (6%)	0	100	100
1	I	249/273 (91%)	235 (94%)	14 (6%)	0	100	100
1	J	250/273 (92%)	235 (94%)	15 (6%)	0	100	100
All	All	2498/2730 (92%)	2355 (94%)	133 (5%)	10 (0%)	30	54

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	216	ILE
1	A	83	GLU
1	B	96	GLY
1	C	86	GLY
1	F	85	GLY
1	F	84	ARG
1	D	212	ASP
1	E	35	LYS
1	E	119	ARG
1	F	212	ASP

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	214/228 (94%)	196 (92%)	18 (8%)	10	26
1	B	211/228 (92%)	198 (94%)	13 (6%)	16	39
1	C	209/228 (92%)	192 (92%)	17 (8%)	11	27
1	D	212/228 (93%)	189 (89%)	23 (11%)	6	16
1	E	209/228 (92%)	198 (95%)	11 (5%)	20	46
1	F	209/228 (92%)	189 (90%)	20 (10%)	8	20
1	G	208/228 (91%)	185 (89%)	23 (11%)	6	15
1	H	209/228 (92%)	193 (92%)	16 (8%)	12	30
1	I	208/228 (91%)	188 (90%)	20 (10%)	8	20
1	J	210/228 (92%)	192 (91%)	18 (9%)	10	25
All	All	2099/2280 (92%)	1920 (92%)	179 (8%)	10	25

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LYS
1	A	49	LEU
1	A	60	ASP
1	A	69	ASP
1	A	72	GLU
1	A	81	VAL
1	A	83	GLU
1	A	94	VAL
1	A	99	ASN
1	A	191	LEU
1	A	210	THR
1	A	218	ILE
1	A	225	LYS
1	A	246	GLU
1	A	265	ARG
1	A	266	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	272	GLU
1	A	273	LEU
1	B	33	ASP
1	B	34	LEU
1	B	36	THR
1	B	67	GLU
1	B	104	ILE
1	B	173	GLU
1	B	210	THR
1	B	212	ASP
1	B	214	HIS
1	B	216	ILE
1	B	223	THR
1	B	237	SER
1	B	266	LEU
1	C	36	THR
1	C	41	TRP
1	C	67	GLU
1	C	69	ASP
1	C	76	SER
1	C	81	VAL
1	C	84	ARG
1	C	124	ILE
1	C	140	THR
1	C	141	ARG
1	C	173	GLU
1	C	261	GLN
1	C	263	GLN
1	C	267	GLN
1	C	269	LEU
1	C	271	SER
1	C	272	GLU
1	D	22	ILE
1	D	25	PHE
1	D	32	LEU
1	D	44	THR
1	D	69	ASP
1	D	76	SER
1	D	78	ILE
1	D	79	LYS
1	D	80	ARG
1	D	93	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	97	THR
1	D	110	LEU
1	D	112	ARG
1	D	113	ASP
1	D	191	LEU
1	D	215	ILE
1	D	216	ILE
1	D	218	ILE
1	D	234	MET
1	D	246	GLU
1	D	267	GLN
1	D	269	LEU
1	D	273	LEU
1	E	31	ASP
1	E	33	ASP
1	E	36	THR
1	E	67	GLU
1	E	112	ARG
1	E	119	ARG
1	E	120	HIS
1	E	131	GLU
1	E	236	LEU
1	E	266	LEU
1	E	273	LEU
1	F	32	LEU
1	F	35	LYS
1	F	36	THR
1	F	40	ASP
1	F	69	ASP
1	F	84	ARG
1	F	94	VAL
1	F	104	ILE
1	F	110	LEU
1	F	112	ARG
1	F	113	ASP
1	F	117	THR
1	F	121	LEU
1	F	124	ILE
1	F	143	THR
1	F	180	GLU
1	F	210	THR
1	F	215	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	230	THR
1	F	261	GLN
1	G	32	LEU
1	G	36	THR
1	G	44	THR
1	G	51	ILE
1	G	67	GLU
1	G	83	GLU
1	G	93	ARG
1	G	97	THR
1	G	111	ILE
1	G	112	ARG
1	G	113	ASP
1	G	121	LEU
1	G	124	ILE
1	G	157	ILE
1	G	220	ARG
1	G	223	THR
1	G	228	ASP
1	G	246	GLU
1	G	265	ARG
1	G	266	LEU
1	G	268	GLU
1	G	269	LEU
1	G	273	LEU
1	H	27	VAL
1	H	36	THR
1	H	55	GLN
1	H	67	GLU
1	H	97	THR
1	H	98	SER
1	H	110	LEU
1	H	112	ARG
1	H	113	ASP
1	H	128	ILE
1	H	141	ARG
1	H	181	LEU
1	H	218	ILE
1	H	220	ARG
1	H	222	VAL
1	H	236	LEU
1	I	27	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	32	LEU
1	I	36	THR
1	I	104	ILE
1	I	110	LEU
1	I	113	ASP
1	I	114	GLU
1	I	119	ARG
1	I	121	LEU
1	I	124	ILE
1	I	175	LEU
1	I	181	LEU
1	I	215	ILE
1	I	216	ILE
1	I	223	THR
1	I	237	SER
1	I	256	LEU
1	I	261	GLN
1	I	268	GLU
1	I	269	LEU
1	J	36	THR
1	J	66	LEU
1	J	88	PHE
1	J	94	VAL
1	J	97	THR
1	J	98	SER
1	J	102	GLN
1	J	121	LEU
1	J	134	VAL
1	J	210	THR
1	J	225	LYS
1	J	260	GLN
1	J	261	GLN
1	J	262	THR
1	J	265	ARG
1	J	266	LEU
1	J	269	LEU
1	J	271	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	186	GLN
1	B	242	GLN
1	C	261	GLN
1	E	120	HIS
1	E	235	HIS
1	E	261	GLN
1	F	186	GLN
1	F	259	HIS
1	G	186	GLN
1	H	267	GLN
1	H	270	GLN
1	I	150	HIS
1	J	261	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](#)

35 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	CYN	C	602	-	1,1,1	0.30	0	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	I	601	1	50,50,50	1.51	8 (16%)	67,82,82	1.64	11 (16%)
2	HEM	F	302	1	50,50,50	1.43	6 (12%)	67,82,82	1.30	8 (11%)
3	CYN	D	304	-	1,1,1	0.25	0	-		
4	GOL	E	604	-	5,5,5	1.06	0	5,5,5	0.99	0
4	GOL	C	603	-	5,5,5	1.02	1 (20%)	5,5,5	1.10	0
4	GOL	H	301	-	5,5,5	1.11	0	5,5,5	1.05	0
4	GOL	J	301	-	5,5,5	1.18	1 (20%)	5,5,5	0.99	0
3	CYN	B	303	-	1,1,1	0.22	0	-		
3	CYN	J	304	-	1,1,1	0.34	0	-		
3	CYN	A	602	-	1,1,1	0.27	0	-		
2	HEM	D	303	1	50,50,50	1.47	9 (18%)	67,82,82	1.43	12 (17%)
4	GOL	A	603	-	5,5,5	1.07	0	5,5,5	1.01	0
4	GOL	J	302	-	5,5,5	0.95	0	5,5,5	1.05	0
3	CYN	F	303	-	1,1,1	0.34	0	-		
4	GOL	F	301	-	5,5,5	1.22	1 (20%)	5,5,5	1.19	0
2	HEM	C	601	1	50,50,50	1.47	10 (20%)	67,82,82	1.79	19 (28%)
2	HEM	E	601	1	50,50,50	1.50	8 (16%)	67,82,82	1.30	8 (11%)
2	HEM	G	601	1	50,50,50	1.44	8 (16%)	67,82,82	1.25	8 (11%)
3	CYN	I	602	-	1,1,1	0.36	0	-		
4	GOL	A	604	-	5,5,5	1.30	0	5,5,5	1.26	0
2	HEM	B	302	1	50,50,50	1.45	10 (20%)	67,82,82	1.32	6 (8%)
2	HEM	J	303	1	50,50,50	1.27	6 (12%)	67,82,82	1.26	7 (10%)
4	GOL	B	301	-	5,5,5	1.40	1 (20%)	5,5,5	1.23	1 (20%)
4	GOL	E	603	-	5,5,5	1.23	0	5,5,5	1.01	0
2	HEM	H	302	1	50,50,50	1.36	5 (10%)	67,82,82	1.50	9 (13%)
4	GOL	D	301	-	5,5,5	1.45	1 (20%)	5,5,5	1.40	1 (20%)
4	GOL	G	604	-	5,5,5	0.99	0	5,5,5	1.22	0
3	CYN	E	602	-	1,1,1	0.29	0	-		
2	HEM	A	601	1	50,50,50	1.38	8 (16%)	67,82,82	1.41	12 (17%)
3	CYN	H	303	-	1,1,1	0.25	0	-		
4	GOL	I	603	-	5,5,5	0.98	0	5,5,5	1.09	0
4	GOL	D	302	-	5,5,5	0.89	0	5,5,5	1.08	0
3	CYN	G	602	-	1,1,1	0.31	0	-		
4	GOL	G	603	-	5,5,5	1.14	0	5,5,5	0.93	0

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
4	GOL	E	604	-	-	2/4/4/4	-
2	HEM	I	601	1	-	6/14/54/54	-
2	HEM	F	302	1	-	3/14/54/54	-
4	GOL	C	603	-	-	2/4/4/4	-
4	GOL	H	301	-	-	2/4/4/4	-
4	GOL	J	301	-	-	2/4/4/4	-
2	HEM	D	303	1	-	6/14/54/54	-
4	GOL	A	603	-	-	0/4/4/4	-
4	GOL	J	302	-	-	2/4/4/4	-
4	GOL	F	301	-	-	1/4/4/4	-
2	HEM	C	601	1	-	9/14/54/54	-
2	HEM	E	601	1	-	2/14/54/54	-
2	HEM	G	601	1	-	5/14/54/54	-
4	GOL	A	604	-	-	1/4/4/4	-
2	HEM	B	302	1	-	6/14/54/54	-
2	HEM	J	303	1	-	5/14/54/54	-
4	GOL	B	301	-	-	0/4/4/4	-
4	GOL	E	603	-	-	2/4/4/4	-
2	HEM	H	302	1	-	8/14/54/54	-
4	GOL	D	301	-	-	2/4/4/4	-
4	GOL	G	604	-	-	0/4/4/4	-
2	HEM	A	601	1	-	5/14/54/54	-
4	GOL	I	603	-	-	2/4/4/4	-
4	GOL	D	302	-	-	1/4/4/4	-
4	GOL	G	603	-	-	2/4/4/4	-

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	601	HEM	FE-NA	5.46	2.13	1.95
2	E	601	HEM	FE-NC	4.79	2.11	1.95
2	G	601	HEM	FE-NB	4.68	2.09	1.94
2	D	303	HEM	FE-NA	4.49	2.10	1.95
2	C	601	HEM	FE-NB	4.44	2.08	1.94
2	F	302	HEM	FE-NC	4.39	2.09	1.95
2	F	302	HEM	FE-NB	4.21	2.07	1.94
2	E	601	HEM	FE-NB	4.14	2.07	1.94
2	I	601	HEM	FE-NB	3.92	2.07	1.94
2	B	302	HEM	FE-NC	3.49	2.06	1.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	303	HEM	FE-NB	3.44	2.05	1.94
2	B	302	HEM	CAC-C3C	3.42	1.56	1.47
2	B	302	HEM	FE-NB	3.39	2.05	1.94
2	H	302	HEM	FE-NB	3.32	2.05	1.94
2	H	302	HEM	FE-NC	3.28	2.06	1.95
2	E	601	HEM	CAC-C3C	3.28	1.56	1.47
2	D	303	HEM	CAC-C3C	3.23	1.56	1.47
2	I	601	HEM	CAC-C3C	3.22	1.56	1.47
2	B	302	HEM	CAB-C3B	3.12	1.55	1.47
2	B	302	HEM	FE-ND	3.12	2.04	1.94
2	A	601	HEM	FE-ND	3.12	2.04	1.94
2	D	303	HEM	CAB-C3B	3.10	1.55	1.47
2	G	601	HEM	CAC-C3C	3.10	1.55	1.47
2	F	302	HEM	CAC-C3C	3.10	1.55	1.47
2	E	601	HEM	CAB-C3B	3.09	1.55	1.47
2	C	601	HEM	FE-NC	3.02	2.05	1.95
2	A	601	HEM	FE-NA	3.02	2.05	1.95
2	A	601	HEM	FE-NB	2.96	2.04	1.94
2	A	601	HEM	CAC-C3C	2.94	1.55	1.47
2	H	302	HEM	CAC-C3C	2.91	1.55	1.47
2	J	303	HEM	CAC-C3C	2.91	1.55	1.47
2	D	303	HEM	CMD-C2D	2.88	1.56	1.50
2	C	601	HEM	CAB-C3B	2.86	1.55	1.47
2	H	302	HEM	CAB-C3B	2.86	1.55	1.47
2	G	601	HEM	CAB-C3B	2.84	1.55	1.47
2	G	601	HEM	FE-NA	2.83	2.04	1.95
2	D	303	HEM	CMA-C3A	2.83	1.56	1.50
2	F	302	HEM	CAB-C3B	2.82	1.54	1.47
2	G	601	HEM	FE-ND	2.81	2.03	1.94
2	J	303	HEM	CAB-C3B	2.75	1.54	1.47
2	I	601	HEM	CAB-C3B	2.73	1.54	1.47
2	D	303	HEM	FE-NC	2.71	2.04	1.95
2	A	601	HEM	CAB-C3B	2.66	1.54	1.47
2	D	303	HEM	CMC-C2C	2.59	1.56	1.50
2	B	302	HEM	CMC-C2C	2.58	1.56	1.50
4	B	301	GOL	O2-C2	-2.57	1.35	1.43
2	D	303	HEM	CMB-C2B	2.53	1.56	1.50
2	A	601	HEM	FE-NC	2.53	2.03	1.95
2	C	601	HEM	FE-ND	2.50	2.02	1.94
2	C	601	HEM	CMA-C3A	2.37	1.55	1.50
2	C	601	HEM	CAC-C3C	2.37	1.53	1.47
2	E	601	HEM	FE-ND	2.37	2.02	1.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	HEM	FE-NA	2.34	2.02	1.95
2	J	303	HEM	FE-NA	2.32	2.02	1.95
2	A	601	HEM	CMD-C2D	2.31	1.55	1.50
2	I	601	HEM	C2A-C3A	-2.27	1.33	1.38
2	E	601	HEM	CMD-C2D	2.27	1.55	1.50
2	I	601	HEM	CMB-C2B	2.27	1.55	1.50
2	I	601	HEM	CMD-C2D	2.26	1.55	1.50
2	H	302	HEM	CMA-C3A	2.26	1.55	1.50
2	D	303	HEM	FE-NB	2.25	2.01	1.94
2	C	601	HEM	CMD-C2D	2.23	1.55	1.50
4	J	301	GOL	O2-C2	-2.22	1.36	1.43
2	C	601	HEM	C3C-C2C	-2.19	1.32	1.37
4	F	301	GOL	O2-C2	-2.18	1.37	1.43
2	G	601	HEM	FE-NC	2.18	2.02	1.95
2	J	303	HEM	CMA-C3A	2.16	1.55	1.50
2	F	302	HEM	CMD-C2D	2.16	1.55	1.50
2	C	601	HEM	C3B-C2B	-2.14	1.32	1.37
2	E	601	HEM	CMA-C3A	2.13	1.55	1.50
2	E	601	HEM	CMC-C2C	2.12	1.55	1.50
4	D	301	GOL	O2-C2	-2.11	1.37	1.43
2	B	302	HEM	CMD-C2D	2.10	1.55	1.50
2	I	601	HEM	CMA-C3A	2.10	1.55	1.50
2	F	302	HEM	CMA-C3A	2.06	1.55	1.50
2	G	601	HEM	CMD-C2D	2.05	1.55	1.50
4	C	603	GOL	O2-C2	-2.04	1.37	1.43
2	J	303	HEM	FE-ND	2.04	2.01	1.94
2	G	601	HEM	CMB-C2B	2.04	1.55	1.50
2	B	302	HEM	CMA-C3A	2.03	1.54	1.50
2	A	601	HEM	CMA-C3A	2.02	1.54	1.50
2	B	302	HEM	CMB-C2B	2.02	1.54	1.50
2	C	601	HEM	CMC-C2C	2.02	1.54	1.50

