



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 11:57 AM BST

PDB ID : 5HY8  
Title : Glycation restrains allosteric transition in hemoglobin: The molecular basis of oxidative stress under hyperglycemic conditions in diabetes  
Authors : Saraswathi, N.T.; Pannu, N.S.; Syakhovich, V.E.; Saurabh, A.; Bokut, S.B.; Moras, D.; Ruff, M.  
Deposited on : 2016-02-01  
Resolution : 2.30 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

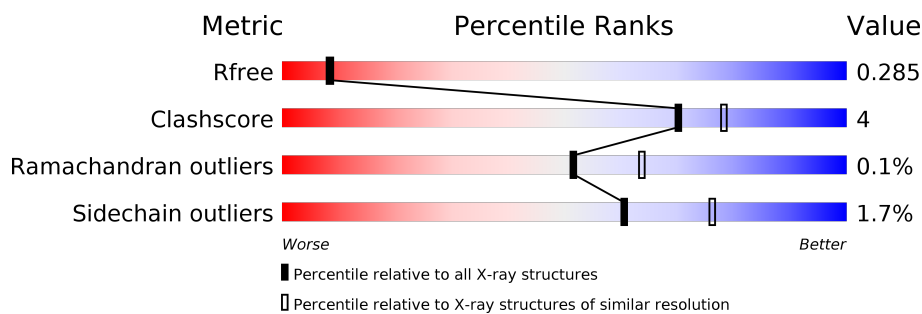
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 Å.

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






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	A	141	96% .
1	C	141	98% .
1	E	141	79% 13% . .
1	G	141	87% 9% . .
1	S	141	96% .
2	B	146	96% .
2	D	146	94% 6%

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Mol	Chain	Length	Quality of chain
2	F	146	 88% 8% . .
2	H	146	 89% 10% .
2	T	146	 96% . .

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11609 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 Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1068	685	187	193	3			
1	C	141	Total	C	N	O	S	0	0	0
			1068	685	187	193	3			
1	E	137	Total	C	N	O	S	0	0	0
			1030	659	180	188	3			
1	G	138	Total	C	N	O	S	0	0	0
			1042	668	181	190	3			
1	S	141	Total	C	N	O	S	0	0	0
			1068	685	187	193	3			

- Molecule 2 is a protein called Hemoglobin subunit beta.

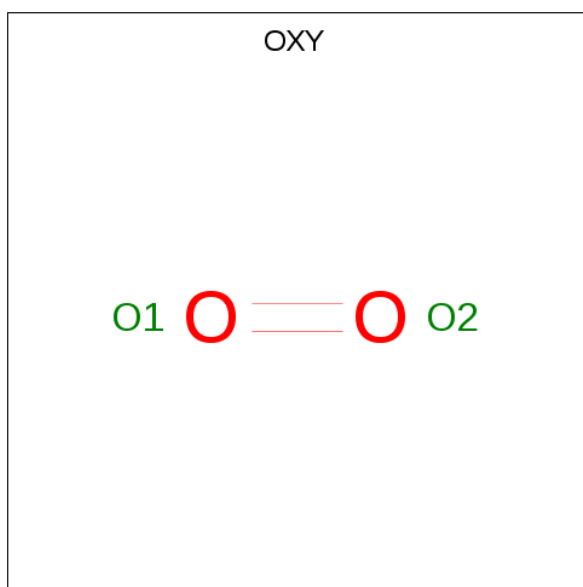
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1122	724	195	200	3			
2	D	146	Total	C	N	O	S	0	0	0
			1122	724	195	200	3			
2	F	146	Total	C	N	O	S	0	0	0
			1122	724	195	200	3			
2	H	146	Total	C	N	O	S	0	0	0
			1122	724	195	200	3			
2	T	146	Total	C	N	O	S	0	0	0
			1122	724	195	200	3			

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



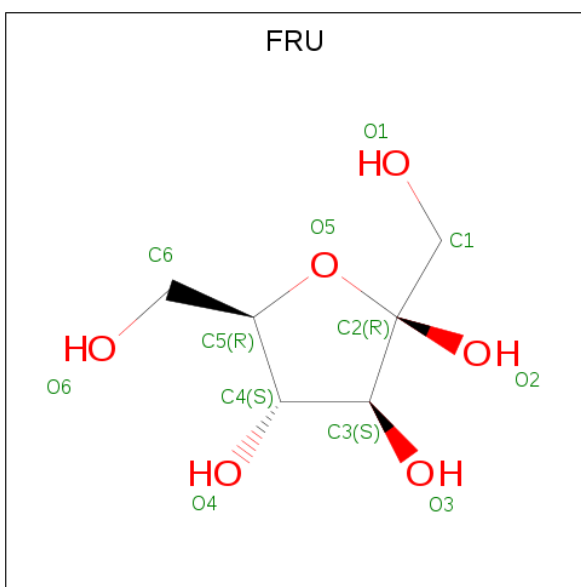
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	D	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	E	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	F	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
3	G	1	Total 43	C 34	Fe 1	N 4	O 4	0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

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O<sub>2</sub>).



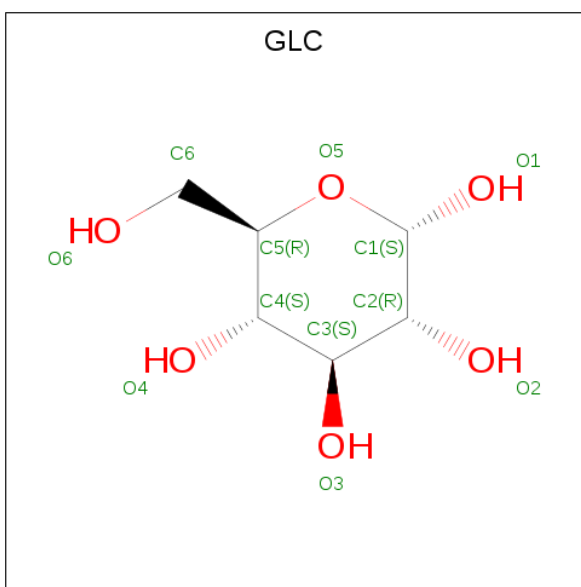
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O 2 2	0	0
4	B	1	Total O 2 2	0	0
4	C	1	Total O 2 2	0	0
4	D	1	Total O 2 2	0	0
4	F	1	Total O 2 2	0	0
4	G	1	Total O 2 2	0	0
4	S	1	Total O 2 2	0	0
4	T	1	Total O 2 2	0	0

- Molecule 5 is beta-D-fructofuranose (three-letter code: FRU) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	C	1	Total	C	O	0	0
			11	6	5		
5	F	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is alpha-D-glucopyranose (three-letter code: GLC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			12	6	6		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	30	Total 30	O 30	0	0
7	B	36	Total 36	O 36	0	0
7	C	39	Total 39	O 39	0	0
7	D	32	Total 32	O 32	0	0
7	E	12	Total 12	O 12	0	0
7	F	26	Total 26	O 26	0	0
7	G	18	Total 18	O 18	0	0
7	H	10	Total 10	O 10	0	0
7	S	15	Total 15	O 15	0	0
7	T	14	Total 14	O 14	0	0



### 3 Residue-property plots

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. 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. 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.

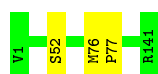
- Molecule 1: Hemoglobin subunit alpha

Chain A:  96% .




- Molecule 1: Hemoglobin subunit alpha

Chain C:  98% .




- Molecule 1: Hemoglobin subunit alpha

Chain E:  79% 13% . .



- Molecule 1: Hemoglobin subunit alpha

Chain G:  87% 9% . .



- Molecule 1: Hemoglobin subunit alpha

Chain S:  96% .



- Molecule 2: Hemoglobin subunit beta

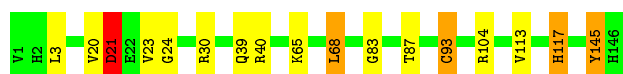
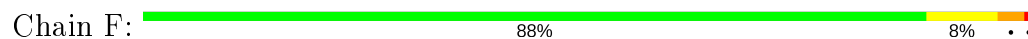
Chain B:  96% .



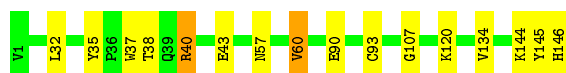
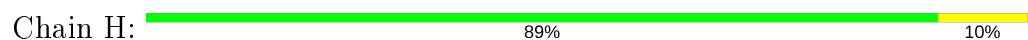
- Molecule 2: Hemoglobin subunit beta



- Molecule 2: Hemoglobin subunit beta



- Molecule 2: Hemoglobin subunit beta



- Molecule 2: Hemoglobin subunit beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	237.99 Å   59.27 Å   137.02 Å 90.00°   125.36°   90.00°	Depositor
Resolution (Å)	112.13 – 2.30 14.89 – 2.30	Depositor EDS
% Data completeness (in resolution range)	87.0 (112.13-2.30) 87.3 (14.89-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 2.29 Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, $R_{free}$	0.203   ,   0.244 0.256   ,   0.285	Depositor DCC
$R_{free}$ test set	3020 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.0	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 42.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h-2*k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11609	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: HEM, GLC, OXY, FRU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.01	1/1096 (0.1%)	0.91	1/1491 (0.1%)
1	C	0.95	0/1096	0.87	0/1491
1	E	0.77	1/1057 (0.1%)	1.13	14/1438 (1.0%)
1	G	0.90	0/1070	0.99	4/1456 (0.3%)
1	S	0.78	0/1096	0.84	1/1491 (0.1%)
2	B	1.10	2/1152 (0.2%)	0.89	1/1566 (0.1%)
2	D	1.03	1/1152 (0.1%)	0.87	2/1566 (0.1%)
2	F	0.99	2/1152 (0.2%)	1.00	9/1566 (0.6%)
2	H	0.81	0/1152	0.86	3/1566 (0.2%)
2	T	0.84	1/1152 (0.1%)	0.81	1/1566 (0.1%)
All	All	0.93	8/11175 (0.1%)	0.92	36/15197 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	37	TRP	CE3-CZ3	7.08	1.50	1.38
1	A	49	SER	CA-CB	6.00	1.61	1.52
2	D	130	TYR	CE1-CZ	-5.67	1.31	1.38
1	E	116	GLU	CD-OE1	-5.59	1.19	1.25
2	B	101	GLU	CG-CD	5.36	1.59	1.51
2	T	101	GLU	CG-CD	5.26	1.59	1.51
2	F	93	CYS	CB-SG	5.25	1.91	1.82
2	F	145	TYR	CG-CD1	5.18	1.45	1.39

