



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 05:48 AM EDT

PDB ID : 9HBA / pdb_00009hba
Title : Crystal structure of C35 bound to Hem
Authors : Brear, P.; Marchesani, F.; De Bei, O.; Spyrakakis, F.; Lazzarato, L.; Ronda, L.
Deposited on : 2024-11-05
Resolution : 1.51 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

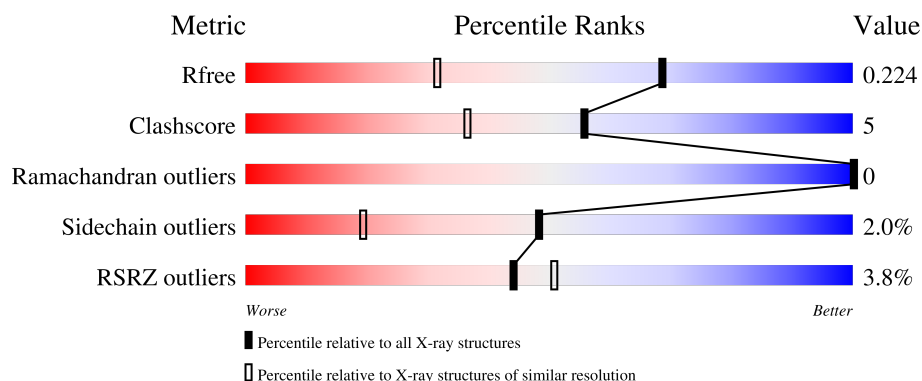
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.51 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	5890 (1.54-1.50)
Clashscore	190562	6116 (1.54-1.50)
Ramachandran outliers	187476	6002 (1.54-1.50)
Sidechain outliers	187428	5999 (1.54-1.50)
RSRZ outliers	180081	5891 (1.54-1.50)

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	141	<div> <div>91%</div> <div>8%</div> <div>.</div> </div>
1	C	141	<div> <div>4%</div> <div>94%</div> <div>5%</div> <div>.</div> </div>
2	B	146	<div> <div>5%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
2	D	146	<div> <div>5%</div> <div>92%</div> <div>6%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	DMS	B	203	-	-	X	-
8	ACY	A	208	-	-	X	-
8	ACY	C	205	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 5136 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.

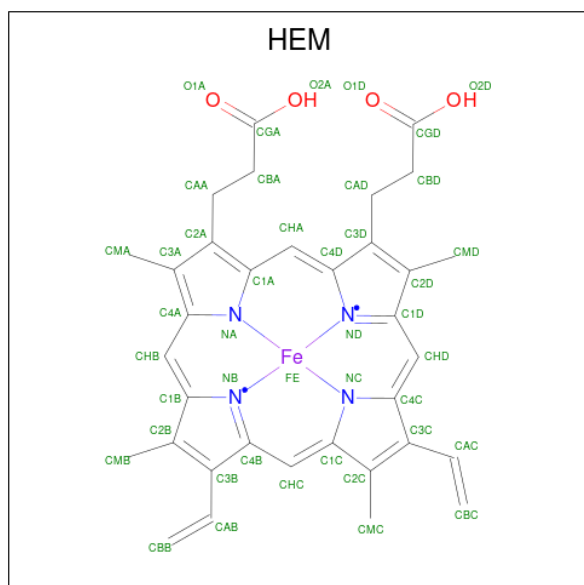
- Molecule 1 is a protein called Hemoglobin subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	141	Total	C	N	O	S	0	0	0
			1069	685	187	194	3			
1	C	141	Total	C	N	O	S	0	2	0
			1088	697	192	196	3			

- Molecule 2 is a protein called Hemoglobin subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	145	Total	C	N	O	S	0	1	0
			1124	724	195	202	3			
2	D	145	Total	C	N	O	S	0	1	0
			1119	720	193	203	3			

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



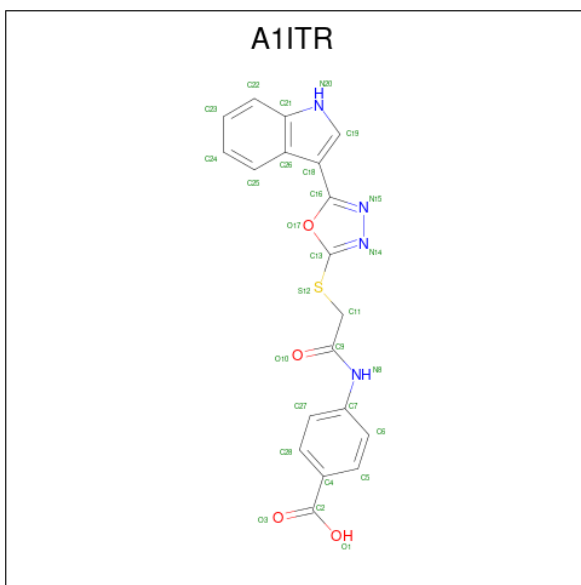
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	C	1	Total	C	Fe	N	O	
			43	34	1	4	4	
3	D	1	Total	C	Fe	N	O	
			43	34	1	4	4	

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



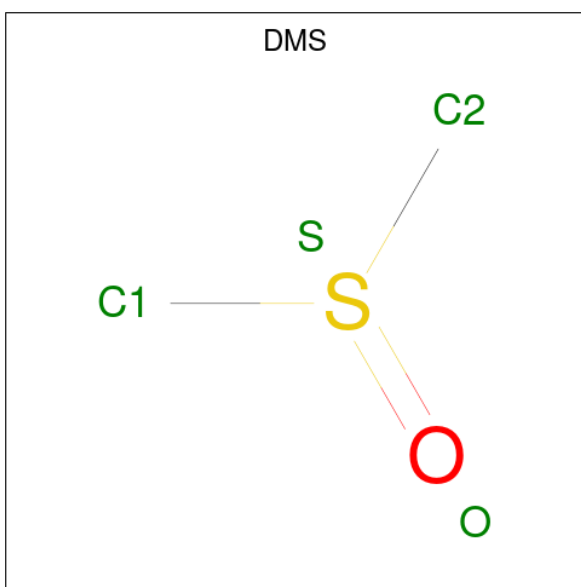
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O		
			6	3	3	0	0
4	A	1	Total	C	O		
			6	3	3	0	0
4	B	1	Total	C	O		
			6	3	3	0	0
4	C	1	Total	C	O		
			6	3	3	0	0
4	C	1	Total	C	O		
			6	3	3	0	0
4	D	1	Total	C	O		
			6	3	3	0	0

- Molecule 5 is 4-[2-[[5-(1H-indol-3-yl)-1,3,4-oxadiazol-2-yl]sulfonyl]ethanoylamino]benzoic acid (CCD ID: A1ITR) (formula: C₁₉H₁₄N₄O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			28	19	4	4	1		
5	B	1	Total	C	N	O		0	0
			10	7	1	2			
5	C	1	Total	C	N	O	S	0	0
			28	19	4	4	1		

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



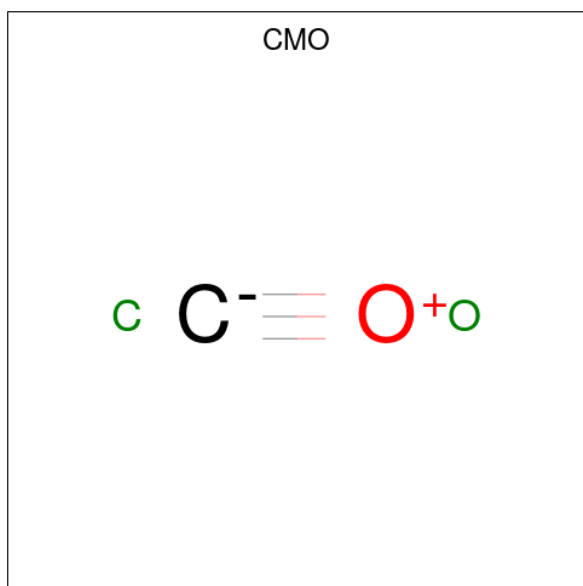
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	O	S	0	0
			4	2	1	1		

Continued on next page...

Continued from previous page...

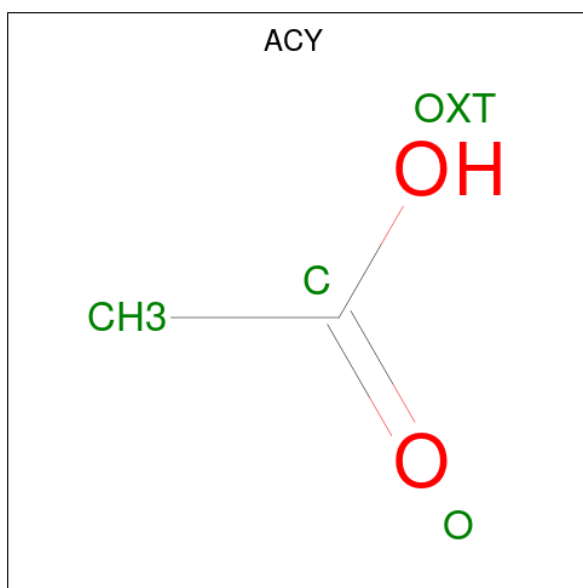
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	A	1	Total 4	C 2	O 1	S 1	0	0
6	B	1	Total 4	C 2	O 1	S 1	0	0
6	B	1	Total 4	C 2	O 1	S 1	0	0
6	B	1	Total 4	C 2	O 1	S 1	0	0
6	B	1	Total 4	C 2	O 1	S 1	0	0
6	D	1	Total 4	C 2	O 1	S 1	0	0

- Molecule 7 is CARBON MONOXIDE (CCD ID: CMO) (formula: CO).



