



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2026 – 04:52 AM JST

PDB ID : 8JS5 / pdb_00008js5
Title : Dimeric PAS domains of oxygen sensor FixL with ferric unliganded heme
Authors : Kamaya, M.; Koteishi, H.; Sawai, H.; Sugimoto, H.; Shiro, Y.
Deposited on : 2023-06-19
Resolution : 2.95 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

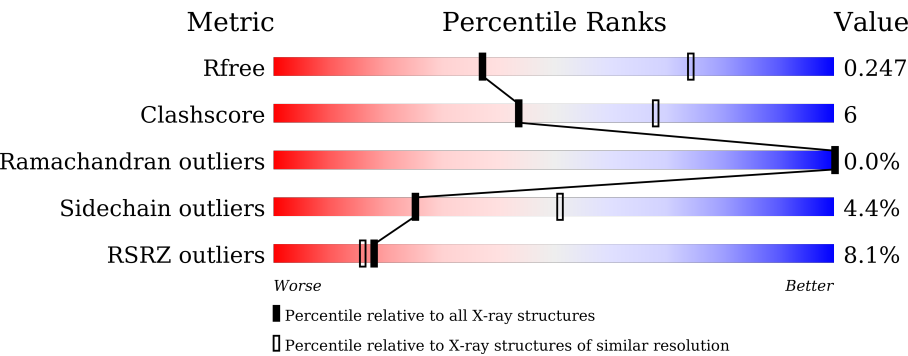
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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% 73% 17% • 8%
1	B	273	4% 76% 16% 7%
1	C	273	8% 75% 16% • 8%
1	D	273	8% 79% 12% • 8%
1	E	273	10% 76% 14% • 8%
1	F	273	6% 78% 12% • 9%

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Mol	Chain	Length	Quality of chain
1	G	273	6% 73% 17% • 9%
1	H	273	7% 73% 16% • 8%
1	I	273	8% 76% 14% • 9%
1	J	273	8% 77% 13% • 9%

2 Entry composition

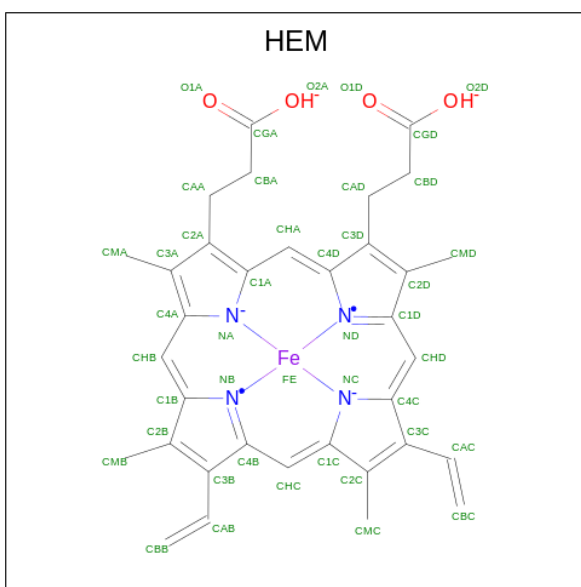
There are 4 unique types of molecules in this entry. The entry contains 20358 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

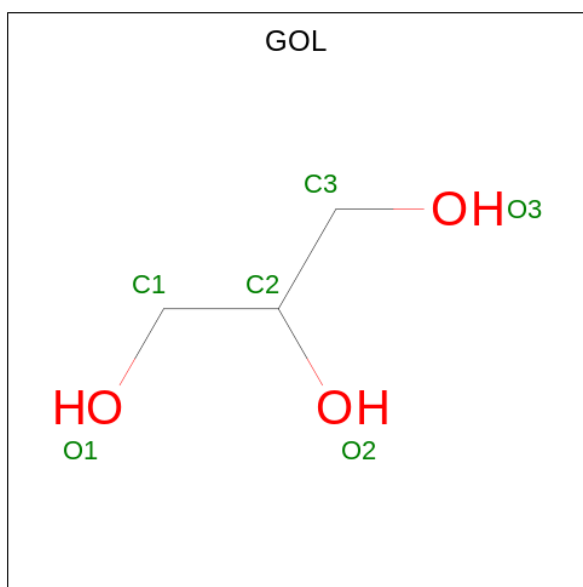
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	1	0
			1985	1237	365	379	4			
1	B	253	Total	C	N	O	S	0	1	0
			2004	1249	365	386	4			
1	C	252	Total	C	N	O	S	0	0	0
			1990	1239	364	383	4			
1	D	250	Total	C	N	O	S	0	1	0
			1984	1237	364	379	4			
1	E	250	Total	C	N	O	S	0	0	0
			1977	1232	362	379	4			
1	F	248	Total	C	N	O	S	0	1	0
			1970	1226	363	377	4			
1	G	249	Total	C	N	O	S	0	1	0
			1974	1228	364	378	4			
1	H	250	Total	C	N	O	S	0	0	0
			1977	1232	362	379	4			
1	I	249	Total	C	N	O	S	0	0	0
			1966	1223	361	378	4			
1	J	249	Total	C	N	O	S	0	1	0
			1974	1228	364	378	4			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
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 GLYCEROL (CCD ID: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

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

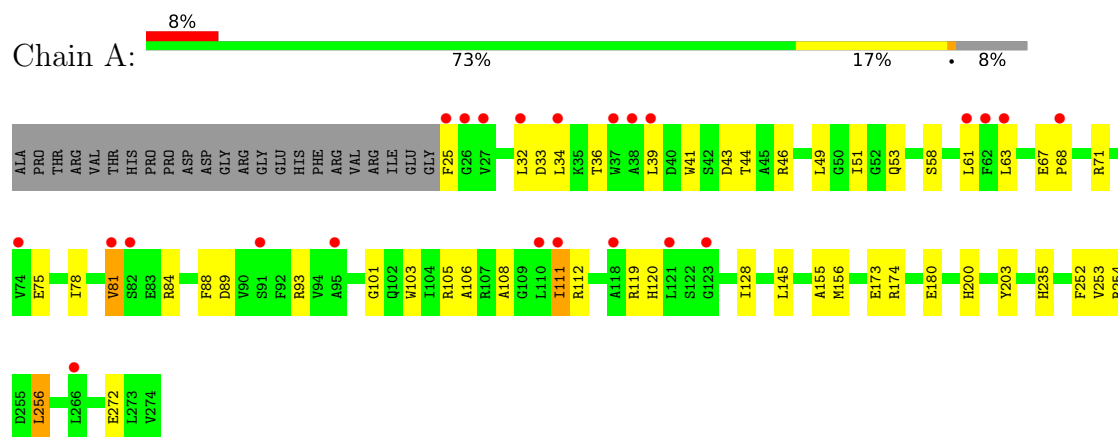
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	4	Total	O	0	0
			4	4		
4	C	3	Total	O	0	0
			3	3		
4	D	5	Total	O	0	0
			5	5		
4	E	5	Total	O	0	0
			5	5		
4	F	5	Total	O	0	0
			5	5		
4	G	1	Total	O	0	0
			1	1		
4	H	2	Total	O	0	0
			2	2		
4	I	3	Total	O	0	0
			3	3		
4	J	3	Total	O	0	0
			3	3		

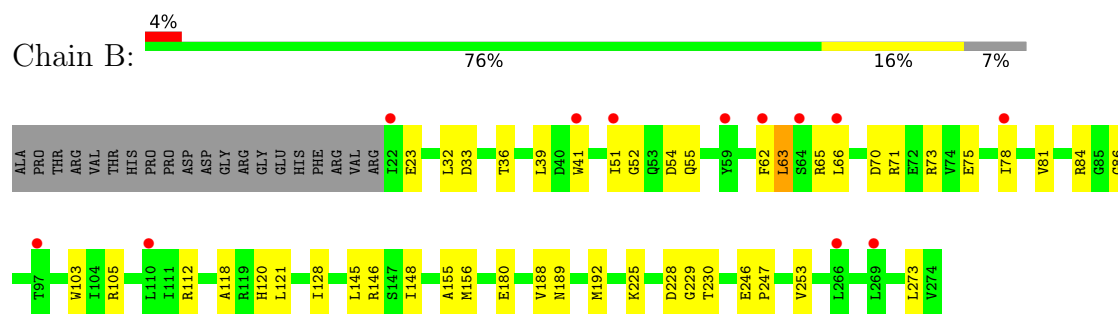
3 Residue-property plots [i](#)

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.

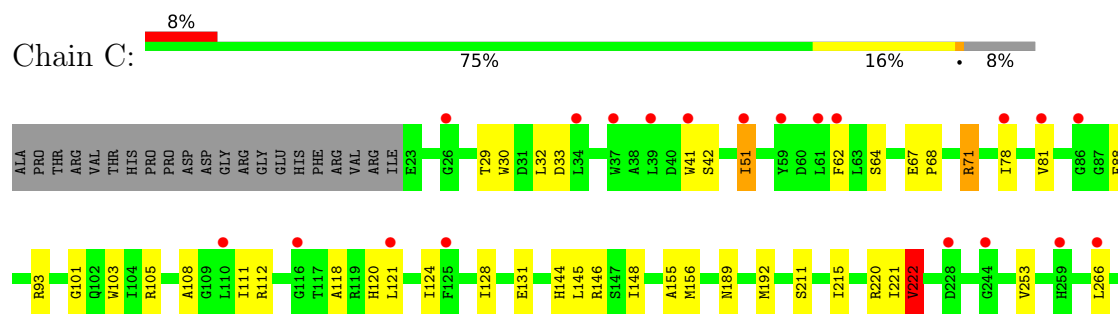
• Molecule 1: Sensor protein FixL



• Molecule 1: Sensor protein FixL

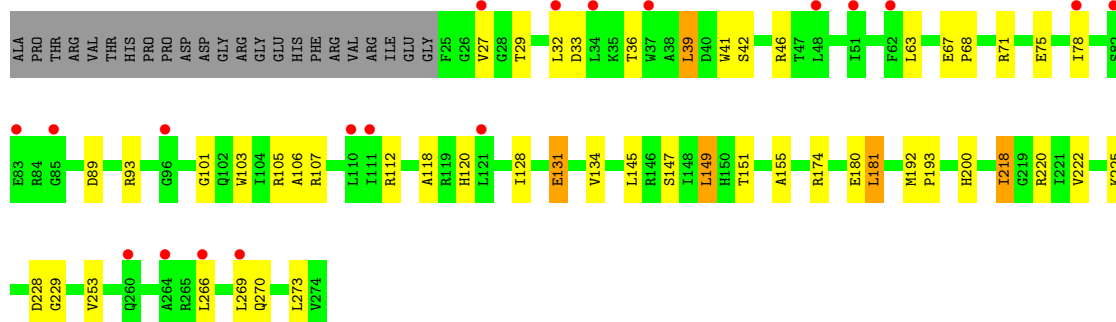
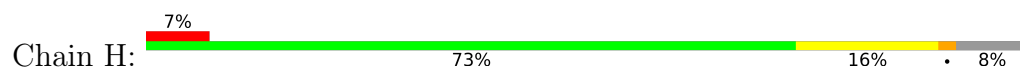


• Molecule 1: Sensor protein FixL

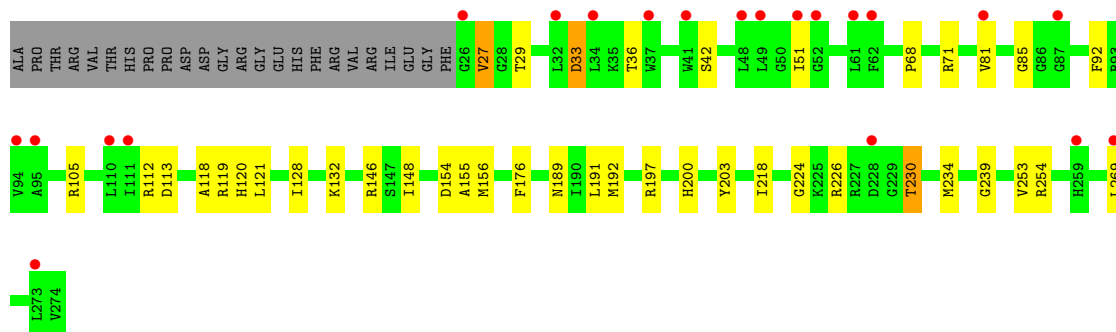
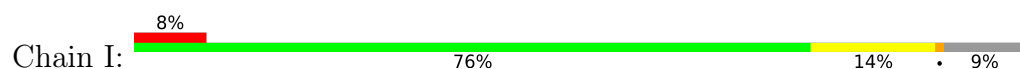




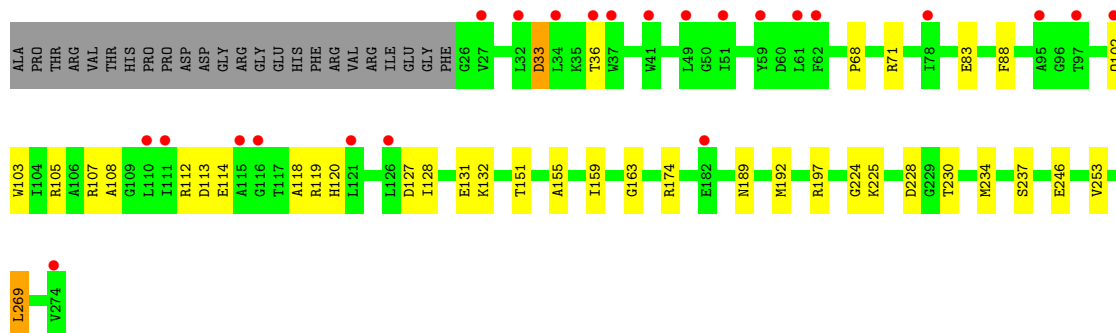
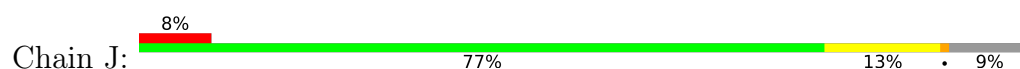
• Molecule 1: Sensor protein FixL



• Molecule 1: Sensor protein FixL



• Molecule 1: Sensor protein FixL



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	190.44Å 194.15Å 269.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.65 – 2.95 28.65 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (28.65-2.95) 99.7 (28.65-2.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.207 , 0.246 0.208 , 0.247	Depositor DCC
R_{free} test set	5304 reflections (2.09%)	wwPDB-VP
Wilson B-factor (Å ²)	84.2	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 115.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.087 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20358	wwPDB-VP
Average B, all atoms (Å ²)	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.28	0/2027	0.53	0/2740
1	B	0.24	0/2046	0.52	0/2766
1	C	0.25	0/2029	0.54	0/2743
1	D	0.25	0/2027	0.51	0/2741
1	E	0.24	0/2016	0.51	0/2726
1	F	0.23	0/2011	0.51	0/2719
1	G	0.24	0/2015	0.54	0/2724
1	H	0.23	0/2016	0.49	0/2726
1	I	0.23	0/2004	0.50	0/2710
1	J	0.24	0/2015	0.55	0/2724
All	All	0.24	0/20206	0.52	0/27319

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

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	1985	0	1940	31	0
1	B	2004	0	1954	24	0
1	C	1990	0	1937	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1984	0	1935	21	0
1	E	1977	0	1928	25	0
1	F	1970	0	1929	17	0
1	G	1974	0	1932	27	0
1	H	1977	0	1928	28	0
1	I	1966	0	1919	25	0
1	J	1974	0	1932	22	0
2	A	43	0	30	1	0
2	B	43	0	30	1	0
2	C	43	0	30	1	0
2	D	43	0	30	1	0
2	E	43	0	30	4	0
2	F	43	0	30	1	0
2	G	43	0	30	2	0
2	H	43	0	30	2	0
2	I	43	0	30	1	0
2	J	43	0	30	2	0
3	A	6	0	8	0	0
3	B	12	0	16	2	0
3	C	6	0	8	0	0
3	D	12	0	16	1	0
3	E	12	0	16	2	0
3	F	6	0	8	0	0
3	G	12	0	16	1	0
3	H	6	0	8	2	0
3	I	12	0	16	0	0
3	J	6	0	8	0	0
4	A	6	0	0	0	0
4	B	4	0	0	1	0
4	C	3	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
4	G	1	0	0	0	0
4	H	2	0	0	1	0
4	I	3	0	0	0	0
4	J	3	0	0	1	0
All	All	20358	0	19754	243	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 6.