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	80	LEU	CB-CG-CD2	10.33	128.56	111.00
1	E	129	LEU	CB-CG-CD2	9.12	126.50	111.00
2	F	68	LEU	CB-CG-CD2	8.13	124.83	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	92	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	E	92	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	E	101	LEU	CB-CG-CD2	-7.53	98.20	111.00
1	G	113	LEU	CA-CB-CG	7.22	131.90	115.30
1	E	32	MET	CG-SD-CE	-7.17	88.72	100.20
2	F	3	LEU	CA-CB-CG	7.11	131.65	115.30
1	G	44	PRO	C-N-CA	-7.10	103.96	121.70
1	E	80	LEU	CB-CG-CD1	-6.68	99.65	111.00
1	E	113	LEU	CA-CB-CG	6.66	130.62	115.30
2	B	40	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	G	98	PHE	CB-CG-CD1	-6.58	116.19	120.80
1	E	101	LEU	CB-CG-CD1	6.52	122.08	111.00
1	E	80	LEU	CA-CB-CG	6.51	130.28	115.30
2	F	68	LEU	CB-CG-CD1	-6.47	99.99	111.00
2	F	117	HIS	CB-CA-C	-6.17	98.05	110.40
1	E	116	GLU	CG-CD-OE2	6.12	130.54	118.30
1	E	129	LEU	CA-CB-CG	6.00	129.09	115.30
2	T	90	GLU	N-CA-CB	5.97	121.35	110.60
1	E	116	GLU	CG-CD-OE1	-5.84	106.61	118.30
1	G	136	LEU	CB-CG-CD1	5.80	120.86	111.00
2	D	9	SER	N-CA-CB	-5.74	101.89	110.50
1	E	136	LEU	CB-CG-CD1	5.60	120.53	111.00
2	F	68	LEU	CB-CA-C	5.58	120.80	110.20
1	A	92	ARG	NE-CZ-NH1	5.58	123.09	120.30
2	H	43	GLU	CG-CD-OE1	-5.56	107.17	118.30
1	S	126	ASP	CB-CG-OD1	5.38	123.14	118.30
2	H	40	ARG	NE-CZ-NH2	5.37	122.99	120.30
2	D	30	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	F	30	ARG	NE-CZ-NH1	5.13	122.86	120.30
2	H	43	GLU	CG-CD-OE2	5.11	128.52	118.30
2	F	104	ARG	NE-CZ-NH1	5.09	122.85	120.30
2	F	113	VAL	N-CA-CB	5.08	122.67	111.50
2	F	21	ASP	N-CA-C	-5.05	97.36	111.00

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	1068	0	1071	2	0
1	C	1068	0	1070	1	0
1	E	1030	0	1028	24	0
1	G	1042	0	1037	7	0
1	S	1068	0	1073	2	0
2	B	1122	0	1118	2	0
2	D	1122	0	1118	3	0
2	F	1122	0	1116	17	0
2	H	1122	0	1118	16	0
2	T	1122	0	1118	2	0
3	A	43	0	30	0	0
3	B	43	0	30	1	0
3	C	43	0	30	1	0
3	D	43	0	30	1	0
3	E	43	0	30	3	0
3	F	43	0	30	2	0
3	G	43	0	30	0	0
3	H	43	0	30	1	0
3	S	43	0	30	1	0
3	T	43	0	30	2	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	S	2	0	0	0	0
4	T	2	0	0	0	0
5	A	11	0	9	1	0
5	C	11	0	9	1	0
5	F	11	0	9	2	0
6	C	12	0	12	0	0
7	A	30	0	0	0	0
7	B	36	0	0	0	0
7	C	39	0	0	0	0
7	D	32	0	0	1	0
7	E	12	0	0	0	0
7	F	26	0	0	1	0
7	G	18	0	0	0	0
7	H	10	0	0	0	0
7	S	15	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	T	14	0	0	0	0
All	All	11609	0	11206	82	0

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

All (82) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:93:CYS:SG	2:H:145:TYR:HE1	1.78	1.05
2:H:93:CYS:SG	2:H:145:TYR:CE1	2.49	1.04
2:H:35:TYR:O	2:H:38:THR:HG22	1.64	0.96
1:E:32:MET:HE1	1:E:101:LEU:HB2	1.50	0.92
2:F:24:GLY:N	2:F:68:LEU:HD12	1.97	0.80
1:G:139:LYS:HD2	1:G:139:LYS:O	1.85	0.77
1:E:32:MET:CE	1:E:101:LEU:HB2	2.14	0.77
2:H:32:LEU:HD23	2:H:38:THR:HG23	1.71	0.73
1:E:92:ARG:CG	2:H:37:TRP:HA	2.20	0.72
1:E:67:THR:O	1:E:70:VAL:HG12	1.91	0.70
1:E:92:ARG:HG2	2:H:37:TRP:HA	1.72	0.70
2:F:24:GLY:CA	2:F:68:LEU:HD12	2.22	0.70
1:E:102:SER:HA	1:E:129:LEU:HD23	1.74	0.69
2:H:93:CYS:SG	2:H:145:TYR:CD1	2.83	0.68
2:H:107:GLY:HA3	2:H:134:VAL:HG13	1.75	0.67
1:G:14:TRP:HE1	1:G:67:THR:HG22	1.61	0.65
1:E:14:TRP:HE1	1:E:67:THR:HG22	1.63	0.64
1:E:32:MET:CE	1:E:101:LEU:CB	2.77	0.63
3:E:201:HEM:HBB2	3:E:201:HEM:HMB2	1.81	0.62
2:F:24:GLY:HA2	2:F:68:LEU:CD1	2.30	0.61
2:H:57:ASN:HB3	2:H:60:VAL:HG13	1.81	0.61
1:E:14:TRP:HE1	1:E:67:THR:CG2	2.15	0.60
1:G:70:VAL:O	1:G:73:VAL:HG23	2.02	0.60
1:G:14:TRP:HE1	1:G:67:THR:CG2	2.15	0.60
1:E:32:MET:HE1	1:E:101:LEU:CB	2.28	0.59
1:S:70:VAL:O	1:S:73:VAL:HG23	2.03	0.59
1:A:70:VAL:O	1:A:73:VAL:HG23	2.03	0.59
2:F:93:CYS:HB2	2:F:145:TYR:CE1	2.38	0.58
1:E:70:VAL:O	1:E:73:VAL:HG23	2.03	0.58
2:F:40:ARG:NH2	7:F:302:HOH:O	2.35	0.58
2:F:24:GLY:CA	2:F:68:LEU:CD1	2.82	0.58
2:B:48:LEU:O	5:C:203:FRU:O3	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:201:HEM:HMB1	3:S:201:HEM:HBB2	1.84	0.57
1:E:101:LEU:HD23	1:E:101:LEU:O	2.05	0.56
1:E:93:VAL:HG23	1:E:98:PHE:HE1	1.71	0.56
1:A:7:LYS:HG2	1:A:73:VAL:HG11	1.87	0.56
2:F:21:ASP:HA	2:F:65:LYS:HG3	1.88	0.56
3:T:201:HEM:HMC2	3:T:201:HEM:HBC2	1.87	0.56
3:H:201:HEM:HBB2	3:H:201:HEM:HHC	1.89	0.54
2:F:20:VAL:HG23	2:F:20:VAL:O	2.07	0.54
3:C:201:HEM:HMB1	3:C:201:HEM:HBB2	1.90	0.52
1:G:7:LYS:HG2	1:G:73:VAL:HG11	1.90	0.52
2:H:107:GLY:HA3	2:H:134:VAL:CG1	2.39	0.52
1:E:7:LYS:HG2	1:E:73:VAL:HG11	1.90	0.52
2:H:35:TYR:O	2:H:38:THR:CG2	2.47	0.52
2:D:26:GLU:OE1	2:D:117:HIS:NE2	2.39	0.51
1:S:7:LYS:HG2	1:S:73:VAL:HG11	1.92	0.51
5:F:203:FRU:C6	2:H:146:HIS:HD2	2.24	0.50
2:T:87:THR:O	2:T:90:GLU:HG3	2.11	0.49
1:E:101:LEU:HD23	1:E:101:LEU:C	2.32	0.49
5:A:203:FRU:H61	2:D:33:VAL:HG13	1.94	0.49
2:F:93:CYS:HB2	2:F:145:TYR:CZ	2.47	0.49
5:F:203:FRU:H62	2:H:146:HIS:HD2	1.78	0.49
2:H:32:LEU:HA	2:H:38:THR:CG2	2.44	0.48
2:F:24:GLY:N	2:F:68:LEU:CD1	2.75	0.48
3:D:201:HEM:HMC1	3:D:201:HEM:HBC2	1.96	0.47
2:H:93:CYS:CB	2:H:145:TYR:CE1	2.96	0.47
1:E:125:LEU:O	1:E:129:LEU:HD13	2.13	0.47
1:E:87:HIS:HE1	3:E:201:HEM:C4C	2.16	0.47
1:E:105:LEU:O	1:E:109:LEU:HD13	2.15	0.47
1:E:42:TYR:CD2	3:E:201:HEM:HBC1	2.50	0.46
2:H:90:GLU:HG3	2:H:144:LYS:HE2	1.96	0.46
1:E:93:VAL:CG2	1:E:98:PHE:HE1	2.28	0.46
1:E:125:LEU:O	1:E:129:LEU:CD1	2.63	0.46
1:E:32:MET:HE3	1:E:101:LEU:HA	1.98	0.45
2:F:20:VAL:O	2:F:21:ASP:CB	2.64	0.45
2:F:20:VAL:O	2:F:21:ASP:CG	2.56	0.44
2:D:87:THR:HG22	7:D:314:HOH:O	2.16	0.44
3:T:201:HEM:HBB2	3:T:201:HEM:HHC	2.00	0.44
2:T:18:VAL:HG13	2:T:23:VAL:HG21	2.00	0.43
1:E:70:VAL:CG1	1:E:71:ALA:N	2.80	0.43
1:G:137:THR:O	1:G:140:TYR:CD2	2.72	0.43
2:F:24:GLY:HA2	2:F:68:LEU:CG	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:39:GLN:OE1	1:G:92:ARG:NH2	2.52	0.42
3:F:201:HEM:HHC	3:F:201:HEM:HBB2	2.03	0.41
2:B:83:GLY:O	2:F:83:GLY:HA3	2.21	0.41
3:F:201:HEM:HBC2	3:F:201:HEM:HMC1	2.02	0.41
2:F:20:VAL:CG2	2:F:20:VAL:O	2.68	0.41
3:B:201:HEM:HMC1	3:B:201:HEM:HBC2	2.03	0.41
1:E:132:VAL:HG12	1:E:136:LEU:HD12	2.02	0.41
2:F:23:VAL:HG12	2:F:68:LEU:HD11	2.03	0.40
1:C:76:MET:N	1:C:77:PRO:CD	2.84	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	139/141 (99%)	138 (99%)	1 (1%)	0	100	100
1	C	139/141 (99%)	136 (98%)	3 (2%)	0	100	100
1	E	135/141 (96%)	133 (98%)	2 (2%)	0	100	100
1	G	136/141 (96%)	134 (98%)	2 (2%)	0	100	100
1	S	139/141 (99%)	137 (99%)	2 (1%)	0	100	100
2	B	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
2	D	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
2	F	144/146 (99%)	137 (95%)	6 (4%)	1 (1%)	22	26
2	H	144/146 (99%)	140 (97%)	4 (3%)	0	100	100
2	T	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
All	All	1408/1435 (98%)	1379 (98%)	28 (2%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	21	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	113/113 (100%)	112 (99%)	1 (1%)	78	89
1	C	113/113 (100%)	112 (99%)	1 (1%)	78	89
1	E	109/113 (96%)	106 (97%)	3 (3%)	43	60
1	G	110/113 (97%)	106 (96%)	4 (4%)	35	49
1	S	113/113 (100%)	111 (98%)	2 (2%)	59	75
2	B	118/118 (100%)	117 (99%)	1 (1%)	81	91
2	D	118/118 (100%)	116 (98%)	2 (2%)	60	76
2	F	118/118 (100%)	116 (98%)	2 (2%)	60	76
2	H	118/118 (100%)	115 (98%)	3 (2%)	47	65
2	T	118/118 (100%)	117 (99%)	1 (1%)	81	91
All	All	1148/1155 (99%)	1128 (98%)	20 (2%)	60	76

