



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 26, 2023 – 04:36 pm BST

PDB ID : 8OUP
Title : Structural characterization of the hexa-coordinated globin from *Spisula solidissima*
Authors : Nardini, M.; Pesce, A.
Deposited on : 2023-04-24
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.33
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) : 2.33

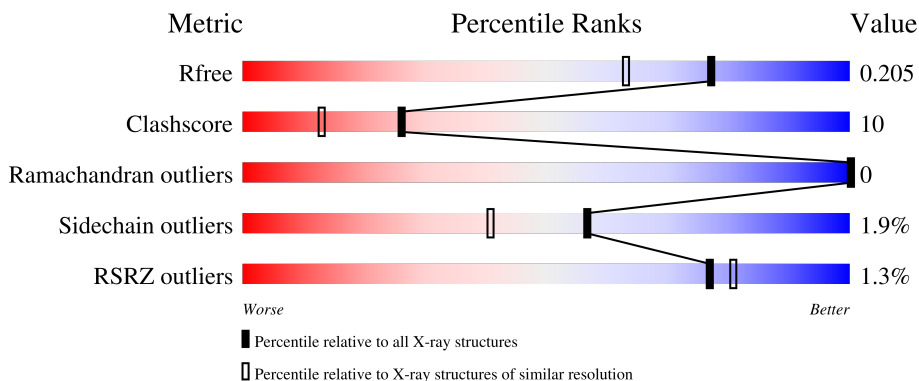
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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

Mol	Chain	Length	Quality of chain
1	A	162	 75% 15% 7%
1	B	162	 80% 11% 7%
1	C	162	 84% 7% 7%
1	D	162	 81% 12% 7%

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
3	GOL	B	204	-	-	X	-

2 Entry composition [i](#)

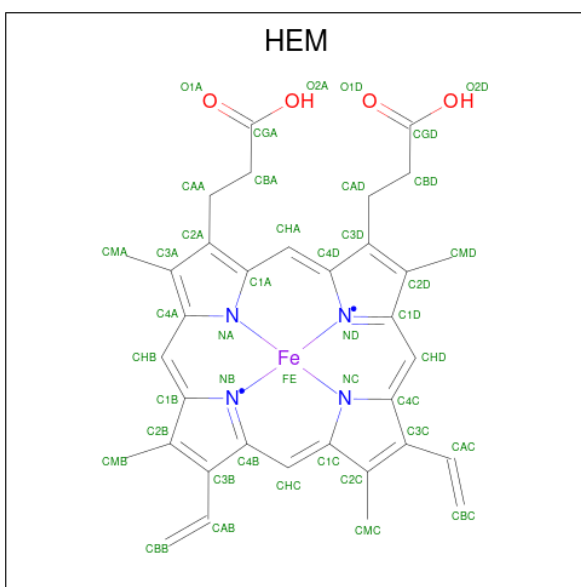
There are 4 unique types of molecules in this entry. The entry contains 6204 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Nerve hemoglobin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	150	Total 1260	C 821	N 212	O 222	S 5	0	8	0
1	B	151	Total 1288	C 838	N 216	O 229	S 5	0	12	0
1	C	151	Total 1250	C 812	N 208	O 226	S 4	0	6	0
1	D	151	Total 1259	C 819	N 211	O 224	S 5	0	8	0

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



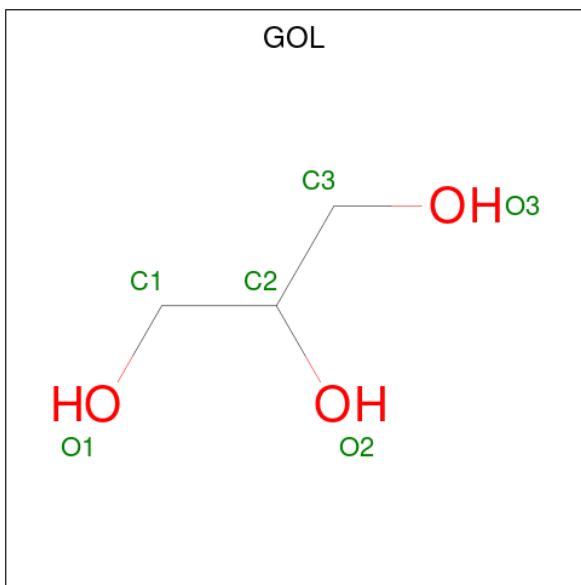
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	Fe	N			O
2	A	1	Total 53	C 40	Fe 1	N 4	O 8	0	1
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	C	1	Total	C	Fe	N	O	0	1
			48	37	1	4	6		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	213	Total	O	0	8
			221	221		
4	B	241	Total	O	0	6
			247	247		
4	C	238	Total	O	0	5
			243	243		

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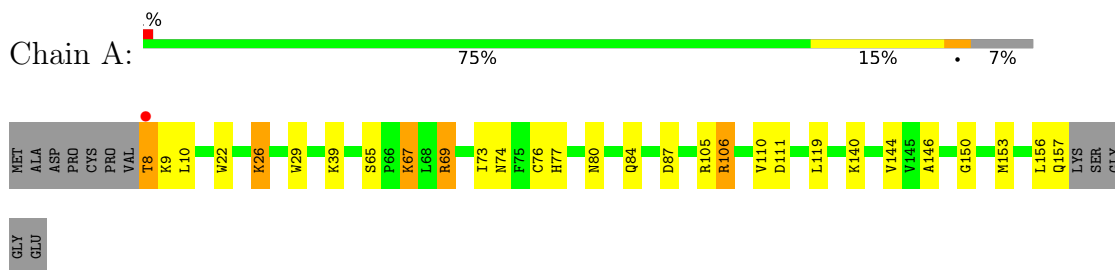
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	216	Total 225	O 225	0	9