All (243) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:PHE:HB3	1:C:108:ALA:HB3	1.71	0.72
1:D:52:GLY:HA2	1:D:55:GLN:HB2	1.72	0.72
1:F:81:VAL:HA	1:F:85:GLY:HA3	1.72	0.72
1:D:155:ALA:HB3	1:D:253:VAL:HB	1.72	0.71
1:D:224:GLY:HA3	1:D:234:MET:HE3	1.74	0.69
1:C:33:ASP:HA	1:C:120:HIS:HA	1.73	0.69
1:C:148:ILE:HG22	1:C:156:MET:HE1	1.76	0.68
1:F:33:ASP:HA	1:F:120:HIS:HA	1.76	0.68
1:I:224:GLY:HA3	1:I:234:MET:HE3	1.76	0.67
1:C:145:LEU:HB2	3:D:302:GOL:H2	1.77	0.66
1:E:29:THR:HG22	1:E:42:SER:HB2	1.77	0.66
1:I:239:GLY:HA3	1:J:151:THR:HG21	1.75	0.66
1:A:93:ARG:HH21	1:A:101:GLY:H	1.42	0.65
1:J:228:ASP:HB2	1:J:230:THR:HG22	1.77	0.65
1:G:33:ASP:HA	1:G:120:HIS:HA	1.77	0.64
1:D:46:ARG:NH1	1:D:55:GLN:O	2.30	0.64
1:B:228:ASP:HB2	1:B:230:THR:HG22	1.79	0.63
1:J:155:ALA:HB3	1:J:253:VAL:HB	1.81	0.63
1:A:67:GLU:HG3	1:A:68:PRO:HD2	1.82	0.62
1:G:63:LEU:O	1:G:71:ARG:NE	2.33	0.62
1:I:155:ALA:HB3	1:I:253:VAL:HB	1.80	0.62
1:G:41:TRP:HZ3	1:G:62:PHE:HB2	1.64	0.62
1:A:58:SER:HB3	1:A:61:LEU:HG	1.80	0.62
1:I:148:ILE:HG22	1:I:156:MET:HE1	1.82	0.61
1:J:224:GLY:HA3	1:J:234:MET:HE3	1.82	0.61
2:C:601:HEM:HHC	2:C:601:HEM:HBB2	1.82	0.61
1:D:68:PRO:HA	1:D:71:ARG:HB3	1.83	0.60
1:D:105:ARG:HB2	1:D:128:ILE:HD13	1.83	0.60
1:F:93:ARG:HE	1:F:101:GLY:HA3	1.67	0.59
1:J:33:ASP:HA	1:J:120:HIS:HA	1.84	0.59
1:C:189:ASN:HA	1:C:192:MET:HE3	1.85	0.59
1:F:105:ARG:HE	1:F:107:ARG:HE	1.50	0.59
1:I:81:VAL:HA	1:I:85:GLY:HA3	1.83	0.59
2:D:303:HEM:HHC	2:D:303:HEM:HBB2	1.84	0.59
1:E:228:ASP:HB2	1:E:230:THR:HG22	1.84	0.59
1:I:269:LEU:HB3	1:J:269:LEU:HB3	1.84	0.59
1:E:189:ASN:HA	1:E:192:MET:HE3	1.84	0.59
1:C:273:LEU:HD23	1:C:274:VAL:HG23	1.83	0.59
1:F:159:ILE:HD12	1:F:163:GLY:HA2	1.85	0.59
1:I:112:ARG:HE	1:I:118:ALA:HB2	1.67	0.58
1:A:155:ALA:HB3	1:A:253:VAL:HB	1.85	0.58
1:H:112:ARG:HE	1:H:118:ALA:HB2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:174:ARG:NH2	4:J:401:HOH:O	2.36	0.58
1:B:66:LEU:HD11	1:B:70:ASP:HB2	1.85	0.58
1:C:93:ARG:HE	1:C:101:GLY:HA3	1.67	0.58
1:B:81:VAL:HG23	1:B:86:GLY:HA3	1.85	0.58
2:E:601:HEM:HHC	2:E:601:HEM:HBB2	1.84	0.58
1:A:51:ILE:HG22	1:A:53:GLN:H	1.69	0.58
1:D:93:ARG:HH21	1:D:101:GLY:H	1.51	0.58
1:E:112:ARG:HG2	1:E:118:ALA:HA	1.86	0.58
1:B:75:GLU:HA	1:B:78:ILE:HG12	1.85	0.57
2:H:302:HEM:HBB2	2:H:302:HEM:HHC	1.86	0.57
1:G:112:ARG:HG2	1:G:118:ALA:HA	1.86	0.57
2:G:601:HEM:HHC	2:G:601:HEM:HBB2	1.87	0.57
1:H:147:SER:O	1:H:151:THR:HG22	2.05	0.57
1:B:112:ARG:HG2	1:B:118:ALA:HA	1.86	0.57
1:E:220:ARG:NH2	2:E:601:HEM:O1A	2.38	0.57
1:E:145:LEU:HB2	3:E:602:GOL:H2	1.88	0.56
1:D:158:VAL:HB	1:D:167:LEU:HB2	1.86	0.56
2:F:302:HEM:HBB2	2:F:302:HEM:HHC	1.87	0.56
1:E:146:ARG:HH11	1:I:146:ARG:HH22	1.51	0.56
1:B:52:GLY:HA2	1:B:55:GLN:HG2	1.87	0.56
1:D:218:ILE:HB	1:H:218:ILE:HG23	1.88	0.56
1:A:32:LEU:HB2	1:A:39:LEU:HG	1.88	0.55
1:B:225:LYS:HE2	1:B:229:GLY:HA2	1.87	0.55
1:I:33:ASP:HA	1:I:120:HIS:HA	1.89	0.55
1:J:159:ILE:HD12	1:J:163:GLY:HA2	1.87	0.55
1:H:67:GLU:HG2	1:H:68:PRO:HD2	1.89	0.55
2:I:601:HEM:HBB2	2:I:601:HEM:HHC	1.88	0.55
1:H:180:GLU:HG3	1:H:181:LEU:HD22	1.89	0.55
1:C:155:ALA:HB3	1:C:253:VAL:HB	1.89	0.54
1:D:200:HIS:HA	1:D:203:TYR:CD2	2.43	0.54
1:C:266:LEU:HD22	1:D:262:THR:HG23	1.89	0.54
1:G:119:ARG:HG3	1:G:120:HIS:H	1.72	0.54
1:B:33:ASP:HA	1:B:120:HIS:HA	1.90	0.54
1:H:174:ARG:NH2	4:H:401:HOH:O	2.39	0.54
1:H:228:ASP:OD1	1:H:229:GLY:N	2.40	0.54
1:F:66:LEU:HB2	1:F:71:ARG:HB3	1.90	0.54
2:A:601:HEM:HHC	2:A:601:HEM:HBB2	1.89	0.53
1:H:192:MET:HE1	1:H:200:HIS:CD2	2.44	0.53
1:C:112:ARG:HG2	1:C:118:ALA:HA	1.90	0.53
1:E:76:SER:HA	1:E:79:LYS:HD2	1.90	0.53
1:I:105:ARG:HB2	1:I:128:ILE:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:246:GLU:HG2	1:G:247:PRO:HD2	1.91	0.53
1:A:105:ARG:HB2	1:A:128:ILE:HD13	1.91	0.53
1:C:105:ARG:HB2	1:C:128:ILE:HD13	1.90	0.53
1:A:112:ARG:NH1	1:B:23:GLU:OE2	2.41	0.52
1:H:29:THR:H	1:H:42:SER:HB3	1.74	0.52
1:H:33:ASP:HA	1:H:120:HIS:HA	1.91	0.52
1:A:84:ARG:HB3	1:A:112:ARG:HH21	1.73	0.52
1:G:88:PHE:HD2	1:G:108:ALA:HB3	1.74	0.52
1:C:30:TRP:HH2	1:C:108:ALA:HB2	1.74	0.52
1:I:189:ASN:HB2	1:I:197:ARG:HG3	1.92	0.52
1:A:200:HIS:HA	1:A:203:TYR:CD2	2.44	0.52
1:F:155:ALA:HB3	1:F:253:VAL:HB	1.91	0.52
1:G:33:ASP:OD1	1:G:33:ASP:N	2.43	0.52
1:E:180:GLU:HG3	1:E:181:LEU:HD12	1.92	0.52
1:J:113:ASP:OD2	1:J:119:ARG:NH2	2.42	0.51
1:G:49:LEU:HD21	1:G:62:PHE:HD1	1.75	0.51
1:A:145:LEU:HB2	3:B:302:GOL:H2	1.93	0.51
1:G:159:ILE:HD12	1:G:163:GLY:HA2	1.92	0.51
1:J:68:PRO:HA	1:J:71:ARG:HG2	1.92	0.51
1:G:103:TRP:HB3	1:G:128:ILE:HG13	1.91	0.51
1:G:252:PHE:HE1	1:H:151:THR:HG23	1.75	0.51
1:I:226:ARG:HE	1:I:230:THR:HG23	1.75	0.51
1:J:131:GLU:N	1:J:131:GLU:OE1	2.39	0.51
1:E:112:ARG:HE	1:E:118:ALA:HB2	1.75	0.51
1:G:141[A]:ARG:HH22	3:G:603:GOL:H12	1.76	0.51
1:B:146:ARG:NH1	4:B:401:HOH:O	2.44	0.50
1:A:78:ILE:HA	1:A:81:VAL:HG12	1.93	0.50
1:A:111:ILE:HG12	1:A:120:HIS:HB2	1.93	0.50
1:D:73:ARG:NH2	1:D:91:SER:O	2.43	0.50
1:J:102:GLN:NE2	1:J:127:ASP:OD1	2.45	0.50
1:D:228:ASP:HB3	1:D:230:THR:H	1.76	0.50
1:B:66:LEU:O	1:B:71:ARG:NH1	2.43	0.50
1:J:105:ARG:HB2	1:J:128:ILE:HD13	1.93	0.50
1:A:33:ASP:HA	1:A:120:HIS:HA	1.93	0.49
1:G:145:LEU:HD13	3:H:301:GOL:H11	1.93	0.49
1:B:51:ILE:HB	1:B:65:ARG:HD2	1.94	0.49
1:A:75:GLU:HA	1:A:78:ILE:HG12	1.94	0.49
1:E:58:SER:HB3	1:E:61:LEU:HG	1.93	0.49
1:E:228:ASP:OD1	1:E:228:ASP:N	2.43	0.49
1:B:189:ASN:HA	1:B:192:MET:HE3	1.93	0.49
1:G:220:ARG:HH21	2:G:601:HEM:HBA2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:602:GOL:H32	1:F:145:LEU:HD13	1.95	0.49
1:B:148:ILE:HG22	1:B:156:MET:HE1	1.94	0.49
1:E:131:GLU:OE1	1:E:131:GLU:N	2.44	0.49
1:I:154:ASP:CG	1:I:254:ARG:HE	2.21	0.49
1:A:25:PHE:HB2	1:A:44:THR:HG21	1.95	0.48
1:H:193:PRO:HD3	1:H:225:LYS:HB2	1.94	0.48
1:A:34:LEU:N	1:A:119:ARG:O	2.45	0.48
1:H:33:ASP:OD1	1:H:33:ASP:N	2.45	0.48
1:J:112:ARG:HE	1:J:118:ALA:HB2	1.78	0.48
1:G:64:SER:HA	1:G:71:ARG:HH21	1.78	0.48
1:G:155:ALA:HB3	1:G:253:VAL:HB	1.95	0.48
1:J:189:ASN:HB2	1:J:197:ARG:HG3	1.96	0.48
1:F:54:ASP:N	1:F:54:ASP:OD1	2.47	0.48
1:I:33:ASP:OD1	1:I:33:ASP:N	2.42	0.48
1:B:32:LEU:HD13	1:B:39:LEU:HD12	1.96	0.48
1:E:273:LEU:HD22	1:F:273:LEU:HD11	1.96	0.48
1:H:270:GLN:HG3	1:H:273:LEU:HD12	1.96	0.48
2:B:303:HEM:HBB2	2:B:303:HEM:HHC	1.96	0.47
1:B:246:GLU:HG3	1:B:247:PRO:HD2	1.96	0.47
1:H:32:LEU:HB3	1:H:39:LEU:HG	1.96	0.47
1:C:146:ARG:HH11	1:G:146:ARG:HH22	1.61	0.47
1:G:200:HIS:HA	1:G:203:TYR:CD2	2.49	0.47
1:H:155:ALA:HB3	1:H:253:VAL:HB	1.96	0.47
1:C:30:TRP:CH2	1:C:108:ALA:HB2	2.50	0.47
1:F:97:THR:O	1:F:97:THR:OG1	2.20	0.47
1:H:131:GLU:HA	1:H:134:VAL:HG12	1.97	0.47
1:J:88:PHE:HD2	1:J:108:ALA:HB3	1.79	0.47
2:J:302:HEM:HHC	2:J:302:HEM:HBB2	1.97	0.47
1:A:41:TRP:NE1	1:A:46:ARG:HB3	2.29	0.47
1:F:246:GLU:HG3	1:F:247:PRO:HD2	1.97	0.47
1:H:105:ARG:HE	1:H:107:ARG:HD2	1.79	0.47
1:I:189:ASN:HA	1:I:192:MET:HE3	1.96	0.47
1:B:105:ARG:HB2	1:B:128:ILE:HD13	1.96	0.47
1:I:29:THR:H	1:I:42:SER:HB3	1.78	0.47
1:C:103:TRP:HB3	1:C:128:ILE:HG13	1.98	0.46
1:G:189:ASN:HA	1:G:192:MET:HE3	1.97	0.46
1:E:192:MET:HB3	2:E:601:HEM:CAB	2.45	0.46
1:H:63:LEU:HB3	1:H:71:ARG:HD3	1.98	0.46
1:F:260:GLN:HA	1:F:263:GLN:HB3	1.98	0.46
1:B:63:LEU:HD13	1:B:71:ARG:HG2	1.97	0.46
1:H:222:VAL:HB	2:H:302:HEM:HMB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:ARG:HH11	1:I:146:ARG:NH2	2.15	0.45
1:I:27:VAL:HG22	1:J:107:ARG:HH21	1.81	0.45
1:I:200:HIS:HA	1:I:203:TYR:CD2	2.51	0.45
1:E:33:ASP:HA	1:E:120:HIS:HA	1.98	0.45
1:G:131:GLU:OE1	1:G:131:GLU:N	2.44	0.45
1:J:113:ASP:OD1	1:J:114:GLU:N	2.47	0.45
1:D:32:LEU:HD11	1:D:59:TYR:CD1	2.52	0.45
1:D:53:GLN:HG2	1:D:54:ASP:H	1.81	0.45
1:A:32:LEU:HD13	1:A:39:LEU:HD12	1.99	0.45
1:A:174:ARG:HE	1:A:174:ARG:HB2	1.52	0.45
1:J:103:TRP:CD2	1:J:132:LYS:HG3	2.52	0.45
1:A:63:LEU:O	1:A:71:ARG:NH1	2.50	0.45
1:G:60:ASP:OD1	1:G:60:ASP:N	2.43	0.45
1:B:145:LEU:HD13	3:B:302:GOL:H32	1.99	0.45
1:E:155:ALA:HB3	1:E:253:VAL:HB	1.98	0.44
1:B:78:ILE:HA	1:B:81:VAL:HG12	1.98	0.44
1:C:78:ILE:HA	1:C:81:VAL:HG12	1.99	0.44
1:F:30:TRP:HA	1:F:41:TRP:HA	1.98	0.44
1:A:103:TRP:HB3	1:A:128:ILE:HG13	2.00	0.44
1:E:200:HIS:HA	1:E:203:TYR:CD2	2.52	0.44
1:G:78:ILE:HA	1:G:81:VAL:HG12	1.99	0.44
1:G:252:PHE:CE1	1:H:151:THR:HG23	2.51	0.44
1:C:29:THR:HG22	1:C:124:ILE:HG22	2.00	0.43
1:C:64:SER:HA	1:C:71:ARG:HH21	1.82	0.43
1:C:67:GLU:HG2	1:C:68:PRO:HD2	2.00	0.43
1:I:113:ASP:OD2	1:I:119:ARG:NH2	2.50	0.43
1:J:189:ASN:HA	1:J:192:MET:HE3	1.99	0.43
1:A:254:ARG:HE	1:A:254:ARG:HB2	1.50	0.43
1:C:41:TRP:HZ3	1:C:62:PHE:HB2	1.83	0.43
1:D:54:ASP:N	1:D:54:ASP:OD1	2.51	0.43
1:A:88:PHE:HD2	1:A:108:ALA:HB3	1.84	0.43
1:D:103:TRP:HB3	1:D:128:ILE:HG13	2.01	0.43
1:G:262:THR:HG23	1:H:266:LEU:HD12	2.00	0.43
1:A:33:ASP:OD1	1:A:33:ASP:N	2.44	0.43
1:A:89:ASP:HA	1:A:106:ALA:O	2.18	0.42
1:B:41:TRP:HZ3	1:B:62:PHE:HB2	1.83	0.42
1:B:103:TRP:HB3	1:B:128:ILE:HG13	2.01	0.42
1:B:155:ALA:HB3	1:B:253:VAL:HB	2.00	0.42
1:C:220:ARG:HD2	1:C:222:VAL:HG12	2.01	0.42
1:D:225:LYS:HE2	1:D:225:LYS:HB3	1.89	0.42
1:D:173:GLU:HG2	1:D:179:SER:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:145:LEU:O	1:H:149:LEU:HD12	2.19	0.42
1:E:63:LEU:HA	1:E:71:ARG:HH21	1.85	0.42
1:F:273:LEU:HD23	1:F:273:LEU:HA	1.91	0.42
1:I:112:ARG:HG2	1:I:118:ALA:HA	2.01	0.42
1:E:192:MET:HB3	2:E:601:HEM:HAB	2.01	0.42
1:G:145:LEU:HB2	3:H:301:GOL:H2	2.01	0.42
1:E:65:ARG:HD2	1:E:65:ARG:HA	1.47	0.42
1:F:110:LEU:H	1:F:110:LEU:HD23	1.85	0.42
1:A:173:GLU:OE2	1:A:180:GLU:N	2.48	0.41
1:I:68:PRO:HA	1:I:71:ARG:HG2	2.01	0.41
1:I:132:LYS:HA	1:I:132:LYS:HD2	1.89	0.41
1:D:93:ARG:HE	1:D:101:GLY:HA3	1.85	0.41
1:E:68:PRO:HA	1:E:71:ARG:HB2	2.03	0.41
1:H:41:TRP:CZ3	1:H:46:ARG:HB2	2.55	0.41
1:I:51:ILE:HD12	1:I:51:ILE:HA	1.98	0.41
1:A:235:HIS:HB2	1:A:256:LEU:HD21	2.02	0.41
1:D:78:ILE:O	1:D:81:VAL:HG22	2.21	0.41
1:E:176:PHE:CE2	1:E:191:LEU:HB3	2.56	0.41
1:H:93:ARG:HD2	1:H:101:GLY:HA3	2.01	0.41
1:I:176:PHE:CG	1:I:191:LEU:HD22	2.56	0.41
1:A:272:GLU:HB3	1:B:273:LEU:HD21	2.03	0.41
1:C:51:ILE:HD12	1:C:51:ILE:HA	1.94	0.41
1:C:144:HIS:CE1	1:C:148:ILE:HD11	2.56	0.41
1:F:189:ASN:HA	1:F:192:MET:HE3	2.02	0.41
1:A:119:ARG:HD3	1:A:120:HIS:CE1	2.56	0.41
1:C:29:THR:O	1:C:42:SER:N	2.50	0.41
1:C:266:LEU:O	1:C:270:GLN:HG2	2.21	0.41
1:A:156:MET:HE2	1:A:252:PHE:CE2	2.56	0.41
1:C:221:ILE:O	1:C:222:VAL:HG22	2.21	0.41
1:H:269:LEU:HD23	1:H:269:LEU:HA	1.91	0.41
1:G:89:ASP:HA	1:G:106:ALA:O	2.21	0.40
1:E:226:ARG:HB2	1:E:230:THR:HG23	2.02	0.40
1:J:234:MET:HB2	1:J:253:VAL:HG13	2.04	0.40
1:H:89:ASP:HA	1:H:106:ALA:O	2.21	0.40
1:H:103:TRP:HB3	1:H:128:ILE:HG13	2.04	0.40
2:J:302:HEM:HMC2	2:J:302:HEM:HBC2	2.02	0.40
1:J:112:ARG:HG2	1:J:118:ALA:HA	2.03	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	249/273 (91%)	243 (98%)	6 (2%)	0	100	100
1	B	252/273 (92%)	246 (98%)	6 (2%)	0	100	100
1	C	250/273 (92%)	240 (96%)	9 (4%)	1 (0%)	30	53
1	D	249/273 (91%)	246 (99%)	3 (1%)	0	100	100
1	E	248/273 (91%)	243 (98%)	5 (2%)	0	100	100
1	F	247/273 (90%)	239 (97%)	8 (3%)	0	100	100
1	G	248/273 (91%)	243 (98%)	5 (2%)	0	100	100
1	H	248/273 (91%)	243 (98%)	5 (2%)	0	100	100
1	I	247/273 (90%)	241 (98%)	6 (2%)	0	100	100
1	J	248/273 (91%)	238 (96%)	10 (4%)	0	100	100
All	All	2486/2730 (91%)	2422 (97%)	63 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	222	VAL