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	302	HEM	CAA-C2A-C1A	-5.33	114.53	124.94
2	H	302	HEM	CAA-C2A-C3A	5.04	138.37	127.07
2	I	601	HEM	CAA-CBA-CGA	-4.74	101.09	113.67
2	I	601	HEM	CAA-C2A-C1A	4.61	133.94	124.94
2	A	601	HEM	CMA-C3A-C4A	-4.53	118.53	125.42
2	C	601	HEM	CHC-C1C-NC	4.38	129.22	124.45
2	C	601	HEM	CMA-C3A-C4A	-4.34	118.81	125.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	601	HEM	C3B-C2B-C1B	4.32	109.66	106.41
2	I	601	HEM	CAA-C2A-C3A	-4.26	117.52	127.07
2	A	601	HEM	CMA-C3A-C2A	3.76	133.59	125.62
2	D	303	HEM	CHB-C1B-NB	3.70	128.94	124.37
2	I	601	HEM	C4D-ND-C1D	3.69	109.57	105.21
2	C	601	HEM	CMA-C3A-C2A	3.64	133.34	125.62
2	I	601	HEM	C3D-C4D-ND	-3.41	106.44	110.17
2	C	601	HEM	CAC-C3C-C4C	3.31	132.72	124.82
2	C	601	HEM	CAA-C2A-C3A	3.28	134.42	127.07
2	C	601	HEM	CHD-C4C-C3C	3.25	130.69	125.21
2	H	302	HEM	CBA-CAA-C2A	3.25	121.51	112.53
2	H	302	HEM	C3B-C2B-C1B	3.22	108.83	106.41
2	F	302	HEM	C3B-C2B-C1B	3.21	108.82	106.41
2	I	601	HEM	C2A-C1A-NA	-3.20	106.60	110.15
2	C	601	HEM	C4D-ND-C1D	3.20	108.99	105.21
2	B	302	HEM	C3B-C2B-C1B	3.13	108.76	106.41
2	F	302	HEM	C3B-C4B-NB	-3.10	107.25	109.47
2	G	601	HEM	C3B-C2B-C1B	3.06	108.71	106.41
2	C	601	HEM	CAC-C3C-C2C	-3.04	118.55	128.43
2	I	601	HEM	CBA-CAA-C2A	2.98	120.78	112.53
2	C	601	HEM	CAA-C2A-C1A	-2.93	119.21	124.94
2	G	601	HEM	CHD-C4C-NC	2.87	127.58	124.45
2	G	601	HEM	C3B-C4B-NB	-2.86	107.41	109.47
2	D	303	HEM	CMA-C3A-C2A	2.83	131.64	125.62
2	C	601	HEM	CAD-C3D-C4D	2.83	129.62	124.70
2	C	601	HEM	C2D-C1D-ND	-2.78	106.69	109.90
2	B	302	HEM	C3B-C4B-NB	-2.78	107.47	109.47
2	J	303	HEM	C3B-C4B-NB	-2.75	107.49	109.47
2	E	601	HEM	C1B-NB-C4B	2.74	108.45	105.21
2	A	601	HEM	C4D-ND-C1D	2.71	108.42	105.21
2	D	303	HEM	CMA-C3A-C4A	-2.71	121.29	125.42
2	B	302	HEM	C1B-NB-C4B	2.71	108.41	105.21
2	G	601	HEM	C1B-NB-C4B	2.67	108.37	105.21
2	F	302	HEM	C4D-ND-C1D	2.67	108.37	105.21
2	C	601	HEM	CAD-C3D-C2D	-2.65	122.91	127.87
2	E	601	HEM	C4D-ND-C1D	2.63	108.32	105.21
2	F	302	HEM	CAA-CBA-CGA	-2.62	106.72	113.67
2	D	303	HEM	CHA-C4D-ND	2.61	127.60	124.37
2	D	303	HEM	C3B-C4B-NB	-2.59	107.61	109.47
2	F	302	HEM	C1B-NB-C4B	2.59	108.28	105.21
2	A	601	HEM	CAA-C2A-C3A	2.59	132.88	127.07
2	H	302	HEM	CHB-C1B-NB	2.58	127.56	124.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	302	HEM	CAA-CBA-CGA	-2.56	106.87	113.67
2	F	302	HEM	CHB-C1B-NB	2.49	127.45	124.37
2	E	601	HEM	CHB-C1B-NB	2.49	127.44	124.37
2	E	601	HEM	C2B-C1B-NB	-2.47	107.00	109.84
2	C	601	HEM	C3B-C2B-C1B	2.46	108.25	106.41
2	J	303	HEM	CMA-C3A-C4A	-2.41	121.75	125.42
2	B	302	HEM	CMA-C3A-C4A	-2.36	121.82	125.42
2	C	601	HEM	C3D-C4D-ND	-2.34	107.60	110.17
2	I	601	HEM	CHD-C1D-ND	2.31	126.91	124.42
4	D	301	GOL	C3-C2-C1	-2.31	103.33	111.80
2	C	601	HEM	CHD-C1D-ND	2.30	126.90	124.42
2	E	601	HEM	C3B-C4B-NB	-2.29	107.83	109.47
2	J	303	HEM	C3B-C2B-C1B	2.28	108.12	106.41
2	J	303	HEM	CMA-C3A-C2A	2.28	130.46	125.62
2	A	601	HEM	C3D-C4D-ND	-2.28	107.67	110.17
2	D	303	HEM	CAC-C3C-C4C	-2.26	119.41	124.82
2	I	601	HEM	CHA-C1A-C2A	2.25	130.22	125.30
2	D	303	HEM	CAA-CBA-CGA	-2.25	107.71	113.67
2	I	601	HEM	C2D-C1D-ND	-2.21	107.35	109.90
2	C	601	HEM	C4C-C3C-C2C	2.20	108.73	106.81
2	D	303	HEM	C4C-C3C-C2C	2.19	108.71	106.81
2	C	601	HEM	CHB-C4A-NA	2.17	127.80	123.86
2	J	303	HEM	CBD-CAD-C3D	-2.17	106.54	112.53
2	B	302	HEM	CBD-CAD-C3D	-2.16	106.55	112.53
2	C	601	HEM	C1D-C2D-C3D	2.16	109.25	106.98
2	H	302	HEM	CMA-C3A-C2A	2.16	130.21	125.62
2	A	601	HEM	CHA-C4D-ND	2.16	127.04	124.37
2	E	601	HEM	C3D-C4D-ND	-2.15	107.81	110.17
2	H	302	HEM	C1B-NB-C4B	2.15	107.75	105.21
2	A	601	HEM	C3B-C4B-NB	-2.14	107.93	109.47
2	D	303	HEM	CHD-C4C-NC	2.14	126.78	124.45
2	A	601	HEM	C1B-NB-C4B	2.14	107.74	105.21
2	G	601	HEM	CHB-C1B-NB	2.13	127.00	124.37
2	A	601	HEM	CAA-C2A-C1A	-2.13	120.78	124.94
2	D	303	HEM	CAA-C2A-C1A	-2.13	120.78	124.94
4	B	301	GOL	C3-C2-C1	-2.12	104.01	111.80
2	D	303	HEM	C3B-C2B-C1B	2.11	108.00	106.41
2	G	601	HEM	C2A-C1A-NA	-2.11	107.81	110.15
2	I	601	HEM	CMB-C2B-C1B	-2.11	121.74	125.03
2	A	601	HEM	O2D-CGD-CBD	2.10	120.63	114.00
2	B	302	HEM	CAA-C2A-C3A	2.10	131.77	127.07
2	G	601	HEM	CAC-C3C-C4C	-2.08	119.84	124.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	C3B-C2B-C1B	2.07	107.97	106.41
2	F	302	HEM	C3D-C4D-ND	-2.07	107.91	110.17
2	H	302	HEM	C3B-C4B-NB	-2.06	107.98	109.47
2	F	302	HEM	CHA-C4D-ND	2.05	126.90	124.37
2	D	303	HEM	C3D-C4D-ND	-2.05	107.92	110.17
2	A	601	HEM	CBA-CAA-C2A	2.05	118.20	112.53
2	G	601	HEM	C4D-ND-C1D	2.05	107.63	105.21
2	J	303	HEM	C4D-ND-C1D	2.05	107.63	105.21
2	C	601	HEM	CBA-CAA-C2A	2.03	118.15	112.53
2	E	601	HEM	C2A-C1A-NA	-2.01	107.93	110.15
2	J	303	HEM	C1B-NB-C4B	2.00	107.58	105.21

There are no chirality outliers.

All (76) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	HEM	C3A-C2A-CAA-CBA
2	D	303	HEM	C1A-C2A-CAA-CBA
2	D	303	HEM	C3A-C2A-CAA-CBA
2	H	302	HEM	C3D-CAD-CBD-CGD
2	I	601	HEM	C1A-C2A-CAA-CBA
4	C	603	GOL	O1-C1-C2-C3
4	E	603	GOL	C1-C2-C3-O3
4	G	603	GOL	C1-C2-C3-O3
4	H	301	GOL	O1-C1-C2-O2
4	H	301	GOL	O1-C1-C2-C3
4	I	603	GOL	C1-C2-C3-O3
4	J	301	GOL	C1-C2-C3-O3
4	J	302	GOL	C1-C2-C3-O3
2	C	601	HEM	C2D-C3D-CAD-CBD
2	C	601	HEM	C3A-C2A-CAA-CBA
2	H	302	HEM	C3A-C2A-CAA-CBA
2	C	601	HEM	C4D-C3D-CAD-CBD
2	A	601	HEM	C1A-C2A-CAA-CBA
2	H	302	HEM	C1A-C2A-CAA-CBA
2	I	601	HEM	C3A-C2A-CAA-CBA
2	C	601	HEM	C1A-C2A-CAA-CBA
2	E	601	HEM	C3D-CAD-CBD-CGD
4	D	301	GOL	C1-C2-C3-O3
4	E	604	GOL	O1-C1-C2-C3
4	E	603	GOL	O2-C2-C3-O3
2	B	302	HEM	C1A-C2A-CAA-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	C	603	GOL	O1-C1-C2-O2
4	G	603	GOL	O2-C2-C3-O3
4	I	603	GOL	O2-C2-C3-O3
4	J	302	GOL	O2-C2-C3-O3
2	B	302	HEM	C3A-C2A-CAA-CBA
4	D	302	GOL	O2-C2-C3-O3
4	J	301	GOL	O2-C2-C3-O3
2	H	302	HEM	C2A-CAA-CBA-CGA
4	D	301	GOL	O1-C1-C2-O2
4	E	604	GOL	O1-C1-C2-O2
2	B	302	HEM	C3D-CAD-CBD-CGD
2	B	302	HEM	C4B-C3B-CAB-CBB
2	C	601	HEM	C4B-C3B-CAB-CBB
2	E	601	HEM	C4B-C3B-CAB-CBB
2	F	302	HEM	C4B-C3B-CAB-CBB
2	G	601	HEM	C4B-C3B-CAB-CBB
2	H	302	HEM	C4B-C3B-CAB-CBB
2	A	601	HEM	CAD-CBD-CGD-O1D
2	D	303	HEM	CAA-CBA-CGA-O1A
2	H	302	HEM	CAA-CBA-CGA-O1A
4	F	301	GOL	O1-C1-C2-C3
2	H	302	HEM	CAA-CBA-CGA-O2A
2	D	303	HEM	CAA-CBA-CGA-O2A
2	B	302	HEM	CAD-CBD-CGD-O1D
2	A	601	HEM	CAD-CBD-CGD-O2D
2	B	302	HEM	CAD-CBD-CGD-O2D
2	I	601	HEM	CAA-CBA-CGA-O2A
2	C	601	HEM	CAD-CBD-CGD-O1D
2	I	601	HEM	CAA-CBA-CGA-O1A
2	C	601	HEM	CAD-CBD-CGD-O2D
2	J	303	HEM	CAD-CBD-CGD-O2D
2	G	601	HEM	C2A-CAA-CBA-CGA
2	D	303	HEM	CAD-CBD-CGD-O1D
2	F	302	HEM	CAD-CBD-CGD-O2D
2	I	601	HEM	CAD-CBD-CGD-O2D
2	D	303	HEM	CAD-CBD-CGD-O2D
2	G	601	HEM	CAD-CBD-CGD-O2D
4	A	604	GOL	O1-C1-C2-C3
2	J	303	HEM	CAD-CBD-CGD-O1D
2	F	302	HEM	CAD-CBD-CGD-O1D
2	I	601	HEM	CAD-CBD-CGD-O1D
2	G	601	HEM	CAD-CBD-CGD-O1D

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	601	HEM	CAA-CBA-CGA-O2A
2	J	303	HEM	C3A-C2A-CAA-CBA
2	C	601	HEM	CAA-CBA-CGA-O1A
2	H	302	HEM	CAD-CBD-CGD-O2D
2	J	303	HEM	CAA-CBA-CGA-O2A
2	J	303	HEM	CAA-CBA-CGA-O1A
2	G	601	HEM	CAA-CBA-CGA-O1A
2	A	601	HEM	CAA-CBA-CGA-O1A

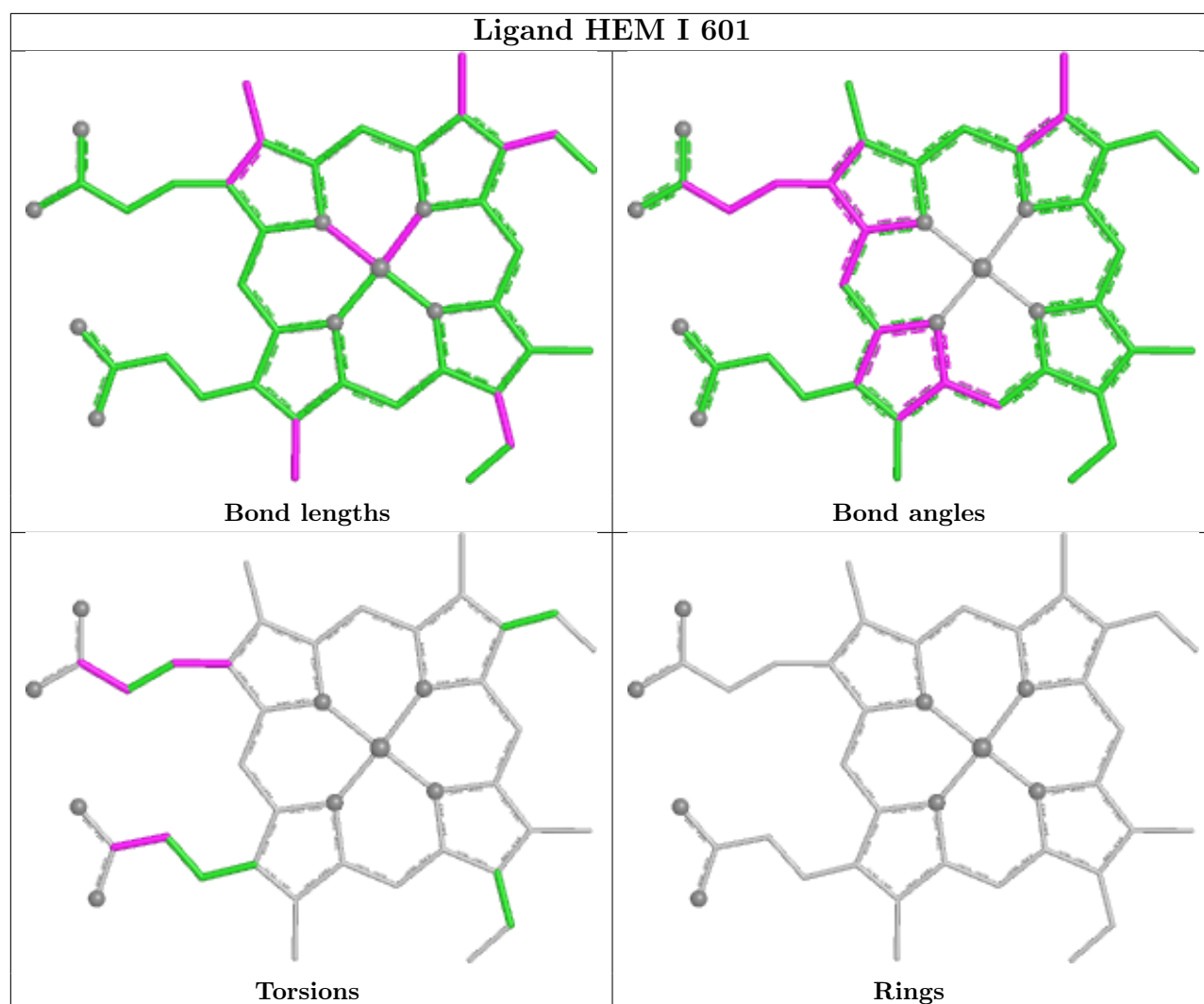
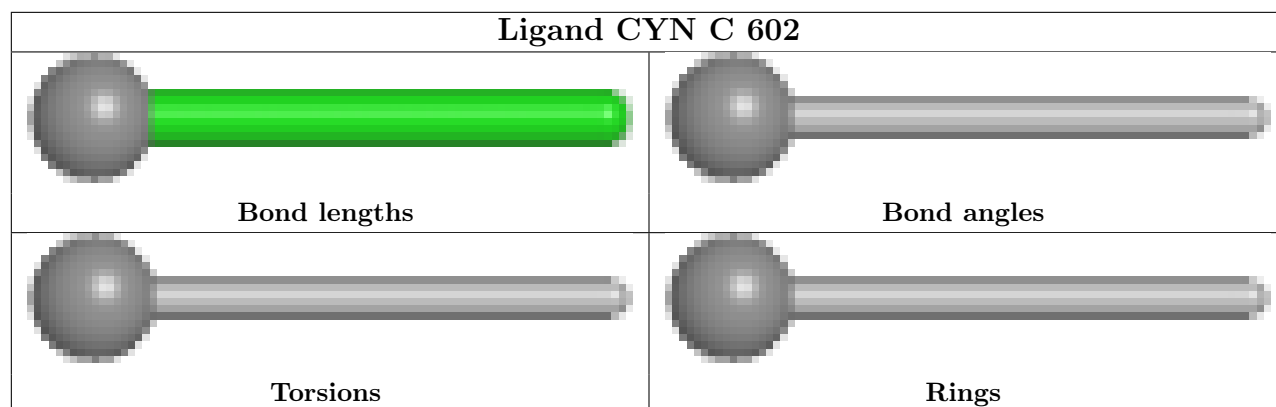
There are no ring outliers.