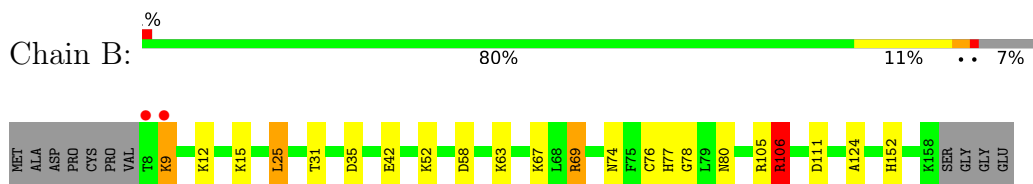
3 Residue-property plots [i](#)

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.

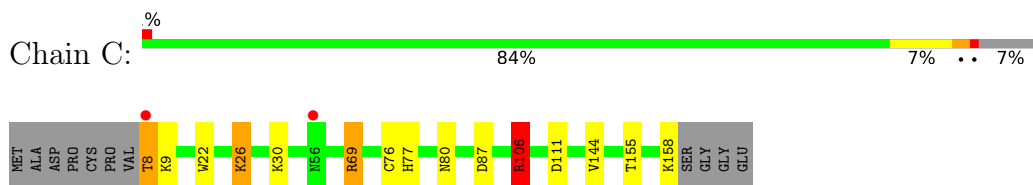
- Molecule 1: Nerve hemoglobin



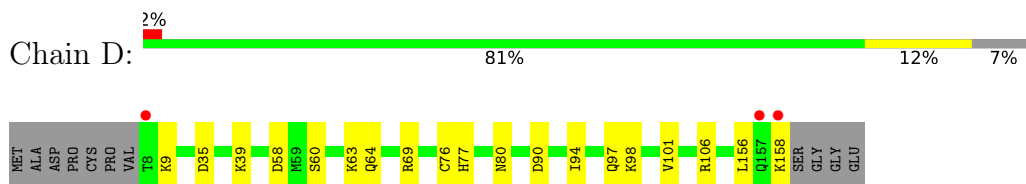
- Molecule 1: Nerve hemoglobin



- Molecule 1: Nerve hemoglobin



- Molecule 1: Nerve hemoglobin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	48.22Å 50.68Å 74.17Å 75.65° 88.09° 85.30°	Depositor
Resolution (Å)	49.01 – 1.70 48.96 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (49.01-1.70) 95.0 (48.96-1.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.44 (at 1.70Å)	Xtrriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.150 , 0.197 0.164 , 0.205	Depositor DCC
R_{free} test set	3579 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtrriage
Anisotropy	0.046	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 56.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6204	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.67% 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 i

5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.48	0/1310	0.83	1/1768 (0.1%)
1	B	0.59	2/1350 (0.1%)	0.91	2/1819 (0.1%)
1	C	0.51	0/1296	0.81	2/1747 (0.1%)
1	D	0.51	0/1312	0.79	0/1769
All	All	0.52	2/5268 (0.0%)	0.84	5/7103 (0.1%)

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
1	A	0	5
1	B	0	5
1	C	0	2
1	D	0	2
All	All	0	14

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	9[A]	LYS	N-CA	5.01	1.56	1.46
1	B	9[B]	LYS	N-CA	5.01	1.56	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	LYS	CB-CA-C	-7.00	96.41	110.40
1	C	26	LYS	CB-CA-C	-6.86	96.67	110.40
1	B	106[A]	ARG	NE-CZ-NH2	-5.49	117.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106[B]	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	C	106	ARG	NE-CZ-NH2	-5.41	117.60	120.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ARG	Sidechain
1	A	106[A]	ARG	Sidechain
1	A	106[B]	ARG	Sidechain
1	A	69[A]	ARG	Sidechain
1	A	69[B]	ARG	Sidechain
1	B	105	ARG	Sidechain
1	B	106[A]	ARG	Sidechain
1	B	106[B]	ARG	Sidechain
1	B	69[A]	ARG	Sidechain
1	B	69[B]	ARG	Sidechain
1	C	106	ARG	Sidechain
1	C	69	ARG	Sidechain
1	D	69[A]	ARG	Sidechain
1	D	69[B]	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	1260	0	1285	40	0
1	B	1288	0	1322	32	0
1	C	1250	0	1264	13	0
1	D	1259	0	1285	18	0
2	A	53	0	16	1	0
2	B	43	0	30	6	0
2	C	48	0	8	1	0
2	D	43	0	30	4	0
3	A	6	0	8	2	0
3	B	18	0	24	8	0
4	A	221	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	247	0	0	14	0
4	C	243	0	0	2	0
4	D	225	0	0	5	0
All	All	6204	0	5272	103	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 10.