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	210/228 (92%)	204 (97%)	6 (3%)	37	61
1	B	212/228 (93%)	204 (96%)	8 (4%)	29	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	210/228 (92%)	201 (96%)	9 (4%)	26	52
1	D	210/228 (92%)	205 (98%)	5 (2%)	43	67
1	E	209/228 (92%)	194 (93%)	15 (7%)	13	33
1	F	209/228 (92%)	199 (95%)	10 (5%)	23	48
1	G	209/228 (92%)	195 (93%)	14 (7%)	15	36
1	H	209/228 (92%)	199 (95%)	10 (5%)	23	48
1	I	208/228 (91%)	201 (97%)	7 (3%)	32	58
1	J	209/228 (92%)	202 (97%)	7 (3%)	33	58
All	All	2095/2280 (92%)	2004 (96%)	91 (4%)	25	52

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	THR
1	A	43	ASP
1	A	49	LEU
1	A	81	VAL
1	A	111	ILE
1	A	256	LEU
1	B	36	THR
1	B	54	ASP
1	B	63	LEU
1	B	73	ARG
1	B	84	ARG
1	B	121	LEU
1	B	180	GLU
1	B	188	VAL
1	C	32	LEU
1	C	51	ILE
1	C	71	ARG
1	C	111	ILE
1	C	121	LEU
1	C	131	GLU
1	C	211	SER
1	C	215	ILE
1	C	222	VAL
1	D	32	LEU
1	D	36	THR
1	D	167	LEU

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Mol	Chain	Res	Type
1	D	174	ARG
1	D	218	ILE
1	E	25	PHE
1	E	27	VAL
1	E	33	ASP
1	E	36	THR
1	E	49	LEU
1	E	65	ARG
1	E	92	PHE
1	E	94	VAL
1	E	121	LEU
1	E	124	ILE
1	E	133	GLN
1	E	208	ARG
1	E	228	ASP
1	E	230	THR
1	E	273	LEU
1	F	34	LEU
1	F	36	THR
1	F	49	LEU
1	F	81	VAL
1	F	84	ARG
1	F	97	THR
1	F	111	ILE
1	F	133	GLN
1	F	220	ARG
1	F	228	ASP
1	G	31	ASP
1	G	32	LEU
1	G	36	THR
1	G	43	ASP
1	G	72	GLU
1	G	94	VAL
1	G	114	GLU
1	G	120	HIS
1	G	121	LEU
1	G	220	ARG
1	G	222	VAL
1	G	256	LEU
1	G	257	THR
1	G	267	GLN
1	H	27	VAL

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Mol	Chain	Res	Type
1	H	36	THR
1	H	39	LEU
1	H	75	GLU
1	H	78	ILE
1	H	131	GLU
1	H	149	LEU
1	H	181	LEU
1	H	218	ILE
1	H	220	ARG
1	I	27	VAL
1	I	33	ASP
1	I	36	THR
1	I	92	PHE
1	I	121	LEU
1	I	218	ILE
1	I	230	THR
1	J	33	ASP
1	J	36	THR
1	J	83	GLU
1	J	225	LYS
1	J	237	SER
1	J	246	GLU
1	J	269	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	270	GLN
1	B	162	HIS
1	C	102	GLN
1	C	162	HIS
1	C	214	HIS
1	C	235	HIS
1	D	120	HIS
1	D	162	HIS
1	D	186	GLN
1	D	260	GLN
1	E	133	GLN
1	E	186	GLN
1	G	242	GLN
1	H	102	GLN
1	H	150	HIS

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Mol	Chain	Res	Type
1	I	166	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

25 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	HEM	D	303	1	50,50,50	1.33	7 (14%)	66,82,82	1.09	2 (3%)
3	GOL	I	603	-	5,5,5	0.94	0	5,5,5	0.94	0
3	GOL	C	602	-	5,5,5	0.96	0	5,5,5	0.95	0
3	GOL	I	602	-	5,5,5	1.13	0	5,5,5	0.97	0
2	HEM	A	601	1	50,50,50	1.34	7 (14%)	66,82,82	1.09	2 (3%)
2	HEM	H	302	1	50,50,50	1.46	6 (12%)	66,82,82	1.29	8 (12%)
2	HEM	F	302	1	50,50,50	1.46	9 (18%)	66,82,82	1.21	6 (9%)
3	GOL	B	301	-	5,5,5	0.78	0	5,5,5	1.09	0
2	HEM	C	601	1	50,50,50	1.35	7 (14%)	66,82,82	1.21	3 (4%)
3	GOL	H	301	-	5,5,5	1.03	0	5,5,5	0.97	0
3	GOL	G	603	-	5,5,5	0.87	0	5,5,5	1.13	0
3	GOL	J	301	-	5,5,5	0.87	0	5,5,5	0.96	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	G	602	-	5,5,5	0.95	0	5,5,5	0.93	0
3	GOL	A	602	-	5,5,5	0.73	0	5,5,5	1.21	1 (20%)
2	HEM	G	601	1	50,50,50	1.48	7 (14%)	66,82,82	1.18	7 (10%)
3	GOL	D	301	-	5,5,5	1.02	0	5,5,5	1.11	0
3	GOL	E	603	-	5,5,5	1.30	1 (20%)	5,5,5	0.75	0
3	GOL	E	602	-	5,5,5	1.03	0	5,5,5	0.93	0
3	GOL	F	301	-	5,5,5	0.79	0	5,5,5	1.09	1 (20%)
2	HEM	I	601	1	50,50,50	1.53	7 (14%)	66,82,82	1.21	6 (9%)
3	GOL	D	302	-	5,5,5	0.99	0	5,5,5	1.03	0
2	HEM	J	302	1	50,50,50	1.66	8 (16%)	66,82,82	1.24	7 (10%)
2	HEM	E	601	1	50,50,50	1.42	8 (16%)	66,82,82	1.26	8 (12%)
3	GOL	B	302	-	5,5,5	0.93	0	5,5,5	1.01	0
2	HEM	B	303	1	50,50,50	1.46	7 (14%)	66,82,82	1.27	8 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	D	303	1	-	1/14/54/54	-
3	GOL	I	603	-	-	2/4/4/4	-
3	GOL	C	602	-	-	2/4/4/4	-
3	GOL	I	602	-	-	1/4/4/4	-
2	HEM	A	601	1	-	4/14/54/54	-
2	HEM	H	302	1	-	3/14/54/54	-
2	HEM	F	302	1	-	3/14/54/54	-
3	GOL	B	301	-	-	4/4/4/4	-
2	HEM	C	601	1	-	4/14/54/54	-
3	GOL	H	301	-	-	2/4/4/4	-
3	GOL	G	603	-	-	2/4/4/4	-
3	GOL	J	301	-	-	2/4/4/4	-
3	GOL	G	602	-	-	1/4/4/4	-
3	GOL	A	602	-	-	4/4/4/4	-
2	HEM	G	601	1	-	2/14/54/54	-
3	GOL	D	301	-	-	0/4/4/4	-
3	GOL	E	603	-	-	0/4/4/4	-
3	GOL	E	602	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	F	301	-	-	2/4/4/4	-
2	HEM	I	601	1	-	1/14/54/54	-
3	GOL	D	302	-	-	2/4/4/4	-
2	HEM	J	302	1	-	4/14/54/54	-
2	HEM	E	601	1	-	4/14/54/54	-
3	GOL	B	302	-	-	0/4/4/4	-
2	HEM	B	303	1	-	4/14/54/54	-