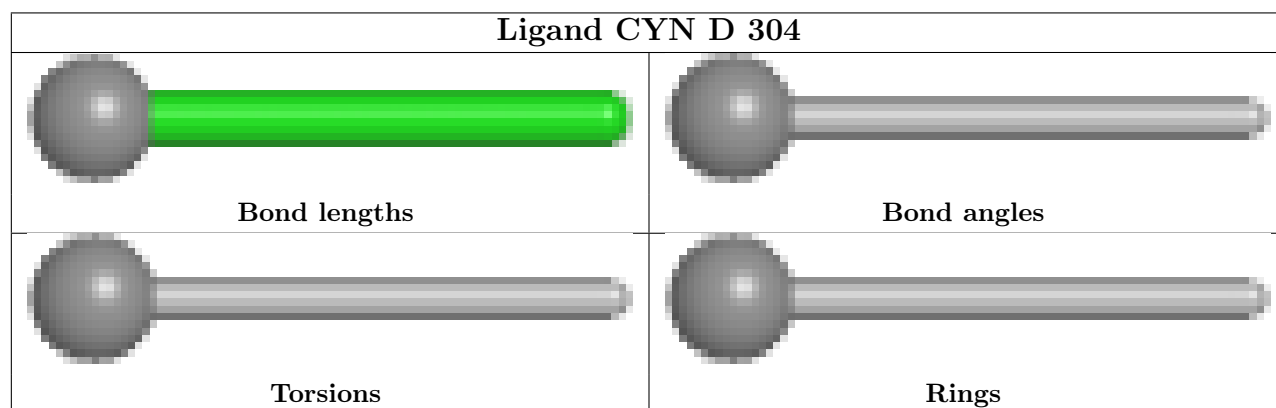
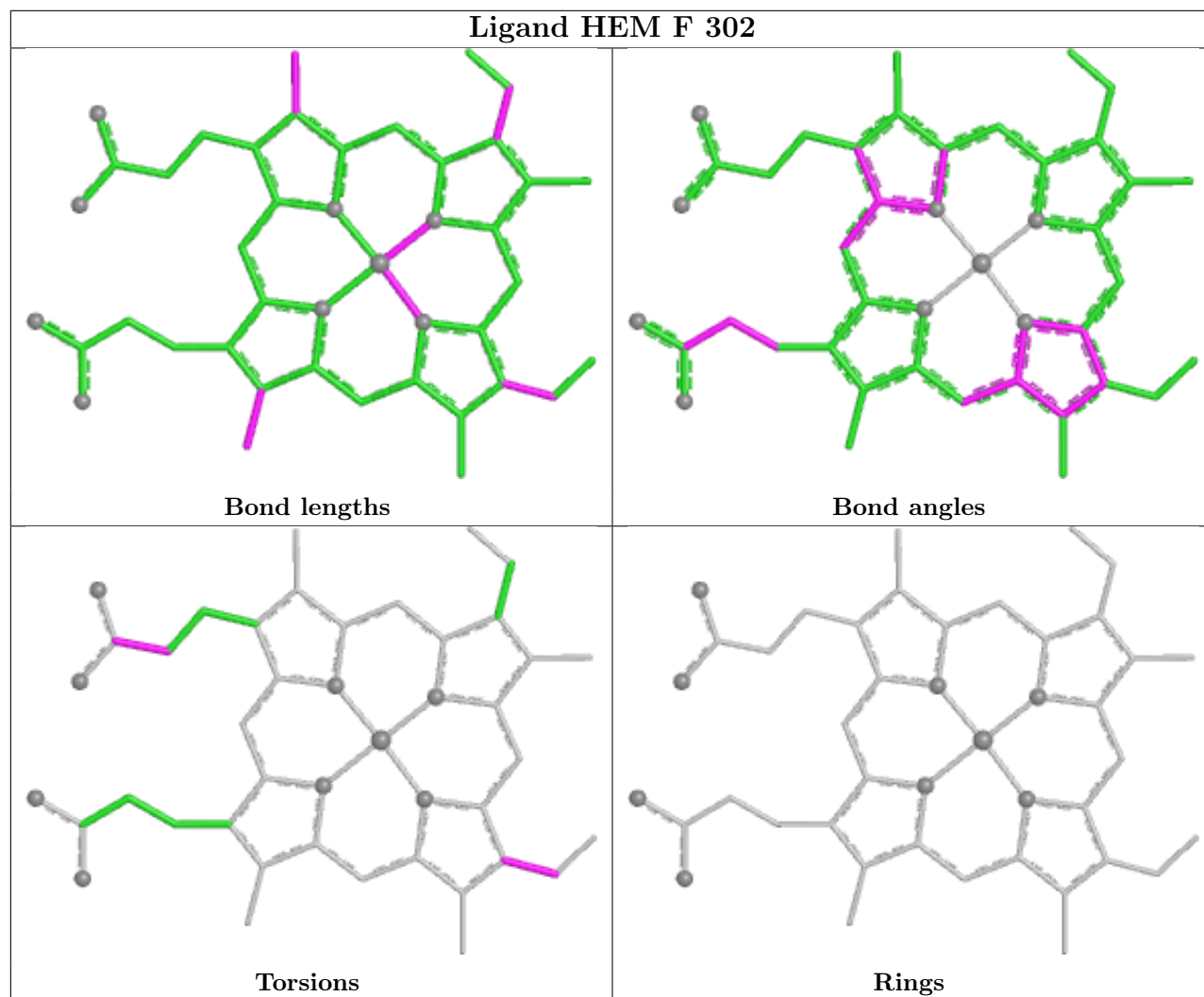
17 monomers are involved in 39 short contacts:

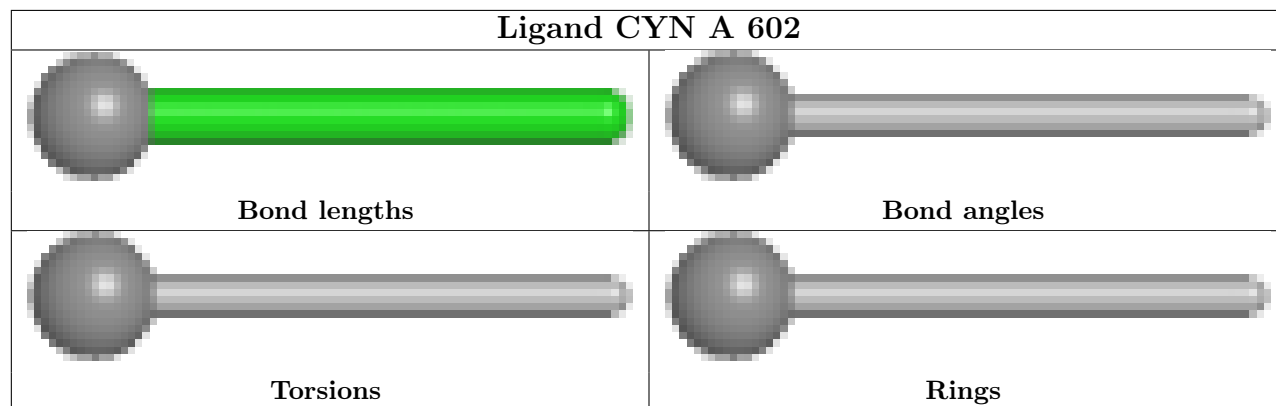
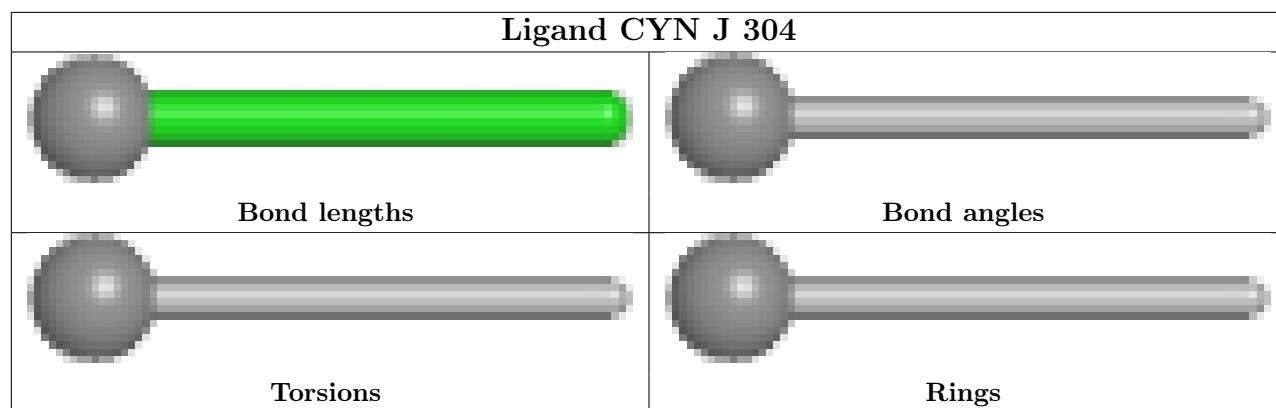
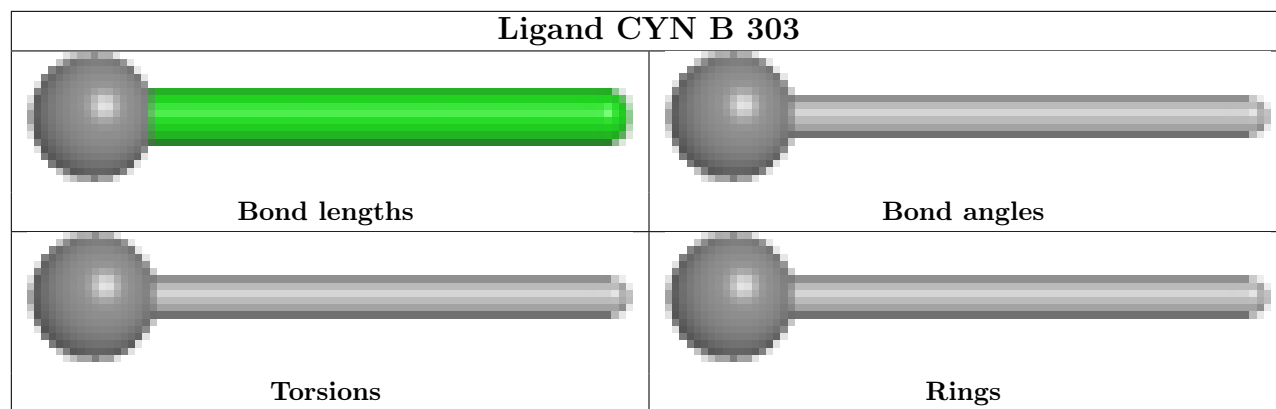
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	601	HEM	2	0
2	F	302	HEM	3	0
2	D	303	HEM	3	0
4	A	603	GOL	3	0
4	J	302	GOL	1	0
4	F	301	GOL	2	0
2	C	601	HEM	5	0
2	E	601	HEM	2	0
2	G	601	HEM	2	0
4	A	604	GOL	1	0
2	B	302	HEM	3	0
2	J	303	HEM	3	0
4	B	301	GOL	1	0
4	E	603	GOL	1	0
2	H	302	HEM	2	0
4	D	302	GOL	3	0
4	G	603	GOL	2	0

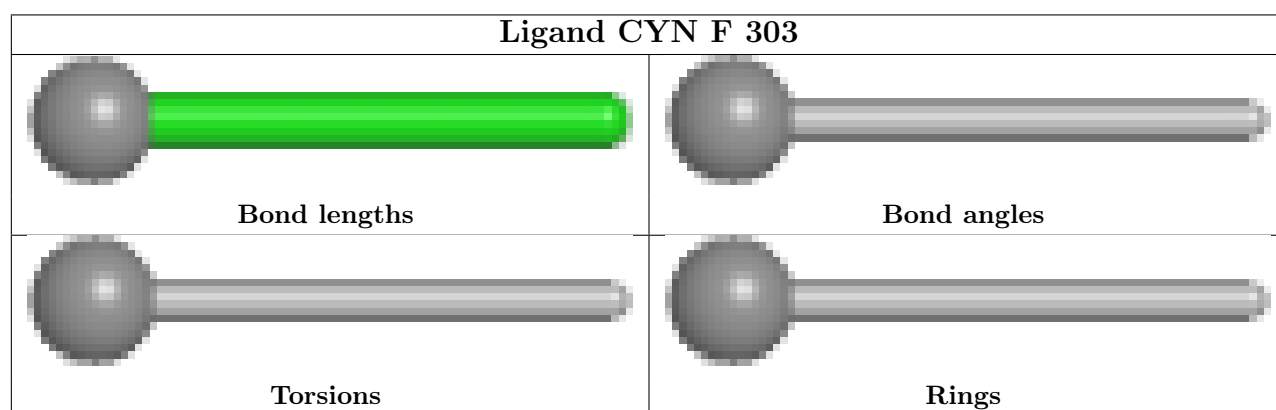
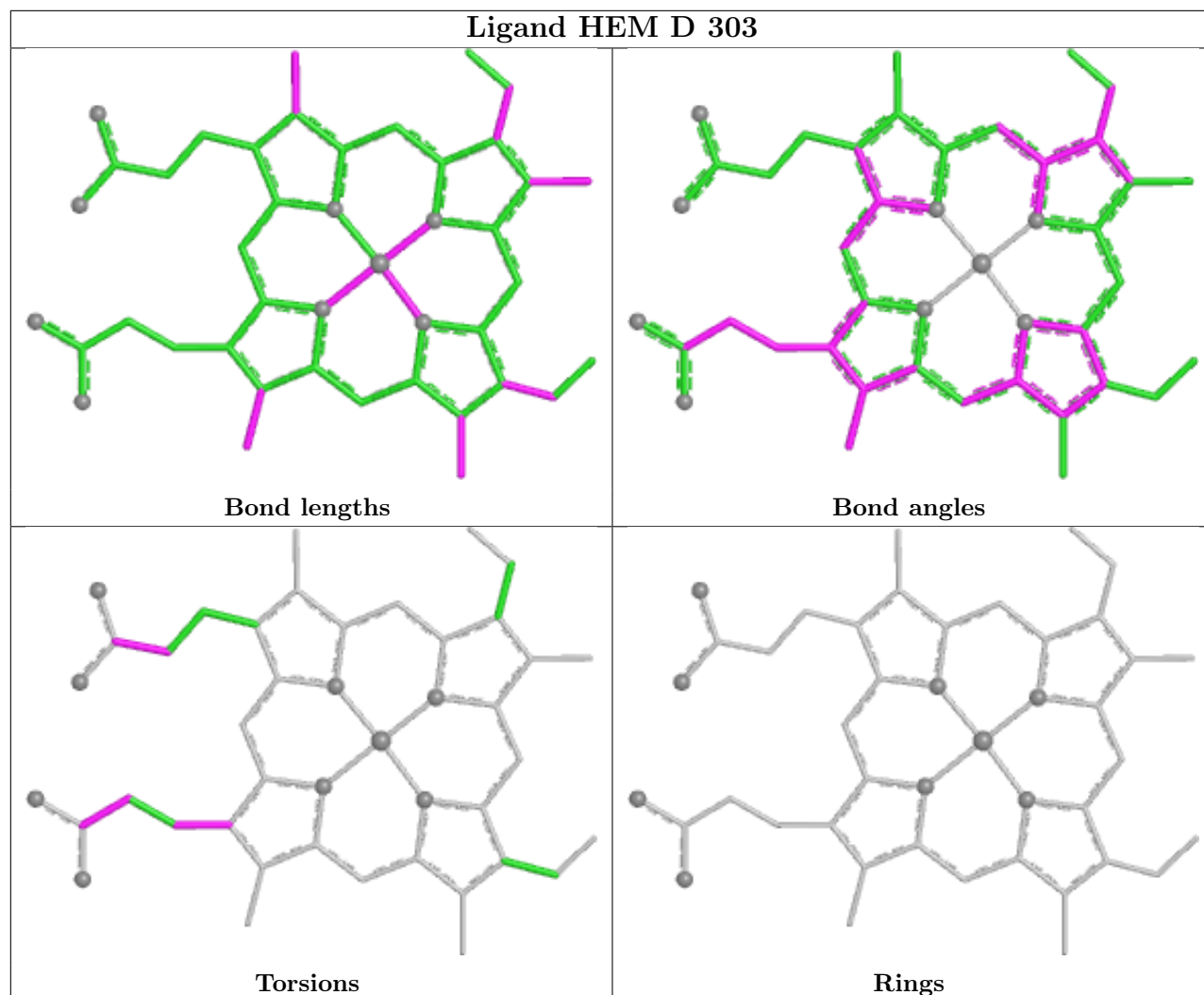
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

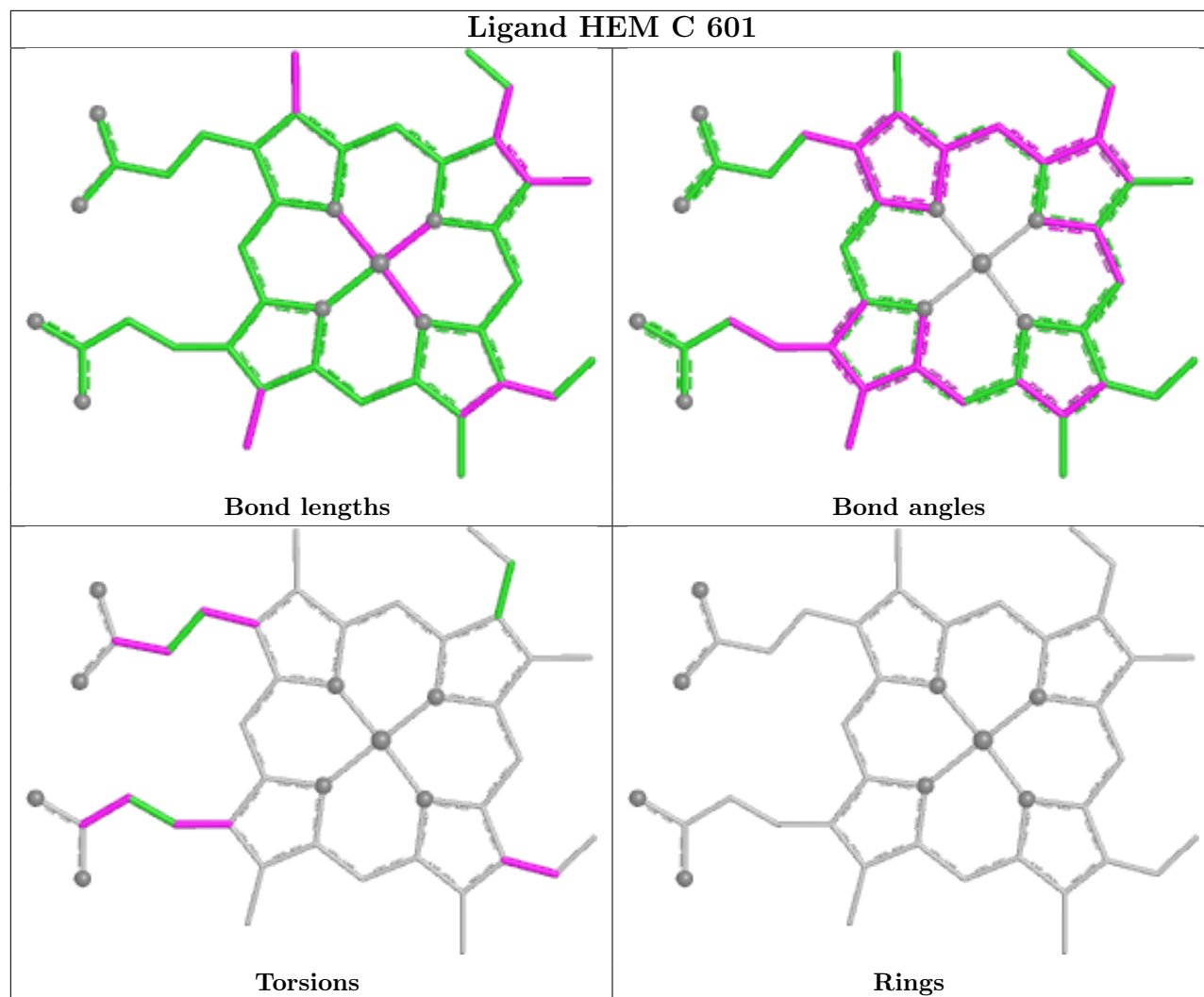
equivalents in the CSD to analyse the geometry.