All (103) 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:69[A]:ARG:NH1	1:A:73[A]:ILE:HD11	1.31	1.45
1:A:69[A]:ARG:CZ	1:A:73[A]:ILE:HD11	1.58	1.33
1:A:69[A]:ARG:NH1	1:A:73[A]:ILE:CD1	2.10	1.13
1:A:110[A]:VAL:HG21	1:A:150:GLY:HA2	1.33	1.09
1:D:98[B]:LYS:NZ	4:D:301:HOH:O	1.61	1.05
1:B:58[B]:ASP:OD1	4:B:301:HOH:O	1.86	0.91
1:B:35[A]:ASP:OD1	1:B:63:LYS:NZ	2.05	0.90
1:D:158:LYS:C	4:D:376:HOH:O	2.12	0.87
1:A:77:HIS:HE1	1:B:80:ASN:HD22	1.25	0.82
3:B:204:GOL:H11	4:B:391:HOH:O	1.80	0.82
1:A:77:HIS:CE1	1:B:80:ASN:HD22	2.03	0.75
1:A:74:ASN:ND2	4:A:301:HOH:O	2.05	0.73
1:C:77:HIS:HE1	1:D:80:ASN:HD22	1.35	0.73
2:B:201:HEM:HMB2	2:B:201:HEM:HBB2	1.71	0.72
1:A:69[A]:ARG:CZ	1:A:73[A]:ILE:CD1	2.54	0.72
1:B:42:GLU:OE1	4:B:302:HOH:O	2.08	0.71
1:C:77:HIS:CE1	1:D:80:ASN:HD22	2.08	0.71
1:C:80:ASN:HD22	1:D:77:HIS:CE1	2.08	0.71
4:A:301:HOH:O	3:B:204:GOL:H32	1.91	0.70
1:C:80:ASN:HD22	1:D:77:HIS:HE1	1.39	0.69
1:A:110[A]:VAL:HG23	4:A:402:HOH:O	1.94	0.68
1:A:80:ASN:HD22	1:B:77:HIS:HE1	1.42	0.68
2:B:201:HEM:HBB2	2:B:201:HEM:CMB	2.23	0.67
2:D:200:HEM:HBB2	2:D:200:HEM:HMB2	1.76	0.67
1:D:64:GLN:HG2	4:D:472:HOH:O	1.95	0.67
1:A:69[A]:ARG:HD2	1:A:73[A]:ILE:HD13	1.76	0.67
1:B:152:HIS:HD2	4:B:366:HOH:O	1.78	0.66
1:A:84:GLN:HE21	1:B:69[B]:ARG:HH22	1.40	0.65
1:D:76[B]:CYS:SG	4:D:448[B]:HOH:O	2.54	0.65
1:A:80:ASN:HD22	1:B:77:HIS:CE1	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:LEU:HD21	1:B:124:ALA:HB1	1.79	0.64
1:A:39[A]:LYS:HE2	1:A:119:LEU:HD11	1.81	0.63
1:D:35:ASP:OD1	1:D:63[B]:LYS:NZ	2.30	0.63
1:B:67:LYS:HG3	4:B:304:HOH:O	1.98	0.62
1:A:67:LYS:H	1:A:67:LYS:HE3	1.63	0.62
1:B:9[A]:LYS:HA	4:B:303:HOH:O	2.03	0.59
1:A:8:THR:HB	1:A:10:LEU:H	1.67	0.58
1:B:9[B]:LYS:HA	4:B:303:HOH:O	2.04	0.57
1:A:69[A]:ARG:HD2	1:A:73[A]:ILE:CD1	2.34	0.57
3:B:204:GOL:H12	4:B:385:HOH:O	2.04	0.57
2:B:201:HEM:CMC	2:B:201:HEM:HBC2	2.35	0.56
2:D:200:HEM:HBB2	2:D:200:HEM:CMB	2.35	0.55
1:A:106[B]:ARG:CZ	2:A:201[B]:HEM:HAD2	2.36	0.55
1:C:76:CYS:SG	1:C:77:HIS:HD2	2.30	0.55
1:B:31:THR:HG23	4:B:388:HOH:O	2.05	0.55
1:C:22:TRP:O	1:C:26:LYS:HG3	2.07	0.55
1:B:12:LYS:HA	1:B:15[A]:LYS:HZ2	1.71	0.54
1:A:69[A]:ARG:HH11	1:A:73[A]:ILE:CD1	2.11	0.54
1:D:106:ARG:NH2	2:D:200:HEM:O1A	2.32	0.53
1:C:30:LYS:HD3	1:C:69:ARG:CZ	2.39	0.53
1:B:12:LYS:HA	1:B:15[A]:LYS:NZ	2.24	0.53
1:B:67:LYS:HE3	4:B:499:HOH:O	2.08	0.52
1:A:146:ALA:C	3:A:202:GOL:H31	2.30	0.52
1:D:35:ASP:OD1	1:D:63[B]:LYS:HE3	2.09	0.52
1:B:15[A]:LYS:NZ	1:B:15[A]:LYS:HB2	2.25	0.52
1:A:8:THR:HG21	1:A:10:LEU:HD12	1.92	0.51
1:A:8:THR:HG23	4:A:320:HOH:O	2.11	0.50
1:C:155:THR:O	1:C:158[A]:LYS:HG2	2.12	0.50
1:D:35:ASP:OD1	1:D:63[B]:LYS:CE	2.59	0.50
2:B:201:HEM:HBC2	2:B:201:HEM:HMC2	1.94	0.50
1:A:9:LYS:HE2	1:A:140:LYS:NZ	2.27	0.49
1:A:8:THR:C	1:A:10:LEU:H	2.15	0.49
1:A:110[A]:VAL:CG2	1:A:150:GLY:HA2	2.24	0.49
1:A:110[A]:VAL:HG21	1:A:150:GLY:CA	2.24	0.49
1:B:76[A]:CYS:SG	3:B:202:GOL:O3	2.66	0.48
1:D:97:GLN:O	1:D:101[A]:VAL:HG23	2.13	0.48
1:B:78:GLY:HA2	3:B:204:GOL:H2	1.95	0.48
1:D:58[B]:ASP:OD2	1:D:60:SER:OG	2.13	0.47
1:C:106:ARG:NH2	2:C:200[A]:HEM:O1A	2.42	0.47
1:A:84:GLN:HE21	1:B:69[B]:ARG:NH2	2.10	0.47
1:B:78:GLY:N	3:B:204:GOL:H2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:GLY:CA	3:B:204:GOL:H2	2.44	0.47
1:C:158[B]:LYS:NZ	4:C:306:HOH:O	2.47	0.47
1:C:22:TRP:CE2	1:C:26:LYS:HG2	2.50	0.46
1:B:35[A]:ASP:CG	1:B:63:LYS:NZ	2.69	0.46
1:A:8:THR:HG22	1:A:144:VAL:HG21	1.99	0.44
1:A:9:LYS:HE2	1:A:140:LYS:HZ1	1.82	0.44
1:A:110[A]:VAL:HG22	1:A:153:MET:SD	2.58	0.44
1:A:87:ASP:HB2	4:A:333:HOH:O	2.17	0.44
2:D:200:HEM:HBC2	2:D:200:HEM:CMC	2.47	0.44
1:B:80:ASN:CB	3:B:202:GOL:H31	2.48	0.43
1:A:65:SER:HB2	1:A:67:LYS:HE3	2.01	0.43
1:B:106[A]:ARG:NH2	2:B:201:HEM:O1A	2.45	0.43
1:B:9[B]:LYS:CA	4:B:303:HOH:O	2.65	0.43
1:A:76[A]:CYS:SG	1:A:77:HIS:HD2	2.42	0.42
1:A:69[A]:ARG:NH1	1:A:73[A]:ILE:HD12	2.20	0.42
1:B:9[A]:LYS:CA	4:B:303:HOH:O	2.66	0.42
1:A:22:TRP:CE2	1:A:26:LYS:HG3	2.54	0.42
1:D:39:LYS:HD3	4:D:423:HOH:O	2.18	0.42
1:A:156:LEU:O	1:A:157:GLN:HB2	2.19	0.42
1:C:87:ASP:HB2	4:C:354:HOH:O	2.20	0.42
1:D:101[B]:VAL:HG12	1:D:156:LEU:HD11	2.02	0.41
1:A:146:ALA:HB1	3:A:202:GOL:H31	2.03	0.41
1:B:52[B]:LYS:NZ	4:B:318:HOH:O	2.54	0.41
1:C:8:THR:HB	1:C:144:VAL:HG21	2.03	0.41
1:B:152:HIS:HE1	4:B:460:HOH:O	2.03	0.41
1:B:74:ASN:HB3	2:B:201:HEM:CMA	2.52	0.40
1:D:94:ILE:HG22	1:D:98[A]:LYS:HD2	2.01	0.40
1:A:29:TRP:CD1	1:A:76[B]:CYS:HB2	2.56	0.40
1:B:9[A]:LYS:HE2	1:B:9[A]:LYS:HB2	1.93	0.40