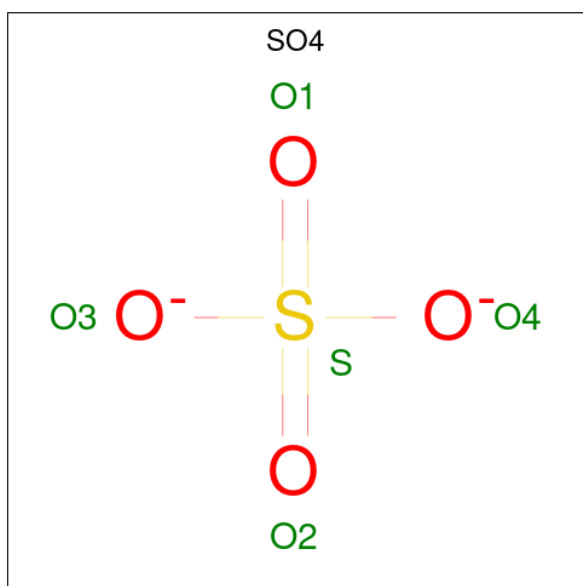
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 2	C 1	O 1	0	0
7	B	1	Total 2	C 1	O 1	0	0
7	C	1	Total 2	C 1	O 1	0	0
7	D	1	Total 2	C 1	O 1	0	0

- Molecule 8 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			4	2	2		
8	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 9 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



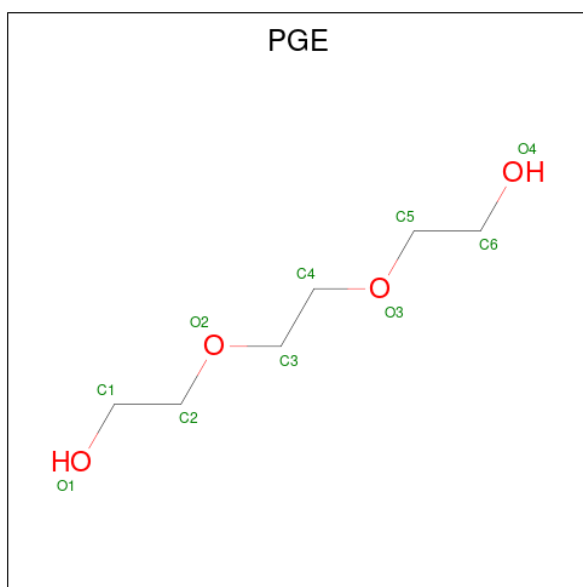
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	A	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	B	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	C	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	88	Total	O	0	0
			88	88		
11	B	79	Total	O	0	0
			79	79		
11	C	83	Total	O	0	1
			84	84		
11	D	73	Total	O	0	0
			73	73		

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.

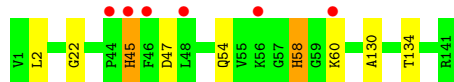
- Molecule 1: Hemoglobin subunit alpha

Chain A:  91% 8% .

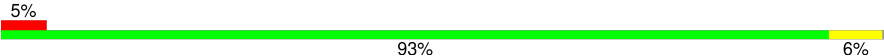


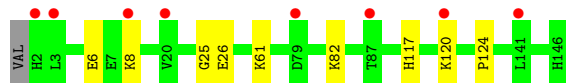
- Molecule 1: Hemoglobin subunit alpha

Chain C:  4% 94% 5% .

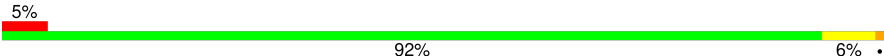


- Molecule 2: Hemoglobin subunit beta

Chain B:  5% 93% 6% .



- Molecule 2: Hemoglobin subunit beta

Chain D:  5% 92% 6% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	92.18Å 92.18Å 142.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	53.26 – 1.51 53.26 – 1.51	Depositor EDS
% Data completeness (in resolution range)	99.4 (53.26-1.51) 99.4 (53.26-1.51)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 1.51Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.184 , 0.215 0.195 , 0.224	Depositor DCC
R_{free} test set	5487 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 37.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5136	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% 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: ACY, DMS, PGE, HEM, CMO, GOL, SO4, A1ITR

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	0.63	0/1097	0.91	0/1491
1	C	0.65	0/1117	0.96	1/1517 (0.1%)
2	B	0.59	0/1154	0.91	1/1566 (0.1%)
2	D	0.62	0/1148	0.98	1/1558 (0.1%)
All	All	0.62	0/4516	0.94	3/6132 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	D	116	HIS	CA-CB-CG	5.72	119.52	113.80
1	C	58	HIS	CA-CB-CG	-5.57	108.23	113.80
2	B	124	PRO	CB-CA-C	5.11	117.15	110.92

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	104	ARG	Sidechain

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	1069	0	1073	10	0
1	C	1088	0	1091	9	0
2	B	1124	0	1111	10	0
2	D	1119	0	1105	7	0
3	A	43	0	30	0	0
3	B	43	0	30	1	0
3	C	43	0	30	0	0
3	D	43	0	30	1	0
4	A	12	0	16	0	0
4	B	6	0	8	1	0
4	C	12	0	16	3	0
4	D	6	0	8	0	0
5	A	28	0	0	0	0
5	B	10	0	0	0	0
5	C	28	0	0	0	0
6	A	12	0	18	0	0
6	B	16	0	24	8	0
6	D	4	0	6	2	0
7	A	2	0	0	1	0
7	B	2	0	0	0	0
7	C	2	0	0	1	0
7	D	2	0	0	0	0
8	A	4	0	3	5	0
8	C	4	0	3	4	0
9	A	20	0	0	0	0
9	B	35	0	0	0	0
9	C	15	0	0	0	0
9	D	10	0	0	0	0
10	B	10	0	14	0	0
11	A	88	0	0	2	1
11	B	79	0	0	1	0
11	C	84	0	0	0	0
11	D	73	0	0	1	1
All	All	5136	0	4616	44	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (44) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:SER:HB3	11:A:302:HOH:O	0.91	1.08
6:D:203:DMS:H13	11:D:317:HOH:O	1.57	1.03
2:B:25:GLY:HA3	6:B:203:DMS:H13	1.49	0.93
1:C:47:ASP:H	1:C:54:GLN:NE2	1.73	0.86
1:A:92:ARG:HG3	1:A:92:ARG:HH11	1.46	0.79
8:A:208:ACY:H3	8:C:205:ACY:H2	1.66	0.77
2:D:26[A]:GLU:OE2	2:D:117:HIS:HE1	1.69	0.73
2:B:26:GLU:OE1	2:B:117:HIS:HE1	1.72	0.73
1:A:92:ARG:HG3	1:A:92:ARG:NH1	2.05	0.72
8:A:208:ACY:H3	8:C:205:ACY:CH3	2.18	0.71
1:C:47:ASP:H	1:C:54:GLN:HE22	1.35	0.71
2:B:61:LYS:HG3	6:B:203:DMS:H11	1.76	0.68
2:D:101:GLU:OE2	2:D:104:ARG:NH1	2.27	0.67
2:B:6:GLU:HG3	11:B:328:HOH:O	1.95	0.66
2:B:25:GLY:CA	6:B:203:DMS:H13	2.24	0.66
1:A:47:ASP:H	1:A:54:GLN:NE2	1.95	0.64
1:A:45:HIS:H	1:A:45:HIS:CD2	2.17	0.60
2:D:19:ASN:HD21	2:D:21:ASP:HB2	1.66	0.60
1:C:22:GLY:HA3	1:C:60:LYS:HE3	1.84	0.59
2:B:82:LYS:H	4:B:208:GOL:H31	1.68	0.58
2:D:20:VAL:HA	2:D:68:LEU:HD23	1.87	0.57
2:B:61:LYS:CB	6:B:203:DMS:H11	2.35	0.57
2:D:51:PRO:HG3	6:D:203:DMS:H11	1.89	0.55
2:B:61:LYS:CG	6:B:203:DMS:H11	2.37	0.54
2:D:20:VAL:HA	2:D:68:LEU:CD2	2.38	0.53
1:A:81:SER:CB	11:A:302:HOH:O	1.77	0.52
1:C:130:ALA:HA	4:C:206:GOL:H32	1.93	0.51
1:A:92:ARG:HH11	1:A:92:ARG:CG	2.18	0.51
2:D:26[A]:GLU:OE2	2:D:117:HIS:CE1	2.59	0.49
1:A:47:ASP:H	1:A:54:GLN:HE22	1.60	0.49
2:B:25:GLY:HA3	6:B:203:DMS:C1	2.32	0.48
1:C:58:HIS:NE2	7:C:204:CMO:C	2.76	0.48
3:D:201:HEM:HBB2	3:D:201:HEM:HHC	1.94	0.48
1:C:47:ASP:HB3	1:C:54:GLN:HE21	1.78	0.48
6:B:201:DMS:H21	4:C:202:GOL:H12	1.95	0.47
8:A:208:ACY:H3	8:C:205:ACY:H1	1.96	0.47
3:B:202:HEM:HBB2	3:B:202:HEM:HHC	1.98	0.46
1:C:134:THR:HG21	8:C:205:ACY:H2	1.98	0.45
1:A:58:HIS:NE2	7:A:206:CMO:C	2.81	0.44
1:A:21:ALA:HB1	1:A:63:ALA:HB1	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:208:ACY:OXT	4:C:202:GOL:H32	2.20	0.42
2:B:61:LYS:HA	6:B:203:DMS:H11	2.01	0.41
8:A:208:ACY:H3	1:C:134:THR:HG21	2.02	0.41
1:C:45[A]:HIS:ND1	1:C:45[A]:HIS:N	2.66	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:361:HOH:O	11:D:353:HOH:O[5_545]	2.04	0.16