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	302	HEM	FE-NB	5.45	2.11	1.94
2	B	303	HEM	FE-NB	5.07	2.10	1.94
2	I	601	HEM	FE-ND	4.70	2.09	1.94
2	G	601	HEM	FE-NB	4.69	2.09	1.94
2	J	302	HEM	FE-NC	4.34	2.09	1.95
2	J	302	HEM	FE-ND	4.32	2.08	1.94
2	F	302	HEM	FE-NB	4.25	2.08	1.94
2	H	302	HEM	FE-NB	4.18	2.07	1.94
2	H	302	HEM	FE-NA	3.75	2.07	1.95
2	I	601	HEM	FE-NC	3.66	2.07	1.95
2	I	601	HEM	FE-NB	3.60	2.06	1.94
2	F	302	HEM	FE-NA	3.56	2.07	1.95
2	E	601	HEM	FE-ND	3.48	2.05	1.94
2	A	601	HEM	FE-NA	3.42	2.06	1.95
2	E	601	HEM	FE-NB	3.30	2.05	1.94
2	F	302	HEM	FE-ND	3.24	2.04	1.94
2	G	601	HEM	FE-NA	3.23	2.06	1.95
2	B	303	HEM	CAC-C3C	3.21	1.56	1.47
2	D	303	HEM	FE-ND	3.20	2.04	1.94
2	F	302	HEM	CAC-C3C	3.19	1.56	1.47
2	C	601	HEM	FE-NA	3.18	2.05	1.95
2	C	601	HEM	FE-NB	3.18	2.04	1.94
2	H	302	HEM	FE-ND	3.17	2.04	1.94
2	H	302	HEM	CAC-C3C	3.16	1.56	1.47
2	D	303	HEM	FE-NC	3.15	2.05	1.95
2	B	303	HEM	FE-NA	3.14	2.05	1.95
2	E	601	HEM	CAC-C3C	3.13	1.56	1.47
2	C	601	HEM	CAC-C3C	3.09	1.55	1.47
2	I	601	HEM	CAC-C3C	3.07	1.55	1.47
2	G	601	HEM	FE-ND	3.05	2.04	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	601	HEM	CAB-C3B	2.98	1.55	1.47
2	C	601	HEM	CAB-C3B	2.97	1.55	1.47
2	D	303	HEM	CAB-C3B	2.97	1.55	1.47
2	G	601	HEM	CAB-C3B	2.95	1.55	1.47
2	C	601	HEM	FE-ND	2.93	2.03	1.94
2	I	601	HEM	FE-NA	2.91	2.05	1.95
2	D	303	HEM	CAC-C3C	2.90	1.55	1.47
2	J	302	HEM	CAB-C3B	2.90	1.55	1.47
2	G	601	HEM	CAC-C3C	2.89	1.55	1.47
2	B	303	HEM	CAB-C3B	2.88	1.55	1.47
2	J	302	HEM	CAC-C3C	2.86	1.55	1.47
2	A	601	HEM	CAC-C3C	2.85	1.55	1.47
2	H	302	HEM	CAB-C3B	2.82	1.55	1.47
2	A	601	HEM	FE-ND	2.81	2.03	1.94
2	A	601	HEM	CAB-C3B	2.77	1.55	1.47
2	E	601	HEM	CAB-C3B	2.74	1.54	1.47
2	J	302	HEM	FE-NA	2.74	2.04	1.95
2	E	601	HEM	FE-NC	2.70	2.04	1.95
2	D	303	HEM	FE-NB	2.68	2.03	1.94
2	A	601	HEM	FE-NC	2.67	2.04	1.95
2	F	302	HEM	CAB-C3B	2.66	1.54	1.47
2	A	601	HEM	FE-NB	2.52	2.02	1.94
2	B	303	HEM	FE-ND	2.51	2.02	1.94
2	H	302	HEM	FE-NC	2.39	2.03	1.95
2	E	601	HEM	CMD-C2D	2.26	1.55	1.50
3	E	603	GOL	C3-C2	2.18	1.60	1.51
2	E	601	HEM	FE-NA	2.16	2.02	1.95
2	J	302	HEM	CMA-C3A	2.15	1.55	1.50
2	F	302	HEM	CMD-C2D	2.13	1.55	1.50
2	G	601	HEM	CMC-C2C	2.13	1.55	1.50
2	D	303	HEM	FE-NA	2.12	2.02	1.95
2	F	302	HEM	CMC-C2C	2.11	1.55	1.50
2	C	601	HEM	CMB-C2B	2.11	1.55	1.50
2	B	303	HEM	CMA-C3A	2.11	1.55	1.50
2	J	302	HEM	CMD-C2D	2.10	1.55	1.50
2	E	601	HEM	C2A-C3A	-2.09	1.33	1.38
2	A	601	HEM	CAD-C3D	2.09	1.56	1.51
2	C	601	HEM	CMA-C3A	2.06	1.55	1.50
2	F	302	HEM	CMA-C3A	2.03	1.55	1.50
2	I	601	HEM	CMD-C2D	2.02	1.55	1.50
2	F	302	HEM	FE-NC	2.01	2.01	1.95
2	G	601	HEM	CMD-C2D	2.01	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	303	HEM	CMD-C2D	2.01	1.55	1.50
2	D	303	HEM	CMC-C2C	2.00	1.55	1.50

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	HEM	C3B-C2B-C1B	3.44	109.04	106.49
2	H	302	HEM	CAA-CBA-CGA	-3.35	106.39	113.60
2	E	601	HEM	CAA-CBA-CGA	-3.32	106.46	113.60
2	D	303	HEM	C3B-C2B-C1B	3.27	108.91	106.49
2	I	601	HEM	CAA-CBA-CGA	-3.25	106.61	113.60
2	E	601	HEM	CBA-CAA-C2A	-3.20	103.74	112.63
2	J	302	HEM	C1B-NB-C4B	3.12	108.29	105.07
2	J	302	HEM	C3B-C2B-C1B	3.11	108.80	106.49
2	H	302	HEM	C3B-C2B-C1B	3.10	108.78	106.49
2	C	601	HEM	CAA-CBA-CGA	-3.08	106.97	113.60
2	I	601	HEM	C1B-NB-C4B	3.08	108.25	105.07
2	H	302	HEM	C4D-ND-C1D	3.00	108.17	105.07
2	H	302	HEM	C1B-NB-C4B	2.97	108.14	105.07
2	J	302	HEM	CAA-CBA-CGA	-2.95	107.26	113.60
2	E	601	HEM	C3B-C2B-C1B	2.92	108.65	106.49
2	B	303	HEM	C3B-C2B-C1B	2.91	108.64	106.49
2	B	303	HEM	CAA-CBA-CGA	-2.90	107.36	113.60
2	I	601	HEM	C3B-C2B-C1B	2.88	108.62	106.49
2	D	303	HEM	CAA-CBA-CGA	-2.79	107.60	113.60
2	F	302	HEM	C4D-ND-C1D	2.79	107.95	105.07
2	C	601	HEM	C1B-NB-C4B	2.74	107.90	105.07
2	G	601	HEM	CHC-C1C-NC	2.68	127.34	124.44
2	B	303	HEM	C1B-NB-C4B	2.68	107.84	105.07
2	I	601	HEM	C4C-NC-C1C	2.67	107.96	105.35
2	G	601	HEM	C1B-NB-C4B	2.63	107.79	105.07
2	E	601	HEM	C2A-C1A-NA	-2.63	107.21	110.15
2	A	601	HEM	C1B-NB-C4B	2.60	107.76	105.07
2	J	302	HEM	C4D-ND-C1D	2.56	107.72	105.07
2	H	302	HEM	C4A-NA-C1A	2.55	107.84	105.35
2	F	302	HEM	C1B-NB-C4B	2.54	107.70	105.07
2	E	601	HEM	C1B-NB-C4B	2.53	107.69	105.07
2	F	302	HEM	C3B-C2B-C1B	2.47	108.32	106.49
2	G	601	HEM	CAA-CBA-CGA	-2.42	108.39	113.60
2	G	601	HEM	C3B-C2B-C1B	2.40	108.27	106.49
2	C	601	HEM	C3B-C2B-C1B	2.40	108.27	106.49
2	B	303	HEM	CHC-C1C-NC	2.37	127.01	124.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	302	HEM	C4C-NC-C1C	2.37	107.67	105.35
2	I	601	HEM	C4D-ND-C1D	2.35	107.50	105.07
2	G	601	HEM	C4D-ND-C1D	2.33	107.48	105.07
2	F	302	HEM	C4A-NA-C1A	2.32	107.62	105.35
2	J	302	HEM	C4C-NC-C1C	2.32	107.62	105.35
2	E	601	HEM	C4A-NA-C1A	2.25	107.55	105.35
2	H	302	HEM	C2A-C1A-NA	-2.23	107.65	110.15
2	G	601	HEM	CMC-C2C-C1C	-2.21	120.81	124.71
2	G	601	HEM	C4C-NC-C1C	2.17	107.47	105.35
2	J	302	HEM	CHC-C1C-NC	2.14	126.75	124.44
2	F	302	HEM	CAA-CBA-CGA	-2.14	109.00	113.60
2	E	601	HEM	C4D-ND-C1D	2.11	107.25	105.07
2	B	303	HEM	CHD-C1D-ND	2.10	126.70	124.42
2	F	302	HEM	C4C-NC-C1C	2.09	107.39	105.35
2	I	601	HEM	C4A-NA-C1A	2.09	107.39	105.35
2	E	601	HEM	CHD-C1D-ND	2.07	126.67	124.42
2	B	303	HEM	CAB-C3B-C2B	-2.07	121.80	128.60
2	J	302	HEM	CMC-C2C-C1C	-2.04	121.11	124.71
2	B	303	HEM	CMC-C2C-C1C	-2.03	121.13	124.71
2	B	303	HEM	CHC-C4B-C3B	2.03	129.50	125.13
2	H	302	HEM	CHD-C1D-ND	2.03	126.62	124.42
3	A	602	GOL	C3-C2-C1	-2.03	103.83	111.70
3	F	301	GOL	C3-C2-C1	-2.02	103.87	111.70

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	GOL	O1-C1-C2-C3
3	B	301	GOL	C1-C2-C3-O3
3	D	302	GOL	C1-C2-C3-O3
3	F	301	GOL	O1-C1-C2-C3
3	H	301	GOL	C1-C2-C3-O3
3	I	603	GOL	C1-C2-C3-O3
3	J	301	GOL	O1-C1-C2-C3
3	A	602	GOL	C1-C2-C3-O3
3	B	301	GOL	O1-C1-C2-C3
3	C	602	GOL	O1-C1-C2-C3
3	G	602	GOL	C1-C2-C3-O3
3	G	603	GOL	C1-C2-C3-O3
3	A	602	GOL	O1-C1-C2-O2
3	D	302	GOL	O2-C2-C3-O3

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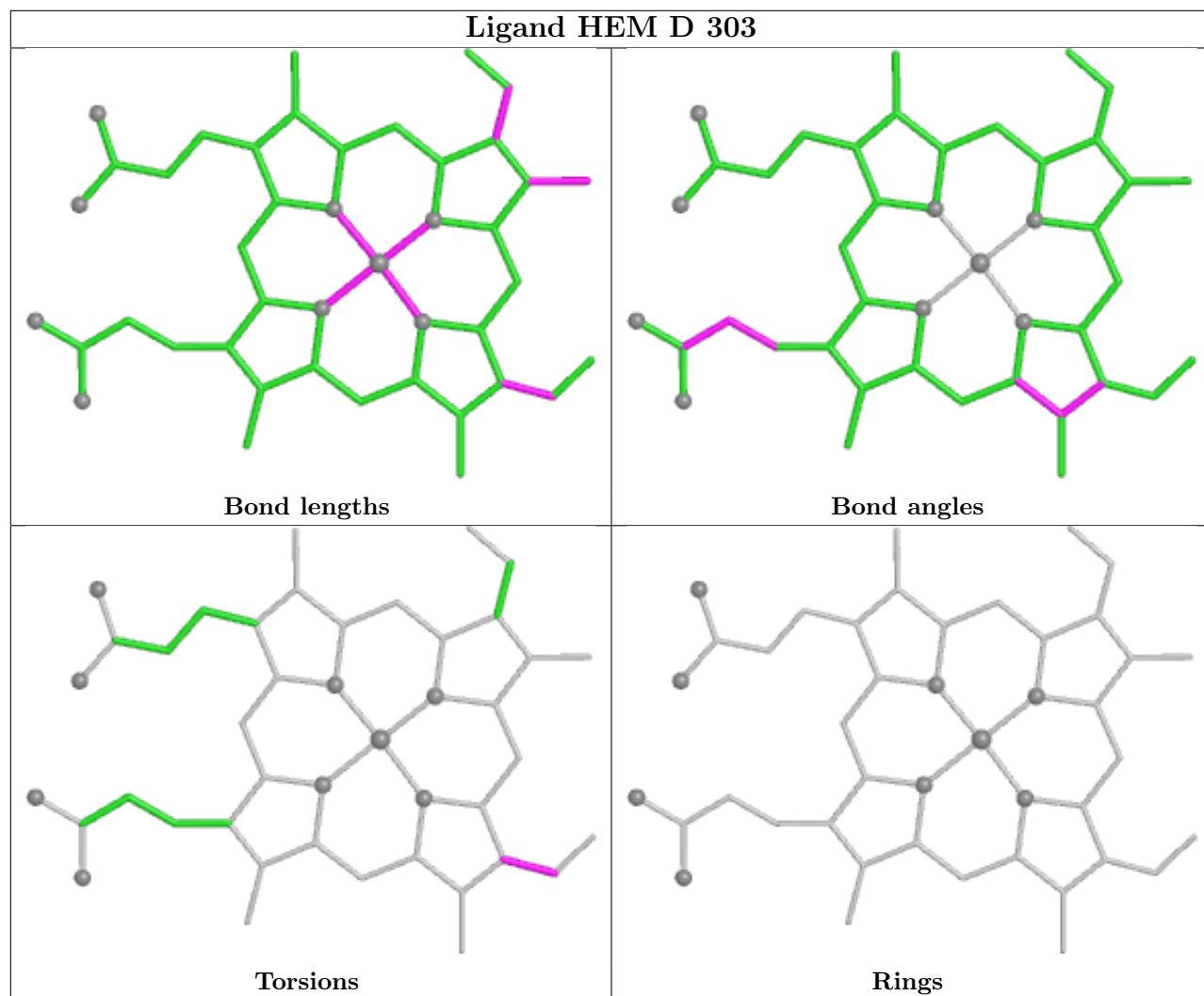
Mol	Chain	Res	Type	Atoms
3	G	603	GOL	O2-C2-C3-O3
3	I	603	GOL	O2-C2-C3-O3
3	J	301	GOL	O1-C1-C2-O2
3	B	301	GOL	O2-C2-C3-O3
3	F	301	GOL	O1-C1-C2-O2
3	H	301	GOL	O2-C2-C3-O3
2	E	601	HEM	C3D-CAD-CBD-CGD
2	F	302	HEM	C3D-CAD-CBD-CGD
2	B	303	HEM	C3D-CAD-CBD-CGD
2	C	601	HEM	C3D-CAD-CBD-CGD
2	H	302	HEM	C3D-CAD-CBD-CGD
3	A	602	GOL	O2-C2-C3-O3
3	I	602	GOL	O2-C2-C3-O3
2	A	601	HEM	C4B-C3B-CAB-CBB
2	B	303	HEM	C4B-C3B-CAB-CBB
2	C	601	HEM	C4B-C3B-CAB-CBB
2	D	303	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	I	601	HEM	C4B-C3B-CAB-CBB
2	J	302	HEM	C4B-C3B-CAB-CBB
3	B	301	GOL	O1-C1-C2-O2
2	G	601	HEM	C3D-CAD-CBD-CGD
2	C	601	HEM	CAA-CBA-CGA-O1A
3	C	602	GOL	O1-C1-C2-O2
2	C	601	HEM	CAA-CBA-CGA-O2A
2	J	302	HEM	C3D-CAD-CBD-CGD
2	A	601	HEM	CAD-CBD-CGD-O2D
2	H	302	HEM	CAA-CBA-CGA-O2A
2	A	601	HEM	CAA-CBA-CGA-O2A
2	B	303	HEM	CAA-CBA-CGA-O2A
2	A	601	HEM	CAD-CBD-CGD-O1D
2	B	303	HEM	CAA-CBA-CGA-O1A
2	F	302	HEM	CAA-CBA-CGA-O2A
2	J	302	HEM	CAA-CBA-CGA-O1A
2	J	302	HEM	CAA-CBA-CGA-O2A
2	E	601	HEM	CAA-CBA-CGA-O2A
2	E	601	HEM	CAA-CBA-CGA-O1A

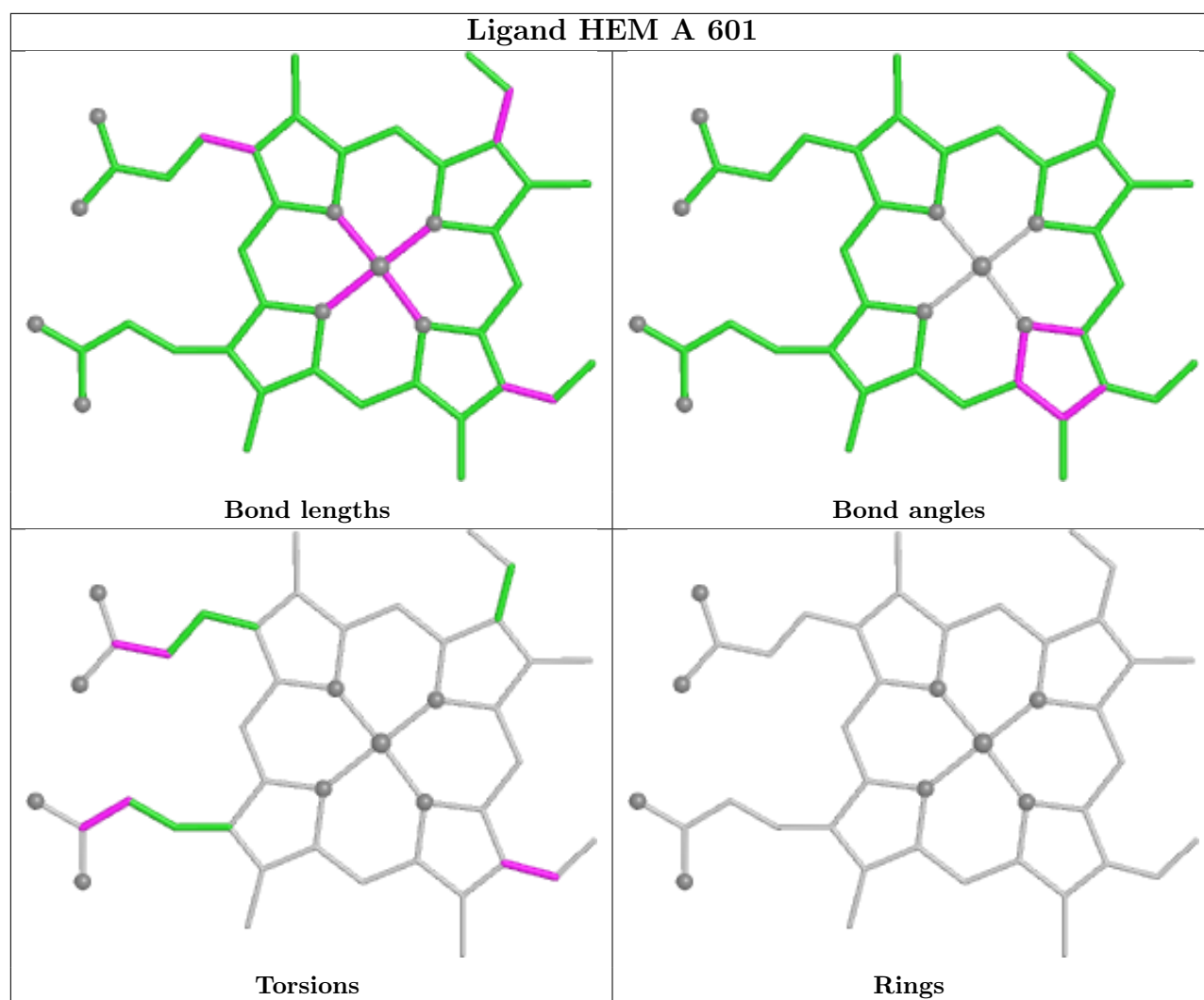
There are no ring outliers.