There are no symmetry-related clashes.

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	156/162 (96%)	156 (100%)	0	0	100	100
1	B	161/162 (99%)	161 (100%)	0	0	100	100
1	C	154/162 (95%)	154 (100%)	0	0	100	100
1	D	157/162 (97%)	157 (100%)	0	0	100	100
All	All	628/648 (97%)	628 (100%)	0	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	137/138 (99%)	134 (98%)	3 (2%)	52	34
1	B	142/138 (103%)	140 (99%)	2 (1%)	67	53
1	C	136/138 (99%)	133 (98%)	3 (2%)	52	34
1	D	138/138 (100%)	136 (99%)	2 (1%)	67	53
All	All	553/552 (100%)	543 (98%)	10 (2%)	57	43

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

Mol	Chain	Res	Type
1	A	8	THR
1	A	67	LYS
1	A	111	ASP
1	B	25	LEU
1	B	111	ASP
1	C	8	THR
1	C	9	LYS
1	C	111	ASP
1	D	9	LYS
1	D	90	ASP

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

Mol	Chain	Res	Type
1	A	46	ASN
1	A	77	HIS
1	A	84	GLN
1	A	102	ASN
1	A	125	GLN
1	B	77	HIS
1	B	125	GLN
1	B	152	HIS
1	C	77	HIS
1	C	154	GLN
1	C	157	GLN
1	D	77	HIS
1	D	84	GLN
1	D	125	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	GOL	B	204	-	5,5,5	0.42	0	5,5,5	1.00	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	C	200[A]	-	41,50,50	1.52	8 (19%)	45,82,82	2.07	18 (40%)
2	HEM	B	201	1	41,50,50	1.48	6 (14%)	45,82,82	2.34	13 (28%)
2	HEM	D	200	1	41,50,50	1.22	4 (9%)	45,82,82	1.72	9 (20%)
3	GOL	B	202	-	5,5,5	0.16	0	5,5,5	0.45	0
3	GOL	B	203	-	5,5,5	0.12	0	5,5,5	0.27	0
2	HEM	A	201[B]	-	41,50,50	1.43	8 (19%)	45,82,82	1.94	13 (28%)
3	GOL	A	202	-	5,5,5	0.14	0	5,5,5	0.58	0
2	HEM	A	201[A]	-	41,50,50	1.45	8 (19%)	45,82,82	2.05	13 (28%)
2	HEM	C	200[B]	-	41,50,50	1.53	8 (19%)	45,82,82	2.11	17 (37%)