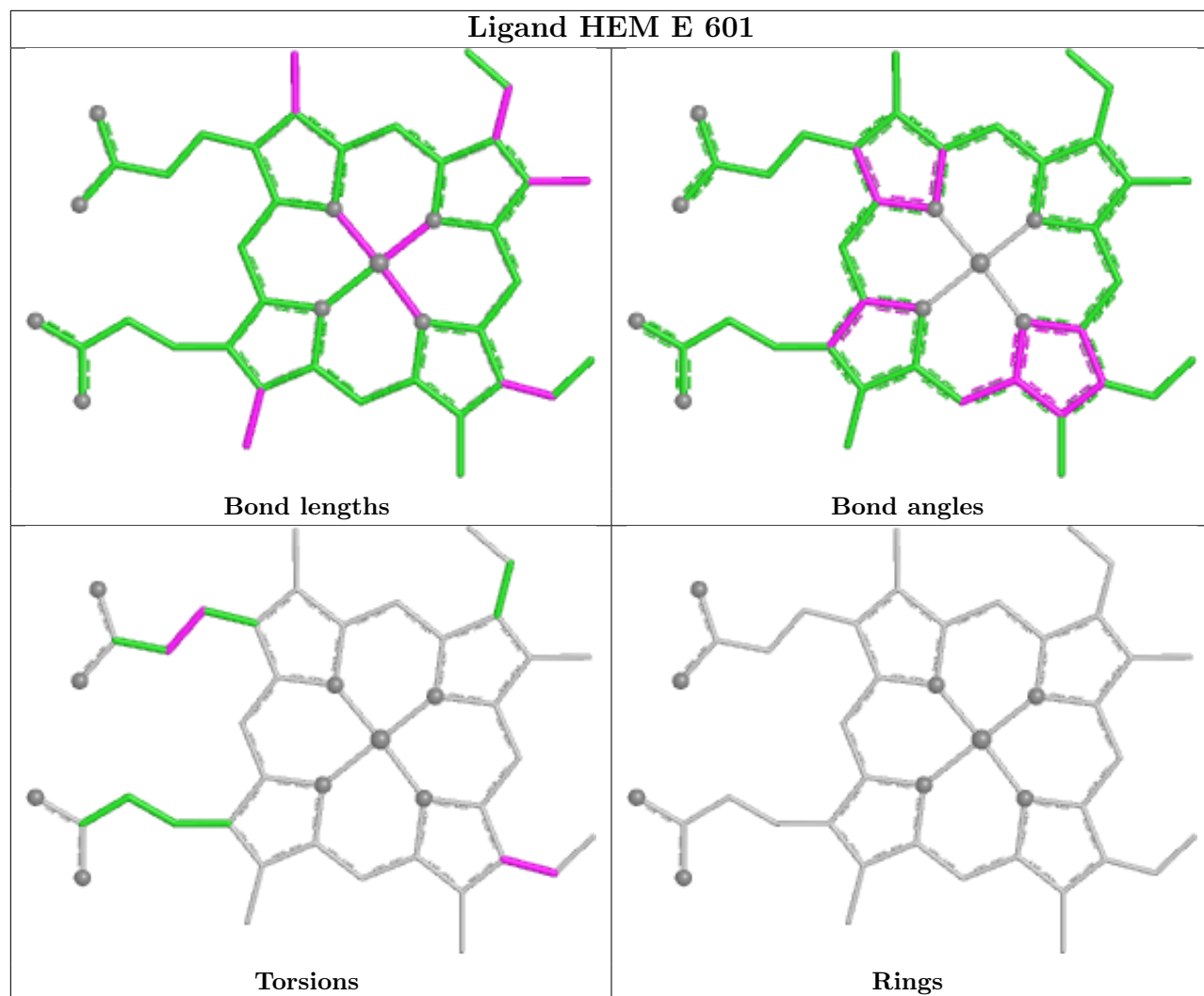


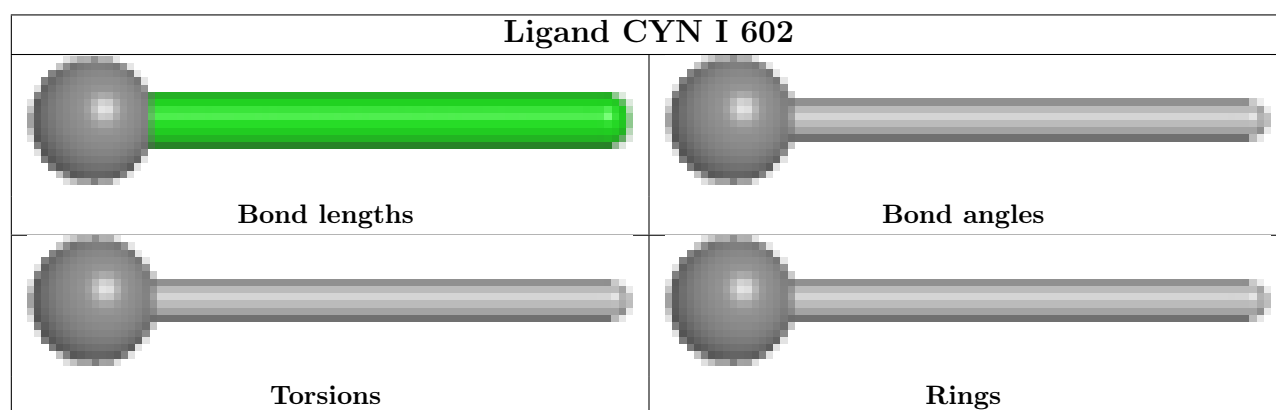
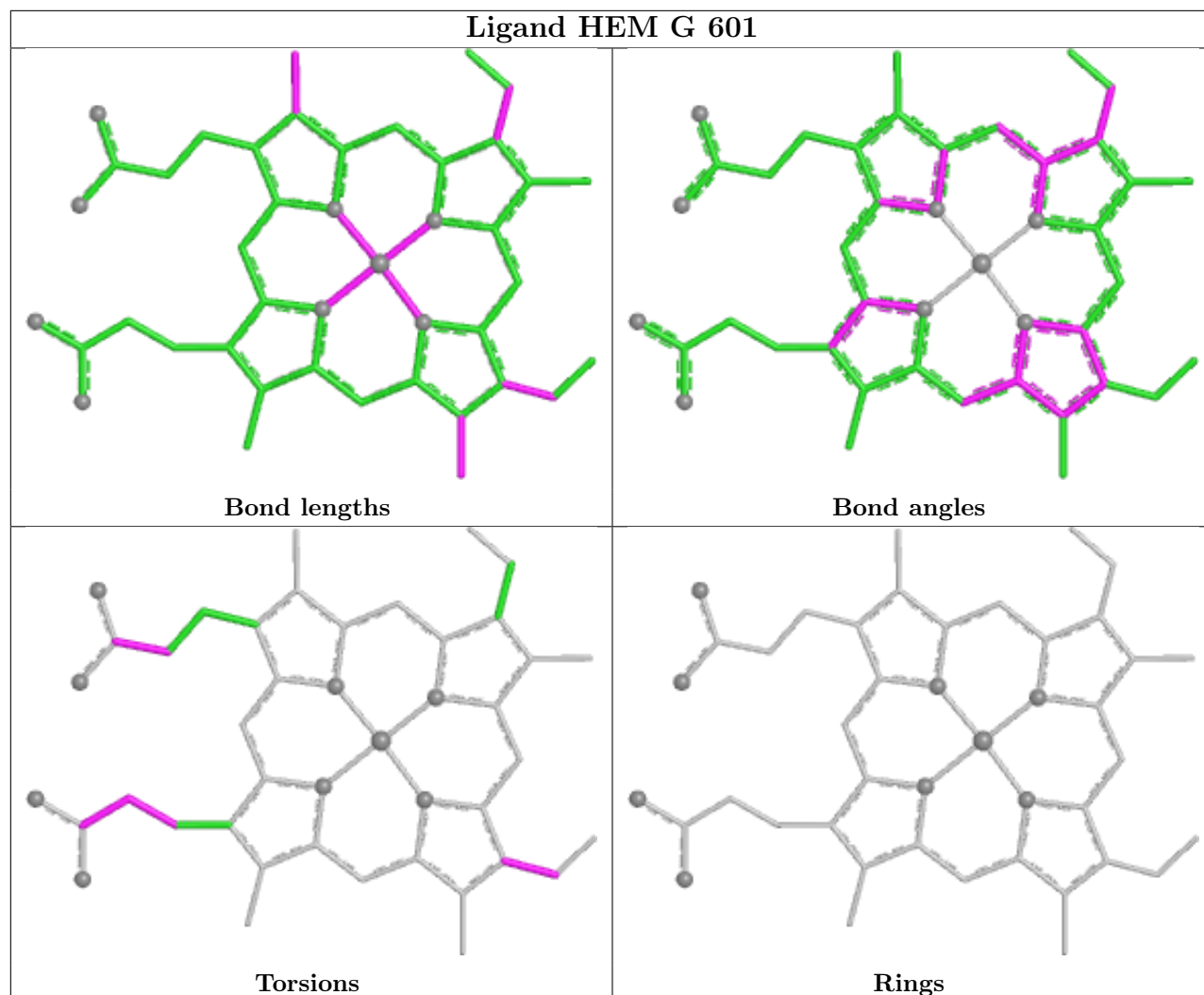