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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%)	137 (99%)	2 (1%)	0	100	100
1	C	141/141 (100%)	140 (99%)	1 (1%)	0	100	100
2	B	144/146 (99%)	142 (99%)	2 (1%)	0	100	100
2	D	144/146 (99%)	141 (98%)	3 (2%)	0	100	100
All	All	568/574 (99%)	560 (99%)	8 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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%)	108 (96%)	5 (4%)	25	4
1	C	115/113 (102%)	112 (97%)	3 (3%)	40	12
2	B	118/118 (100%)	116 (98%)	2 (2%)	53	24
2	D	117/118 (99%)	117 (100%)	0	100	100
All	All	463/462 (100%)	453 (98%)	10 (2%)	48	16

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	16	LYS
1	A	92	ARG
1	A	116	GLU
1	A	136	LEU
2	B	8	LYS
2	B	120	LYS
1	C	2	LEU
1	C	45[A]	HIS
1	C	45[B]	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	HIS
1	A	54	GLN
2	B	97	HIS
2	B	117	HIS
2	B	146	HIS
1	C	54	GLN
2	D	19	ASN
2	D	97	HIS
2	D	117	HIS

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 ⓘ

44 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	$\# Z > 2$
7	CMO	D	202	-	0,1,1	-	-	-		
9	SO4	B	216	-	4,4,4	0.30	0	6,6,6	0.12	0
5	A1ITR	A	203	-	31,31,31	0.69	0	41,43,43	0.60	1 (2%)
8	ACY	A	208	-	3,3,3	0.84	0	3,3,3	1.10	0
5	A1ITR	C	201	-	31,31,31	0.78	0	41,43,43	0.60	0
9	SO4	A	213	-	4,4,4	0.35	0	6,6,6	0.20	0
9	SO4	B	210	-	4,4,4	0.24	0	6,6,6	0.14	0
9	SO4	B	213	-	4,4,4	0.34	0	6,6,6	0.11	0
6	DMS	B	209	-	3,3,3	0.36	0	3,3,3	0.05	0
3	HEM	C	203	1	50,50,50	1.50	7 (14%)	67,82,82	1.78	14 (20%)
9	SO4	B	212	-	4,4,4	0.30	0	6,6,6	0.15	0
9	SO4	B	215	-	4,4,4	0.22	0	6,6,6	0.19	0
3	HEM	D	201	2	50,50,50	1.39	7 (14%)	67,82,82	1.70	21 (31%)
9	SO4	D	205	-	4,4,4	0.31	0	6,6,6	0.12	0
5	A1ITR	B	204	-	10,10,31	0.78	0	13,13,43	0.60	0
3	HEM	B	202	2	50,50,50	1.58	9 (18%)	67,82,82	1.72	14 (20%)
9	SO4	A	212	-	4,4,4	0.31	0	6,6,6	0.12	0
9	SO4	C	208	-	4,4,4	0.29	0	6,6,6	0.09	0
7	CMO	A	206	-	0,1,1	-	-	-		
6	DMS	B	205	-	3,3,3	0.36	0	3,3,3	0.07	0
7	CMO	B	206	-	0,1,1	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	DMS	A	209	-	3,3,3	0.54	0	3,3,3	0.18	0
6	DMS	B	201	-	3,3,3	0.63	0	3,3,3	0.40	0
6	DMS	B	203	-	3,3,3	0.90	0	3,3,3	0.62	0
3	HEM	A	201	1	50,50,50	1.53	10 (20%)	67,82,82	1.74	12 (17%)
4	GOL	B	208	-	5,5,5	0.20	0	5,5,5	0.54	0
7	CMO	C	204	-	0,1,1	-	-	-	-	-
4	GOL	C	202	-	5,5,5	0.19	0	5,5,5	0.63	0
6	DMS	A	205	-	3,3,3	0.39	0	3,3,3	0.12	0
4	GOL	A	207	-	5,5,5	0.15	0	5,5,5	0.56	0
9	SO4	A	210	-	4,4,4	0.32	0	6,6,6	0.25	0
9	SO4	A	211	-	4,4,4	0.28	0	6,6,6	0.25	0
9	SO4	B	211	-	4,4,4	0.27	0	6,6,6	0.18	0
4	GOL	A	202	-	5,5,5	0.31	0	5,5,5	0.56	0
4	GOL	C	206	-	5,5,5	0.14	0	5,5,5	0.30	0
9	SO4	D	204	-	4,4,4	0.16	0	6,6,6	0.21	0
6	DMS	D	203	-	3,3,3	0.56	0	3,3,3	0.30	0
9	SO4	B	214	-	4,4,4	0.32	0	6,6,6	0.09	0
8	ACY	C	205	-	3,3,3	1.04	0	3,3,3	0.88	0
6	DMS	A	204	-	3,3,3	0.46	0	3,3,3	0.11	0
10	PGE	B	207	-	9,9,9	0.33	0	8,8,8	0.45	0
9	SO4	C	209	-	4,4,4	0.31	0	6,6,6	0.15	0
4	GOL	D	206	-	5,5,5	0.15	0	5,5,5	0.15	0
9	SO4	C	207	-	4,4,4	0.30	0	6,6,6	0.08	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
5	A1ITR	A	203	-	-	2/17/17/17	0/4/4/4
3	HEM	A	201	1	-	2/14/54/54	-
3	HEM	D	201	2	-	4/14/54/54	-
4	GOL	B	208	-	-	4/4/4/4	-
5	A1ITR	B	204	-	-	0/4/4/17	0/1/1/4
3	HEM	B	202	2	-	2/14/54/54	-
4	GOL	C	202	-	-	0/4/4/4	-
5	A1ITR	C	201	-	-	2/17/17/17	0/4/4/4
4	GOL	A	207	-	-	4/4/4/4	-
10	PGE	B	207	-	-	2/7/7/7	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	202	-	-	4/4/4/4	-
3	HEM	C	203	1	-	2/14/54/54	-
4	GOL	C	206	-	-	1/4/4/4	-
4	GOL	D	206	-	-	2/4/4/4	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	202	HEM	FE-NB	4.90	2.10	1.94
3	A	201	HEM	FE-NB	4.63	2.09	1.94
3	C	203	HEM	FE-NB	4.60	2.09	1.94
3	D	201	HEM	FE-NC	3.96	2.08	1.95
3	C	203	HEM	C1B-NB	-3.89	1.33	1.40
3	B	202	HEM	C1B-NB	-3.47	1.34	1.40
3	B	202	HEM	FE-NC	3.41	2.06	1.95
3	D	201	HEM	C1B-NB	-3.29	1.34	1.40
3	A	201	HEM	FE-NC	3.27	2.06	1.95
3	C	203	HEM	FE-NC	3.18	2.05	1.95
3	A	201	HEM	C4D-ND	-3.05	1.35	1.40
3	B	202	HEM	C4B-NB	-2.93	1.33	1.38
3	B	202	HEM	C1C-C2C	-2.74	1.39	1.45
3	B	202	HEM	CHB-C1B	2.71	1.43	1.38
3	D	201	HEM	FE-NA	2.68	2.04	1.95
3	D	201	HEM	C4C-NC	-2.66	1.34	1.39
3	A	201	HEM	C1D-C2D	2.64	1.49	1.44
3	C	203	HEM	C4D-ND	-2.62	1.35	1.40
3	D	201	HEM	FE-NB	2.55	2.02	1.94
3	A	201	HEM	C1B-NB	-2.52	1.35	1.40
3	B	202	HEM	C4D-C3D	2.49	1.49	1.45
3	A	201	HEM	O2D-CGD	-2.45	1.22	1.30
3	A	201	HEM	C4B-NB	-2.44	1.34	1.38
3	B	202	HEM	C3B-C4B	2.42	1.49	1.44
3	A	201	HEM	C1D-ND	-2.30	1.34	1.38
3	C	203	HEM	C4B-NB	-2.30	1.34	1.38
3	C	203	HEM	C1C-NC	-2.25	1.35	1.39
3	D	201	HEM	C1D-C2D	2.24	1.49	1.44
3	A	201	HEM	C4D-C3D	2.17	1.48	1.45
3	C	203	HEM	C3B-C4B	2.15	1.49	1.44
3	B	202	HEM	C1D-C2D	2.14	1.48	1.44
3	D	201	HEM	C1B-C2B	-2.11	1.40	1.44
3	A	201	HEM	C1C-C2C	-2.04	1.41	1.45