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	SER
2	B	1	VAL
1	C	52	SER
2	D	1	VAL
2	D	61	LYS
1	E	52	SER
1	E	70	VAL
1	E	75	ASP
2	F	87	THR
2	F	117	HIS
1	G	52	SER
1	G	84	SER
1	G	92	ARG

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Mol	Chain	Res	Type
1	G	139	LYS
2	H	40	ARG
2	H	60	VAL
2	H	120	LYS
1	S	52	SER
1	S	75	ASP
2	T	50	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	87	HIS
2	H	63	HIS
2	H	143	HIS
2	H	146	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

22 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	HEM	D	201	2,4	27,50,50	0.76	0	17,82,82	1.62	4 (23%)
3	HEM	F	201	2,4	27,50,50	1.10	2 (7%)	17,82,82	1.82	5 (29%)
5	FRU	C	203	1	11,11,12	0.93	1 (9%)	15,17,18	1.44	4 (26%)
3	HEM	A	201	1,4	27,50,50	0.85	1 (3%)	17,82,82	1.63	4 (23%)
4	OXY	D	202	3	1,1,1	0.17	0	-		
3	HEM	B	201	2,4	27,50,50	1.20	2 (7%)	17,82,82	1.50	2 (11%)
3	HEM	G	201	1,4	27,50,50	0.88	1 (3%)	17,82,82	1.66	2 (11%)
6	GLC	C	204	-	12,12,12	1.67	3 (25%)	17,17,17	1.79	5 (29%)
5	FRU	F	203	2	11,11,12	0.76	0	15,17,18	1.27	3 (20%)
3	HEM	H	201	2	27,50,50	1.05	2 (7%)	17,82,82	1.36	2 (11%)
5	FRU	A	203	1	11,11,12	0.84	0	15,17,18	3.36	2 (13%)
3	HEM	S	201	1,4	27,50,50	1.02	1 (3%)	17,82,82	1.50	3 (17%)
4	OXY	T	202	3	1,1,1	0.18	0	-		
4	OXY	F	202	3	1,1,1	0.13	0	-		
4	OXY	S	202	3	1,1,1	0.06	0	-		
3	HEM	E	201	1	27,50,50	1.12	1 (3%)	17,82,82	1.66	4 (23%)
4	OXY	G	202	3	1,1,1	0.10	0	-		
4	OXY	C	202	3	1,1,1	0.04	0	-		
4	OXY	A	202	3	1,1,1	0.06	0	-		
3	HEM	T	201	2,4	27,50,50	0.85	1 (3%)	17,82,82	1.21	2 (11%)
3	HEM	C	201	1,4	27,50,50	1.01	1 (3%)	17,82,82	1.83	3 (17%)
4	OXY	B	202	3	1,1,1	0.26	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
3	HEM	B	201	2,4	-	0/6/54/54	-
5	FRU	A	203	1	-	2/2/21/24	0/1/1/1
3	HEM	D	201	2,4	-	0/6/54/54	-
3	HEM	S	201	1,4	-	0/6/54/54	-
3	HEM	F	201	2,4	-	0/6/54/54	-
3	HEM	G	201	1,4	-	0/6/54/54	-
6	GLC	C	204	-	-	0/2/22/22	0/1/1/1
5	FRU	C	203	1	-	0/2/21/24	0/1/1/1
3	HEM	A	201	1,4	-	0/6/54/54	-
3	HEM	T	201	2,4	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	C	201	1,4	-	3/6/54/54	-
5	FRU	F	203	2	-	2/2/21/24	0/1/1/1
3	HEM	H	201	2	-	0/6/54/54	-
3	HEM	E	201	1	-	3/6/54/54	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	HEM	C3B-C2B	-3.34	1.35	1.40
3	B	201	HEM	C4D-C3D	3.16	1.49	1.42
3	G	201	HEM	C4D-C3D	3.08	1.49	1.42
3	E	201	HEM	C3C-C2C	-2.70	1.36	1.40
3	A	201	HEM	C3B-C2B	-2.68	1.36	1.40
3	H	201	HEM	C4D-C3D	2.65	1.48	1.42
3	C	201	HEM	C3B-C2B	-2.65	1.36	1.40
3	T	201	HEM	C4D-C3D	2.63	1.48	1.42
6	C	204	GLC	O5-C1	2.61	1.49	1.42
6	C	204	GLC	O4-C4	2.52	1.48	1.43
3	F	201	HEM	C4D-C3D	2.48	1.48	1.42
3	S	201	HEM	C4D-C3D	2.38	1.48	1.42
3	H	201	HEM	C3B-C2B	-2.34	1.37	1.40
5	C	203	FRU	C1-C2	2.21	1.55	1.52
6	C	204	GLC	O2-C2	2.17	1.48	1.43
3	F	201	HEM	C1D-ND	-2.11	1.31	1.36

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	203	FRU	O5-C2-C1	9.32	113.70	107.46
5	A	203	FRU	O2-C2-O5	-8.34	104.51	109.99
3	C	201	HEM	CBA-CAA-C2A	4.96	121.63	112.49
3	G	201	HEM	CAA-CBA-CGA	-4.78	104.64	112.67
3	D	201	HEM	CBD-CAD-C3D	-4.67	103.87	112.48
3	A	201	HEM	CBD-CAD-C3D	-4.02	105.07	112.48
3	F	201	HEM	CBD-CAD-C3D	-3.67	105.72	112.48
3	H	201	HEM	CAA-CBA-CGA	-3.62	106.59	112.67
3	E	201	HEM	CAD-CBD-CGD	3.61	118.73	112.67
5	C	203	FRU	O2-C2-O5	3.37	112.20	109.99
6	C	204	GLC	O5-C1-C2	3.34	116.24	110.28
6	C	204	GLC	O2-C2-C1	3.31	116.83	109.16
3	F	201	HEM	C4C-C3C-C2C	-3.27	104.62	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	201	HEM	C1D-C2D-C3D	-2.81	105.04	107.00
3	C	201	HEM	CMA-C3A-C4A	-2.75	124.23	128.46
3	A	201	HEM	CBA-CAA-C2A	-2.72	107.48	112.49
6	C	204	GLC	C4-C3-C2	-2.71	106.08	110.82
6	C	204	GLC	O4-C4-C5	2.71	116.02	109.30
3	B	201	HEM	CBD-CAD-C3D	-2.69	107.52	112.48
3	E	201	HEM	CBA-CAA-C2A	2.62	117.32	112.49
3	F	201	HEM	C3B-C4B-NB	-2.62	105.82	109.21
3	F	201	HEM	CMA-C3A-C4A	-2.61	124.45	128.46
3	A	201	HEM	CAD-CBD-CGD	-2.58	108.35	112.67
3	T	201	HEM	C3B-C4B-NB	-2.52	105.95	109.21
3	F	201	HEM	C1D-C2D-C3D	-2.49	105.27	107.00
3	B	201	HEM	C3B-C4B-NB	-2.49	106.00	109.21
3	S	201	HEM	CAD-CBD-CGD	-2.42	108.61	112.67
3	E	201	HEM	CMA-C3A-C4A	-2.35	124.85	128.46
5	F	203	FRU	O5-C5-C6	2.32	115.31	108.85
5	C	203	FRU	O2-C2-C1	-2.32	107.53	111.87
3	C	201	HEM	CBD-CAD-C3D	-2.23	108.37	112.48
6	C	204	GLC	C1-O5-C5	2.23	117.86	113.66
3	T	201	HEM	CMA-C3A-C4A	-2.20	125.08	128.46
5	F	203	FRU	O2-C2-O5	2.20	111.43	109.99
3	S	201	HEM	CMB-C2B-C3B	2.17	128.75	124.68
5	F	203	FRU	O2-C2-C3	2.17	114.46	109.31
3	E	201	HEM	C4A-C3A-C2A	2.16	108.50	107.00
3	D	201	HEM	CBA-CAA-C2A	-2.15	108.52	112.49
5	C	203	FRU	O2-C2-C3	-2.13	104.25	109.31
3	G	201	HEM	C3B-C4B-NB	-2.11	106.48	109.21
3	H	201	HEM	C4C-C3C-C2C	-2.10	105.43	106.90
3	A	201	HEM	C1D-C2D-C3D	-2.08	105.55	107.00
3	D	201	HEM	CAA-CBA-CGA	-2.07	109.20	112.67
3	D	201	HEM	CMA-C3A-C4A	-2.03	125.35	128.46
5	C	203	FRU	O3-C3-C4	-2.02	106.34	113.32

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	201	HEM	C1A-C2A-CAA-CBA
3	E	201	HEM	C3A-C2A-CAA-CBA
3	E	201	HEM	C2A-CAA-CBA-CGA
3	C	201	HEM	C1A-C2A-CAA-CBA
3	C	201	HEM	C3A-C2A-CAA-CBA

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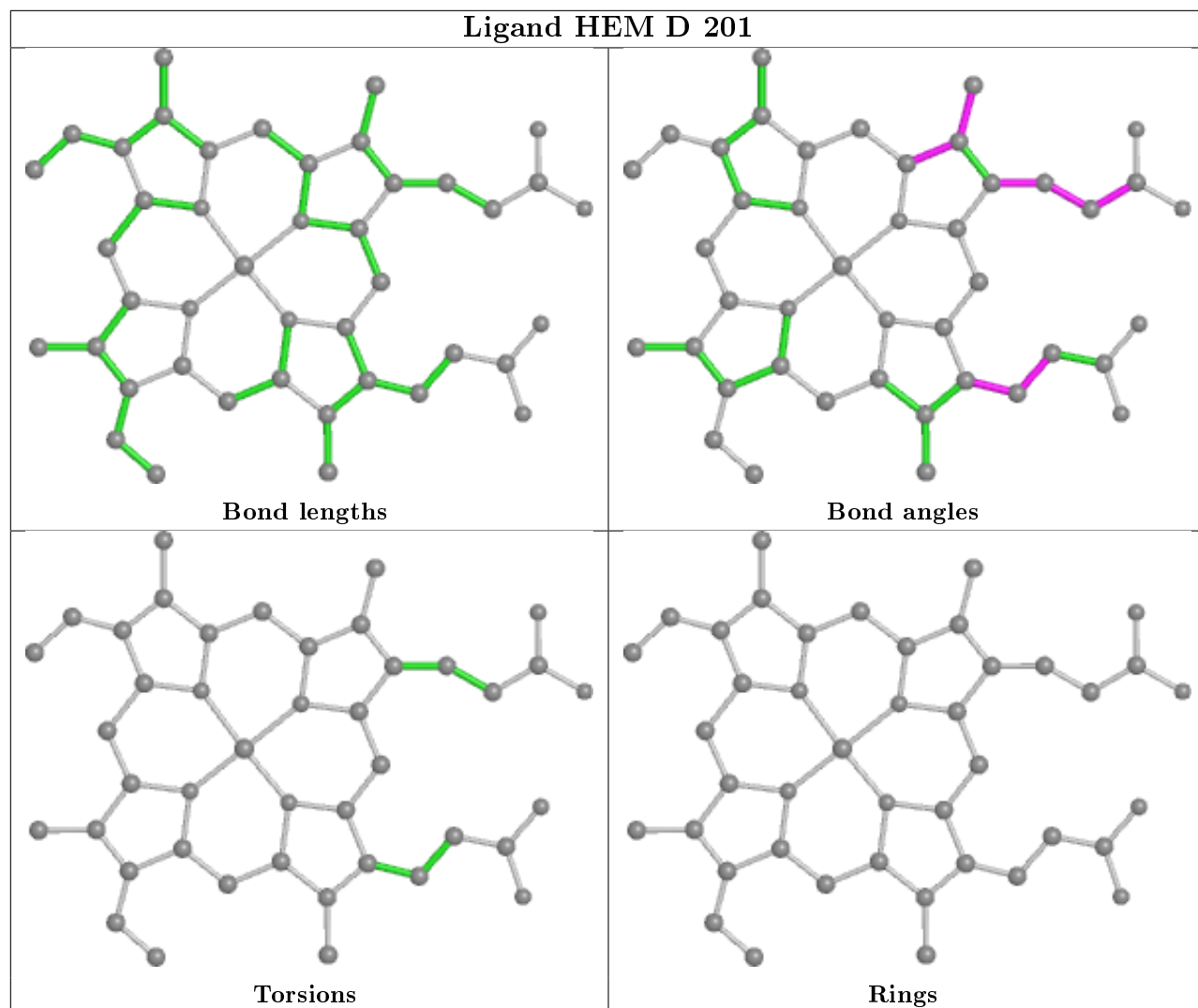
Mol	Chain	Res	Type	Atoms
3	C	201	HEM	C2A-CAA-CBA-CGA
5	F	203	FRU	O5-C5-C6-O6
5	A	203	FRU	O5-C5-C6-O6
5	A	203	FRU	C4-C5-C6-O6
5	F	203	FRU	C4-C5-C6-O6