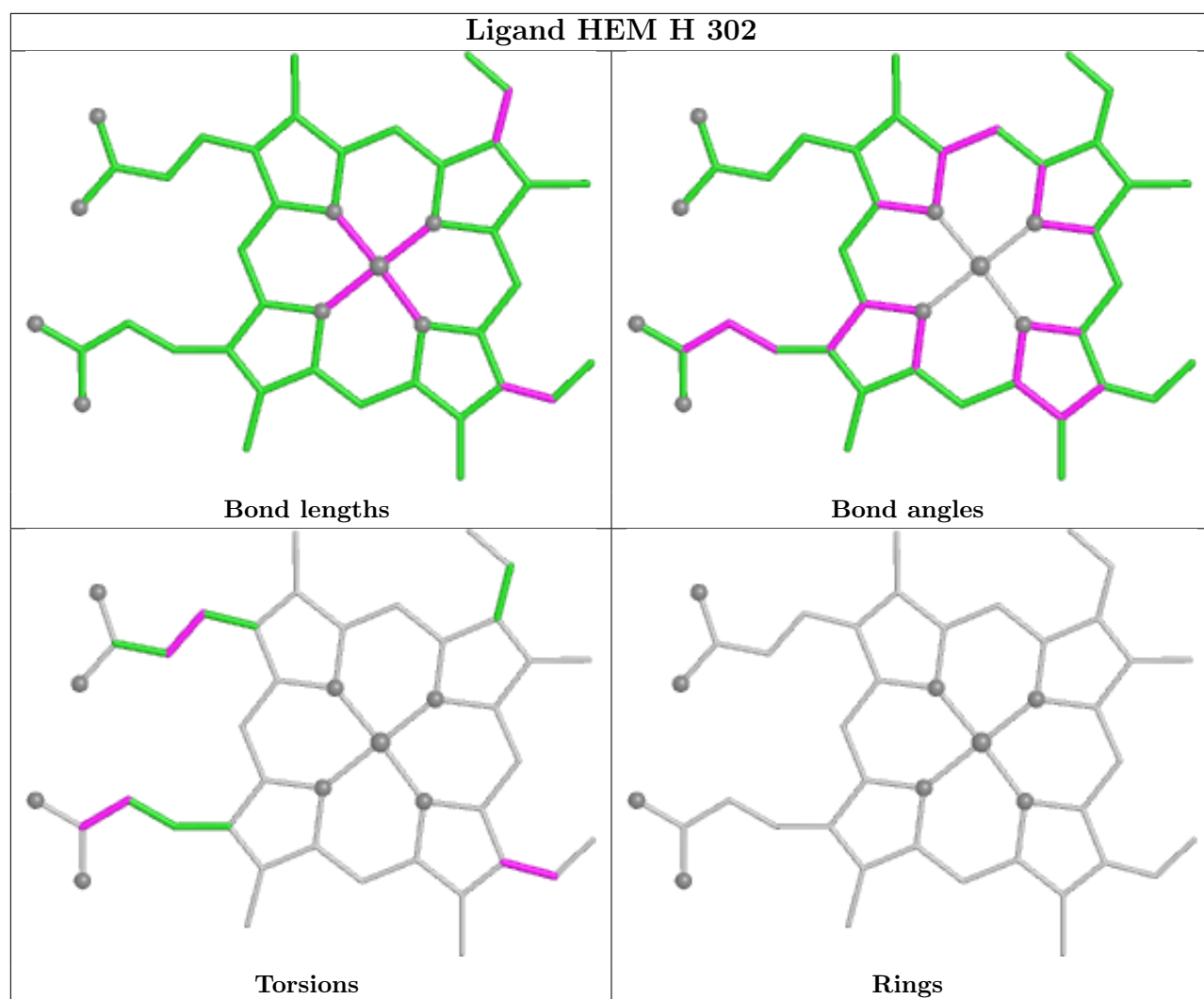
15 monomers are involved in 24 short contacts:

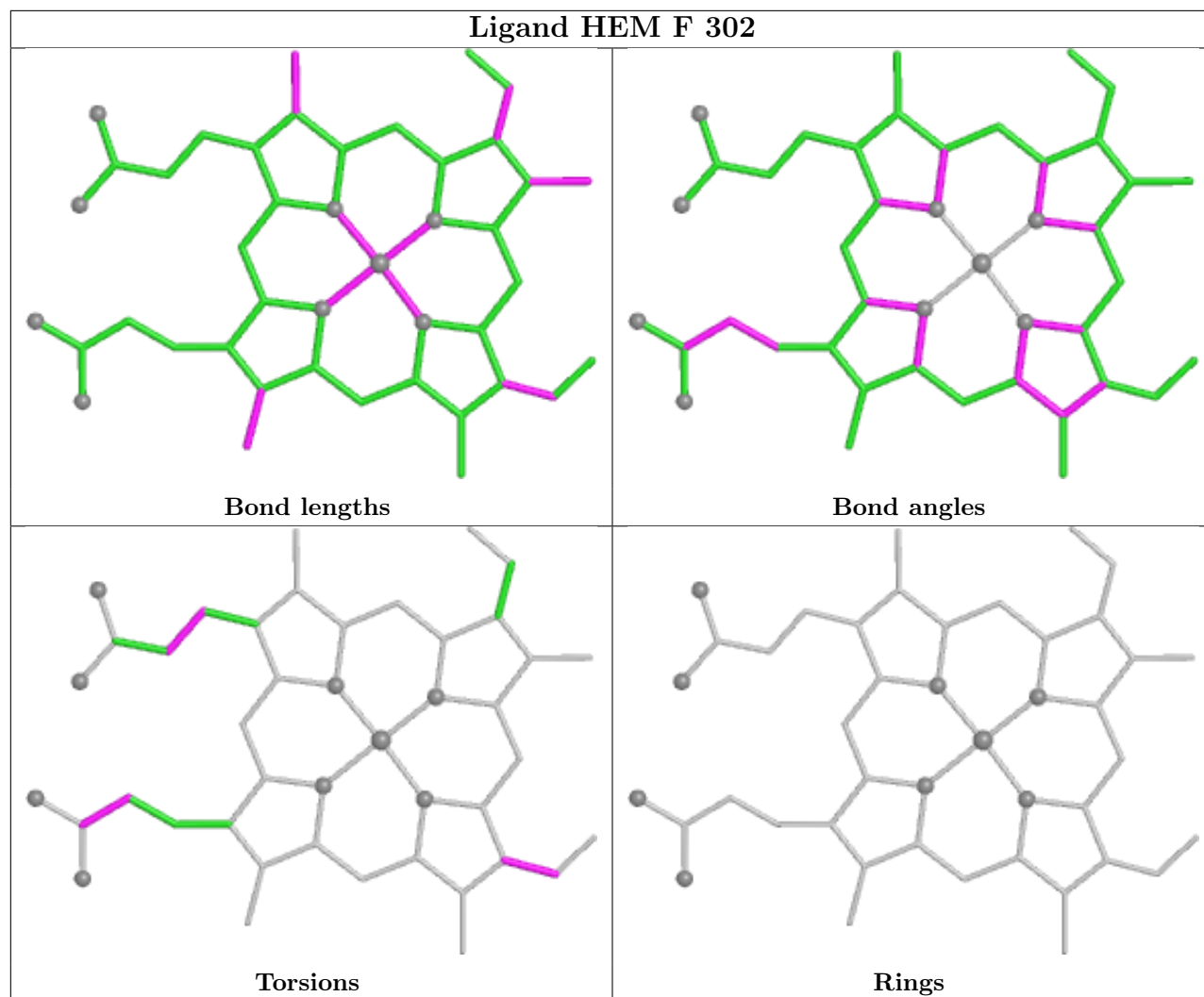
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	303	HEM	1	0
2	A	601	HEM	1	0
2	H	302	HEM	2	0
2	F	302	HEM	1	0
2	C	601	HEM	1	0
3	H	301	GOL	2	0
3	G	603	GOL	1	0
2	G	601	HEM	2	0
3	E	602	GOL	2	0
2	I	601	HEM	1	0
3	D	302	GOL	1	0
2	J	302	HEM	2	0
2	E	601	HEM	4	0
3	B	302	GOL	2	0
2	B	303	HEM	1	0

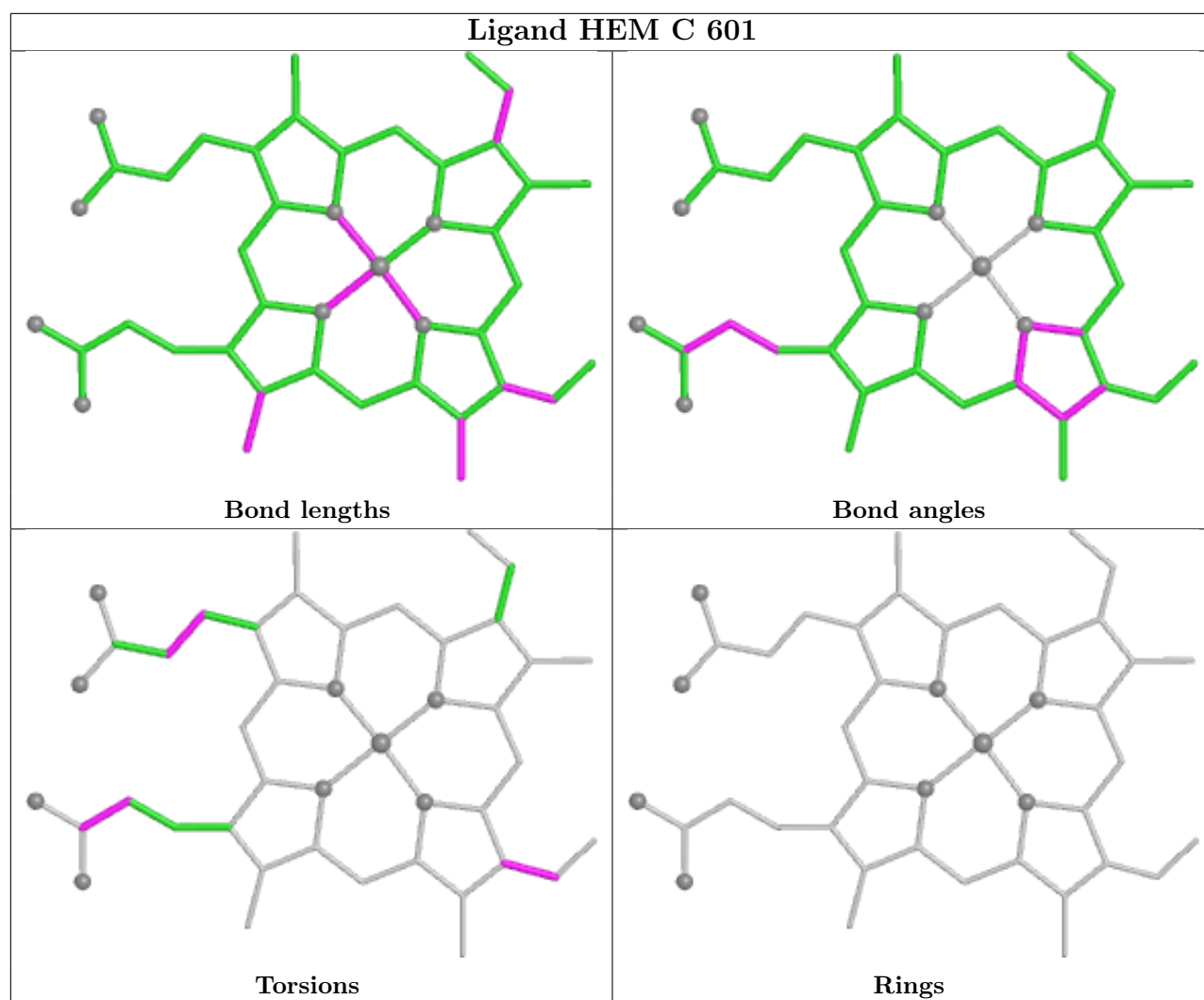
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