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	GOL	B	204	-	-	2/4/4/4	-
2	HEM	C	200[A]	-	-	4/12/54/54	-
2	HEM	B	201	1	-	4/12/54/54	-
2	HEM	D	200	1	-	4/12/54/54	-
3	GOL	B	202	-	-	4/4/4/4	-
3	GOL	B	203	-	-	2/4/4/4	-
2	HEM	A	201[B]	-	-	4/12/54/54	-
3	GOL	A	202	-	-	3/4/4/4	-
2	HEM	A	201[A]	-	-	4/12/54/54	-
2	HEM	C	200[B]	-	-	4/12/54/54	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201[A]	HEM	C1B-NB	-4.85	1.32	1.40
2	A	201[B]	HEM	C1B-NB	-4.85	1.32	1.40
2	C	200[A]	HEM	CHB-C1B	3.58	1.44	1.35
2	C	200[B]	HEM	CHB-C1B	3.58	1.44	1.35
2	C	200[A]	HEM	C1B-NB	-3.49	1.34	1.40
2	C	200[B]	HEM	C1B-NB	-3.49	1.34	1.40
2	B	201	HEM	C4D-ND	-3.39	1.34	1.40
2	B	201	HEM	C1B-NB	-3.38	1.34	1.40
2	B	201	HEM	C3C-C2C	-3.17	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	200[A]	HEM	C4D-ND	-2.81	1.35	1.40
2	C	200[B]	HEM	C4D-ND	-2.81	1.35	1.40
2	D	200	HEM	C1B-NB	-2.63	1.35	1.40
2	A	201[A]	HEM	C3B-C4B	2.60	1.50	1.44
2	A	201[B]	HEM	C3B-C4B	2.60	1.50	1.44
2	D	200	HEM	C4B-NB	-2.49	1.33	1.38
2	C	200[A]	HEM	C1B-C2B	-2.33	1.40	1.44
2	C	200[B]	HEM	C1B-C2B	-2.33	1.40	1.44
2	A	201[A]	HEM	C4A-NA	2.31	1.40	1.36
2	A	201[B]	HEM	C4A-NA	2.31	1.40	1.36
2	C	200[A]	HEM	C1A-CHA	-2.25	1.34	1.41
2	C	200[B]	HEM	C1A-CHA	-2.25	1.34	1.41
2	C	200[A]	HEM	C2C-C1C	2.20	1.47	1.42
2	C	200[B]	HEM	C2C-C1C	2.20	1.47	1.42
2	A	201[A]	HEM	C3C-C2C	-2.20	1.37	1.40
2	A	201[B]	HEM	C3C-C2C	-2.20	1.37	1.40
2	B	201	HEM	CBD-CGD	2.19	1.55	1.50
2	A	201[A]	HEM	C1A-CHA	-2.19	1.34	1.41
2	A	201[B]	HEM	C1A-CHA	-2.19	1.34	1.41
2	D	200	HEM	C4D-C3D	2.19	1.48	1.45
2	A	201[A]	HEM	FE-NB	2.17	2.07	1.96
2	A	201[B]	HEM	FE-NB	2.17	2.07	1.96
2	B	201	HEM	CBD-CAD	2.16	1.58	1.52
2	B	201	HEM	CMD-C2D	2.12	1.55	1.50
2	D	200	HEM	CBA-CGA	-2.10	1.45	1.50
2	C	200[A]	HEM	C3C-C2C	-2.09	1.37	1.40
2	C	200[B]	HEM	C3C-C2C	-2.09	1.37	1.40
2	A	201[A]	HEM	C3D-C2D	-2.08	1.32	1.36
2	A	201[B]	HEM	C3D-C2D	-2.08	1.32	1.36
2	C	200[A]	HEM	C1A-NA	2.07	1.40	1.36
2	C	200[B]	HEM	C1A-NA	2.07	1.40	1.36
2	A	201[A]	HEM	C4D-ND	-2.02	1.36	1.40
2	A	201[B]	HEM	C4D-ND	-2.02	1.36	1.40