There are no ring outliers.

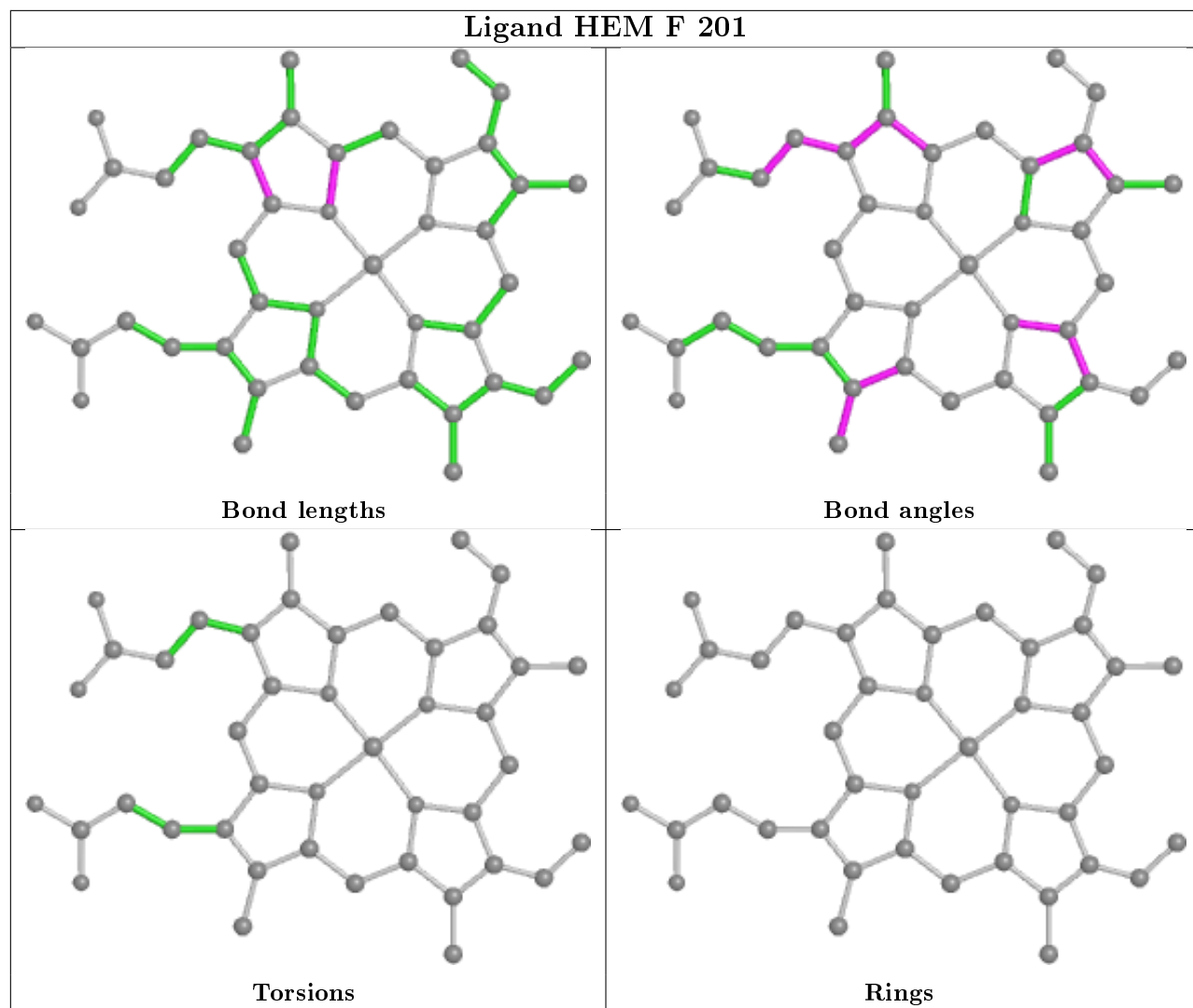
11 monomers are involved in 16 short contacts:

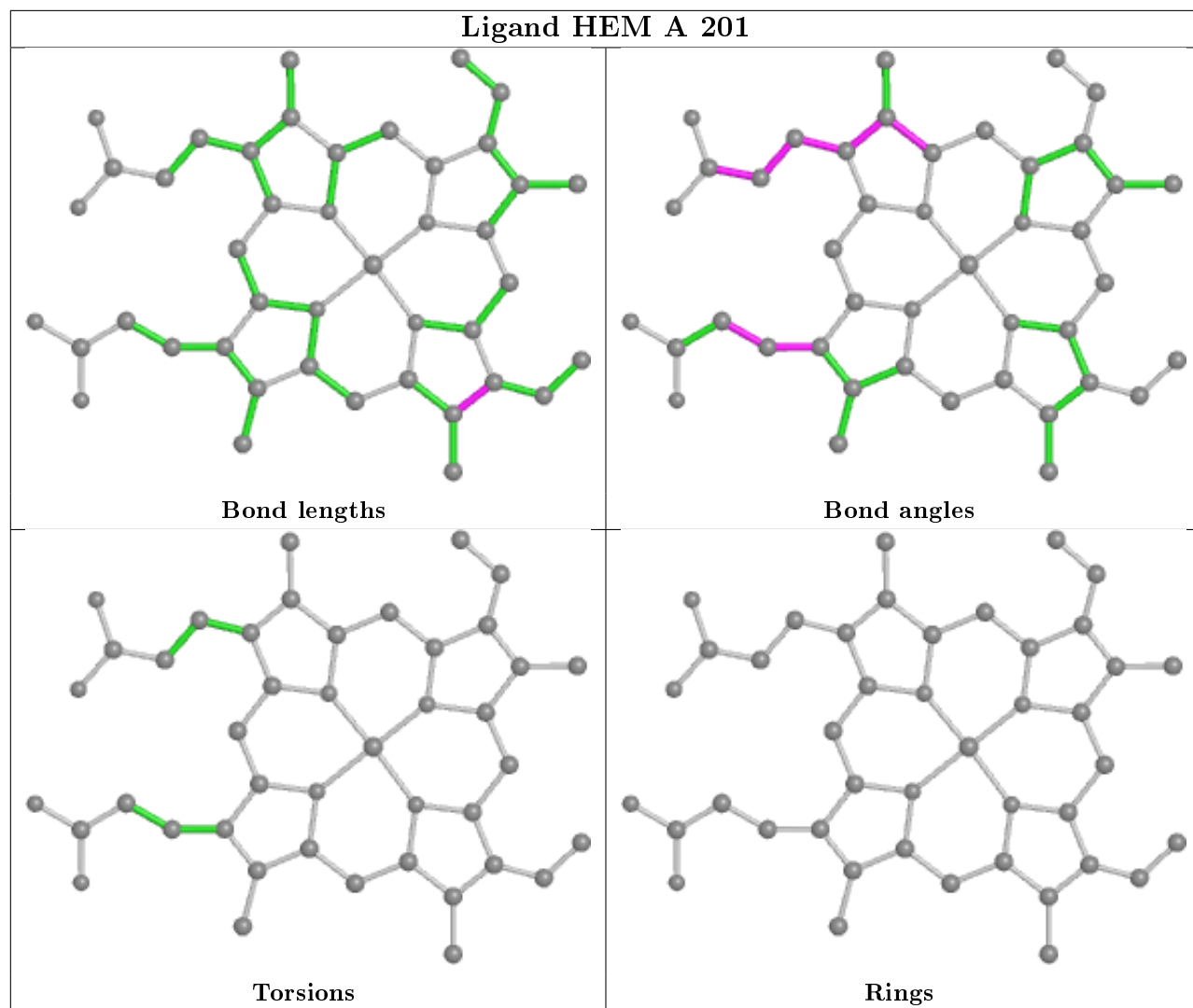
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	201	HEM	1	0
3	F	201	HEM	2	0
5	C	203	FRU	1	0
3	B	201	HEM	1	0
5	F	203	FRU	2	0
3	H	201	HEM	1	0
5	A	203	FRU	1	0
3	S	201	HEM	1	0
3	E	201	HEM	3	0
3	T	201	HEM	2	0
3	C	201	HEM	1	0