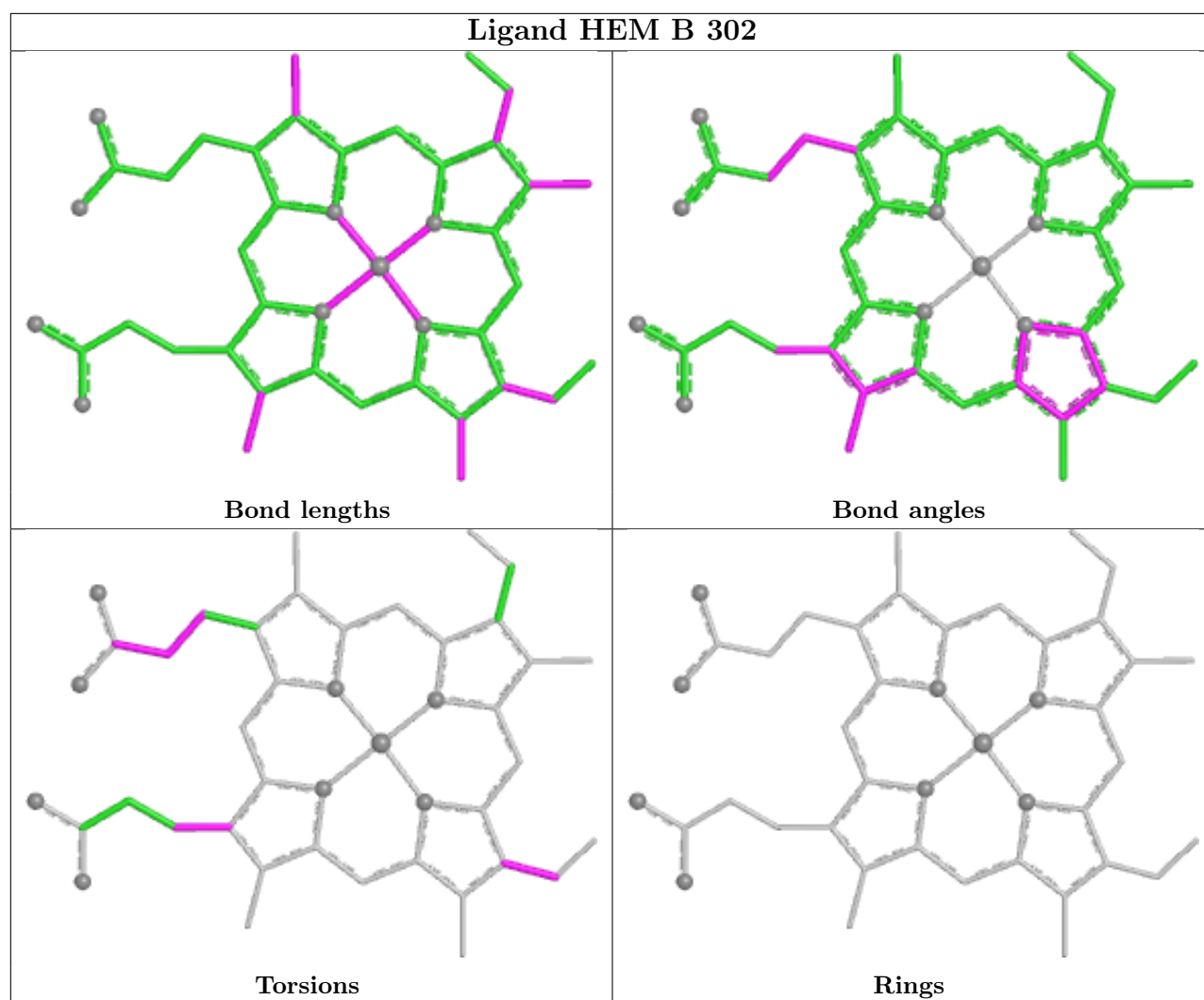




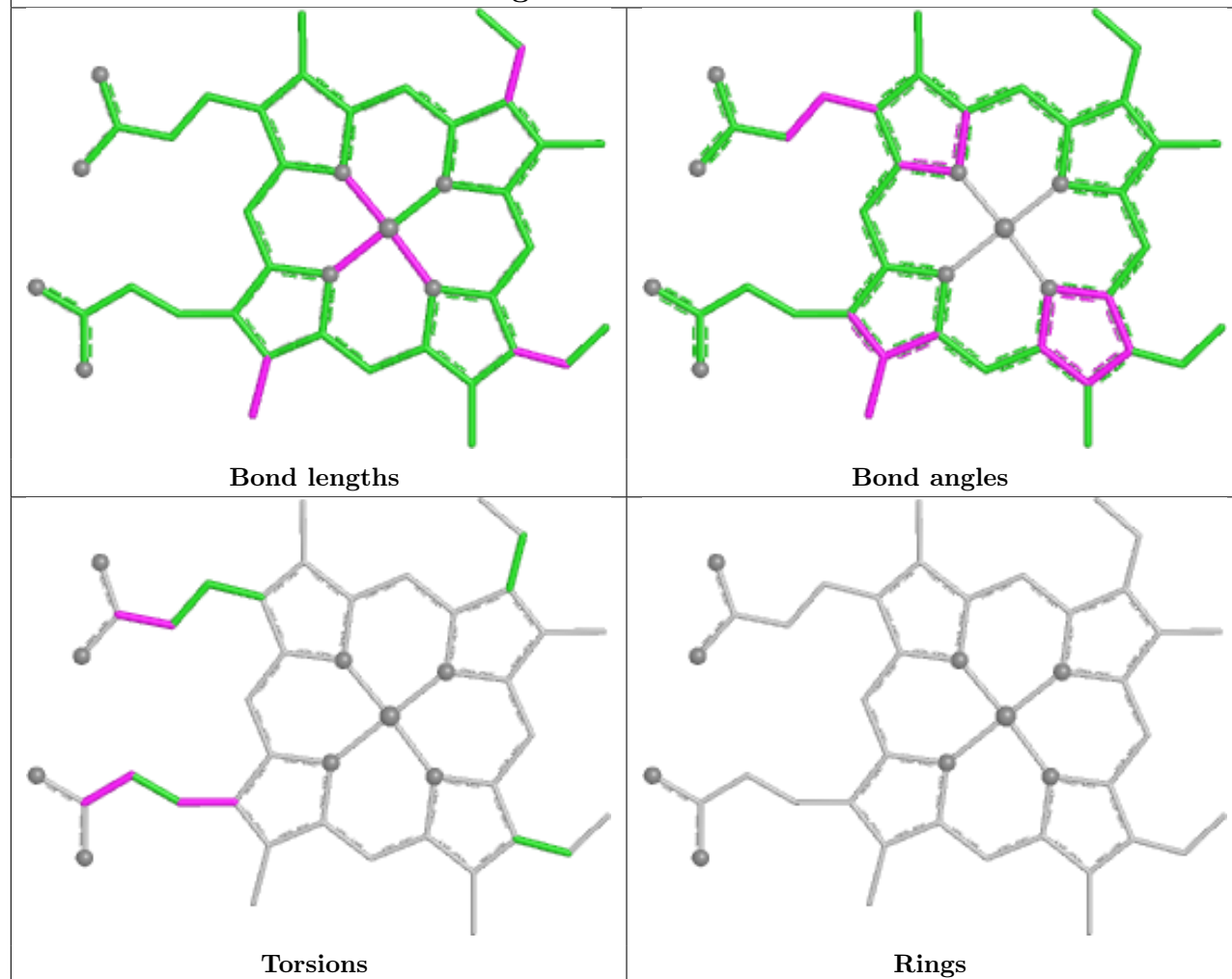


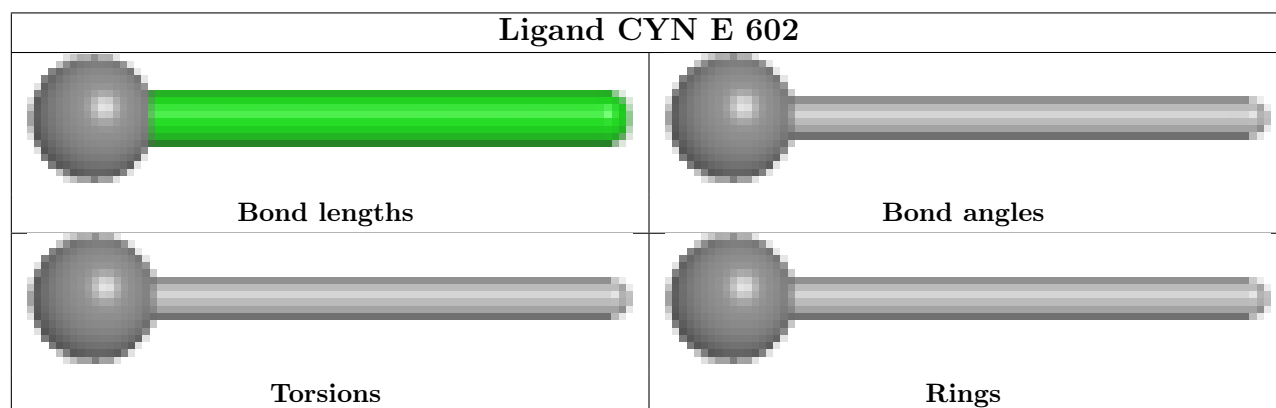
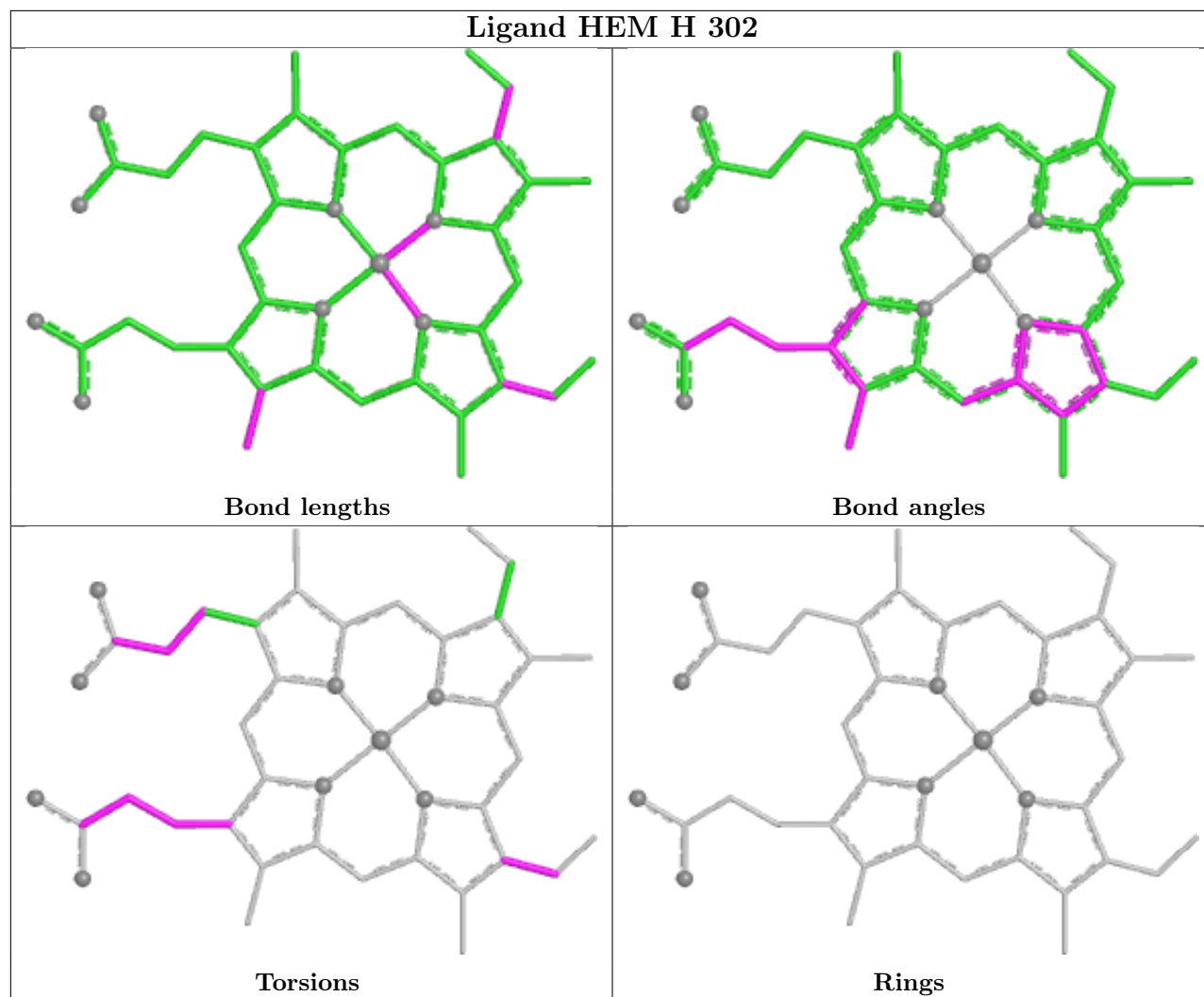


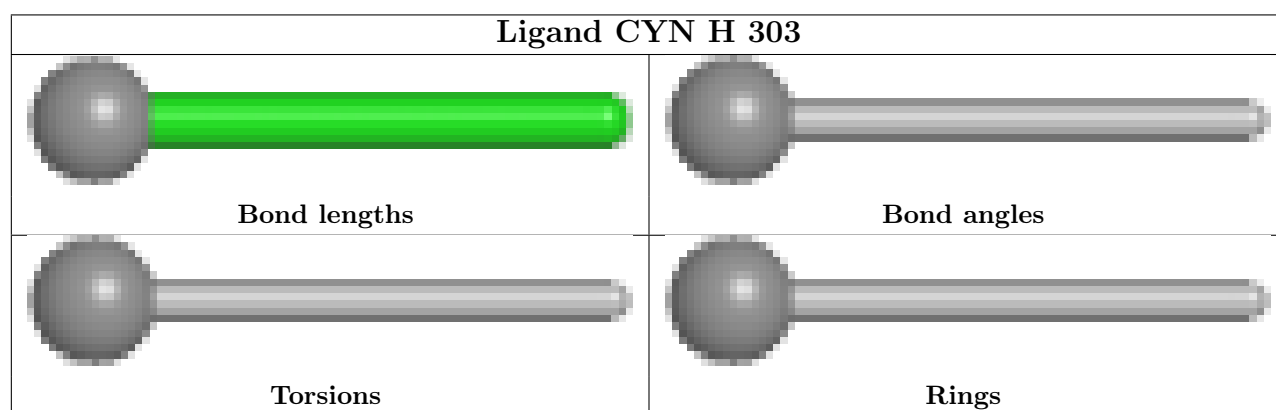
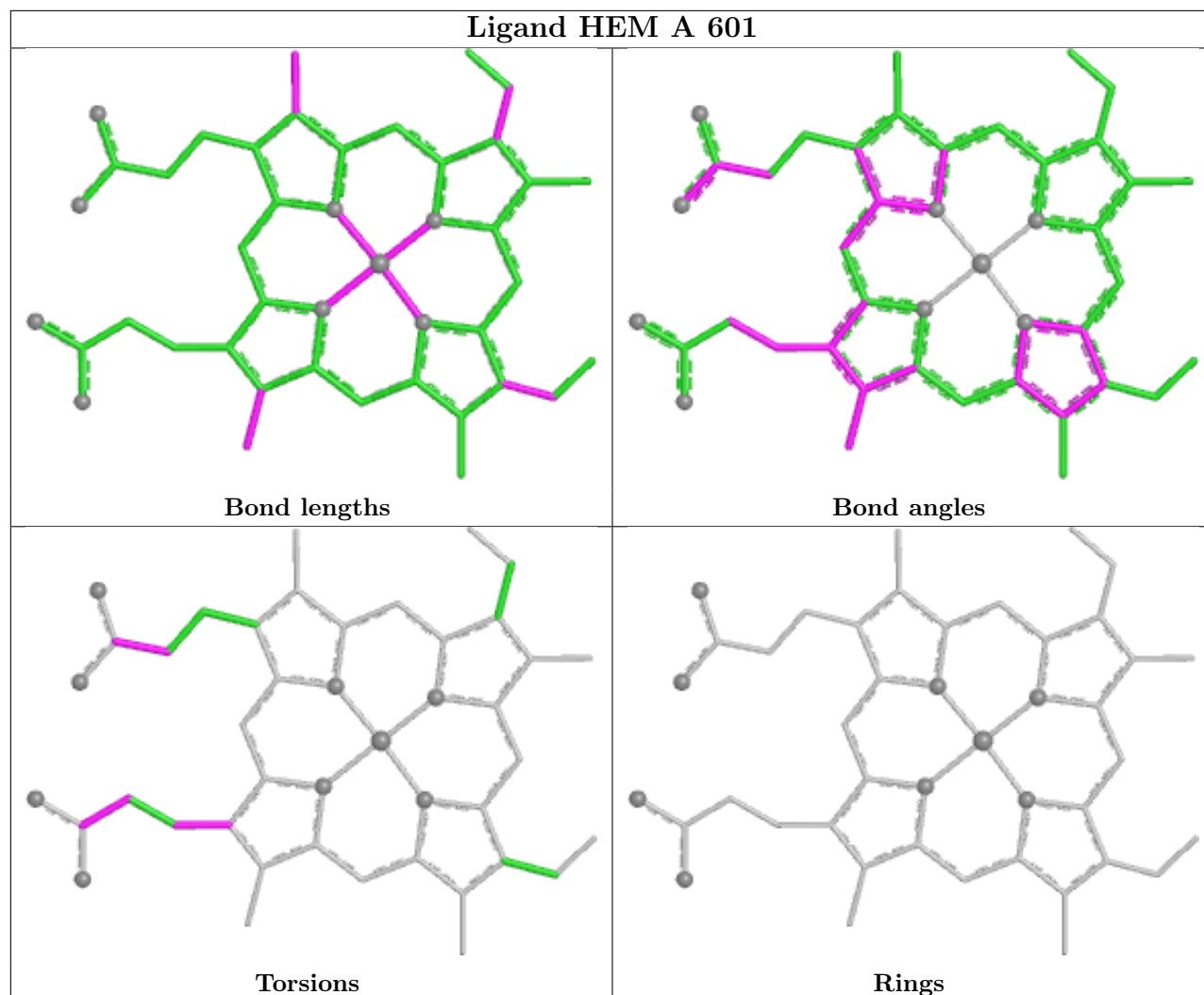


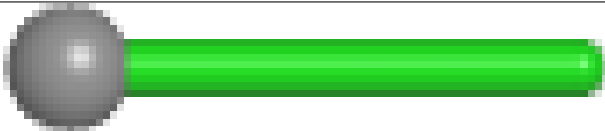
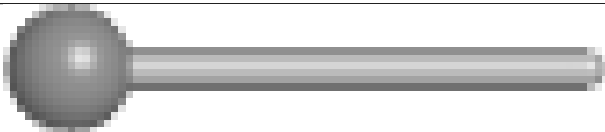
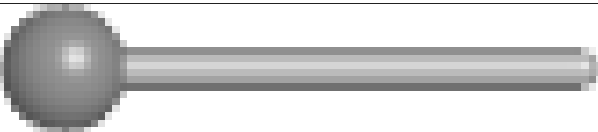


Ligand HEM J 303







Ligand CYN G 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	253/273 (92%)	0.49	22 (8%) 16 13	41, 92, 208, 288	3 (1%)
1	B	253/273 (92%)	0.62	26 (10%) 12 10	56, 113, 225, 261	0
1	C	251/273 (91%)	0.66	25 (9%) 12 10	60, 112, 228, 313	0
1	D	253/273 (92%)	0.41	19 (7%) 20 17	45, 89, 196, 255	1 (0%)
1	E	251/273 (91%)	0.61	21 (8%) 17 14	68, 112, 240, 277	0
1	F	251/273 (91%)	0.80	35 (13%) 6 5	66, 137, 246, 305	0
1	G	249/273 (91%)	0.75	26 (10%) 11 10	69, 136, 231, 309	0
1	H	249/273 (91%)	0.68	23 (9%) 14 12	53, 134, 250, 339	1 (0%)
1	I	251/273 (91%)	0.74	31 (12%) 8 7	73, 168, 266, 333	0
1	J	251/273 (91%)	0.83	35 (13%) 6 5	53, 159, 279, 356	1 (0%)
All	All	2512/2730 (92%)	0.66	263 (10%) 11 9	41, 119, 247, 356	6 (0%)

All (263) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	216	ILE	9.9
1	A	215	ILE	9.7
1	B	214	HIS	7.8
1	F	110	LEU	6.7
1	J	78	ILE	6.6
1	D	22	ILE	6.2
1	J	62	PHE	6.2
1	B	51	ILE	6.1
1	E	274	VAL	5.8
1	B	215	ILE	5.4
1	G	215	ILE	5.4
1	J	110	LEU	5.3
1	C	51	ILE	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	62	PHE	4.9
1	A	210	THR	4.8
1	D	215	ILE	4.7
1	A	34	LEU	4.6
1	G	110	LEU	4.6
1	H	51	ILE	4.5
1	I	34	LEU	4.5
1	F	215	ILE	4.5
1	C	95	ALA	4.5
1	A	212	ASP	4.4
1	C	215	ILE	4.4
1	G	78	ILE	4.4
1	H	26	GLY	4.3
1	H	110	LEU	4.3
1	F	34	LEU	4.2
1	C	271	SER	4.2
1	E	51	ILE	4.2
1	J	81	VAL	4.2
1	I	51	ILE	4.1
1	C	214	HIS	4.1
1	E	273	LEU	4.1
1	J	34	LEU	4.1
1	D	51	ILE	4.1
1	G	51	ILE	4.1
1	J	32	LEU	4.0
1	F	111	ILE	4.0
1	B	211	SER	3.9
1	I	30	TRP	3.9
1	C	213	PRO	3.8
1	F	37	TRP	3.8
1	J	218	ILE	3.8
1	I	217	GLY	3.8
1	H	32	LEU	3.8
1	I	78	ILE	3.8
1	B	62	PHE	3.8
1	G	273	LEU	3.7
1	D	213	PRO	3.7
1	F	214	HIS	3.7
1	F	269	LEU	3.6
1	I	41	TRP	3.6
1	A	211	SER	3.6
1	F	62	PHE	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	273	LEU	3.6
1	D	216	ILE	3.6
1	A	96	GLY	3.6
1	J	95	ALA	3.6
1	H	116	GLY	3.5
1	J	217	GLY	3.5
1	D	37	TRP	3.5
1	F	213	PRO	3.5
1	I	88	PHE	3.5
1	E	110	LEU	3.5
1	I	100	ALA	3.5
1	E	88	PHE	3.5
1	C	212	ASP	3.5
1	A	269	LEU	3.5
1	I	49	LEU	3.5
1	F	27	VAL	3.5
1	H	59	TYR	3.4
1	J	216	ILE	3.4
1	C	211	SER	3.4
1	C	216	ILE	3.4
1	B	49	LEU	3.4
1	H	49	LEU	3.4
1	H	274	VAL	3.4
1	E	100	ALA	3.4
1	A	218	ILE	3.4
1	J	37	TRP	3.4
1	H	260	GLN	3.4
1	H	27	VAL	3.4
1	J	51	ILE	3.3
1	E	264	ALA	3.3
1	H	88	PHE	3.3
1	F	51	ILE	3.3
1	J	59	TYR	3.3
1	H	125	PHE	3.3
1	J	74	VAL	3.3
1	D	97	THR	3.2
1	G	218	ILE	3.2
1	B	95	ALA	3.2
1	J	215	ILE	3.2
1	A	100	ALA	3.2
1	B	269	LEU	3.2
1	C	96	GLY	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	22	ILE	3.2
1	A	146[A]	ARG	3.1
1	E	118	ALA	3.1
1	J	118	ALA	3.1
1	D	214	HIS	3.1
1	I	215	ILE	3.1
1	C	88	PHE	3.1
1	F	88	PHE	3.1
1	J	111	ILE	3.1
1	A	266	LEU	3.0
1	D	273	LEU	3.0
1	B	213	PRO	3.0
1	A	209	THR	3.0
1	F	24	GLY	3.0
1	G	213	PRO	3.0
1	H	120	HIS	3.0
1	F	212	ASP	3.0
1	F	266	LEU	2.9
1	G	132	LYS	2.9
1	G	26	GLY	2.9
1	F	36	THR	2.9
1	I	74	VAL	2.9
1	E	260	GLN	2.9
1	G	124	ILE	2.9
1	G	59	TYR	2.9
1	C	210	THR	2.9
1	I	110	LEU	2.9
1	J	61	LEU	2.9
1	G	30	TRP	2.8
1	C	100	ALA	2.8
1	E	267	GLN	2.8
1	J	126	LEU	2.8
1	J	27	VAL	2.8
1	H	218	ILE	2.8
1	D	211	SER	2.8
1	I	59	TYR	2.8
1	C	91	SER	2.8
1	E	271	SER	2.8
1	G	34	LEU	2.8
1	G	217	GLY	2.8
1	J	48	LEU	2.8
1	J	273	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	56	PRO	2.7
1	I	212	ASP	2.7
1	I	213	PRO	2.7
1	A	97	THR	2.7
1	B	34	LEU	2.6
1	F	48	LEU	2.6
1	G	115	ALA	2.6
1	B	29	THR	2.6
1	A	37	TRP	2.6
1	C	62	PHE	2.6
1	E	62	PHE	2.6
1	F	92	PHE	2.6
1	G	106	ALA	2.6
1	C	269	LEU	2.6
1	B	81	VAL	2.6
1	E	263	GLN	2.6
1	B	37	TRP	2.5
1	C	64	SER	2.5
1	J	124	ILE	2.5
1	A	214	HIS	2.5
1	J	150[A]	HIS	2.5
1	B	77	ALA	2.5
1	C	34	LEU	2.5
1	G	36	THR	2.5
1	F	103	TRP	2.5
1	G	214	HIS	2.5
1	F	219	GLY	2.5
1	C	94	VAL	2.5
1	G	74	VAL	2.5
1	I	48	LEU	2.4
1	J	211	SER	2.4
1	J	24	GLY	2.4
1	I	126	LEU	2.4
1	I	219	GLY	2.4
1	B	212	ASP	2.4
1	F	125	PHE	2.4
1	F	97	THR	2.4
1	F	98	SER	2.4
1	B	52	GLY	2.4
1	A	38	ALA	2.4
1	B	48	LEU	2.3
1	J	121	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	97	THR	2.3
1	C	68	PRO	2.3
1	H	109	GLY	2.3
1	J	116	GLY	2.3
1	B	266	LEU	2.3
1	I	39	LEU	2.3
1	F	59	TYR	2.3
1	F	87	GLY	2.3
1	I	90	VAL	2.3
1	B	25	PHE	2.3
1	J	97	THR	2.3
1	D	54	ASP	2.3
1	I	24	GLY	2.3
1	I	81	VAL	2.3
1	F	49	LEU	2.3
1	E	78	ILE	2.3
1	F	95	ALA	2.3
1	F	262	THR	2.3
1	D	23	GLU	2.3
1	B	274	VAL	2.3
1	E	34	LEU	2.3
1	J	49	LEU	2.3
1	H	118	ALA	2.2
1	J	174	ARG	2.2
1	H	68	PRO	2.2
1	C	49	LEU	2.2
1	F	100	ALA	2.2
1	G	95	ALA	2.2
1	I	124	ILE	2.2
1	E	24	GLY	2.2
1	E	26	GLY	2.2
1	E	86	GLY	2.2
1	F	228	ASP	2.2
1	B	32	LEU	2.2
1	G	61	LEU	2.2
1	D	94	VAL	2.2
1	C	32	LEU	2.2
1	F	25	PHE	2.2
1	J	68	PRO	2.2
1	E	52	GLY	2.2
1	I	273	LEU	2.2
1	J	120	HIS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	29	THR	2.1
1	H	79	LYS	2.1
1	H	34	LEU	2.1
1	A	274	VAL	2.1
1	A	95	ALA	2.1
1	I	38	ALA	2.1
1	J	41	TRP	2.1
1	G	117	THR	2.1
1	A	273	LEU	2.1
1	B	59	TYR	2.1
1	I	52	GLY	2.1
1	I	274	VAL	2.1
1	H	62	PHE	2.1
1	B	45	ALA	2.1
1	D	84	ARG	2.1
1	D	262	THR	2.1
1	H	217	GLY	2.1
1	A	216	ILE	2.1
1	G	27	VAL	2.1
1	H	115	ALA	2.1
1	I	211	SER	2.1
1	F	117	THR	2.1
1	I	61	LEU	2.1
1	I	269	LEU	2.1
1	B	41	TRP	2.0
1	E	257	THR	2.0
1	D	269	LEU	2.0
1	C	25	PHE	2.0
1	J	25	PHE	2.0
1	E	95	ALA	2.0
1	F	79	LYS	2.0
1	F	211	SER	2.0
1	C	262	THR	2.0
1	A	121	LEU	2.0
1	D	55	GLN	2.0
1	F	273	LEU	2.0
1	G	266	LEU	2.0
1	B	111	ILE	2.0
1	D	78	ILE	2.0
1	D	218	ILE	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($\text{\AA}^2$)	Q<0.9
3	CYN	G	602	2/2	0.88	0.22	101,101,101,102	0
4	GOL	C	603	6/6	0.88	0.19	63,83,85,88	0
4	GOL	J	302	6/6	0.90	0.17	91,94,99,107	0
3	CYN	J	304	2/2	0.93	0.17	112,112,112,113	0
4	GOL	I	603	6/6	0.93	0.16	93,103,107,117	0
4	GOL	A	604	6/6	0.93	0.14	75,80,87,90	0
3	CYN	B	303	2/2	0.94	0.20	74,74,74,80	0
4	GOL	E	603	6/6	0.94	0.33	79,83,85,89	0
4	GOL	E	604	6/6	0.94	0.15	82,98,98,98	0
4	GOL	F	301	6/6	0.94	0.13	84,85,94,95	0
4	GOL	G	604	6/6	0.94	0.14	90,98,99,101	0
3	CYN	A	602	2/2	0.94	0.21	68,68,68,76	0
4	GOL	J	301	6/6	0.94	0.14	89,90,91,98	0
4	GOL	B	301	6/6	0.94	0.13	70,81,83,83	0
3	CYN	D	304	2/2	0.95	0.21	74,74,74,98	0
4	GOL	D	302	6/6	0.95	0.37	73,75,82,84	0
4	GOL	A	603	6/6	0.95	0.26	74,78,83,83	0
3	CYN	I	602	2/2	0.96	0.14	101,101,101,114	0
4	GOL	H	301	6/6	0.96	0.10	84,95,95,96	0
3	CYN	F	303	2/2	0.96	0.17	98,98,98,106	0
3	CYN	E	602	2/2	0.96	0.14	79,79,79,83	0
4	GOL	D	301	6/6	0.96	0.11	72,79,81,82	0
2	HEM	D	303	43/43	0.97	0.11	56,74,102,118	0
2	HEM	G	601	43/43	0.97	0.11	76,98,128,137	0
3	CYN	C	602	2/2	0.97	0.15	89,89,89,91	0
3	CYN	H	303	2/2	0.97	0.16	98,98,98,102	0
2	HEM	J	303	43/43	0.97	0.12	88,112,136,147	0