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	203	HEM	CHC-C4B-NB	5.49	130.34	124.42
3	A	201	HEM	C1B-NB-C4B	5.39	111.59	105.21
3	A	201	HEM	CHC-C4B-NB	5.06	129.87	124.42
3	B	202	HEM	C1B-NB-C4B	5.06	111.20	105.21
3	C	203	HEM	C1B-NB-C4B	4.75	110.83	105.21
3	A	201	HEM	C3B-C4B-NB	-4.52	106.22	109.47
3	B	202	HEM	C3B-C4B-NB	-4.35	106.34	109.47
3	A	201	HEM	CHD-C1D-ND	4.10	128.84	124.42
3	B	202	HEM	CHC-C4B-NB	3.98	128.70	124.42
3	C	203	HEM	CHD-C1D-ND	3.86	128.58	124.42
3	D	201	HEM	CHC-C4B-NB	3.76	128.47	124.42
3	B	202	HEM	CHB-C1B-NB	3.60	128.82	124.37
3	D	201	HEM	C3D-C4D-ND	3.59	114.11	110.17
3	B	202	HEM	CHA-C4D-ND	3.54	128.74	124.37
3	C	203	HEM	CHD-C4C-NC	3.53	128.30	124.45
3	D	201	HEM	CHA-C4D-C3D	-3.27	119.20	125.23
3	C	203	HEM	CHA-C4D-ND	3.26	128.40	124.37
3	D	201	HEM	CHD-C4C-NC	3.24	127.98	124.45
3	A	201	HEM	CHA-C4D-ND	3.22	128.35	124.37
3	C	203	HEM	C3B-C4B-NB	-3.15	107.20	109.47
3	B	202	HEM	CBD-CAD-C3D	-3.09	103.98	112.53
3	A	201	HEM	CMD-C2D-C1D	-3.00	120.35	125.03
3	B	202	HEM	CHD-C1D-ND	2.99	127.64	124.42
3	C	203	HEM	CHB-C1B-NB	2.98	128.05	124.37
3	A	201	HEM	CHB-C1B-NB	2.87	127.92	124.37
3	A	201	HEM	CHA-C4D-C3D	-2.83	120.00	125.23
3	C	203	HEM	CHD-C1D-C2D	-2.82	120.58	125.03
3	C	203	HEM	CHA-C1A-NA	2.75	128.85	123.86
3	A	201	HEM	CBD-CAD-C3D	-2.75	104.94	112.53
3	D	201	HEM	C3B-C2B-C1B	2.66	108.41	106.41
3	D	201	HEM	C4D-ND-C1D	-2.62	102.10	105.21
3	C	203	HEM	CBD-CAD-C3D	-2.55	105.47	112.53
3	C	203	HEM	O1D-CGD-CBD	-2.55	115.00	123.09
3	B	202	HEM	CHA-C4D-C3D	-2.51	120.59	125.23
3	A	201	HEM	CMD-C2D-C3D	2.49	132.88	126.15
3	D	201	HEM	CAB-C3B-C2B	-2.49	120.34	128.43
3	D	201	HEM	O1A-CGA-CBA	-2.48	115.22	123.09
3	B	202	HEM	CHD-C1D-C2D	-2.47	121.12	125.03
3	D	201	HEM	C2D-C1D-ND	2.44	112.72	109.90
3	A	201	HEM	O2A-CGA-CBA	2.43	121.66	114.00
3	D	201	HEM	C3B-C4B-NB	-2.38	107.76	109.47
3	D	201	HEM	CMB-C2B-C1B	2.37	128.75	125.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	203	HEM	C1A-CHA-C4D	-2.37	120.68	126.25
3	A	201	HEM	CHD-C1D-C2D	-2.34	121.33	125.03
3	D	201	HEM	CMB-C2B-C3B	-2.33	122.78	128.43
5	A	203	A1ITR	C11-S12-C13	2.29	100.54	97.84
3	B	202	HEM	O2A-CGA-CBA	2.26	121.14	114.00
3	D	201	HEM	C4C-NC-C1C	2.20	109.41	105.82
3	D	201	HEM	O2D-CGD-CBD	2.19	120.93	114.00
3	D	201	HEM	C1B-NB-C4B	2.19	107.80	105.21
3	D	201	HEM	O2A-CGA-CBA	2.19	120.91	114.00
3	D	201	HEM	C1A-CHA-C4D	-2.17	121.16	126.25
3	B	202	HEM	CAC-C3C-C4C	-2.14	119.72	124.82
3	D	201	HEM	CHD-C1D-C2D	-2.13	121.66	125.03
3	D	201	HEM	C2A-C1A-NA	-2.13	107.79	110.15
3	B	202	HEM	C1A-CHA-C4D	-2.13	121.25	126.25
3	D	201	HEM	CAB-C3B-C4B	2.12	133.76	124.39
3	C	203	HEM	C4C-NC-C1C	2.12	109.27	105.82
3	B	202	HEM	CHD-C4C-NC	2.08	126.72	124.45
3	D	201	HEM	C4D-C3D-C2D	-2.07	103.88	106.89
3	B	202	HEM	C4C-NC-C1C	2.05	109.16	105.82
3	C	203	HEM	CHA-C4D-C3D	-2.01	121.53	125.23

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	202	GOL	O1-C1-C2-C3
4	A	202	GOL	C1-C2-C3-O3
4	A	207	GOL	C1-C2-C3-O3
4	B	208	GOL	O1-C1-C2-C3
4	D	206	GOL	O1-C1-C2-C3
10	B	207	PGE	O1-C1-C2-O2
4	A	207	GOL	O1-C1-C2-C3
4	B	208	GOL	C1-C2-C3-O3
4	C	206	GOL	O1-C1-C2-C3
4	A	202	GOL	O1-C1-C2-O2
4	A	202	GOL	O2-C2-C3-O3
4	A	207	GOL	O2-C2-C3-O3
4	B	208	GOL	O2-C2-C3-O3
4	B	208	GOL	O1-C1-C2-O2
4	D	206	GOL	O1-C1-C2-O2
10	B	207	PGE	O2-C3-C4-O3
5	A	203	A1ITR	O17-C13-S12-C11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	C	201	A1ITR	O17-C13-S12-C11
5	A	203	A1ITR	N14-C13-S12-C11
5	C	201	A1ITR	N14-C13-S12-C11
4	A	207	GOL	O1-C1-C2-O2
3	A	201	HEM	CAD-CBD-CGD-O1D
3	B	202	HEM	CAD-CBD-CGD-O2D
3	B	202	HEM	CAD-CBD-CGD-O1D
3	A	201	HEM	CAD-CBD-CGD-O2D
3	D	201	HEM	CAD-CBD-CGD-O1D
3	D	201	HEM	CAD-CBD-CGD-O2D
3	D	201	HEM	CAA-CBA-CGA-O2A
3	D	201	HEM	CAA-CBA-CGA-O1A
3	C	203	HEM	CAD-CBD-CGD-O1D
3	C	203	HEM	CAD-CBD-CGD-O2D

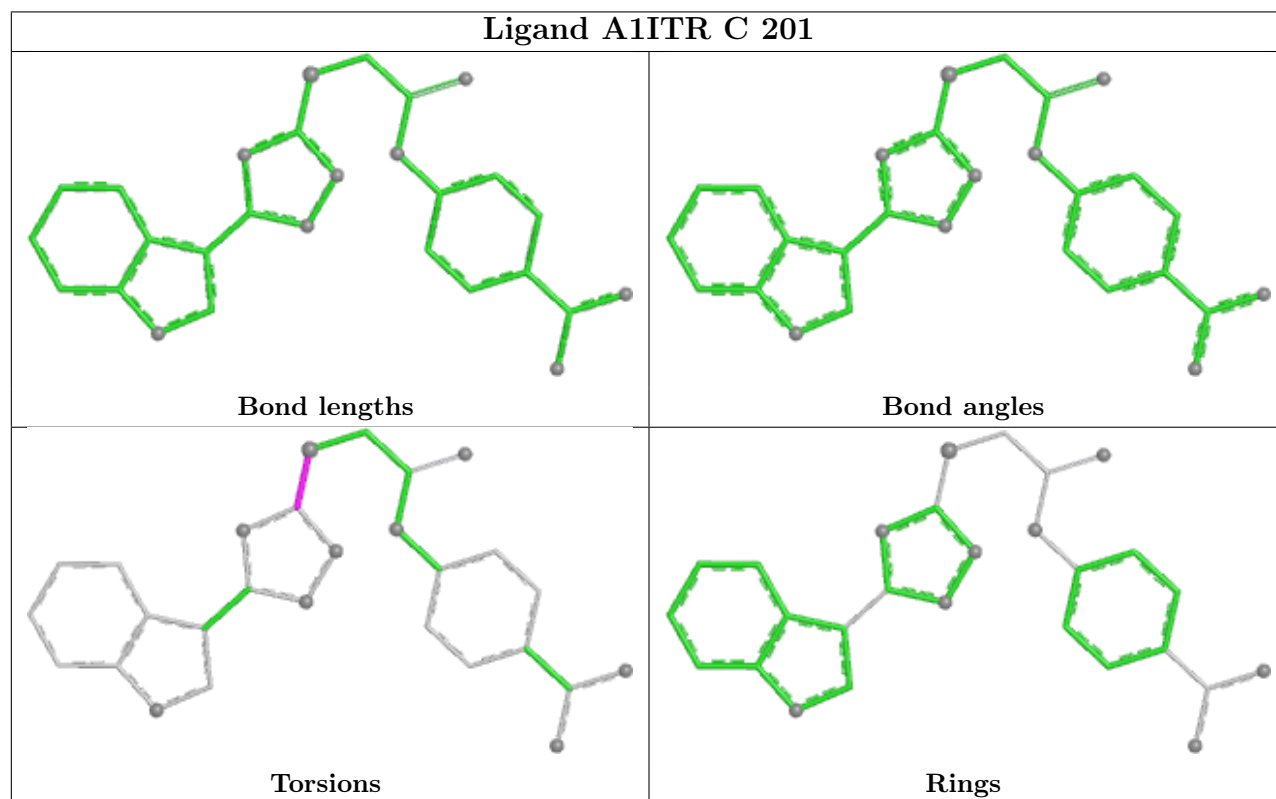
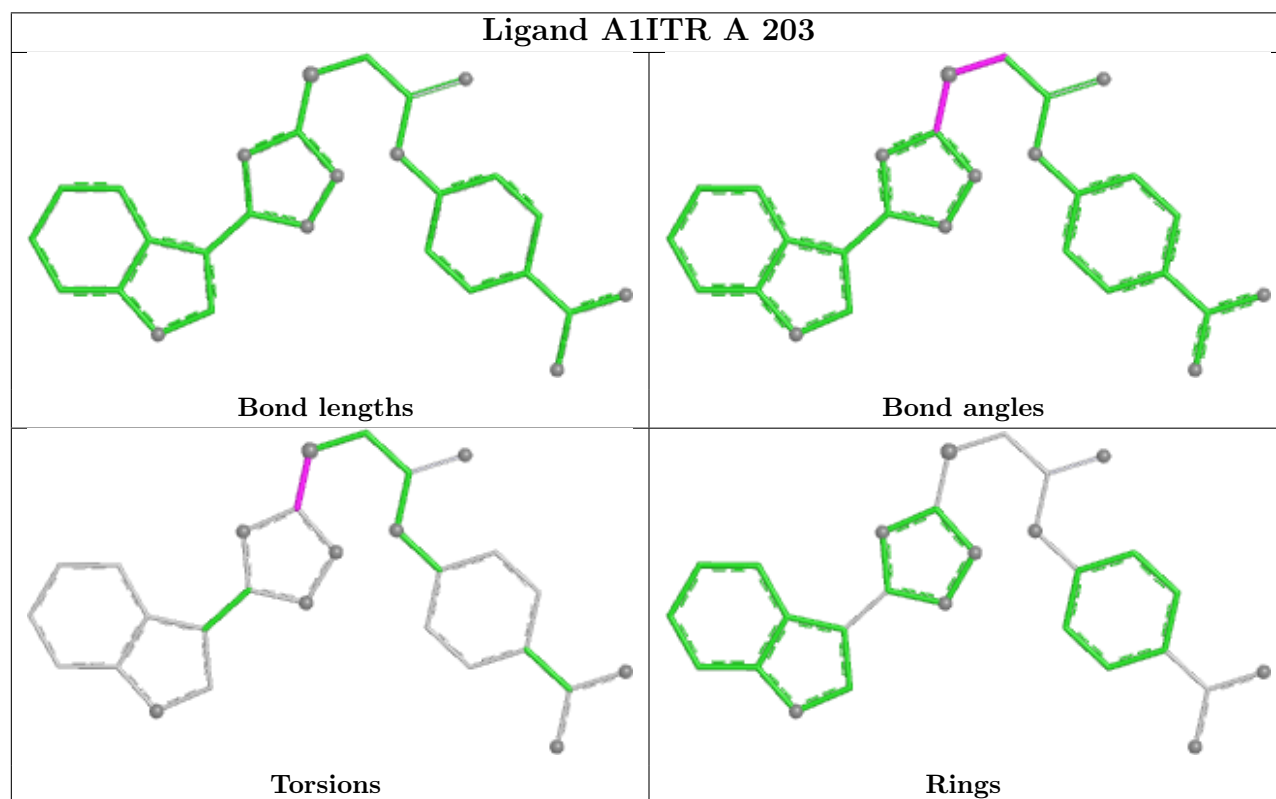
There are no ring outliers.