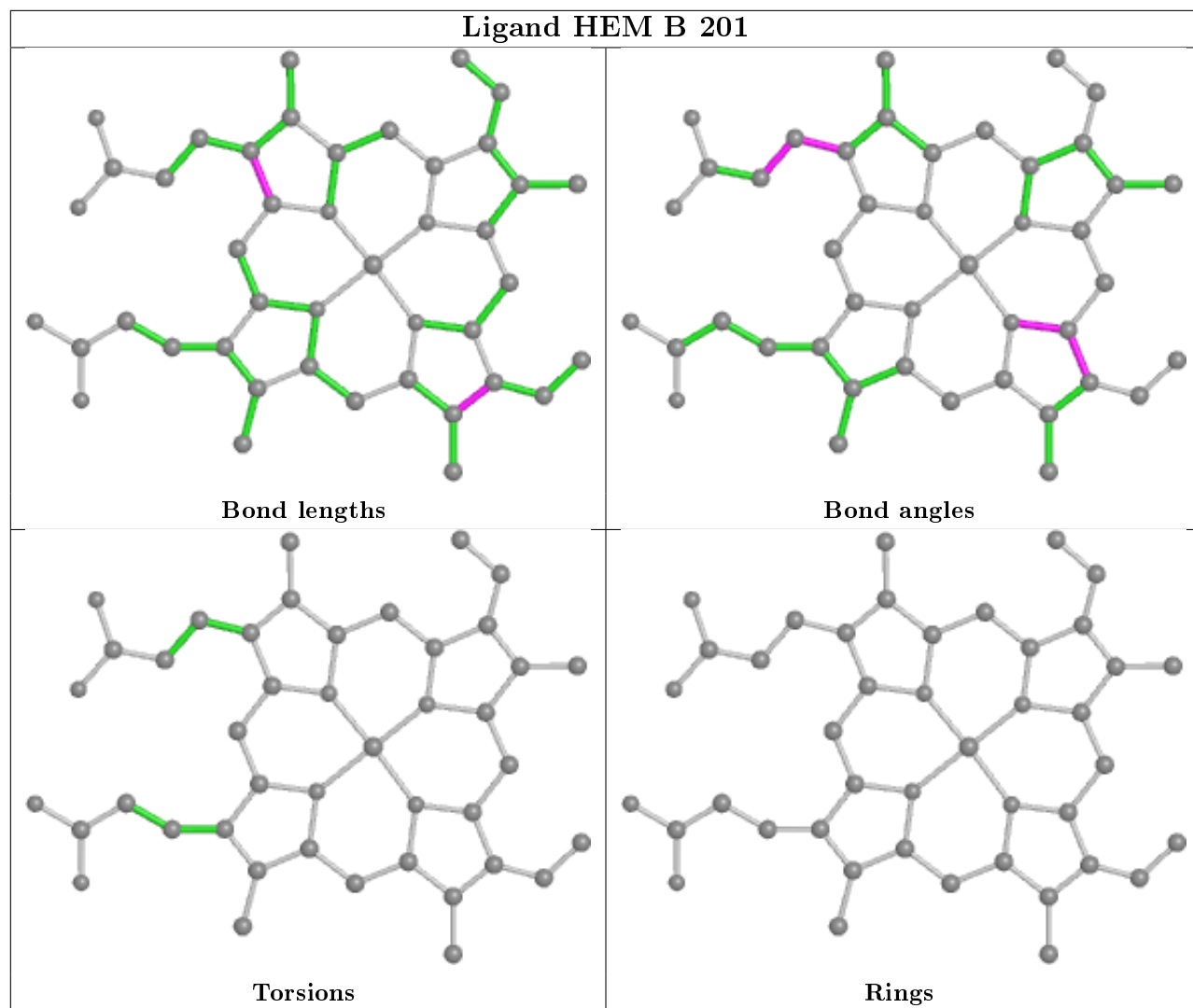
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