Continued on next page...

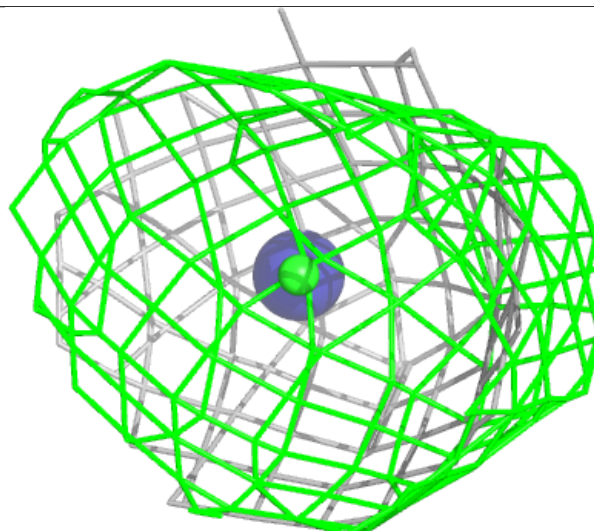
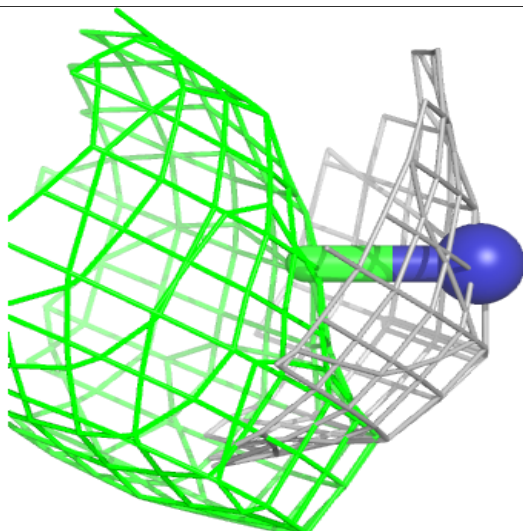
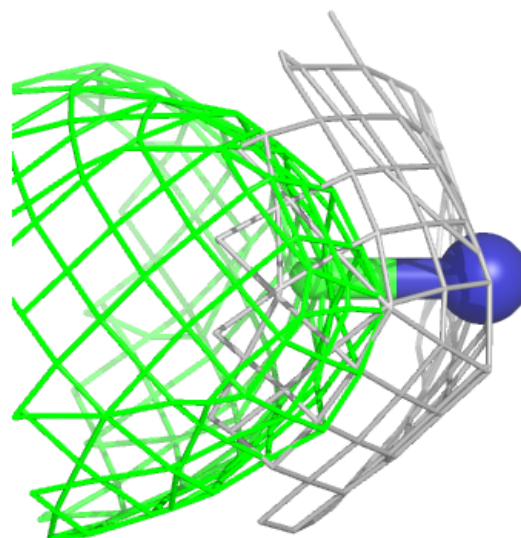
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HEM	B	302	43/43	0.98	0.10	65,80,103,114	0
2	HEM	H	302	43/43	0.98	0.11	77,92,115,126	0
4	GOL	G	603	6/6	0.98	0.16	84,86,87,94	0
2	HEM	I	601	43/43	0.98	0.10	86,108,129,141	0
2	HEM	C	601	43/43	0.98	0.10	67,85,128,133	0
2	HEM	A	601	43/43	0.98	0.10	53,69,97,109	0
2	HEM	E	601	43/43	0.98	0.10	76,82,99,109	0
2	HEM	F	302	43/43	0.98	0.11	80,98,120,131	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.

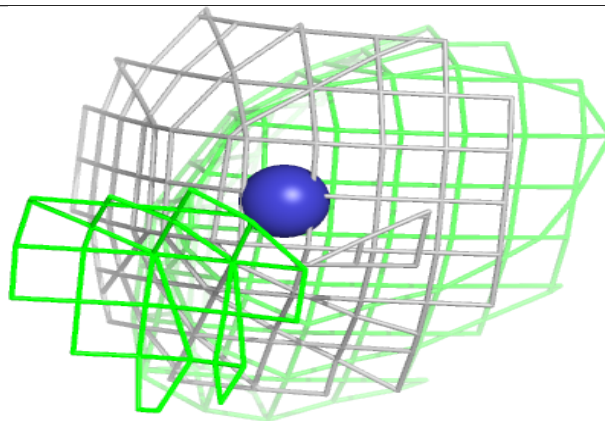
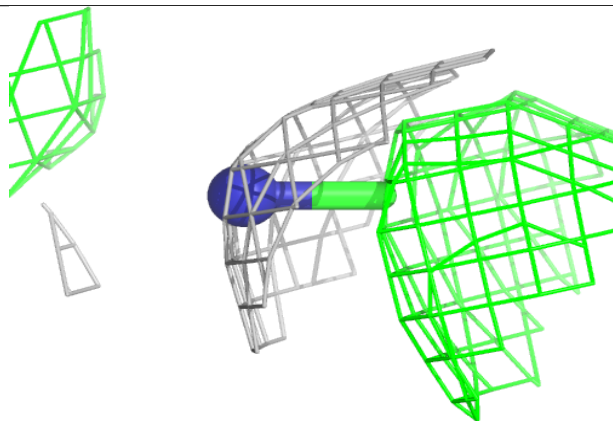
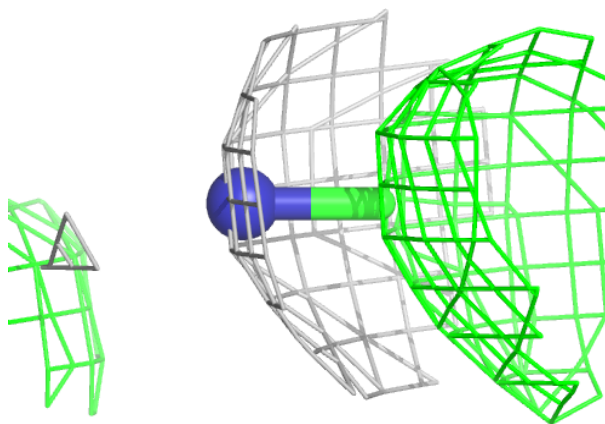
Electron density around CYN G 602:

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



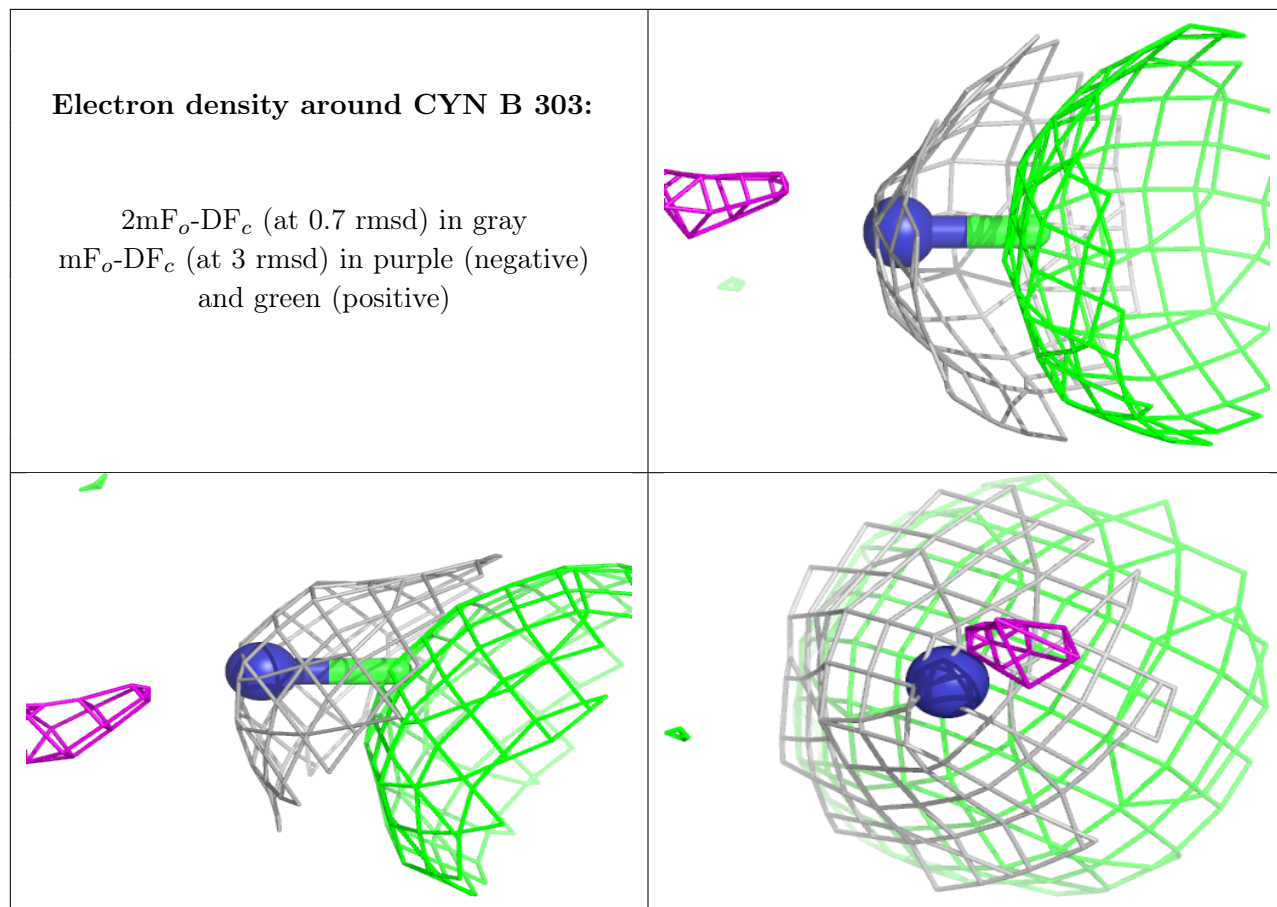
Electron density around CYN J 304:

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



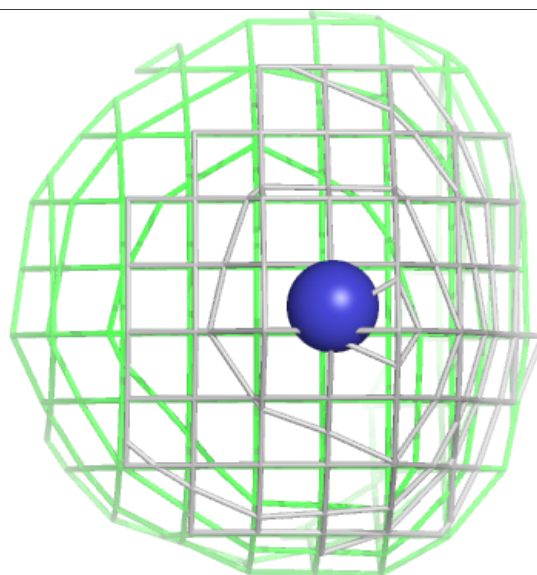
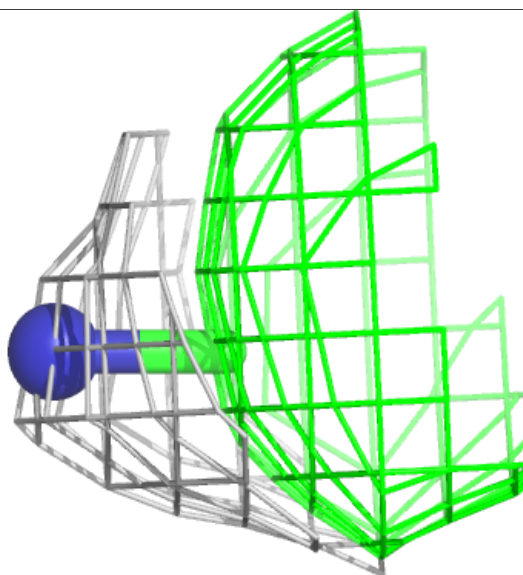
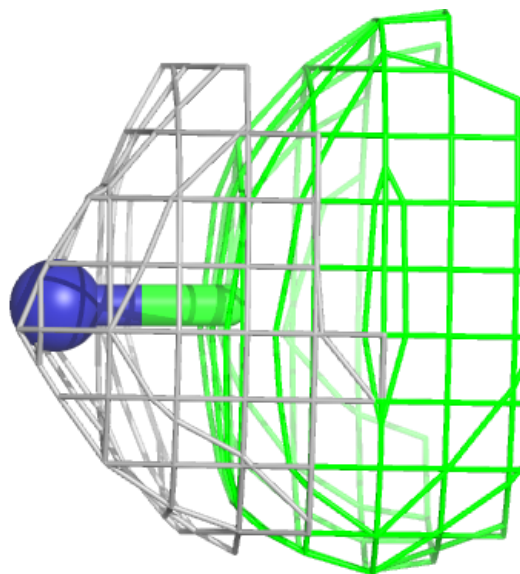
Electron density around CYN B 303:

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



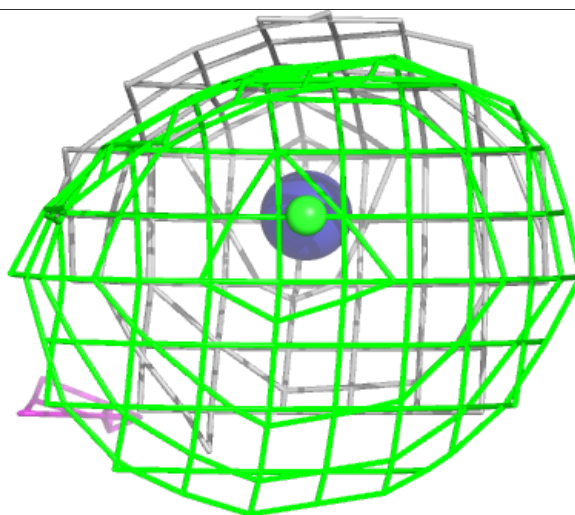
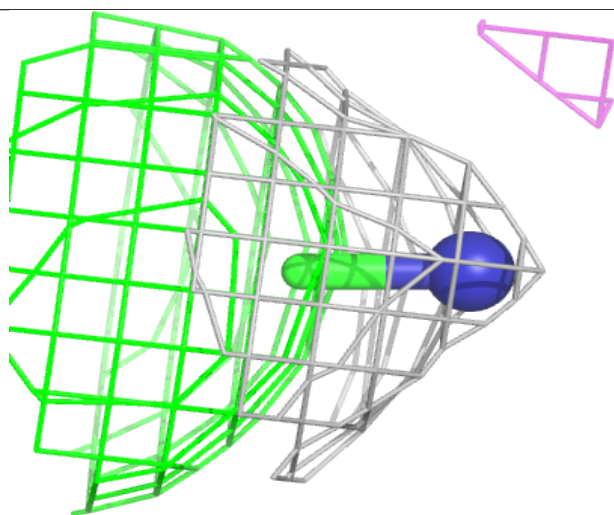
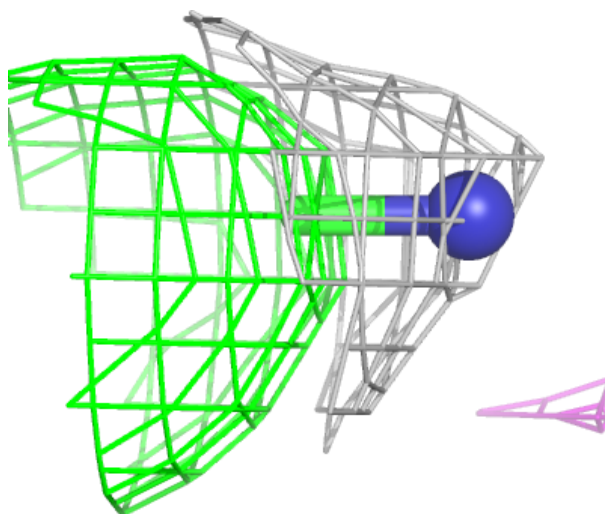
Electron density around CYN A 602:

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



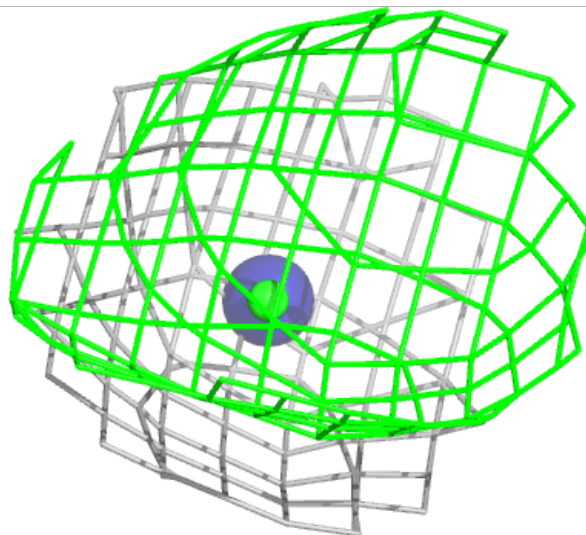
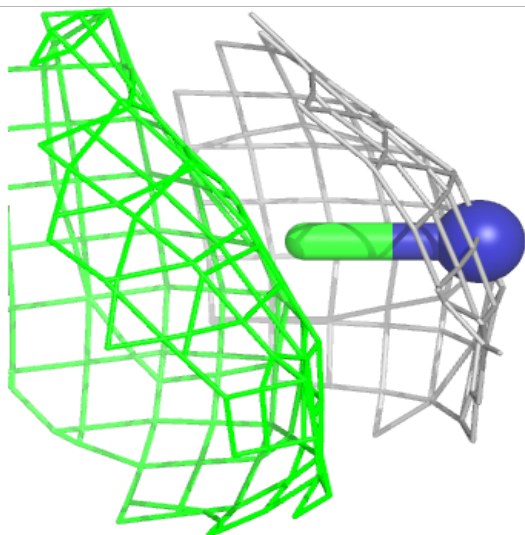
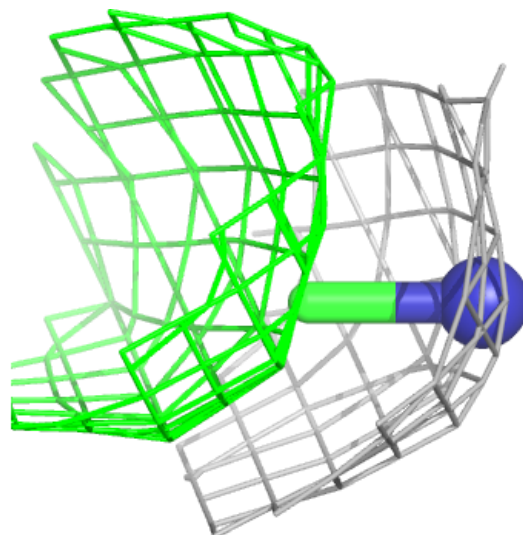
Electron density around CYN D 304:

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



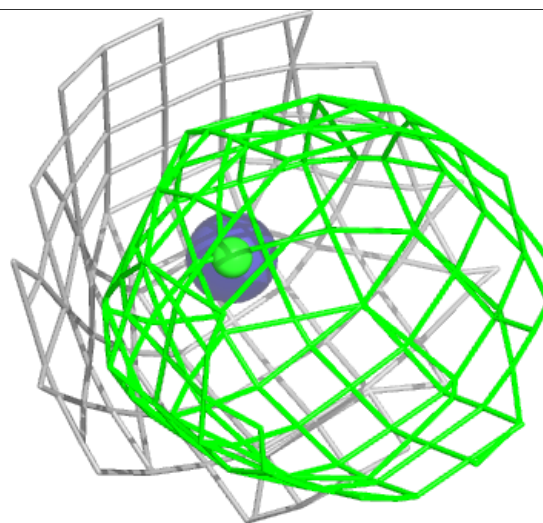
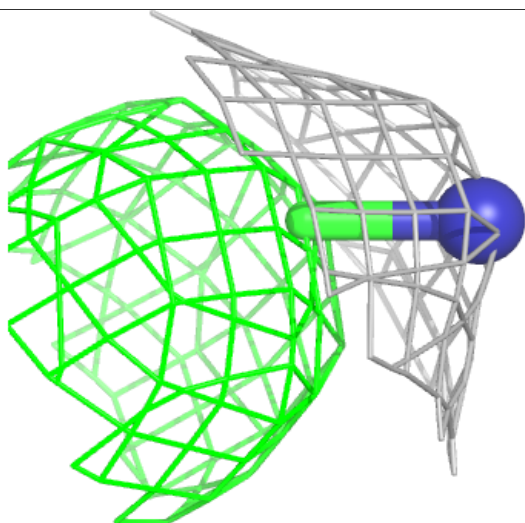
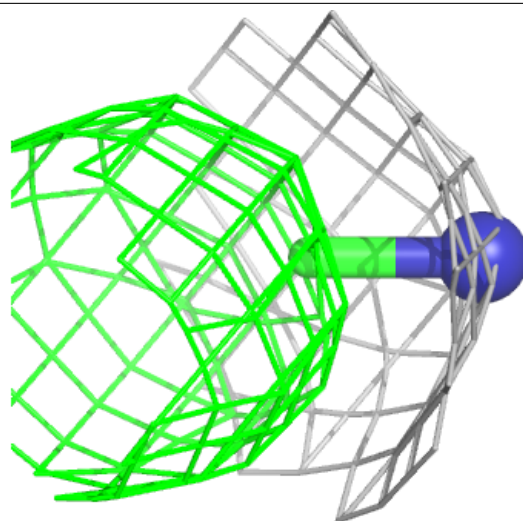
Electron density around CYN I 602:

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



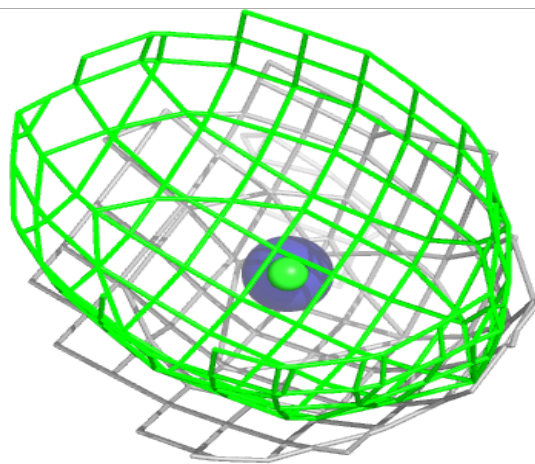
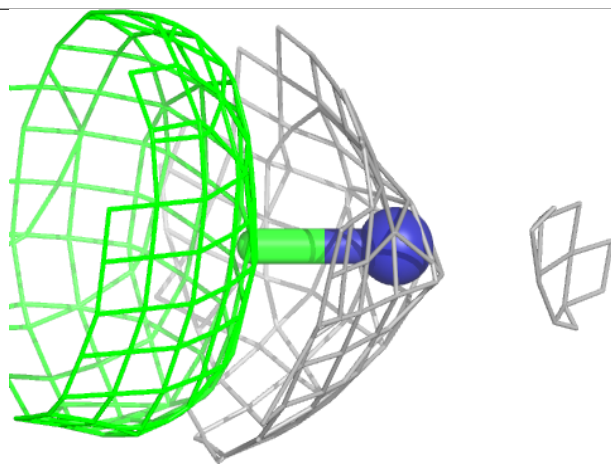
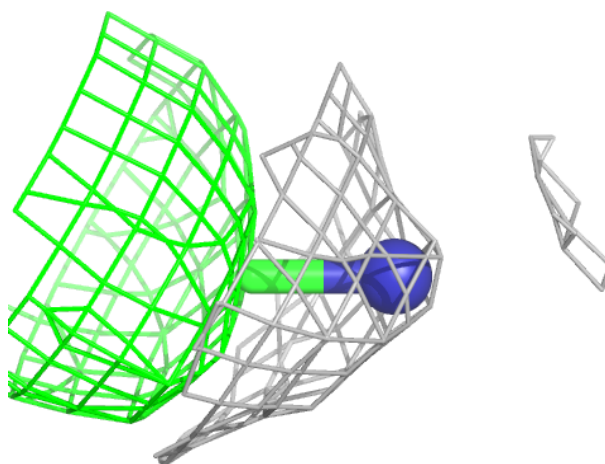
Electron density around CYN F 303:

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



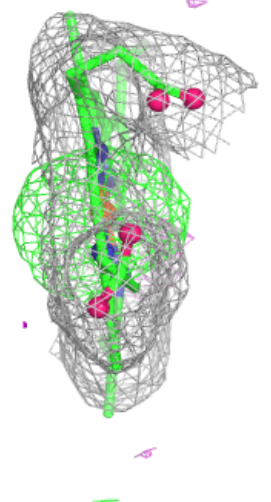
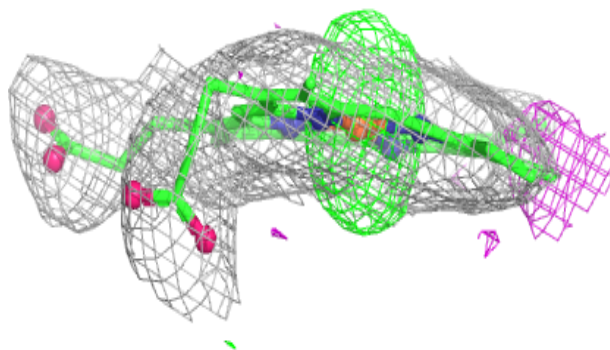
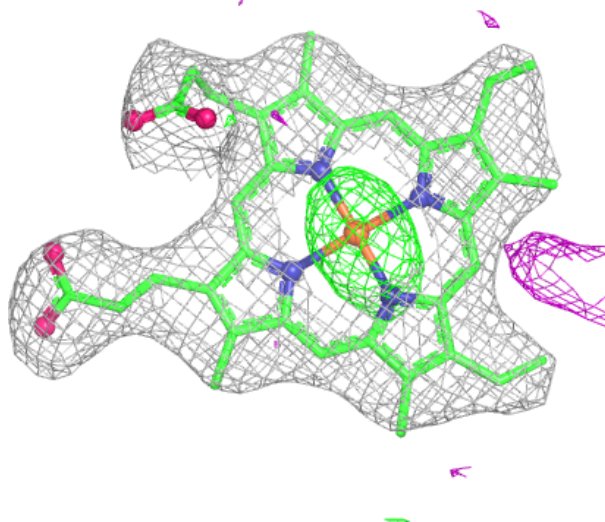
Electron density around CYN E 602:

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



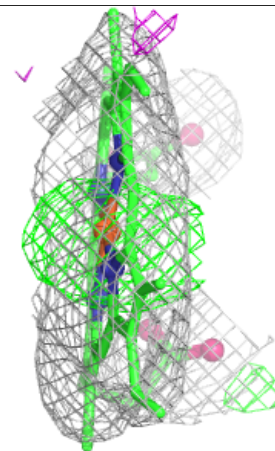
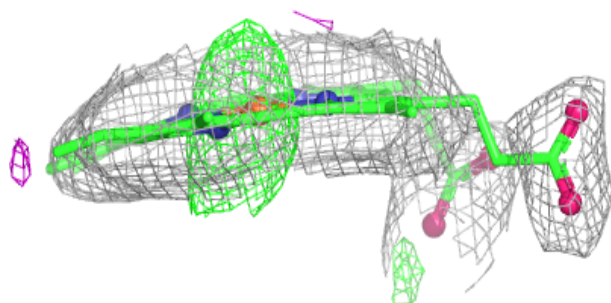
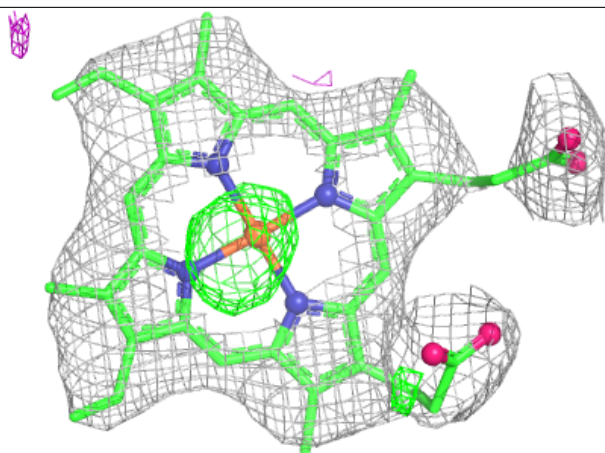
Electron density around HEM D 303:

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



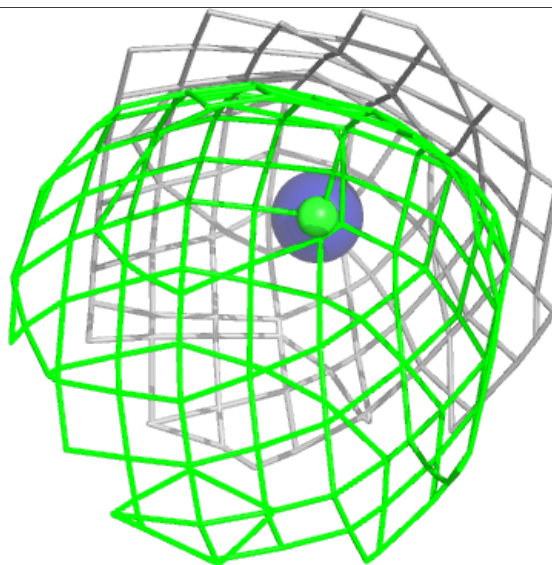
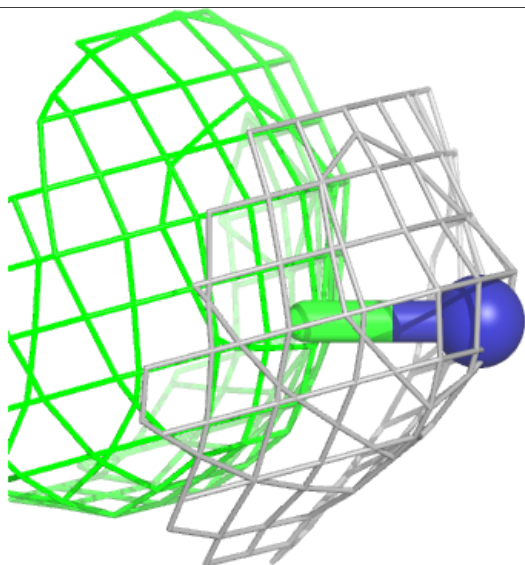
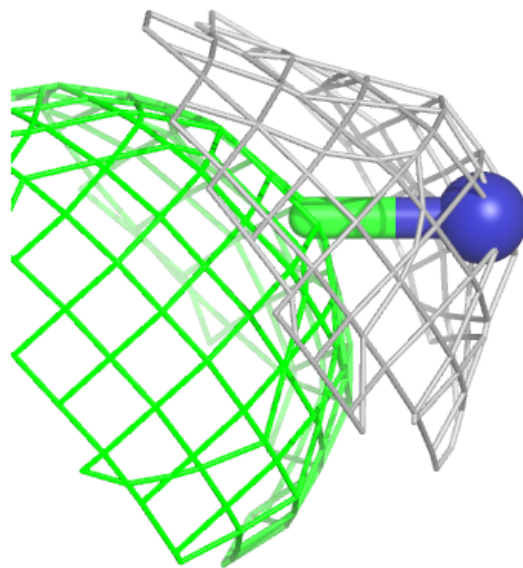
Electron density around HEM G 601:

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



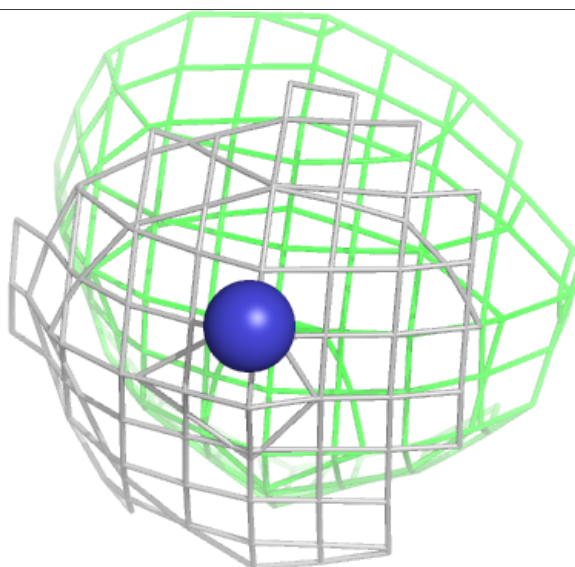
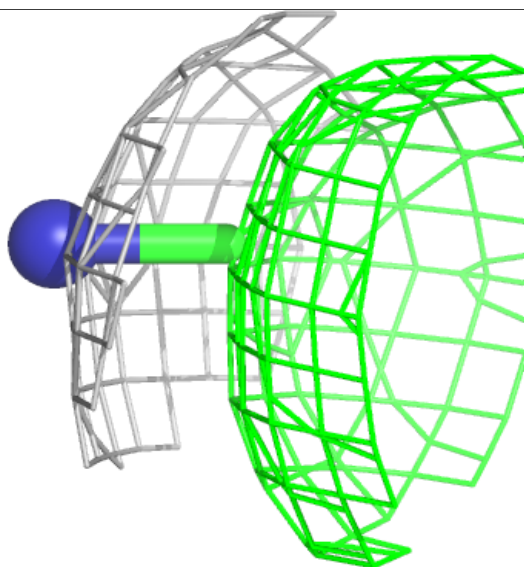
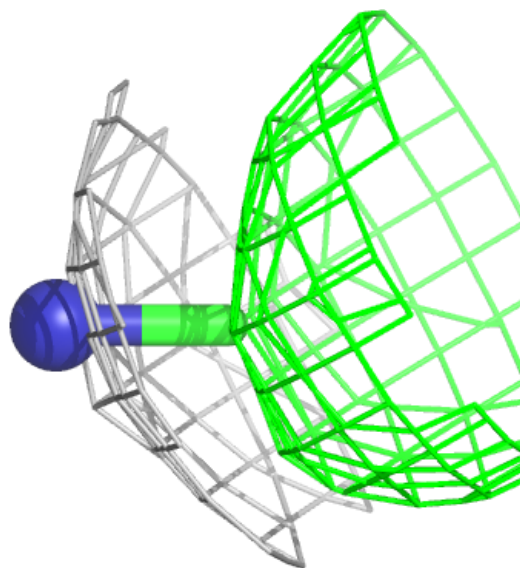
Electron density around CYN C 602:

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



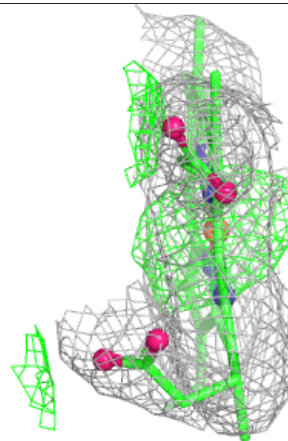
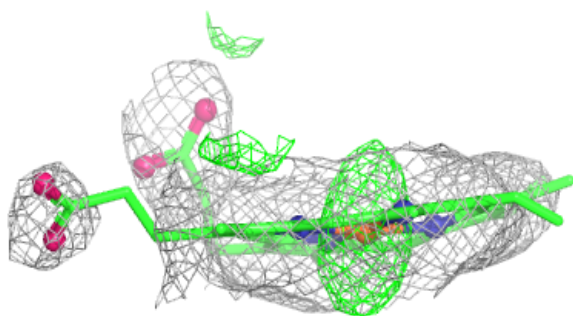
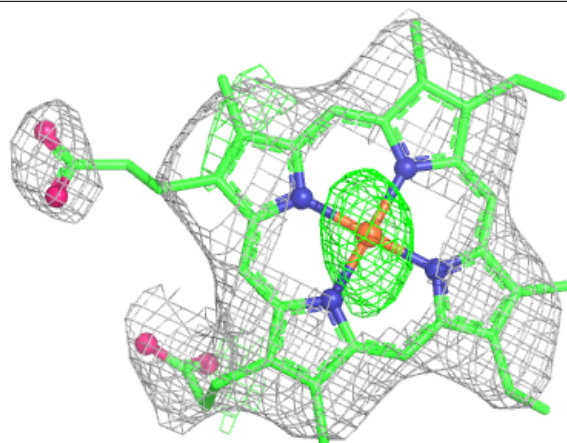
Electron density around CYN H 303:

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



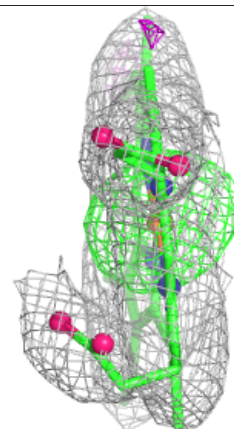
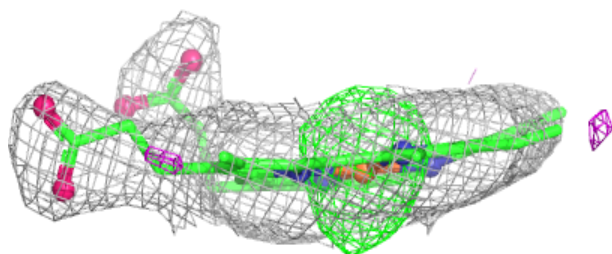
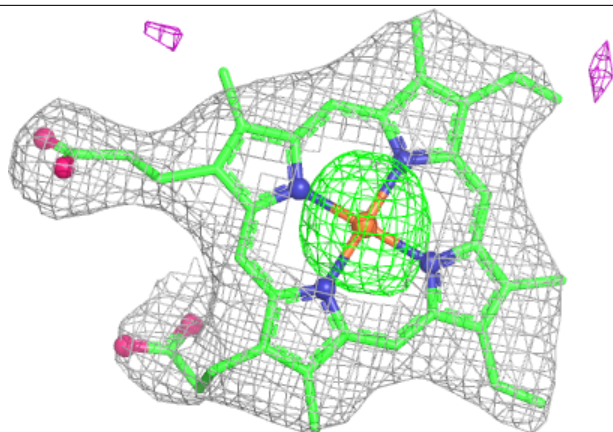
Electron density around HEM J 303:

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

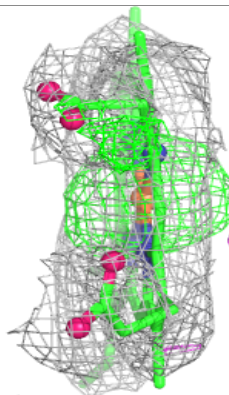
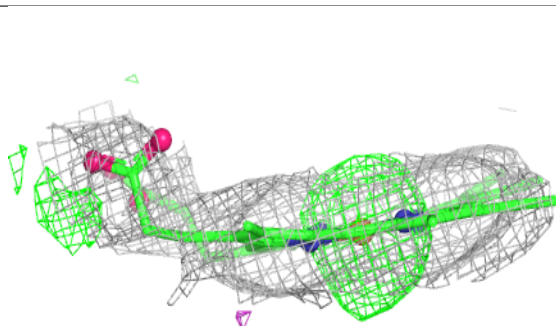
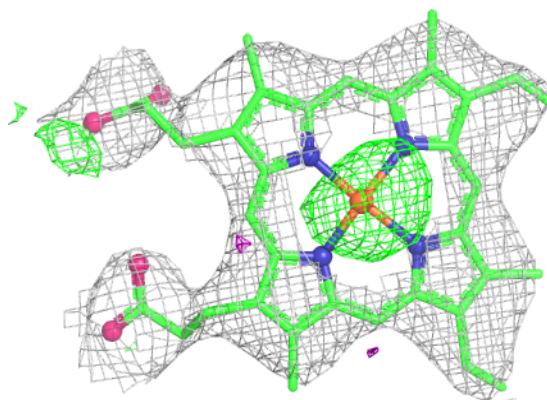


Electron density around HEM B 302:

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

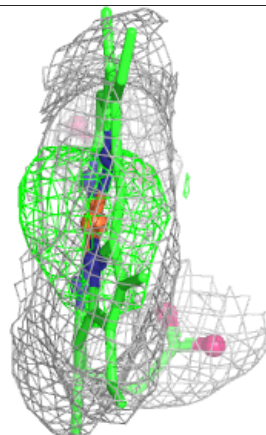
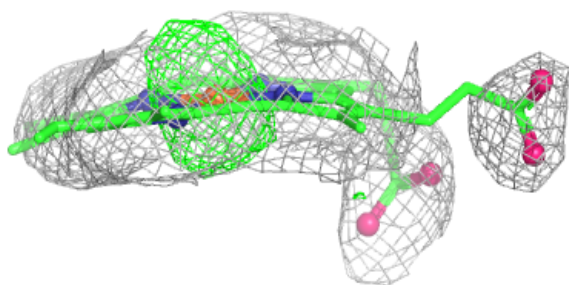
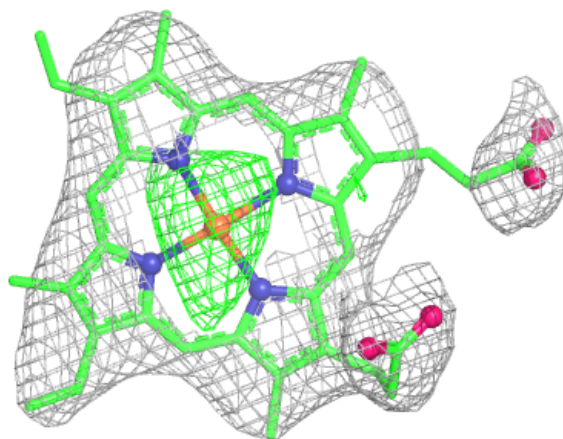
**Electron density around HEM H 302:**

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



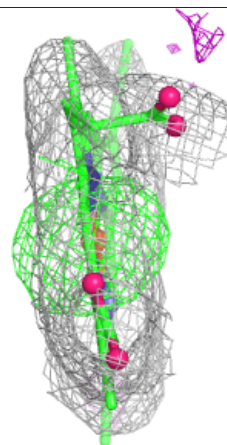
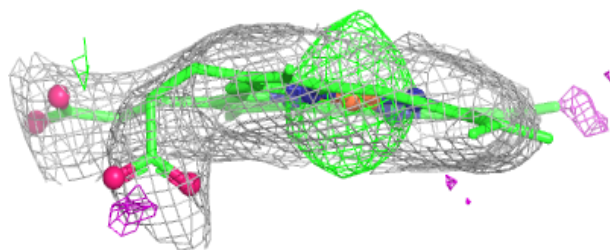
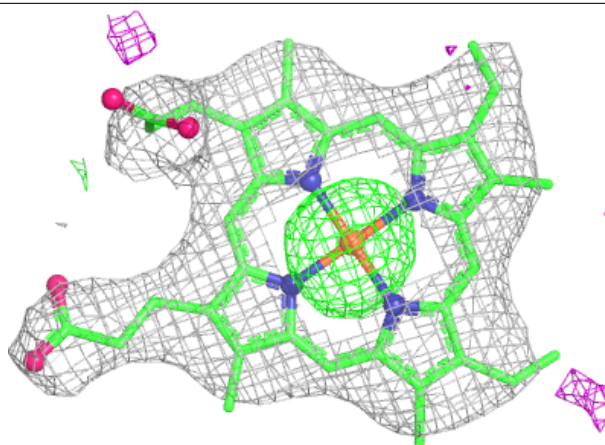
Electron density around HEM I 601:

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



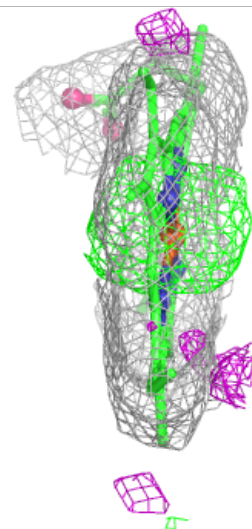
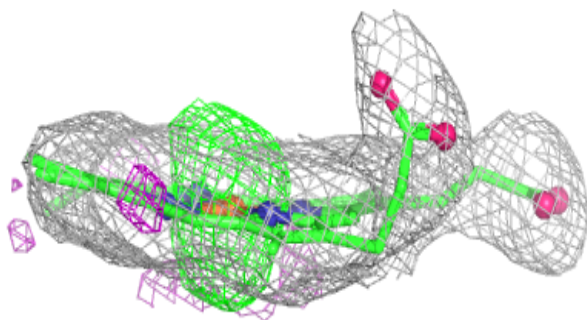
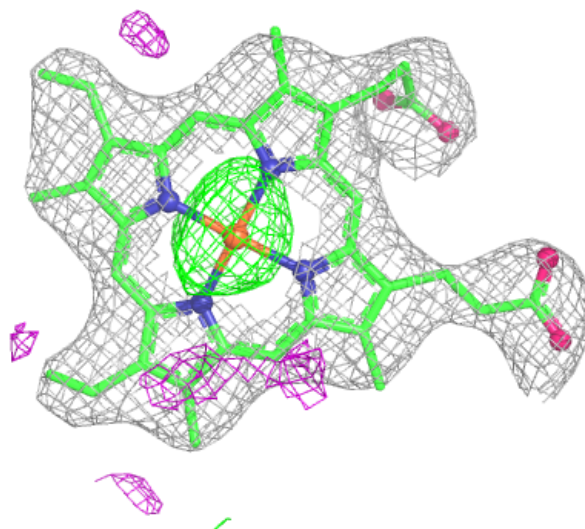
Electron density around HEM C 601:

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



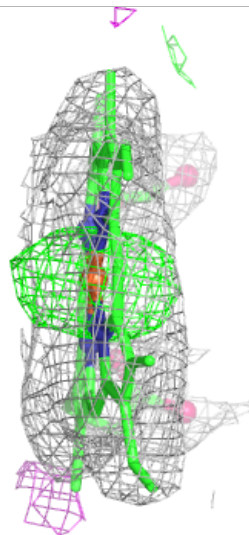
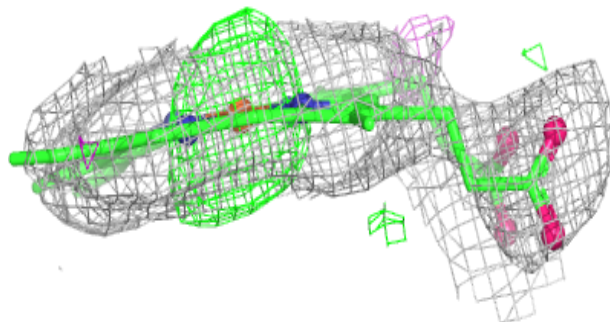
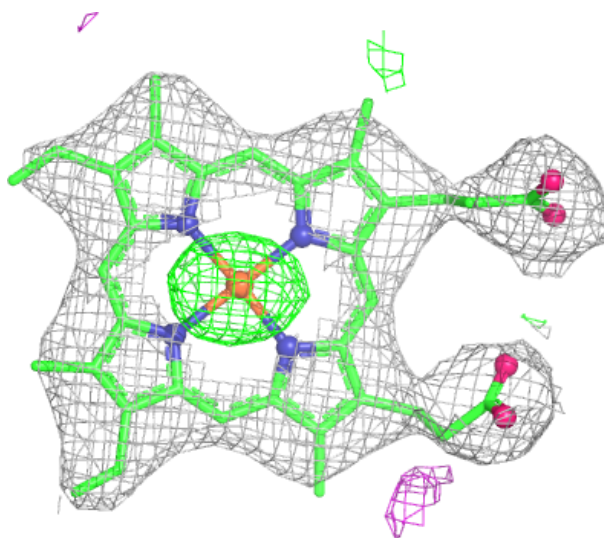
Electron density around HEM A 601:

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



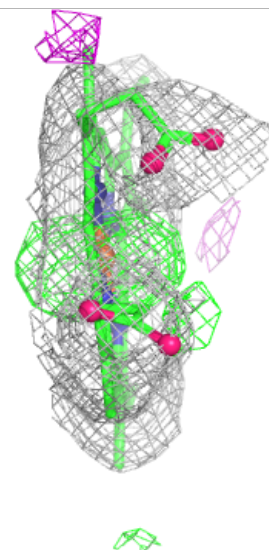
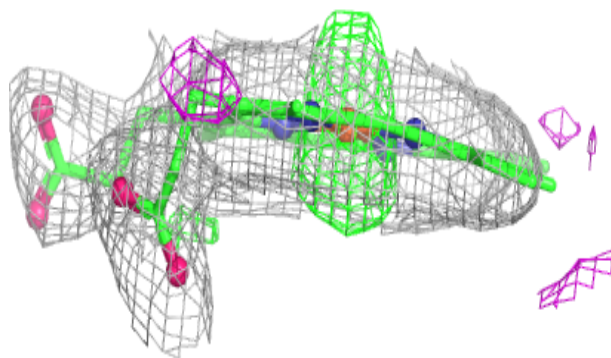
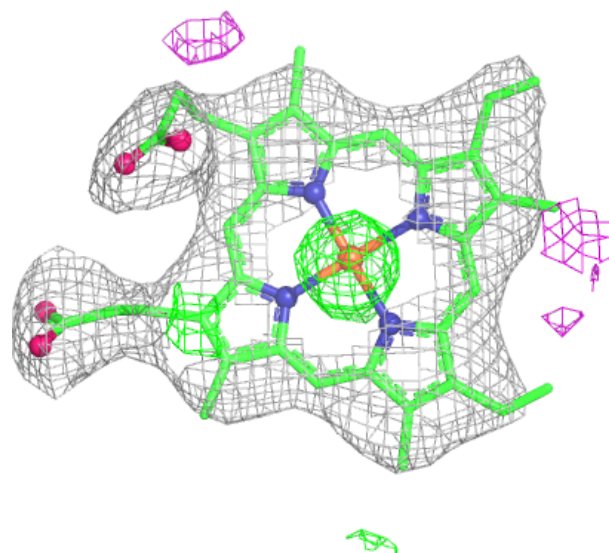
Electron density around HEM E 601:

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



Electron density around HEM F 302:

$2mF_o-DF_c$ (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.