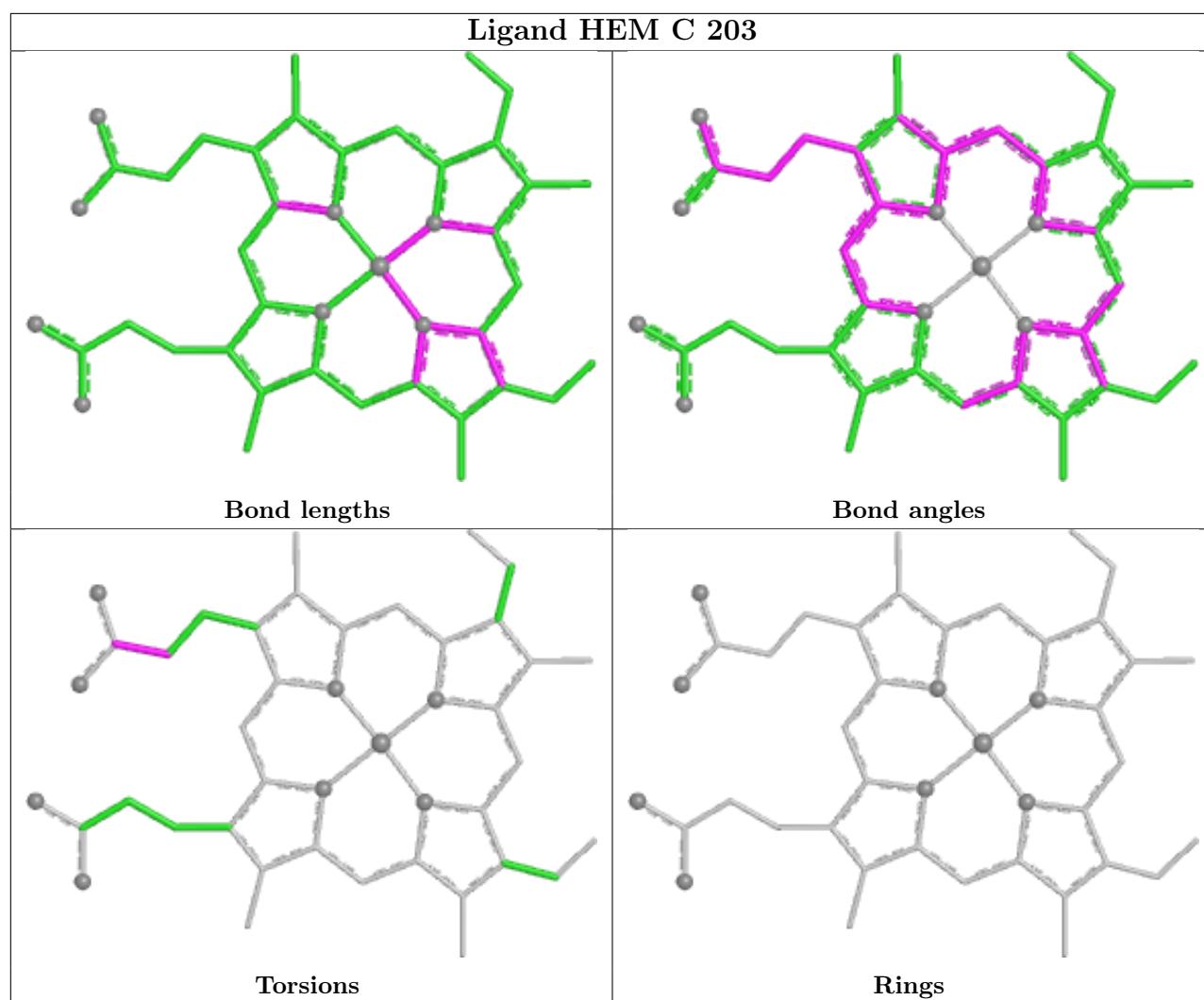
12 monomers are involved in 22 short contacts:

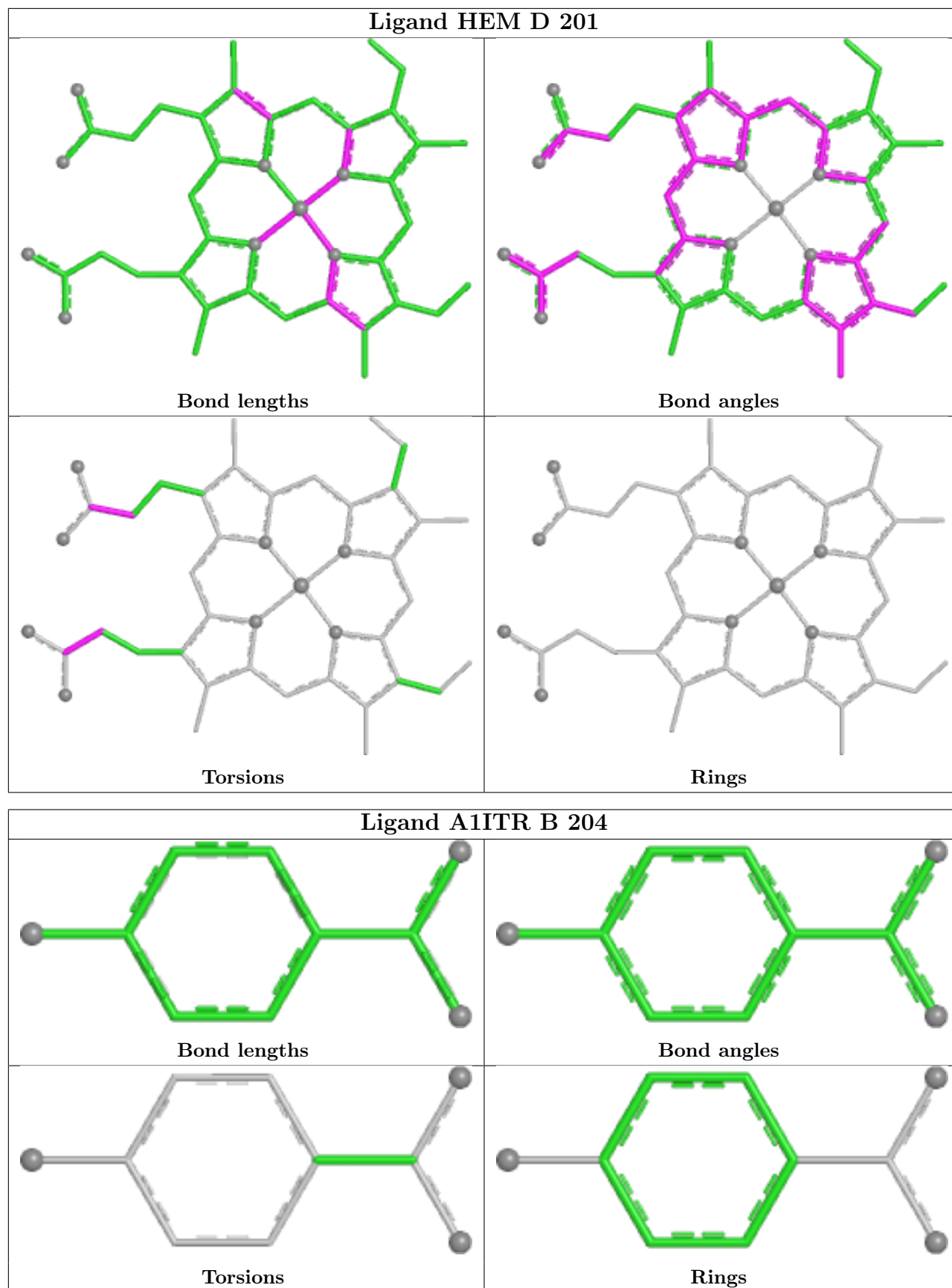
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	208	ACY	5	0
3	D	201	HEM	1	0
3	B	202	HEM	1	0
7	A	206	CMO	1	0
6	B	201	DMS	1	0
6	B	203	DMS	7	0
4	B	208	GOL	1	0
7	C	204	CMO	1	0
4	C	202	GOL	2	0
4	C	206	GOL	1	0
6	D	203	DMS	2	0
8	C	205	ACY	4	0