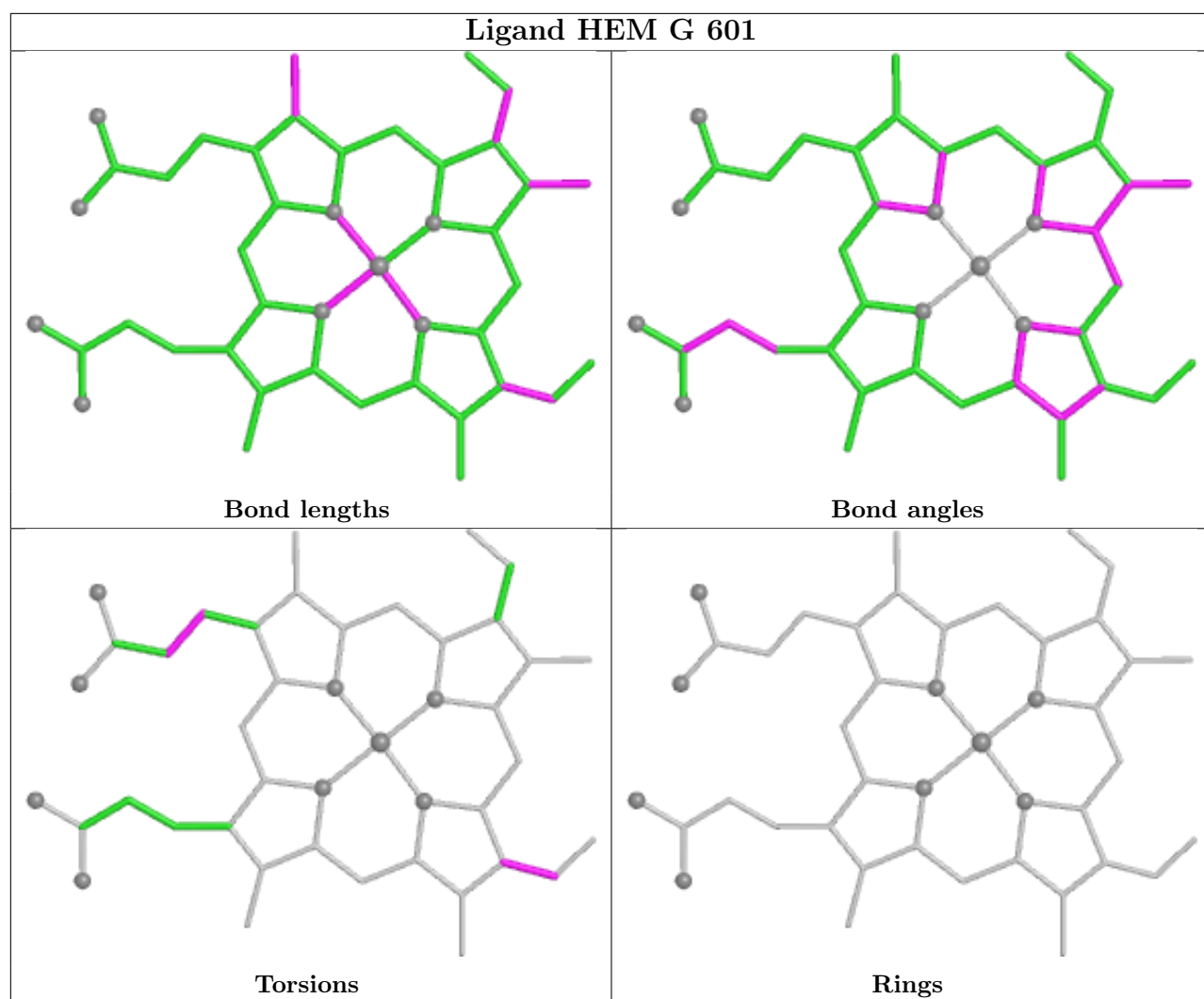


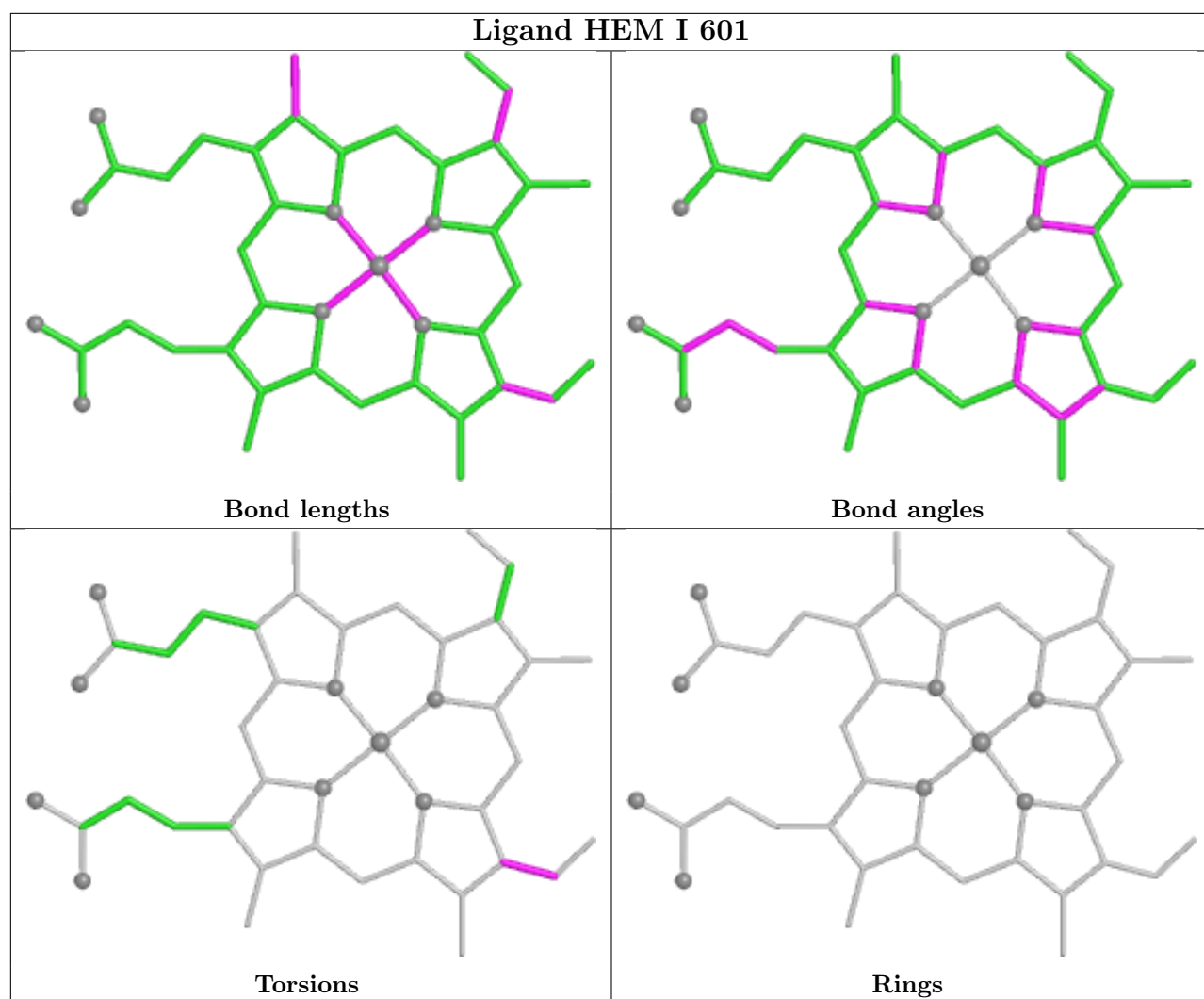


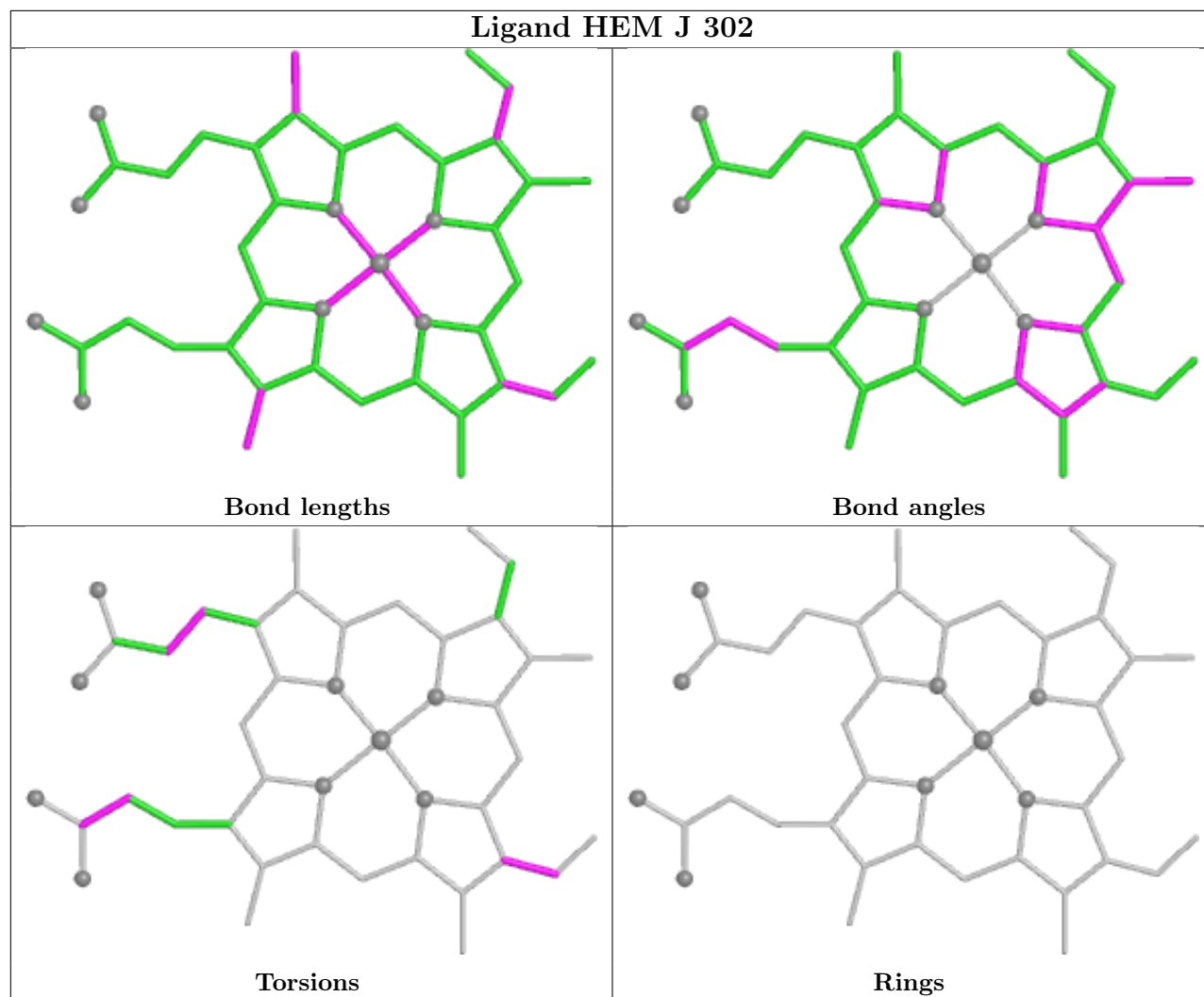


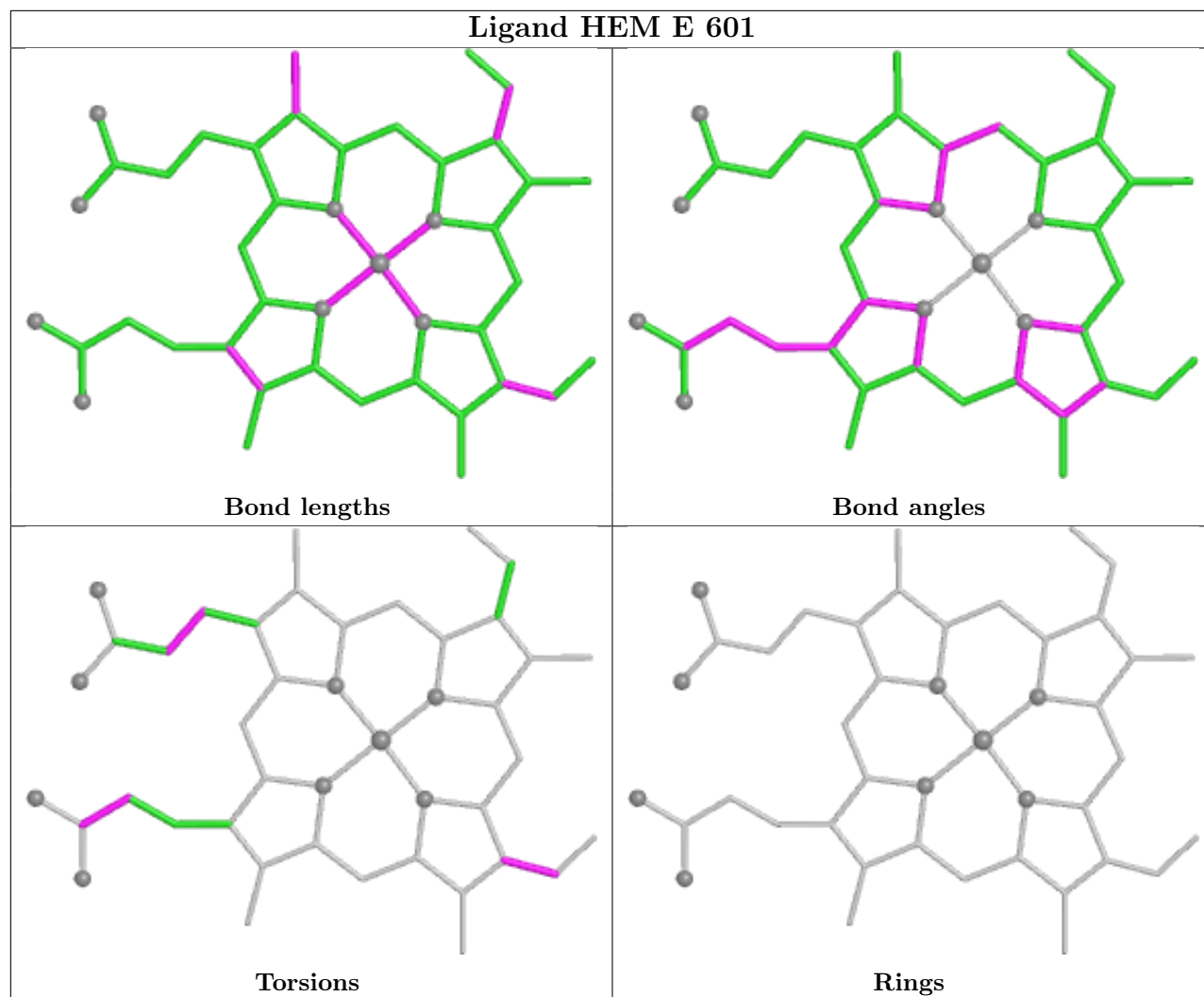


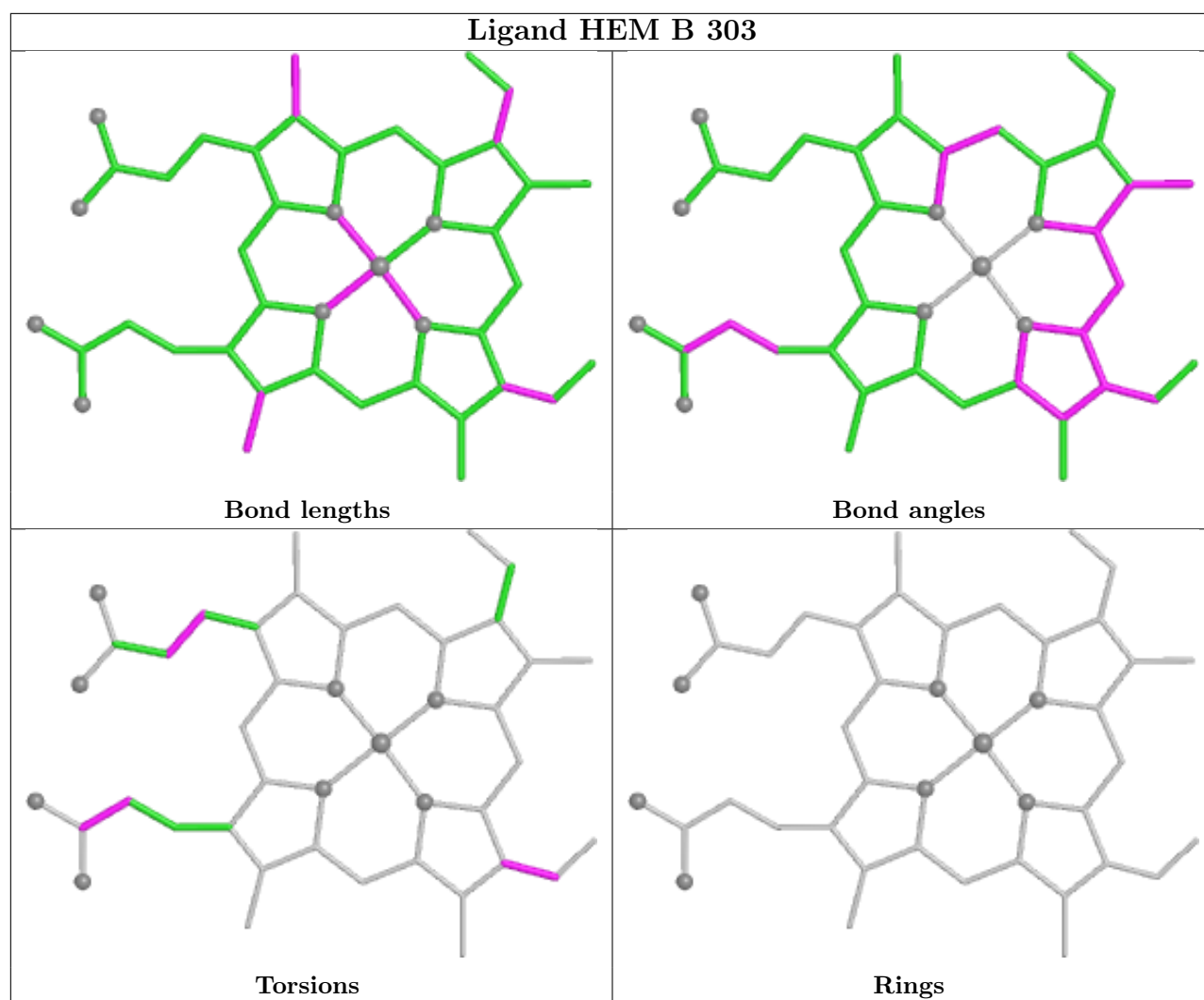












5.7 Other polymers [i](#)

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	250/273 (91%)	0.49	23 (9%)	14	13	46, 117, 245, 307	1 (0%)
1	B	253/273 (92%)	0.41	12 (4%)	36	30	52, 131, 254, 312	1 (0%)
1	C	252/273 (92%)	0.52	23 (9%)	15	13	66, 130, 249, 387	0
1	D	250/273 (91%)	0.45	21 (8%)	17	15	48, 114, 259, 303	1 (0%)
1	E	250/273 (91%)	0.67	27 (10%)	11	10	72, 136, 288, 334	0
1	F	248/273 (90%)	0.53	17 (6%)	23	19	57, 126, 233, 288	1 (0%)
1	G	249/273 (91%)	0.47	16 (6%)	25	21	49, 122, 241, 317	1 (0%)
1	H	250/273 (91%)	0.52	19 (7%)	20	18	71, 133, 272, 343	0
1	I	249/273 (91%)	0.51	21 (8%)	17	15	77, 145, 262, 363	0
1	J	249/273 (91%)	0.44	23 (9%)	14	13	57, 148, 263, 362	1 (0%)
All	All	2500/2730 (91%)	0.50	202 (8%)	18	16	46, 128, 262, 387	6 (0%)