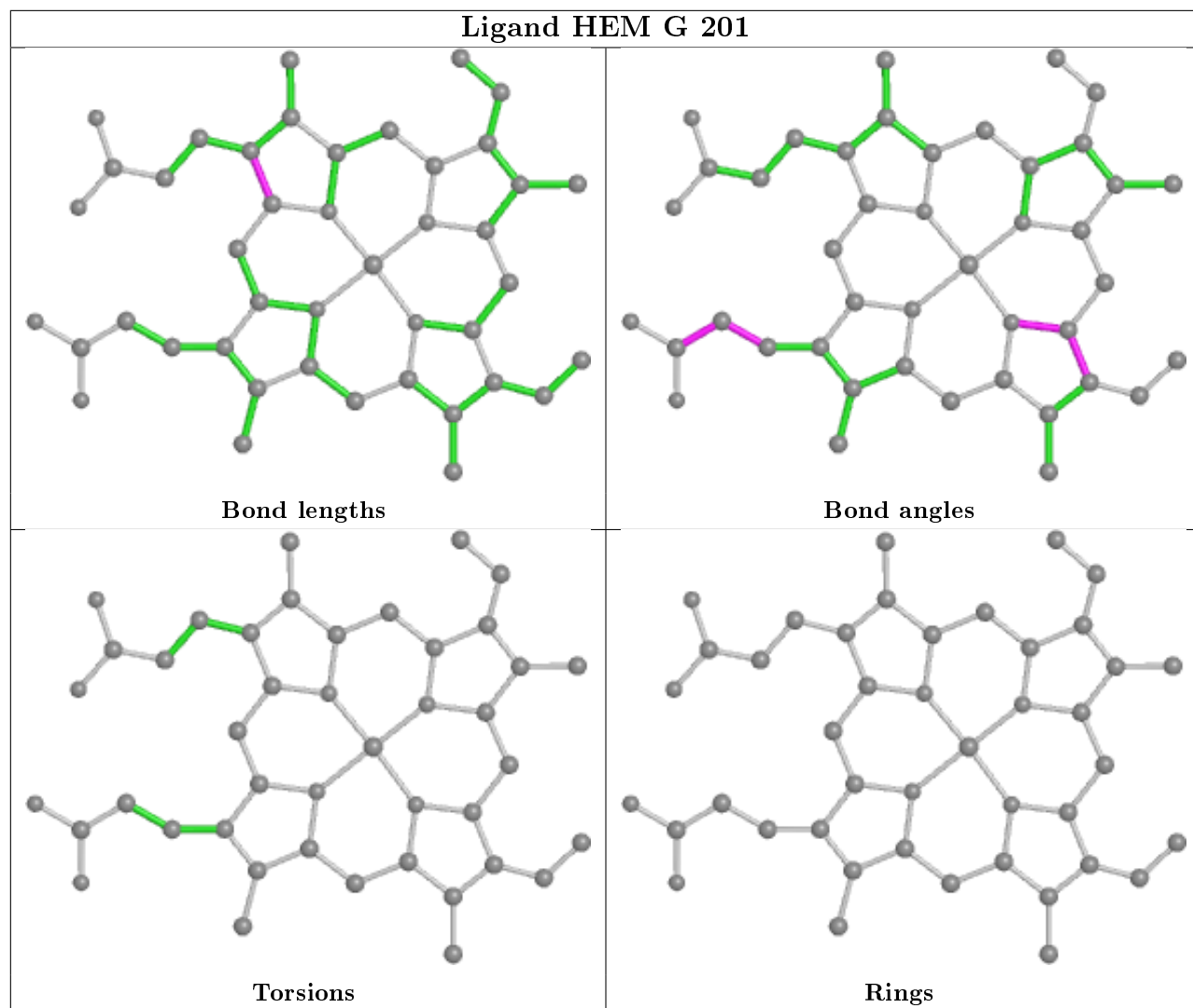


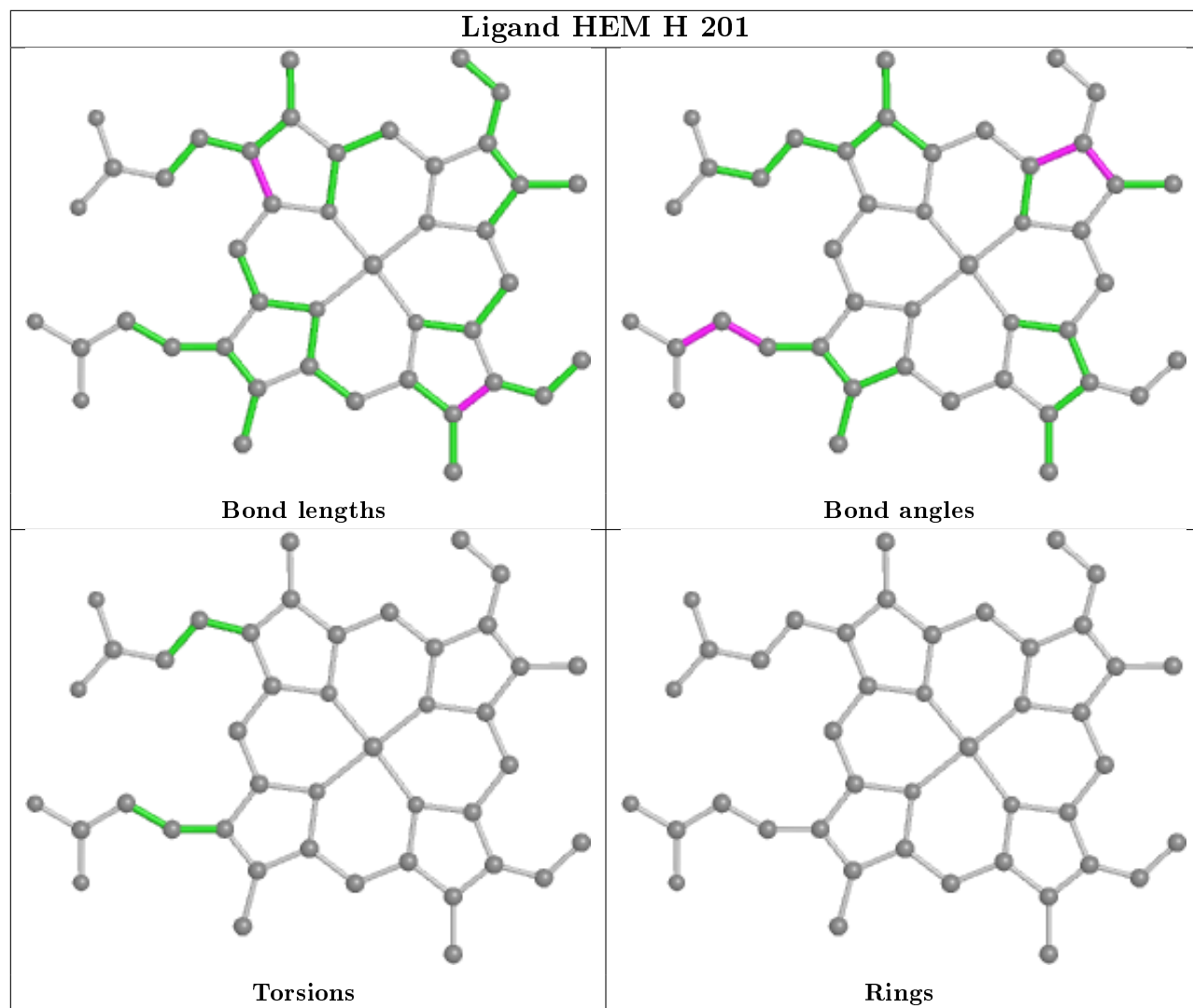


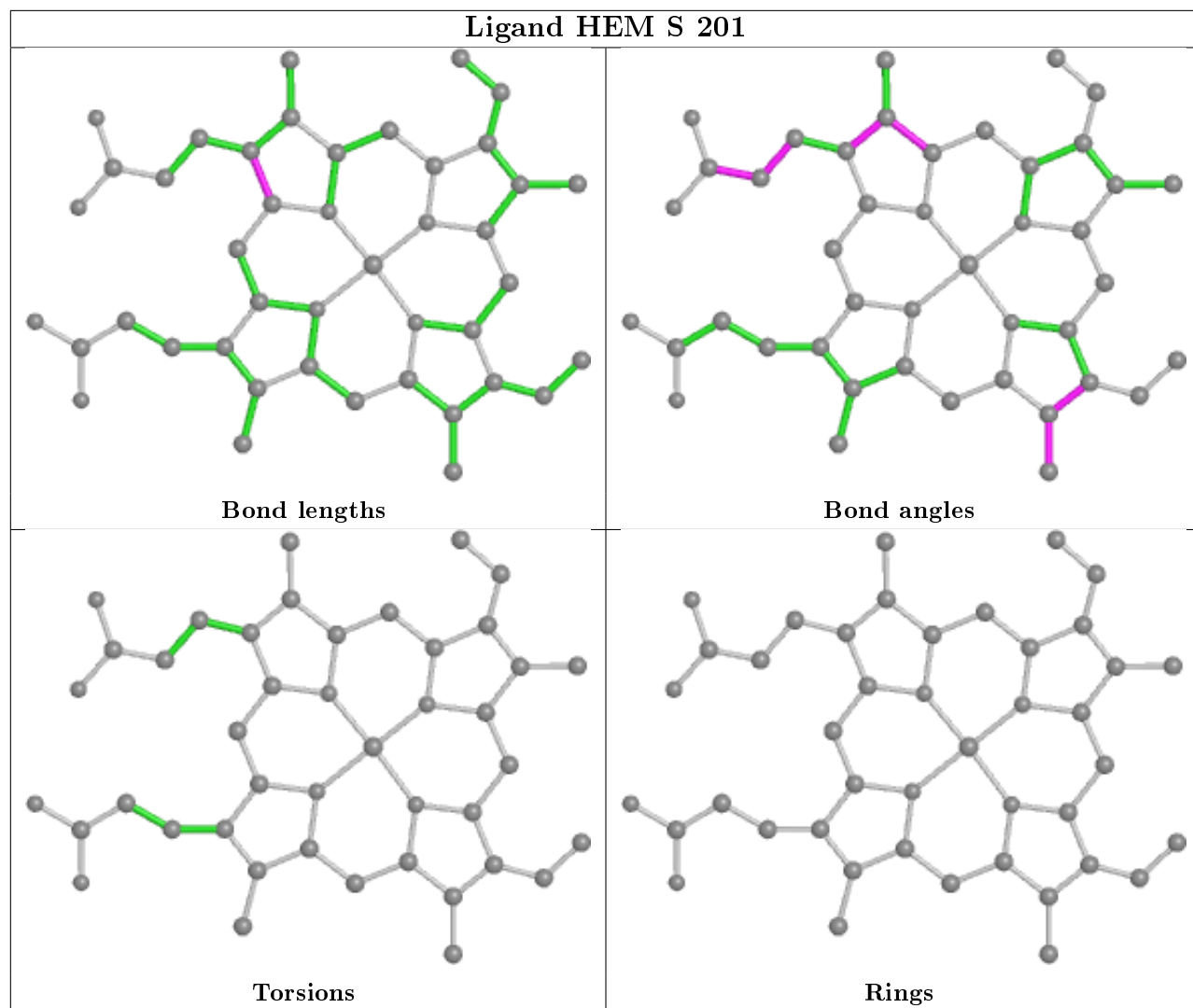


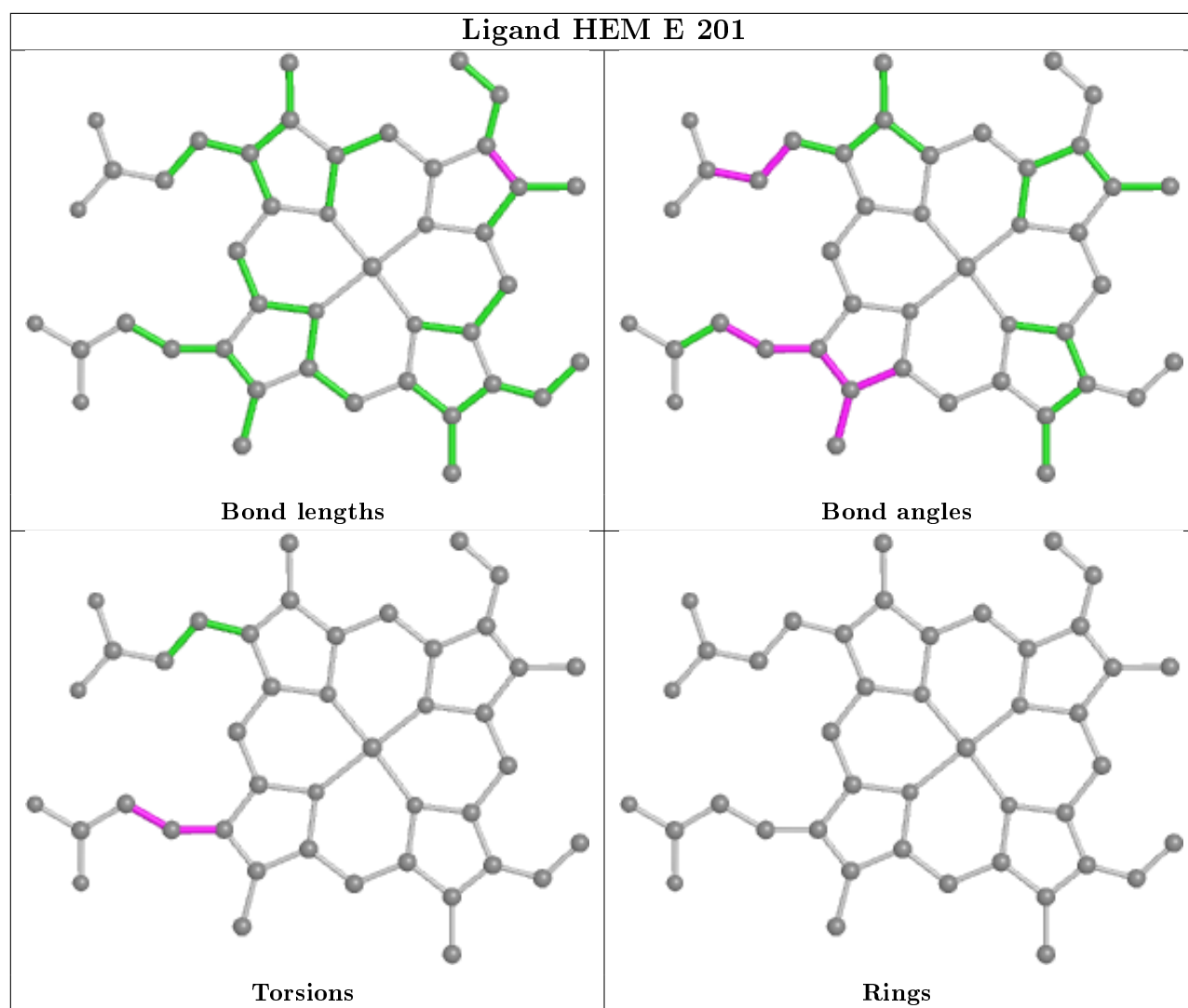


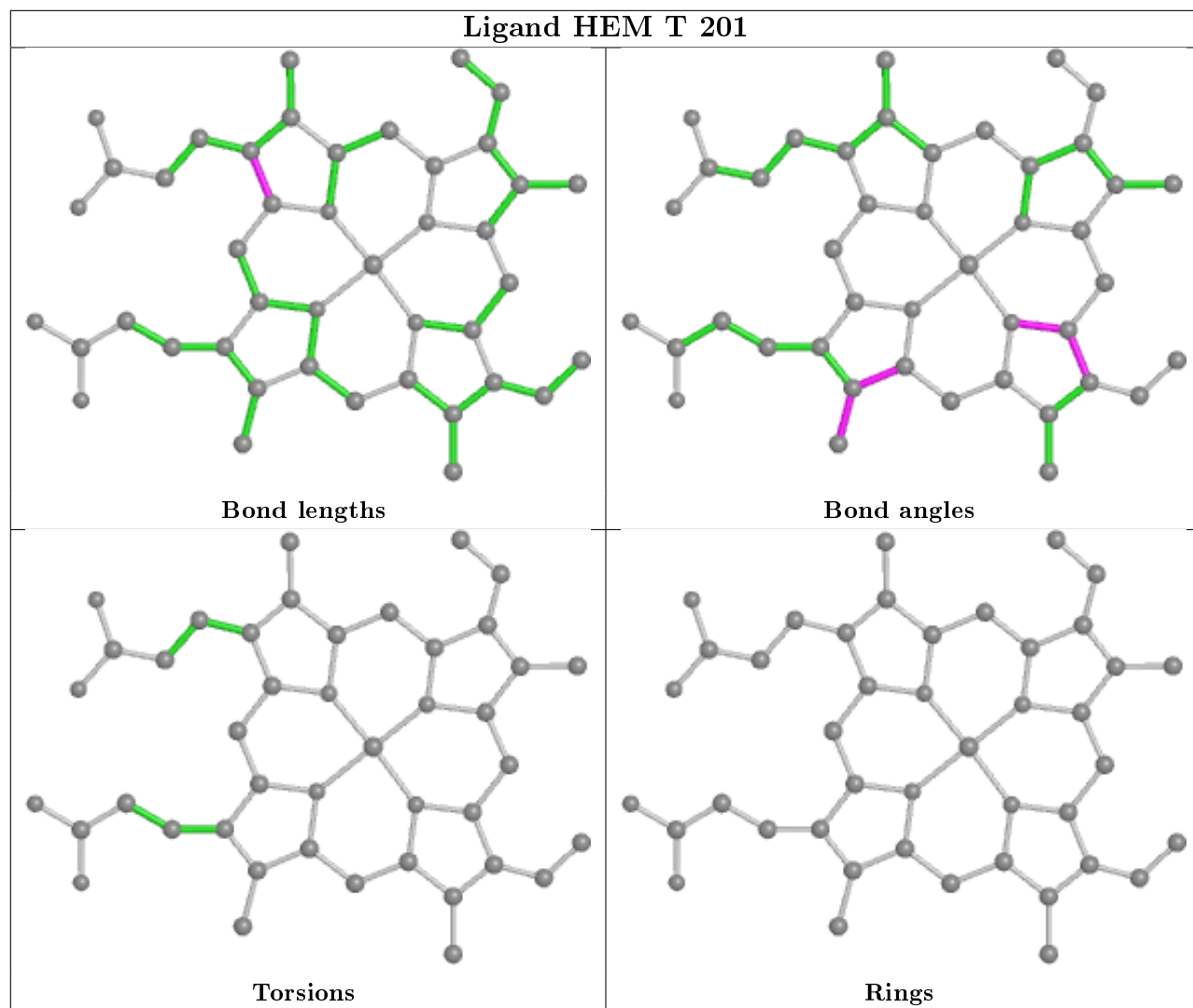




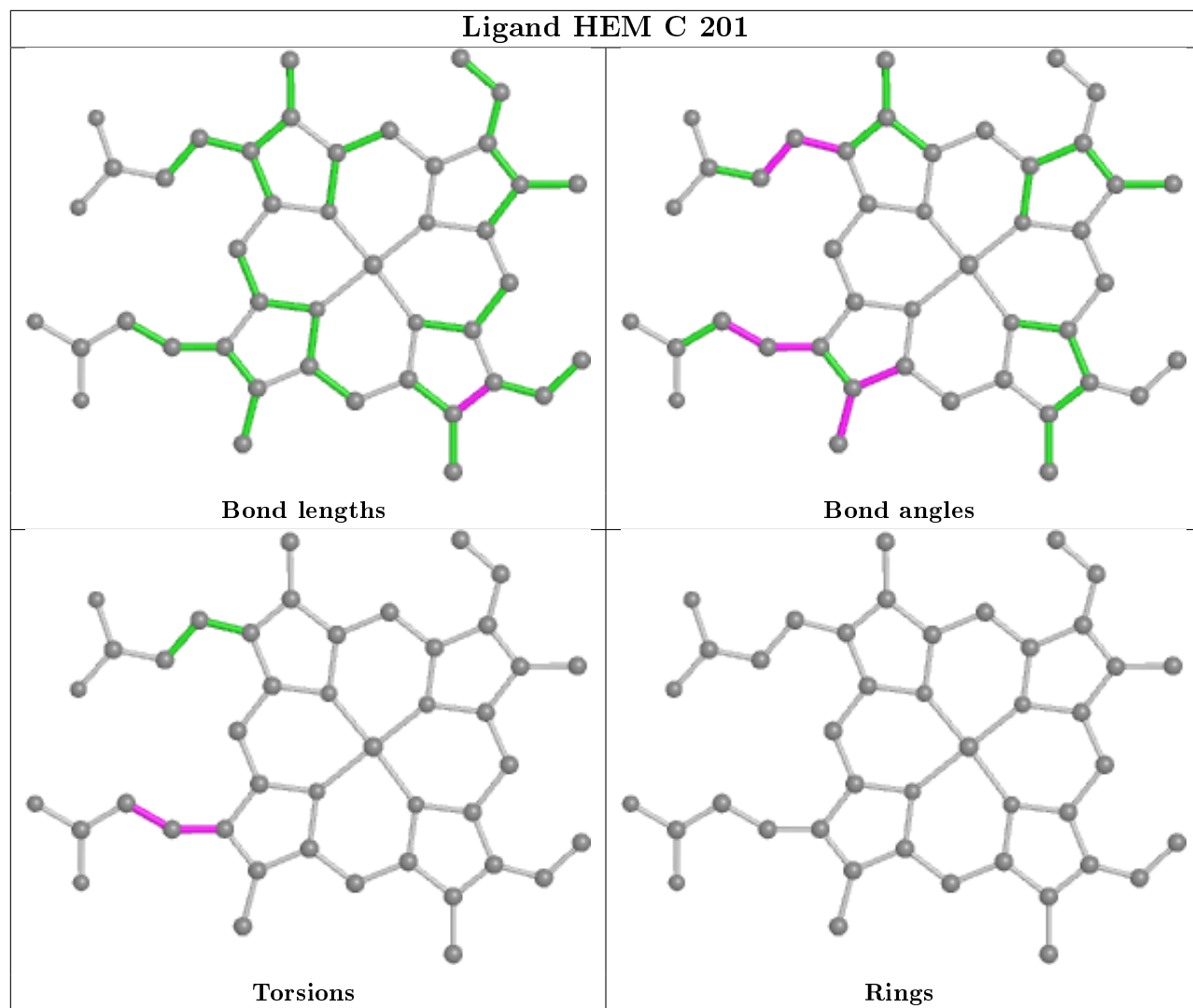












## 5.7 Other polymers [i](#)

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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

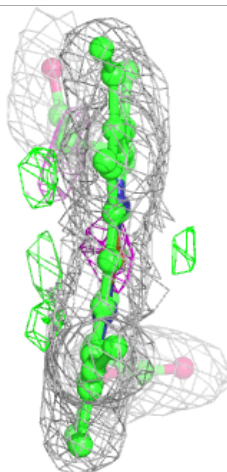
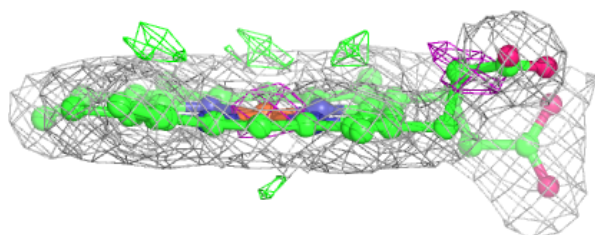
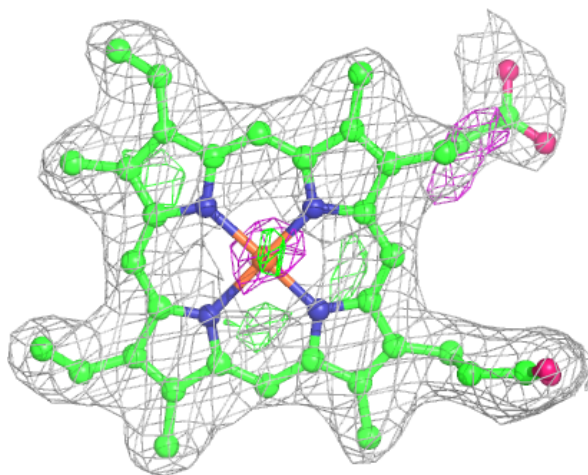
### 6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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.

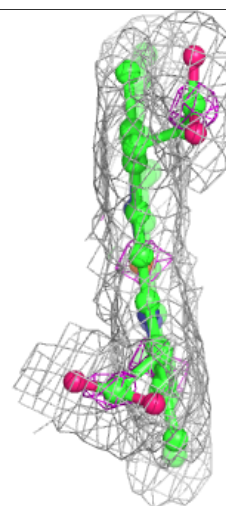