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	HEM	CHC-C4B-NB	6.63	131.63	124.43
2	B	201	HEM	C1B-NB-C4B	6.39	111.67	105.07
2	B	201	HEM	C2C-C3C-C4C	5.75	110.91	106.90
2	A	201[A]	HEM	CBA-CAA-C2A	-5.42	103.37	112.62
2	A	201[A]	HEM	C1B-NB-C4B	5.30	110.55	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201[B]	HEM	C1B-NB-C4B	5.30	110.55	105.07
2	A	201[A]	HEM	C4B-CHC-C1C	5.01	129.17	122.56
2	A	201[B]	HEM	C4B-CHC-C1C	5.01	129.17	122.56
2	C	200[B]	HEM	CBA-CAA-C2A	-4.44	105.04	112.62
2	C	200[A]	HEM	CMA-C3A-C4A	-3.97	122.37	128.46
2	C	200[B]	HEM	CMA-C3A-C4A	-3.97	122.37	128.46
2	C	200[A]	HEM	CMD-C2D-C1D	3.84	130.89	125.04
2	C	200[B]	HEM	CMD-C2D-C1D	3.84	130.89	125.04
2	D	200	HEM	CHB-C1B-NB	3.78	129.05	124.38
2	B	201	HEM	CHB-C1B-NB	3.72	128.98	124.38
2	D	200	HEM	CAA-CBA-CGA	-3.68	103.44	113.76
2	D	200	HEM	CMC-C2C-C3C	3.63	131.48	124.68
2	D	200	HEM	C1B-NB-C4B	3.51	108.69	105.07
2	B	201	HEM	CHA-C4D-ND	3.47	128.67	124.38
2	C	200[A]	HEM	C4A-C3A-C2A	3.35	109.33	107.00
2	C	200[B]	HEM	C4A-C3A-C2A	3.35	109.33	107.00
2	A	201[A]	HEM	CBD-CAD-C3D	-3.33	103.38	112.63
2	A	201[A]	HEM	CHC-C4B-NB	3.31	128.03	124.43
2	A	201[B]	HEM	CHC-C4B-NB	3.31	128.03	124.43
2	B	201	HEM	CMC-C2C-C3C	3.30	130.84	124.68
2	C	200[A]	HEM	CMB-C2B-C1B	-3.25	120.10	125.04
2	C	200[B]	HEM	CMB-C2B-C1B	-3.25	120.10	125.04
2	C	200[A]	HEM	C2D-C1D-ND	3.23	113.75	109.88
2	C	200[B]	HEM	C2D-C1D-ND	3.23	113.75	109.88
2	C	200[A]	HEM	C4B-CHC-C1C	3.08	126.62	122.56
2	C	200[B]	HEM	C4B-CHC-C1C	3.08	126.62	122.56
2	C	200[A]	HEM	C1D-C2D-C3D	-3.05	103.75	106.96
2	C	200[B]	HEM	C1D-C2D-C3D	-3.05	103.75	106.96
2	A	201[A]	HEM	CMC-C2C-C3C	3.05	130.38	124.68
2	A	201[B]	HEM	CMC-C2C-C3C	3.05	130.38	124.68
2	B	201	HEM	CMD-C2D-C1D	-3.02	120.43	125.04
2	A	201[B]	HEM	CAD-C3D-C4D	3.01	129.92	124.66
2	D	200	HEM	CHD-C1D-ND	2.99	127.68	124.43
2	C	200[A]	HEM	C2C-C3C-C4C	2.95	108.96	106.90
2	C	200[B]	HEM	C2C-C3C-C4C	2.95	108.96	106.90
2	C	200[A]	HEM	CHD-C1D-C2D	-2.94	120.39	124.98
2	C	200[B]	HEM	CHD-C1D-C2D	-2.94	120.39	124.98
2	B	201	HEM	CMA-C3A-C4A	-2.93	123.97	128.46
2	C	200[A]	HEM	CAA-CBA-CGA	-2.84	105.80	113.76
2	A	201[B]	HEM	CBD-CAD-C3D	-2.82	104.78	112.63
2	B	201	HEM	C4D-ND-C1D	2.73	107.89	105.07
2	A	201[B]	HEM	CAA-CBA-CGA	-2.71	106.16	113.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	200	HEM	CHD-C1D-C2D	-2.67	120.80	124.98
2	B	201	HEM	CBD-CAD-C3D	-2.66	105.24	112.63
2	C	200[A]	HEM	C4C-CHD-C1D	2.61	126.00	122.56
2	C	200[B]	HEM	C4C-CHD-C1D	2.61	126.00	122.56
2	D	200	HEM	C4B-CHC-C1C	2.55	125.93	122.56
2	C	200[A]	HEM	CBB-CAB-C3B	-2.55	114.95	127.62
2	C	200[B]	HEM	CBB-CAB-C3B	-2.55	114.95	127.62
2	C	200[A]	HEM	O2A-CGA-CBA	2.54	122.19	114.03
2	A	201[A]	HEM	O2D-CGD-CBD	2.48	122.01	114.03
2	B	201	HEM	CHA-C4D-C3D	-2.47	120.69	125.33
2	C	200[A]	HEM	CAD-C3D-C4D	2.47	128.97	124.66
2	C	200[B]	HEM	CAD-C3D-C4D	2.47	128.97	124.66
2	A	201[A]	HEM	C2D-C1D-ND	2.43	112.79	109.88
2	A	201[B]	HEM	C2D-C1D-ND	2.43	112.79	109.88
2	C	200[A]	HEM	CAD-C3D-C2D	-2.40	123.42	127.88
2	C	200[B]	HEM	CAD-C3D-C2D	-2.40	123.42	127.88
2	C	200[A]	HEM	O2A-CGA-O1A	-2.39	117.35	123.30
2	D	200	HEM	C2C-C3C-C4C	2.36	108.55	106.90
2	A	201[A]	HEM	CAD-C3D-C4D	2.35	128.76	124.66
2	D	200	HEM	CHC-C4B-NB	2.33	126.96	124.43
2	A	201[A]	HEM	CBB-CAB-C3B	-2.30	116.16	127.62
2	A	201[B]	HEM	CBB-CAB-C3B	-2.30	116.16	127.62
2	C	200[A]	HEM	C4D-ND-C1D	-2.28	102.72	105.07
2	C	200[B]	HEM	C4D-ND-C1D	-2.28	102.72	105.07
2	C	200[A]	HEM	C1B-NB-C4B	2.21	107.36	105.07
2	C	200[B]	HEM	C1B-NB-C4B	2.21	107.36	105.07
2	C	200[B]	HEM	O2A-CGA-O1A	-2.17	117.89	123.30
2	A	201[A]	HEM	O2D-CGD-O1D	-2.16	117.90	123.30
2	B	201	HEM	C3C-C4C-NC	-2.16	106.86	110.94
2	B	201	HEM	CHD-C1D-ND	2.15	126.77	124.43
2	A	201[B]	HEM	CAD-C3D-C2D	-2.12	123.93	127.88
2	A	201[A]	HEM	CHD-C1D-C2D	-2.10	121.70	124.98
2	A	201[B]	HEM	CHD-C1D-C2D	-2.10	121.70	124.98
2	A	201[B]	HEM	CAD-CBD-CGD	-2.09	109.11	113.60
2	A	201[A]	HEM	C4D-ND-C1D	-2.01	103.00	105.07
2	A	201[B]	HEM	C4D-ND-C1D	-2.01	103.00	105.07