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	62	PHE	6.9
1	I	51	ILE	6.6
1	A	62	PHE	5.8
1	B	269	LEU	5.7
1	H	62	PHE	5.7
1	H	121	LEU	5.7
1	G	110	LEU	5.5
1	I	61	LEU	5.5
1	C	51	ILE	5.5
1	F	110	LEU	5.3
1	H	110	LEU	5.1
1	G	51	ILE	4.9
1	E	49	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	H	266	LEU	4.8
1	A	121	LEU	4.7
1	C	110	LEU	4.5
1	I	94	VAL	4.5
1	E	34	LEU	4.4
1	C	266	LEU	4.3
1	D	37	TRP	4.3
1	I	49	LEU	4.3
1	J	51	ILE	4.2
1	E	121	LEU	4.1
1	I	110	LEU	4.1
1	C	59	TYR	4.1
1	H	51	ILE	4.1
1	J	62	PHE	4.0
1	B	110	LEU	4.0
1	J	111	ILE	3.9
1	B	51	ILE	3.9
1	C	125	PHE	3.8
1	D	38	ALA	3.8
1	F	269	LEU	3.8
1	A	34	LEU	3.7
1	A	25	PHE	3.7
1	D	36	THR	3.6
1	H	111	ILE	3.6
1	B	22	ILE	3.5
1	E	266	LEU	3.5
1	E	62	PHE	3.5
1	I	48	LEU	3.5
1	E	63	LEU	3.5
1	A	110	LEU	3.4
1	D	111	ILE	3.3
1	I	62	PHE	3.3
1	J	32	LEU	3.3
1	D	95	ALA	3.3
1	E	125	PHE	3.3
1	B	78	ILE	3.3
1	H	269	LEU	3.3
1	C	269	LEU	3.2
1	D	34	LEU	3.2
1	I	32	LEU	3.2
1	F	116	GLY	3.2
1	E	51	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	I	111	ILE	3.2
1	A	32	LEU	3.2
1	F	266	LEU	3.2
1	D	86	GLY	3.2
1	J	34	LEU	3.1
1	A	118	ALA	3.1
1	D	62	PHE	3.1
1	E	48	LEU	3.1
1	B	66	LEU	3.1
1	A	63	LEU	3.1
1	D	273	LEU	3.1
1	G	116	GLY	3.1
1	C	61	LEU	3.0
1	B	59	TYR	3.0
1	J	121	LEU	3.0
1	J	126	LEU	3.0
1	C	78	ILE	3.0
1	B	62	PHE	3.0
1	E	88	PHE	3.0
1	A	37	TRP	3.0
1	I	269	LEU	3.0
1	F	259	HIS	3.0
1	J	61	LEU	2.9
1	A	95	ALA	2.9
1	A	74	VAL	2.9
1	E	74	VAL	2.9
1	H	32	LEU	2.9
1	D	269	LEU	2.9
1	J	110	LEU	2.9
1	H	96	GLY	2.9
1	J	78	ILE	2.9
1	H	34	LEU	2.9
1	H	260	GLN	2.8
1	D	121	LEU	2.8
1	D	59	TYR	2.8
1	A	27	VAL	2.8
1	F	111	ILE	2.8
1	G	96	GLY	2.8
1	F	98	SER	2.8
1	J	274	VAL	2.8
1	D	110	LEU	2.8
1	E	273	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	G	111	ILE	2.7
1	I	259	HIS	2.7
1	C	228	ASP	2.7
1	E	61	LEU	2.6
1	I	41	TRP	2.6
1	E	110	LEU	2.6
1	A	111	ILE	2.6
1	F	69	ASP	2.6
1	H	82	SER	2.6
1	C	81	VAL	2.6
1	D	27	VAL	2.6
1	J	182	GLU	2.6
1	C	86	GLY	2.6
1	A	39	LEU	2.5
1	I	26	GLY	2.5
1	E	223	THR	2.5
1	G	260	GLN	2.5
1	F	120	HIS	2.5
1	D	100	ALA	2.5
1	E	264	ALA	2.5
1	J	116	GLY	2.5
1	H	27	VAL	2.5
1	B	97	THR	2.5
1	G	97	THR	2.4
1	C	259	HIS	2.4
1	G	273	LEU	2.4
1	H	78	ILE	2.4
1	C	244	GLY	2.4
1	H	264	ALA	2.4
1	E	97	THR	2.4
1	A	61	LEU	2.4
1	H	48	LEU	2.4
1	A	81	VAL	2.4
1	H	85	GLY	2.4
1	H	37	TRP	2.4
1	A	266	LEU	2.4
1	I	81	VAL	2.3
1	C	116	GLY	2.3
1	D	26	GLY	2.3
1	I	228	ASP	2.3
1	F	74	VAL	2.3
1	C	34	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	59	TYR	2.3
1	D	56	PRO	2.3
1	E	274	VAL	2.3
1	G	274	VAL	2.3
1	G	115	ALA	2.3
1	C	39	LEU	2.3
1	C	273	LEU	2.3
1	E	260	GLN	2.3
1	J	49	LEU	2.3
1	A	38	ALA	2.3
1	E	36	THR	2.3
1	F	103	TRP	2.3
1	J	97	THR	2.3
1	F	72	GLU	2.2
1	E	111	ILE	2.2
1	B	64	SER	2.2
1	C	26	GLY	2.2
1	C	121	LEU	2.2
1	E	39	LEU	2.2
1	H	83	GLU	2.2
1	G	120	HIS	2.2
1	F	68	PRO	2.2
1	G	269	LEU	2.2
1	C	41	TRP	2.2
1	G	47	THR	2.2
1	J	41	TRP	2.2
1	I	52	GLY	2.2
1	I	34	LEU	2.2
1	I	273	LEU	2.2
1	A	26	GLY	2.2
1	E	37	TRP	2.2
1	G	103	TRP	2.2
1	I	37	TRP	2.2
1	I	87	GLY	2.2
1	J	37	TRP	2.2
1	A	82	SER	2.2
1	B	266	LEU	2.2
1	G	82	SER	2.2
1	E	118	ALA	2.2
1	F	115	ALA	2.2
1	J	95	ALA	2.2
1	J	102	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	27	VAL	2.1
1	A	123	GLY	2.1
1	D	78	ILE	2.1
1	F	51	ILE	2.1
1	B	41	TRP	2.1
1	I	95	ALA	2.1
1	A	91	SER	2.1
1	D	259	HIS	2.1
1	A	68	PRO	2.1
1	C	37	TRP	2.1
1	J	115	ALA	2.1
1	E	82	SER	2.1
1	E	91	SER	2.1
1	G	117	THR	2.1
1	D	61	LEU	2.0
1	J	36	THR	2.0
1	C	274	VAL	2.0
1	F	260	GLN	2.0
1	E	115	ALA	2.0
1	F	100	ALA	2.0
1	D	274	VAL	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	D	301	6/6	0.90	0.19	76,87,97,108	0
3	GOL	I	603	6/6	0.90	0.20	98,103,110,113	0

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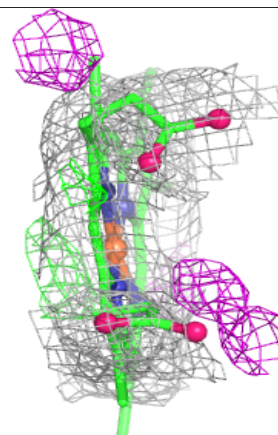
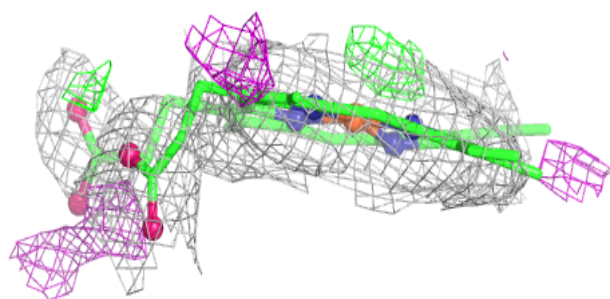
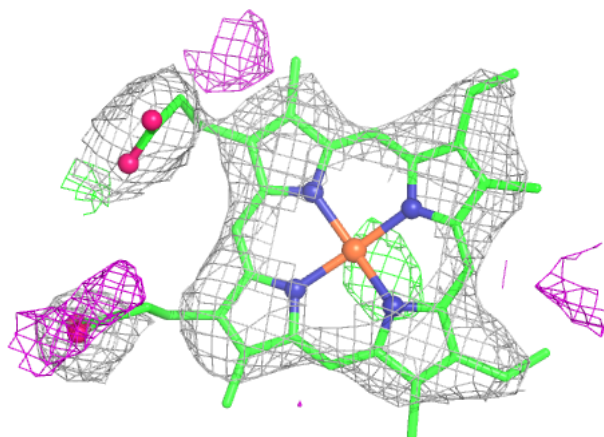
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	G	602	6/6	0.92	0.14	84,94,104,112	0
3	GOL	G	603	6/6	0.92	0.17	78,105,112,113	0
3	GOL	A	602	6/6	0.92	0.17	75,92,99,99	0
3	GOL	E	603	6/6	0.94	0.12	81,85,97,98	0
3	GOL	B	302	6/6	0.95	0.18	83,98,100,100	0
3	GOL	B	301	6/6	0.95	0.14	80,90,93,105	0
3	GOL	J	301	6/6	0.95	0.11	86,99,106,110	0
3	GOL	H	301	6/6	0.96	0.25	78,86,93,97	0
3	GOL	I	602	6/6	0.96	0.27	92,98,107,111	0
3	GOL	D	302	6/6	0.96	0.20	81,96,97,98	0
3	GOL	F	301	6/6	0.96	0.10	83,94,98,110	0
2	HEM	E	601	43/43	0.97	0.11	76,103,136,149	0
3	GOL	E	602	6/6	0.97	0.27	87,95,99,99	0
2	HEM	G	601	43/43	0.97	0.12	76,96,131,140	0
3	GOL	C	602	6/6	0.97	0.10	74,83,87,111	0
2	HEM	A	601	43/43	0.97	0.11	60,82,102,121	0
2	HEM	B	303	43/43	0.98	0.09	64,83,118,124	0
2	HEM	F	302	43/43	0.98	0.09	73,98,130,150	0
2	HEM	C	601	43/43	0.98	0.09	64,86,123,127	0
2	HEM	H	302	43/43	0.98	0.10	69,100,115,134	0
2	HEM	I	601	43/43	0.98	0.09	73,99,131,149	0
2	HEM	J	302	43/43	0.98	0.09	76,100,130,147	0
2	HEM	D	303	43/43	0.98	0.09	65,81,98,120	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.

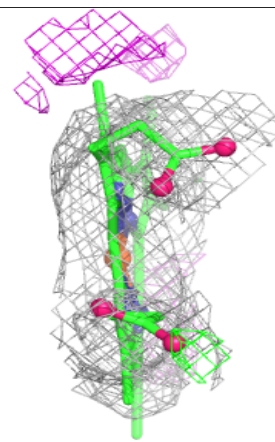
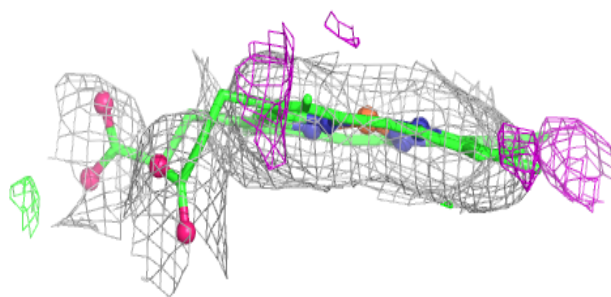
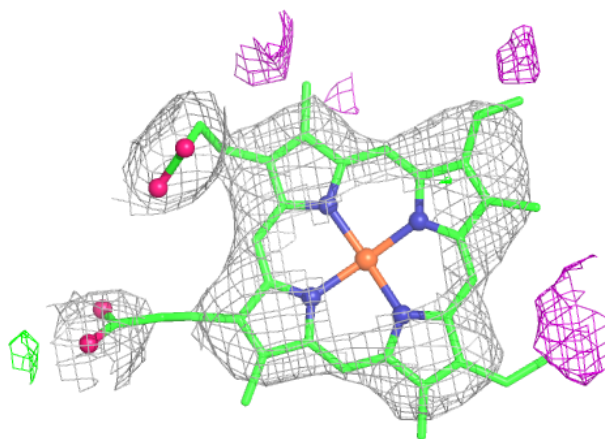
Electron density around HEM E 601:

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



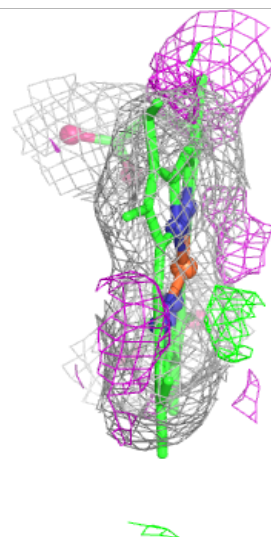
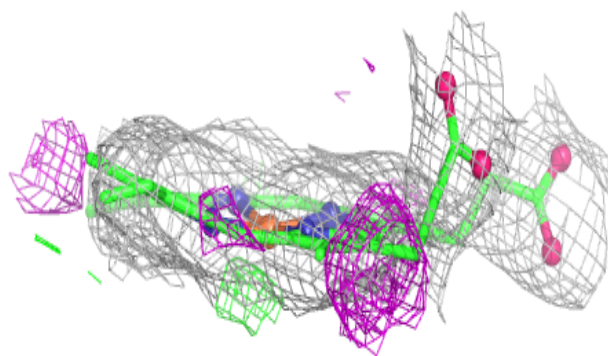
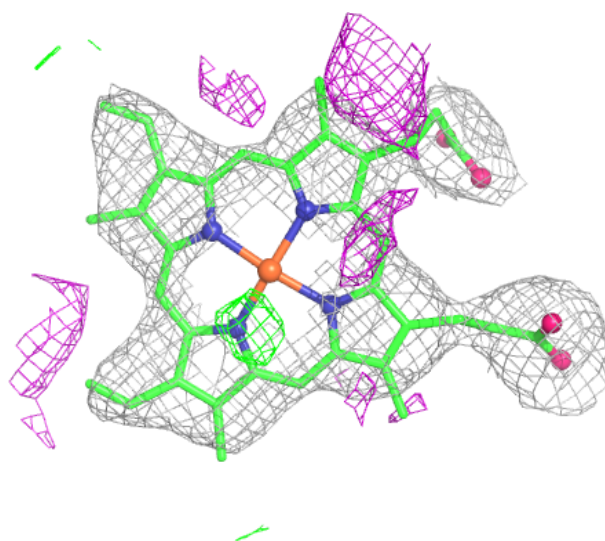
Electron density around HEM G 601:

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



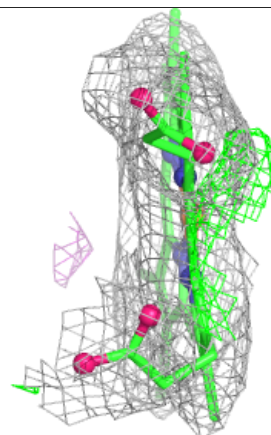
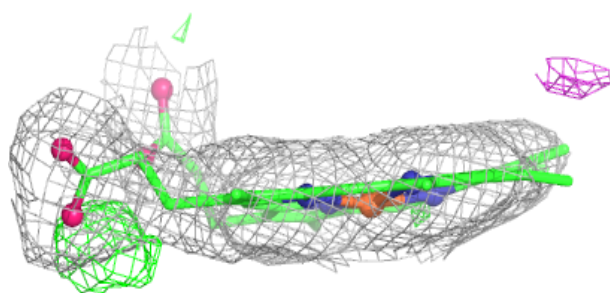
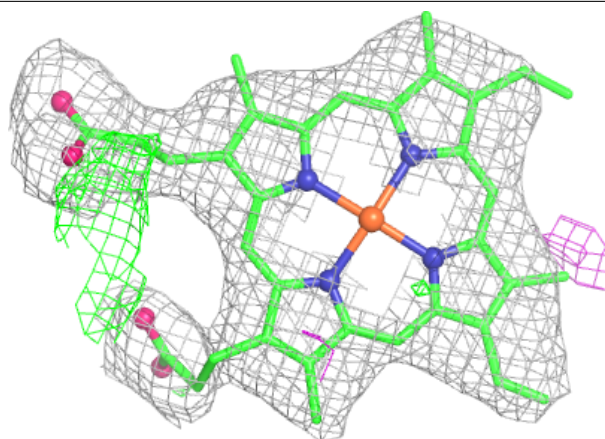
Electron density around HEM A 601:

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



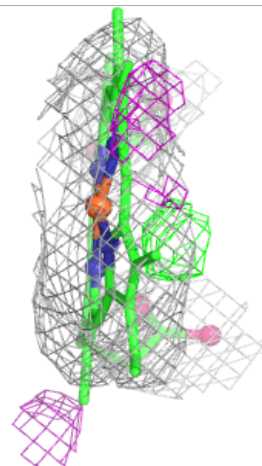
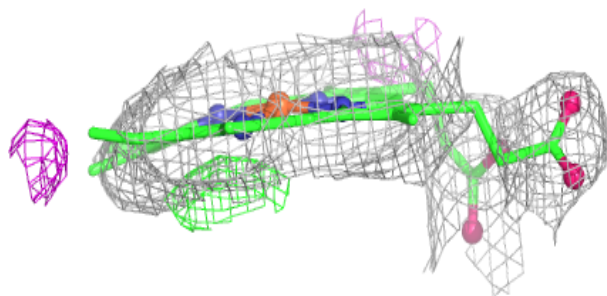
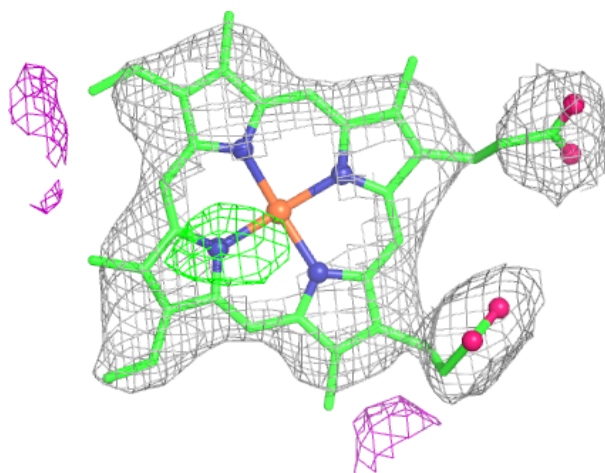
Electron density around HEM B 303:

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and green (positive)



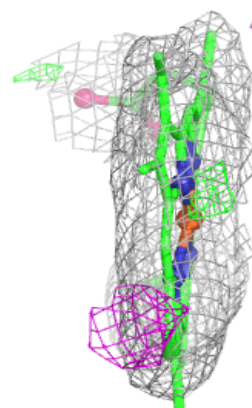
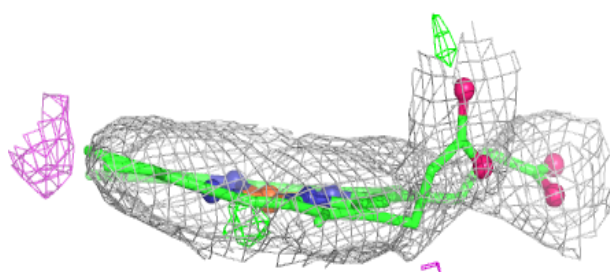
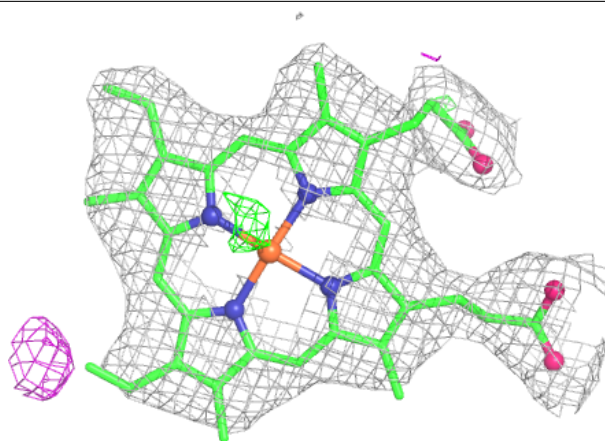
Electron density around HEM F 302:

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



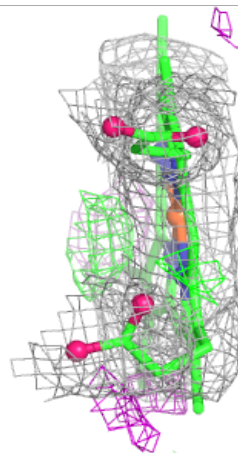
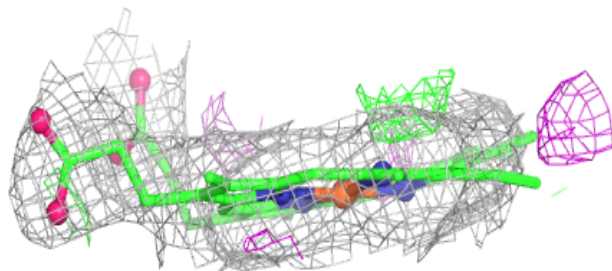
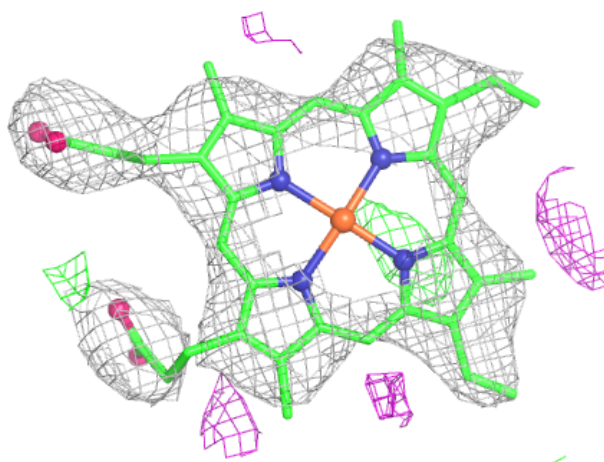
Electron density around HEM C 601:

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



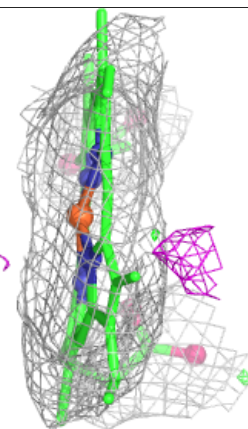
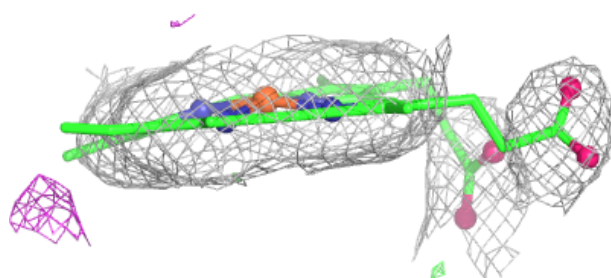
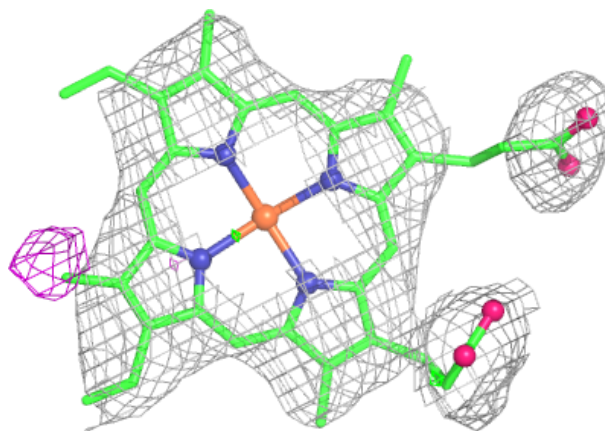
Electron density around HEM H 302:

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



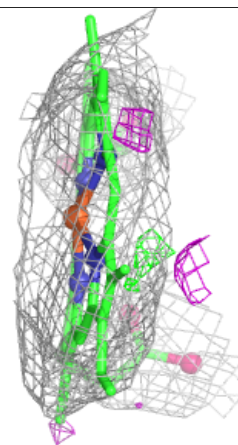
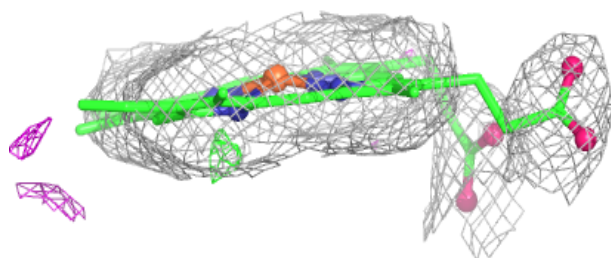
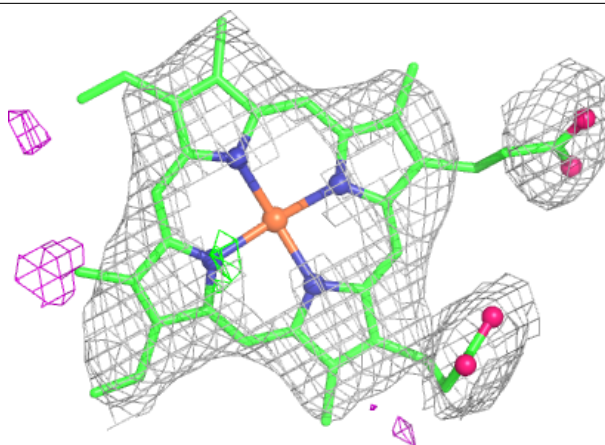
Electron density around HEM I 601:

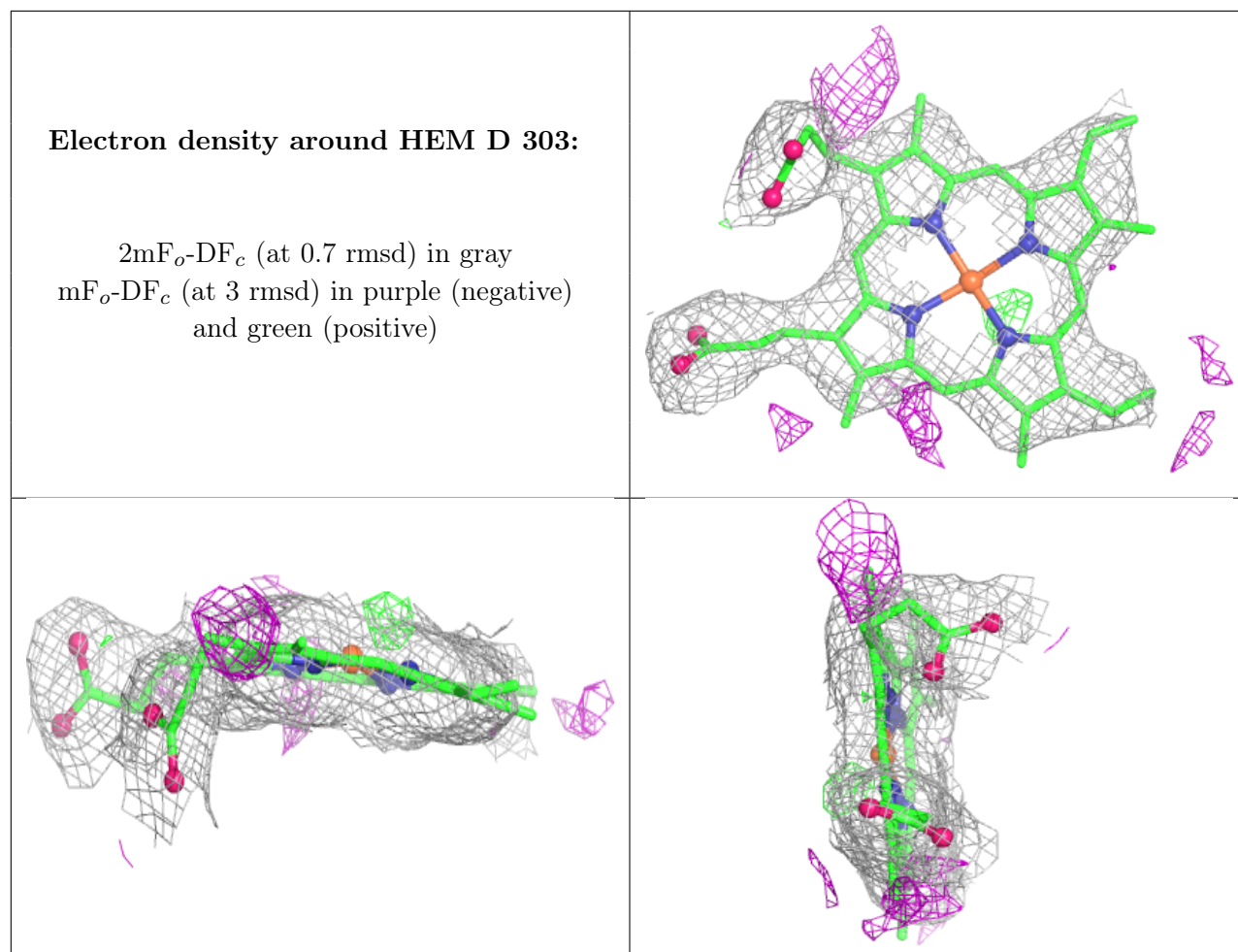
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM J 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.