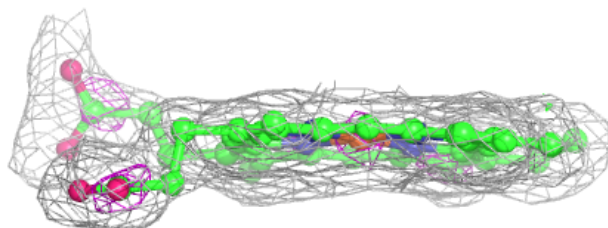
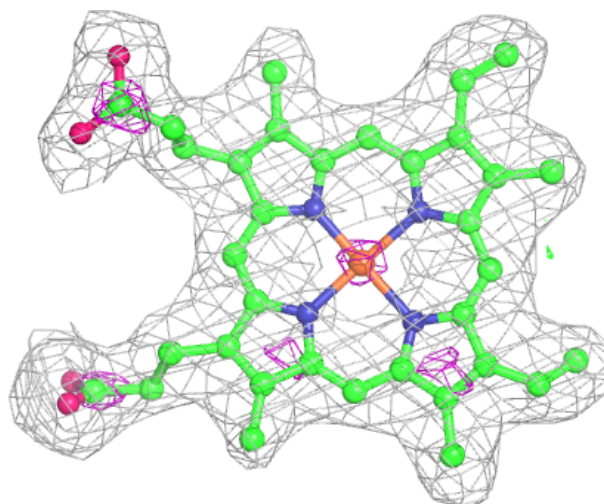
**Electron density around HEM D 201:**

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



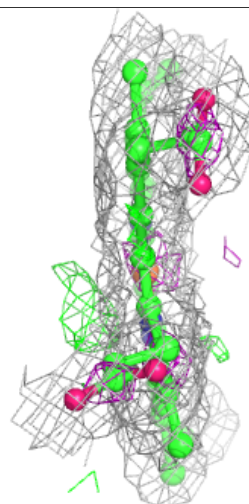
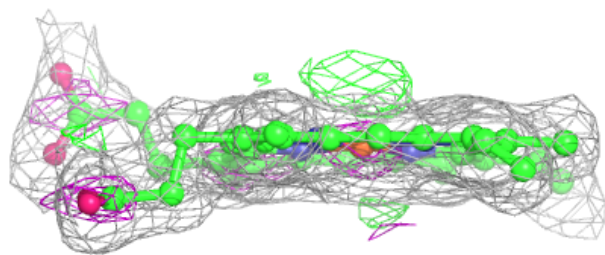
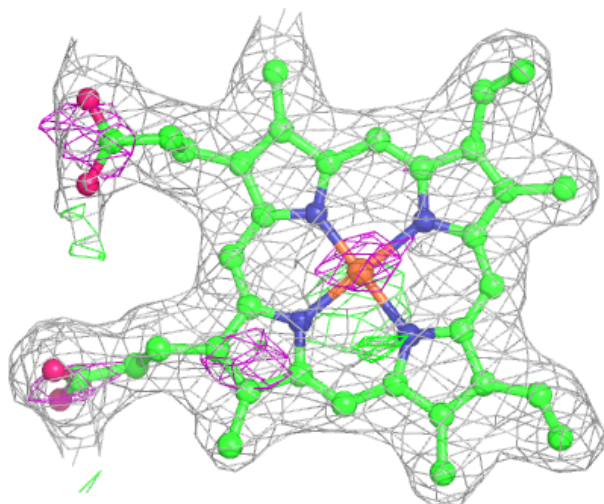
**Electron density around HEM F 201:**

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



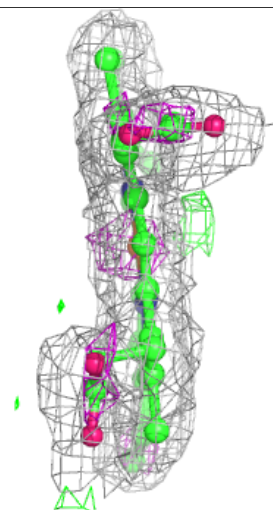
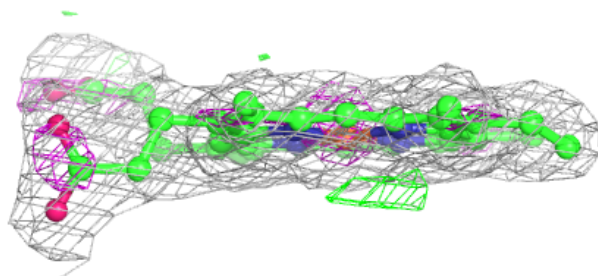
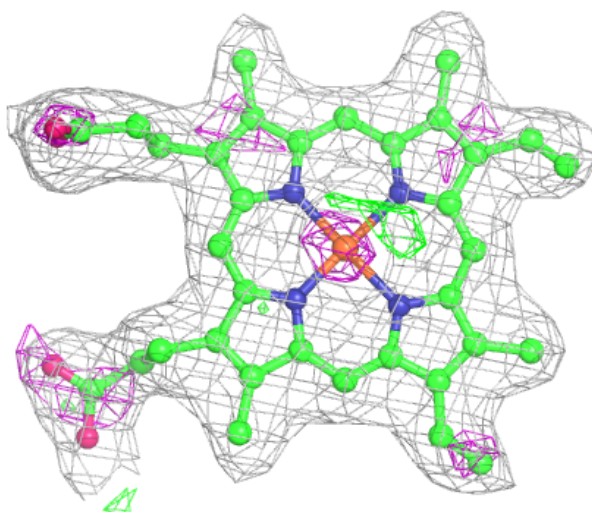
**Electron density around HEM A 201:**