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	202	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
3	B	202	GOL	C1-C2-C3-O3
3	B	202	GOL	O2-C2-C3-O3
3	B	203	GOL	O1-C1-C2-C3
3	B	204	GOL	C1-C2-C3-O3
3	A	202	GOL	C1-C2-C3-O3
3	B	202	GOL	O1-C1-C2-O2
3	B	204	GOL	O2-C2-C3-O3
3	B	203	GOL	O1-C1-C2-O2
2	C	200[A]	HEM	CAA-CBA-CGA-O1A
2	A	201[A]	HEM	CAA-CBA-CGA-O1A
2	C	200[B]	HEM	CAA-CBA-CGA-O1A
2	A	201[A]	HEM	CAA-CBA-CGA-O2A
2	A	201[B]	HEM	CAA-CBA-CGA-O1A
2	B	201	HEM	CAD-CBD-CGD-O2D
2	C	200[A]	HEM	CAA-CBA-CGA-O2A
2	C	200[B]	HEM	CAA-CBA-CGA-O2A
2	D	200	HEM	CAA-CBA-CGA-O2A
2	A	201[A]	HEM	CAD-CBD-CGD-O2D
2	A	201[B]	HEM	CAA-CBA-CGA-O2A
2	A	201[A]	HEM	CAD-CBD-CGD-O1D
2	D	200	HEM	CAD-CBD-CGD-O1D
3	A	202	GOL	O2-C2-C3-O3
2	B	201	HEM	CAA-CBA-CGA-O1A
2	D	200	HEM	CAA-CBA-CGA-O1A
2	B	201	HEM	CAA-CBA-CGA-O2A
2	A	201[B]	HEM	CAD-CBD-CGD-O1D
2	C	200[A]	HEM	CAD-CBD-CGD-O1D
2	C	200[B]	HEM	CAD-CBD-CGD-O1D
3	A	202	GOL	O1-C1-C2-C3
2	B	201	HEM	CAD-CBD-CGD-O1D
2	D	200	HEM	CAD-CBD-CGD-O2D
2	C	200[A]	HEM	CAD-CBD-CGD-O2D
2	C	200[B]	HEM	CAD-CBD-CGD-O2D
2	A	201[B]	HEM	CAD-CBD-CGD-O2D

There are no ring outliers.

7 monomers are involved in 22 short contacts:

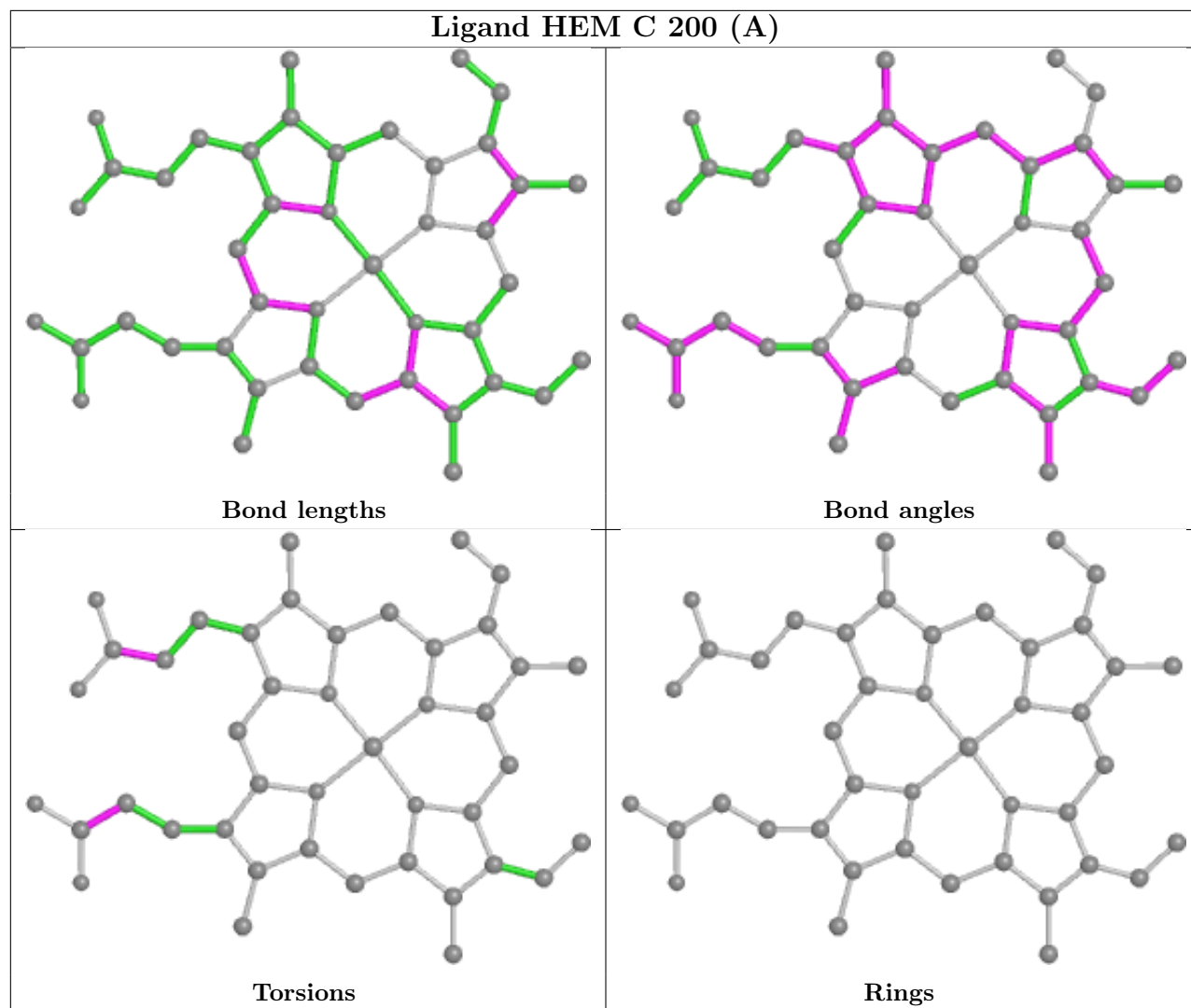
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	204	GOL	6	0
2	C	200[A]	HEM	1	0
2	B	201	HEM	6	0