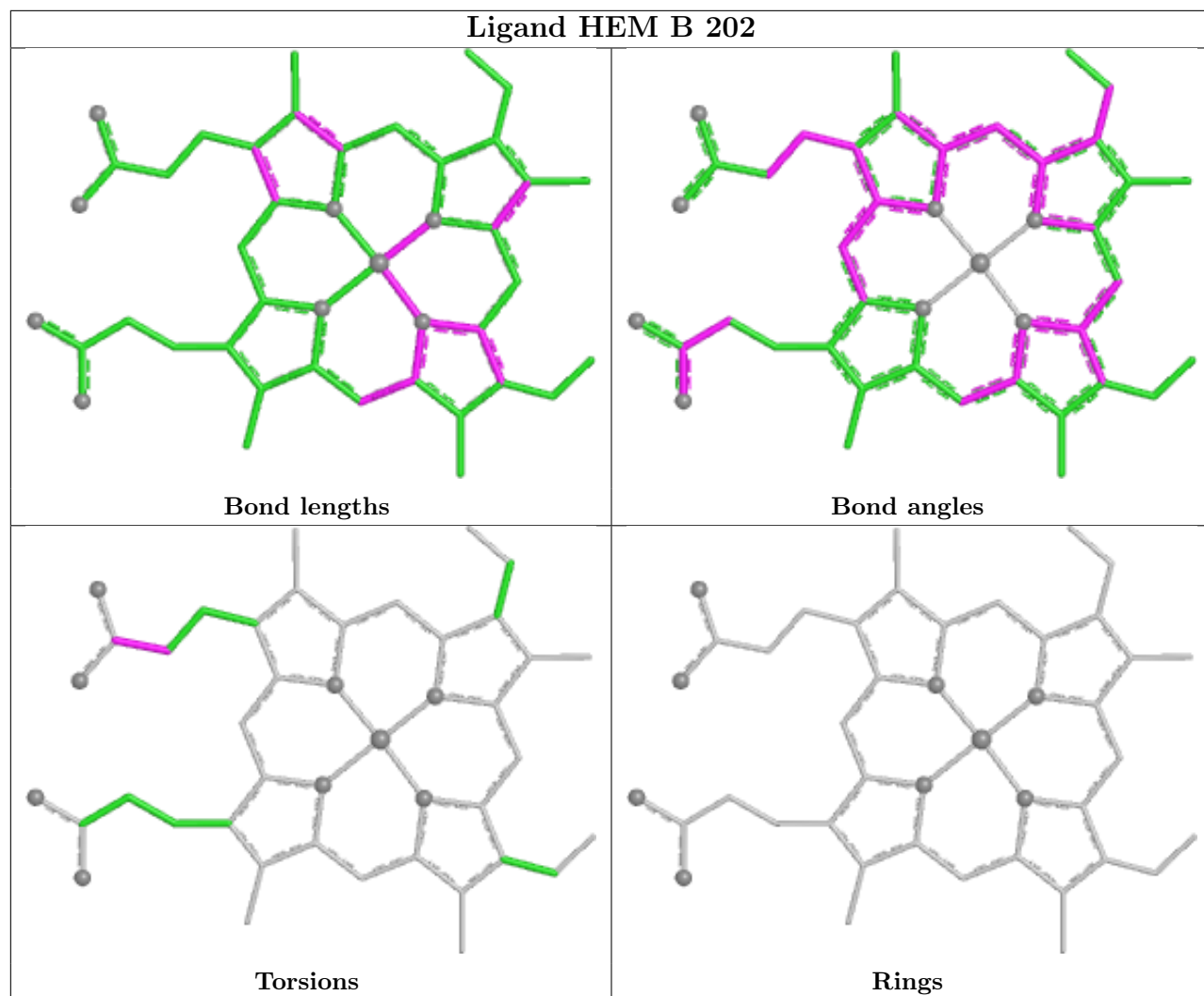
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

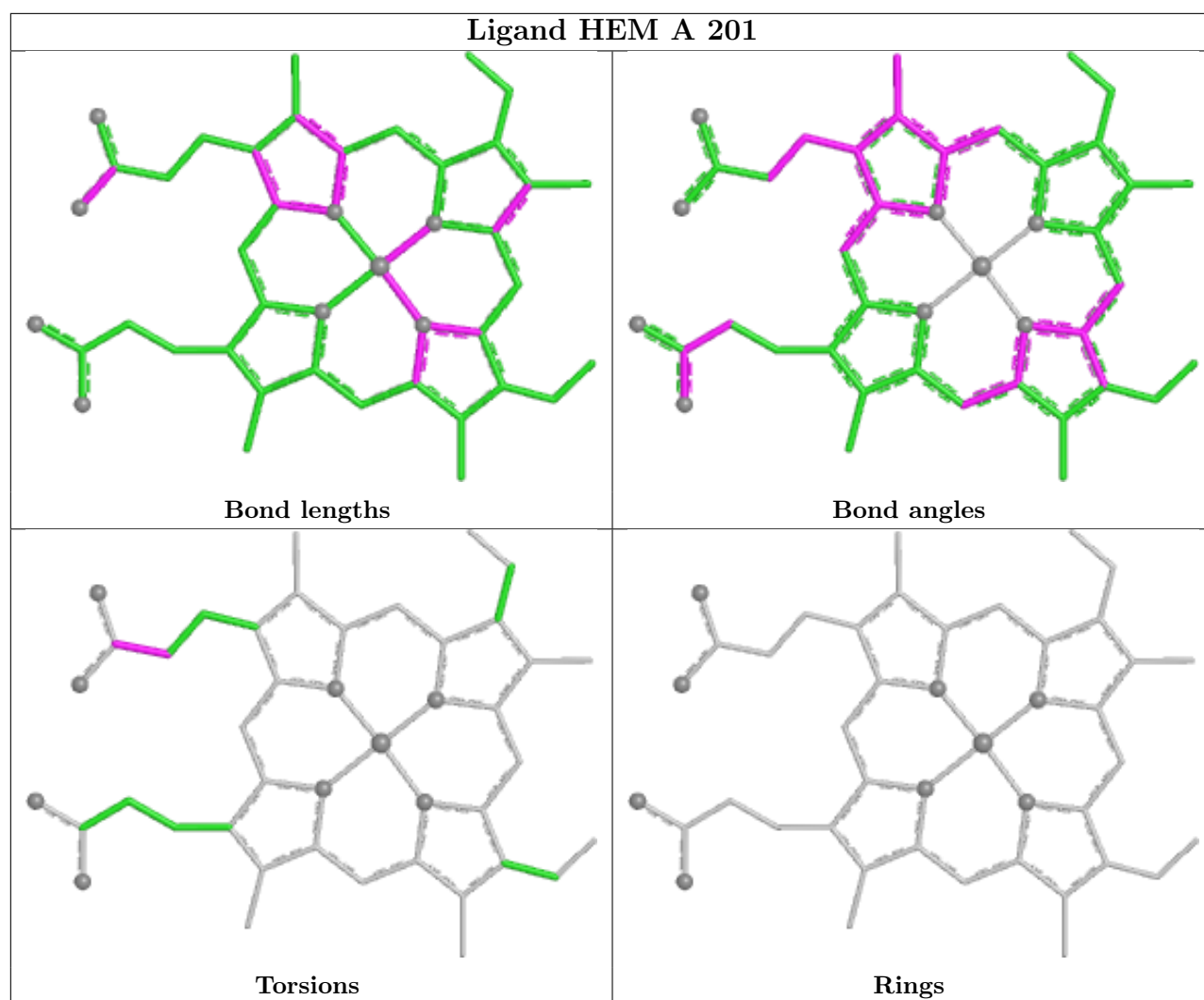
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