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



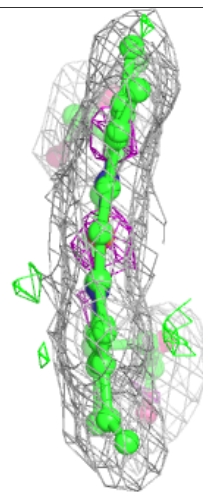
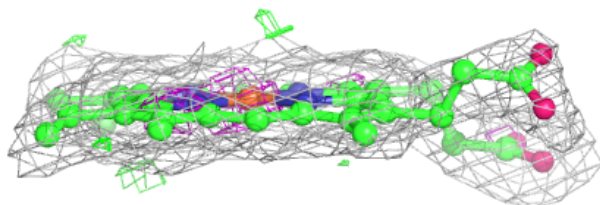
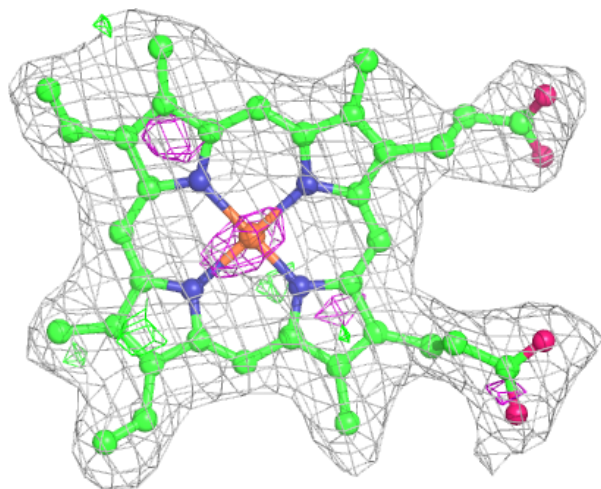
**Electron density around HEM B 201:**

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



**Electron density around HEM G 201:**

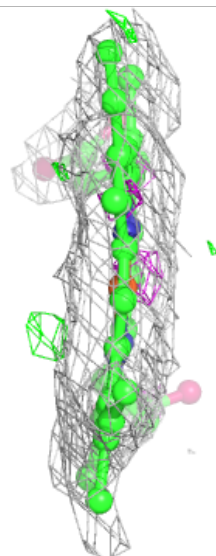
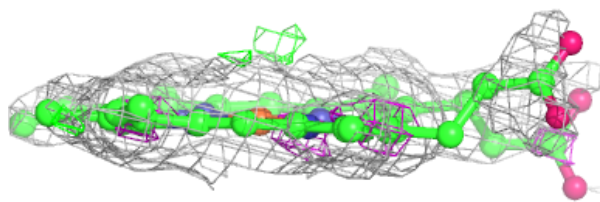
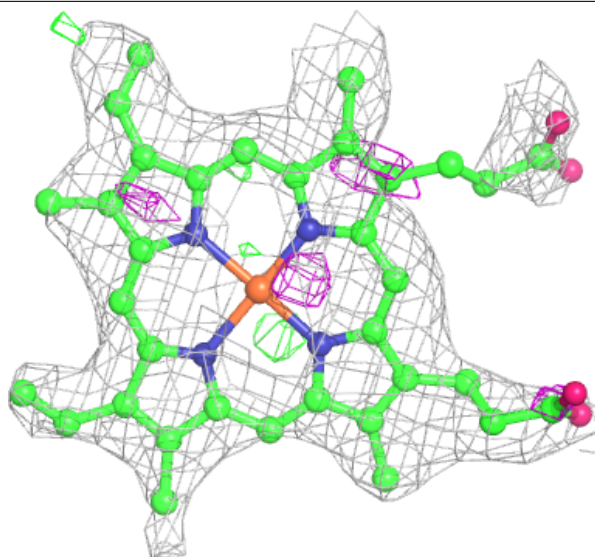
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around HEM H 201:**

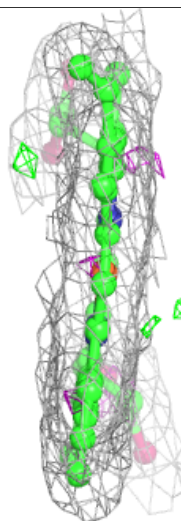
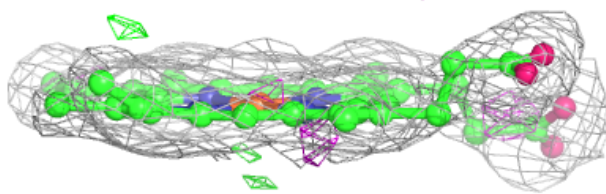
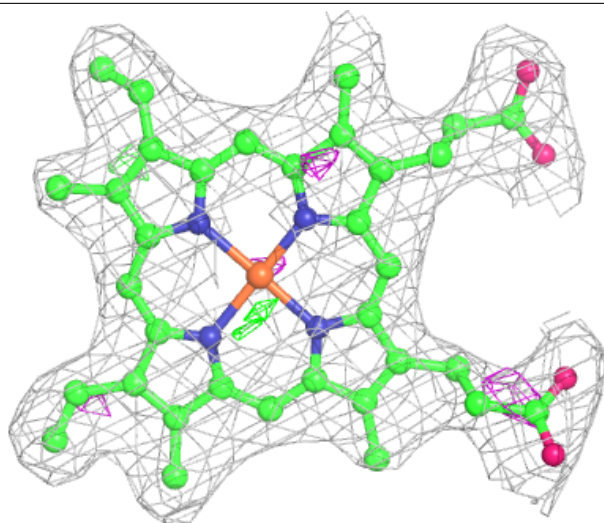
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





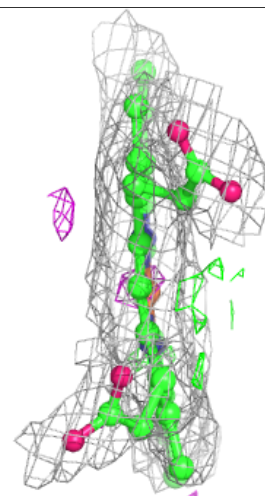
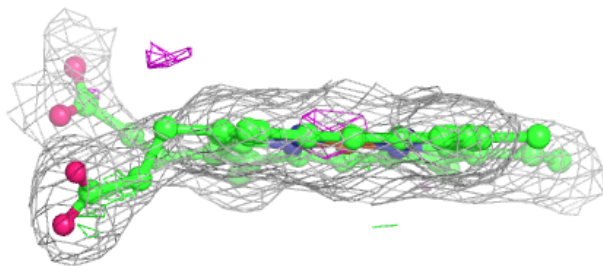
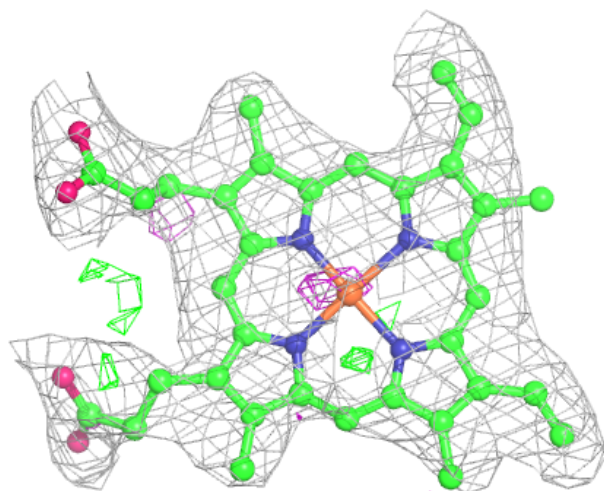
**Electron density around HEM S 201:**

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



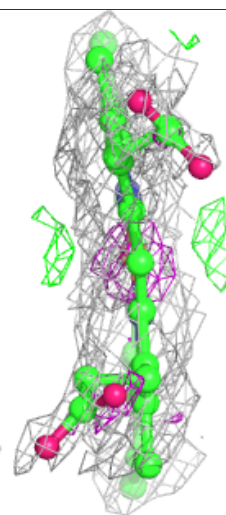
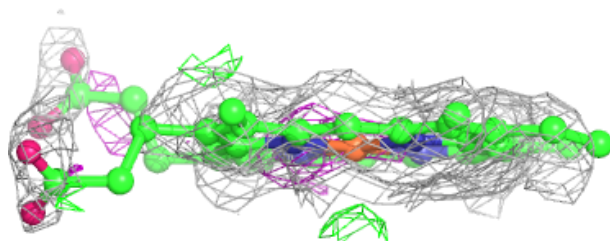
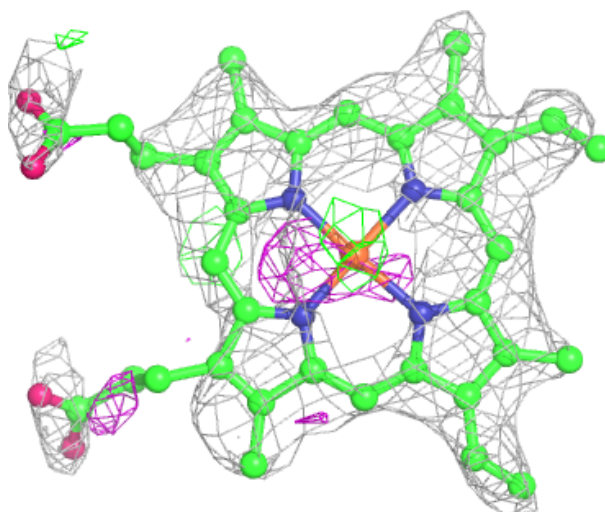
**Electron density around HEM E 201:**

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



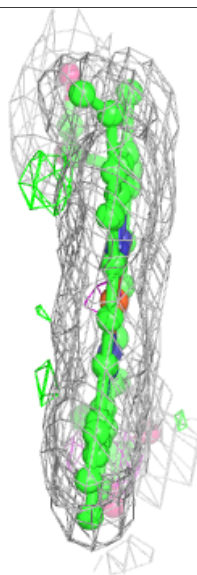
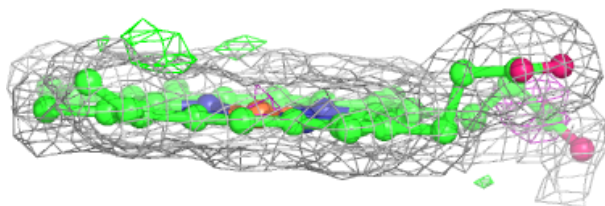
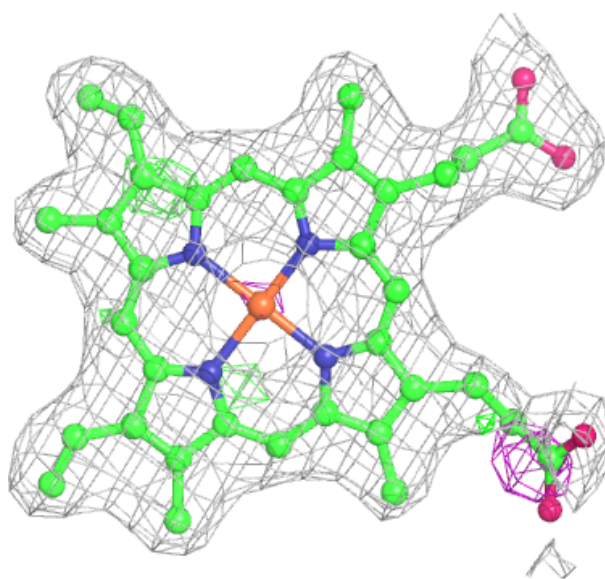
**Electron density around HEM T 201:**

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



**Electron density around HEM C 201:**

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



## 6.5 Other polymers [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.