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	141/141 (100%)	0.24	0	100	100	24, 29, 39, 49	0
1	C	141/141 (100%)	0.31	6 (4%)	40	46	16, 28, 43, 53	2 (1%)
2	B	145/146 (99%)	0.56	8 (5%)	30	36	18, 31, 47, 58	1 (0%)
2	D	145/146 (99%)	0.55	8 (5%)	30	36	15, 33, 54, 64	1 (0%)
All	All	572/574 (99%)	0.42	22 (3%)	44	51	15, 30, 47, 64	4 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	45[A]	HIS	5.0
2	D	2	HIS	4.0
1	C	48	LEU	3.4
1	C	46	PHE	3.4
2	D	3	LEU	3.2
2	B	8	LYS	2.8
2	B	141	LEU	2.8
2	B	87	THR	2.6
2	B	2	HIS	2.5
2	D	14	LEU	2.5
2	D	97	HIS	2.5
2	D	10	ALA	2.4
1	C	56[A]	LYS	2.4
2	B	3	LEU	2.3
2	D	20	VAL	2.3
2	B	120	LYS	2.3
2	D	16	GLY	2.2
2	B	20	VAL	2.2
1	C	44	PRO	2.1
2	D	79	ASP	2.1
2	B	79	ASP	2.0
1	C	60	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	SO4	B	211	5/5	0.67	0.17	65,78,85,87	0
9	SO4	B	210	5/5	0.77	0.12	62,65,81,87	0
5	AlITR	B	204	10/28	0.77	0.18	48,51,61,67	0
4	GOL	D	206	6/6	0.79	0.17	51,56,67,70	0
9	SO4	D	205	5/5	0.80	0.11	76,78,88,99	0
9	SO4	D	204	5/5	0.82	0.12	45,48,60,63	0
4	GOL	A	207	6/6	0.83	0.15	48,50,56,57	0
9	SO4	C	207	5/5	0.83	0.10	71,84,87,89	0
9	SO4	A	213	5/5	0.83	0.10	48,52,68,71	0
4	GOL	A	202	6/6	0.83	0.16	38,39,47,51	0
6	DMS	B	209	4/4	0.84	0.21	68,74,79,83	0
9	SO4	B	214	5/5	0.84	0.09	85,86,94,98	0
9	SO4	A	212	5/5	0.84	0.14	65,71,77,81	0
4	GOL	B	208	6/6	0.84	0.14	41,52,57,71	0
4	GOL	C	206	6/6	0.84	0.15	40,51,55,56	0
9	SO4	C	209	5/5	0.85	0.15	59,61,72,72	0
10	PGE	B	207	10/10	0.86	0.15	50,58,63,63	0
4	GOL	C	202	6/6	0.87	0.17	42,59,64,68	0
9	SO4	C	208	5/5	0.87	0.10	66,73,78,79	0
9	SO4	B	212	5/5	0.88	0.11	81,82,91,94	0
9	SO4	B	213	5/5	0.88	0.10	74,83,93,94	0
9	SO4	A	210	5/5	0.88	0.13	36,41,45,45	0
9	SO4	B	216	5/5	0.88	0.12	85,95,101,101	0
9	SO4	A	211	5/5	0.88	0.08	51,53,55,57	0
6	DMS	B	205	4/4	0.89	0.17	52,59,59,64	0
9	SO4	B	215	5/5	0.90	0.13	40,47,60,66	0
8	ACY	A	208	4/4	0.91	0.12	40,44,49,54	0

Continued on next page...

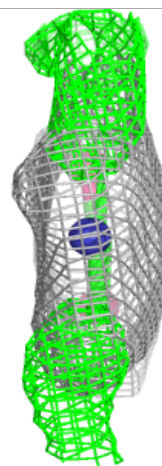
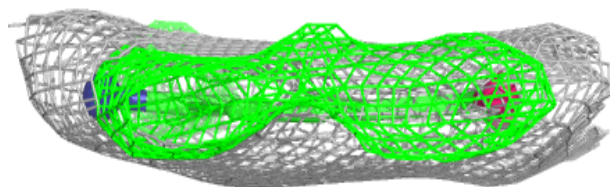
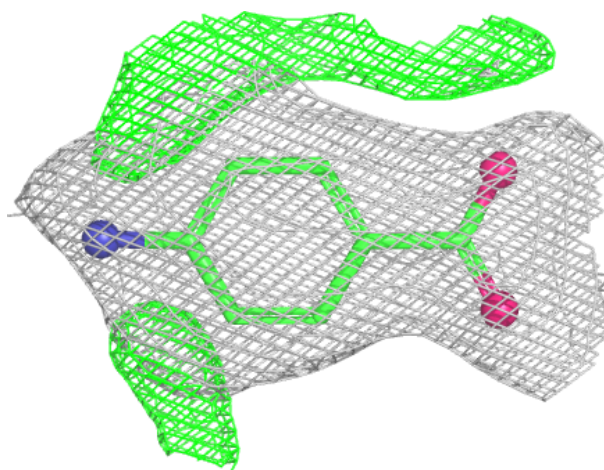
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	DMS	A	204	4/4	0.91	0.13	47,54,55,61	0
6	DMS	A	209	4/4	0.91	0.16	35,37,41,41	0
6	DMS	A	205	4/4	0.92	0.15	44,47,51,52	0
6	DMS	B	201	4/4	0.92	0.16	47,47,54,56	0
6	DMS	D	203	4/4	0.92	0.13	35,48,49,55	0
8	ACY	C	205	4/4	0.94	0.10	41,47,51,51	0
7	CMO	B	206	2/2	0.95	0.12	23,23,23,40	0
6	DMS	B	203	4/4	0.95	0.11	37,38,39,42	0
7	CMO	D	202	2/2	0.96	0.09	22,22,22,44	0
7	CMO	C	204	2/2	0.97	0.10	17,17,17,36	0
7	CMO	A	206	2/2	0.97	0.09	21,21,21,40	0
5	A1ITR	A	203	28/28	0.97	0.06	24,26,30,31	0
3	HEM	B	202	43/43	0.98	0.07	26,29,41,54	0
3	HEM	C	203	43/43	0.98	0.07	24,26,48,55	0
3	HEM	D	201	43/43	0.98	0.08	24,28,46,52	0
5	A1ITR	C	201	28/28	0.98	0.05	23,27,30,31	0
3	HEM	A	201	43/43	0.98	0.07	22,26,37,40	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.

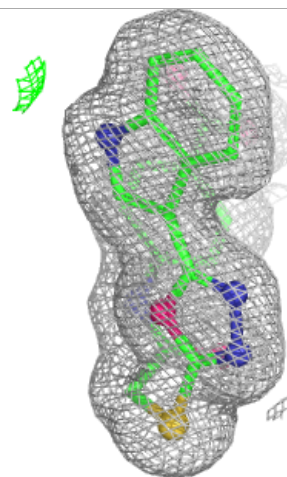
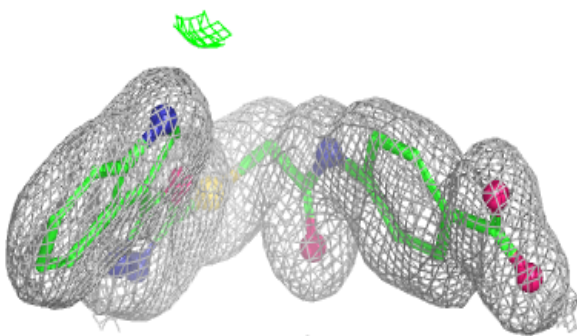
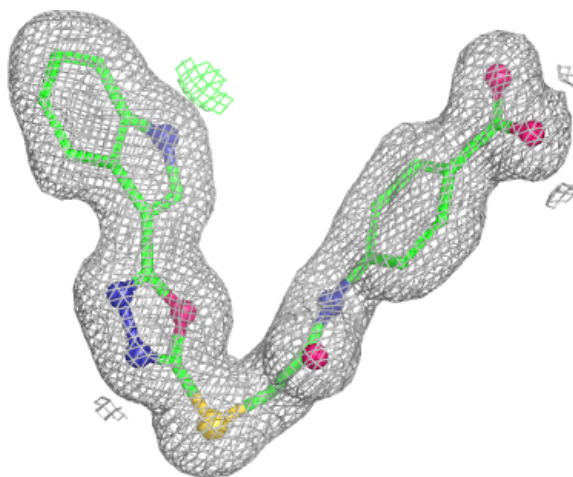
Electron density around A1ITR B 204:

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



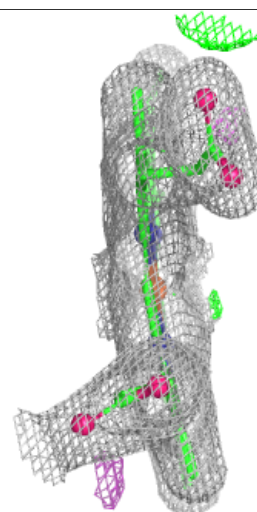
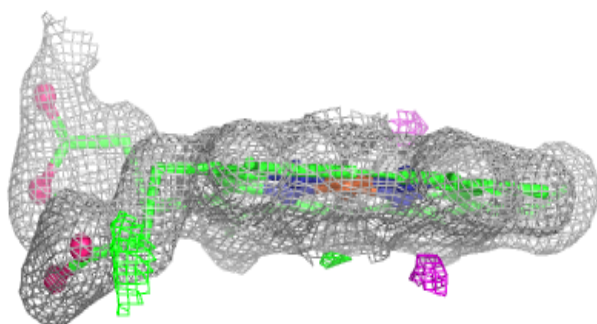
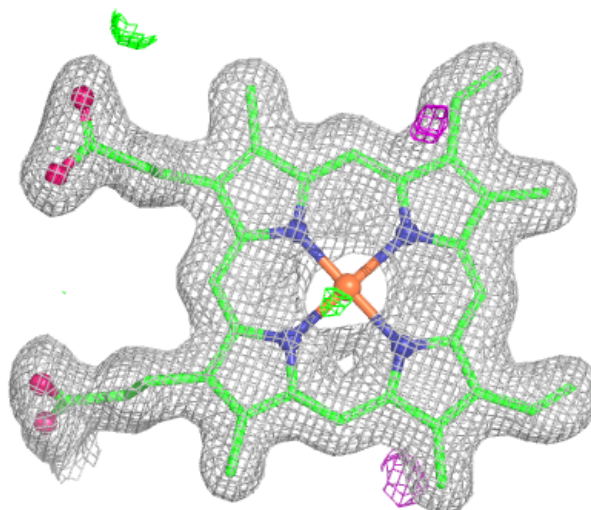
Electron density around A1ITR A 203:

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



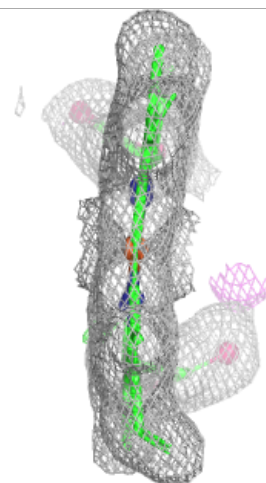
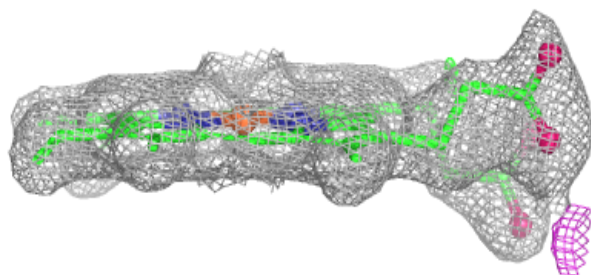
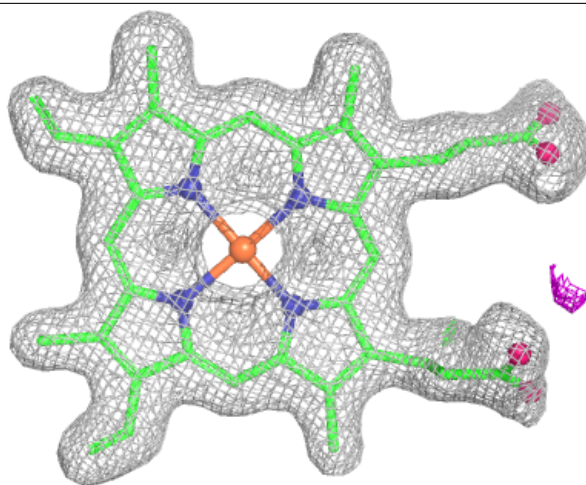
Electron density around HEM B 202:

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



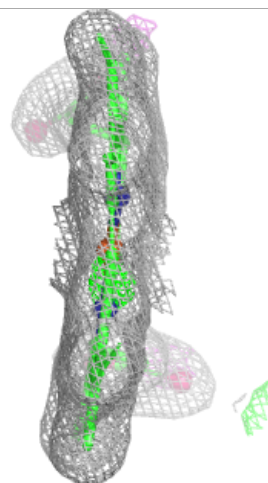
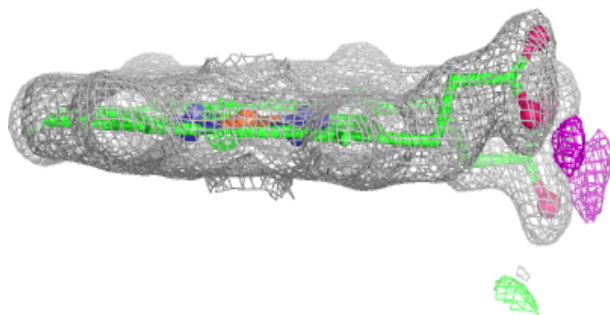
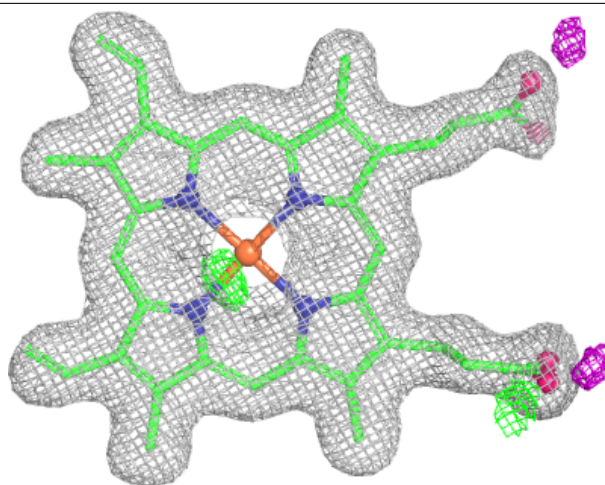
Electron density around HEM C 203:

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



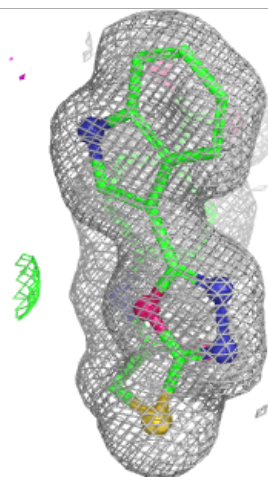
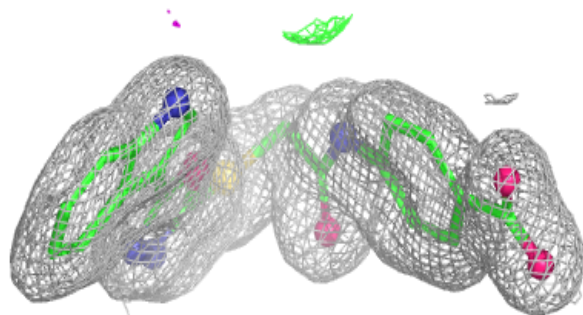
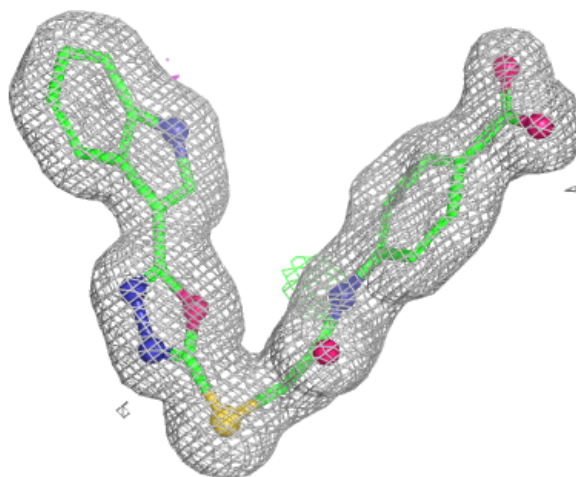
Electron density around HEM D 201:

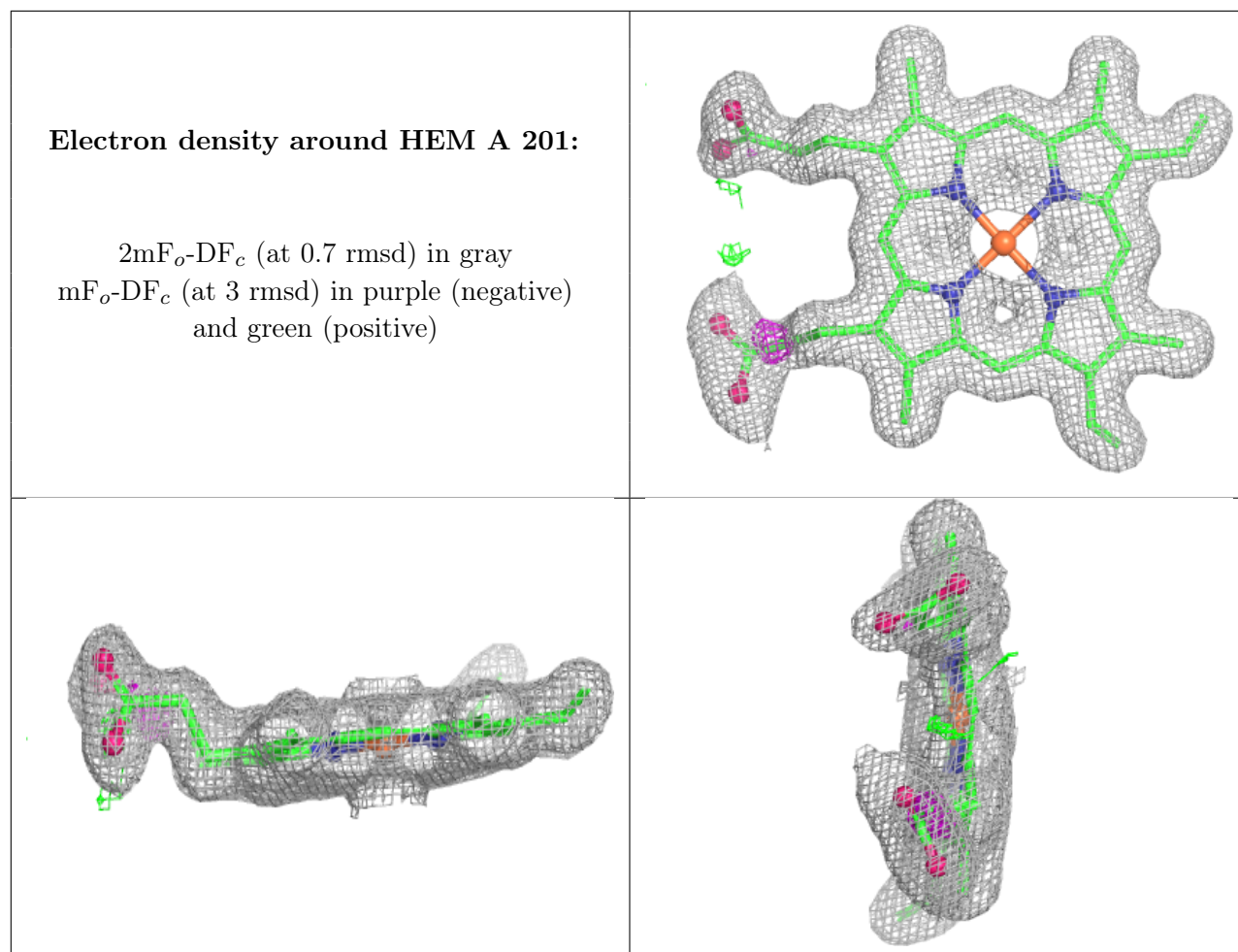
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around A1ITR 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](#)

There are no such residues in this entry.