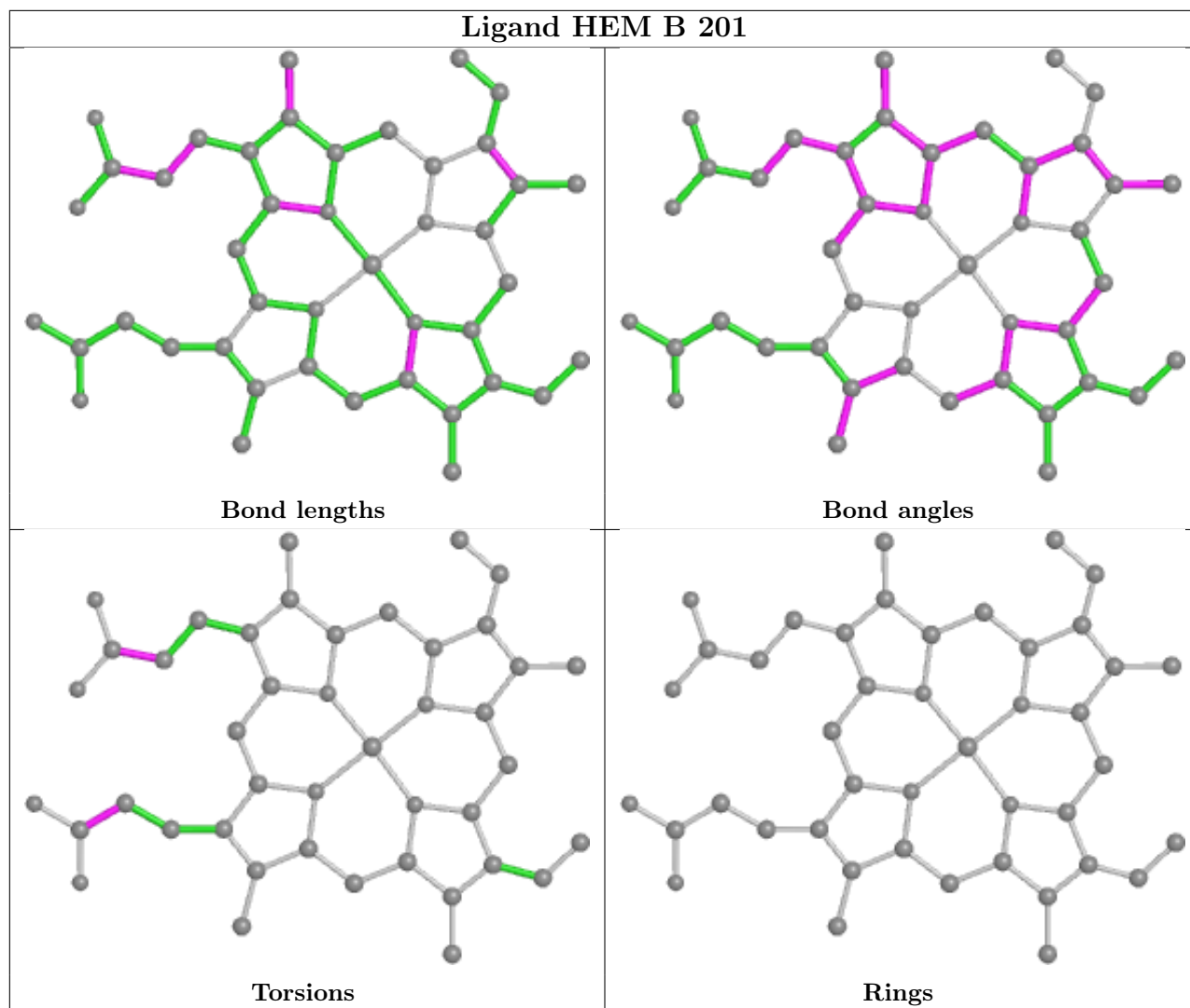
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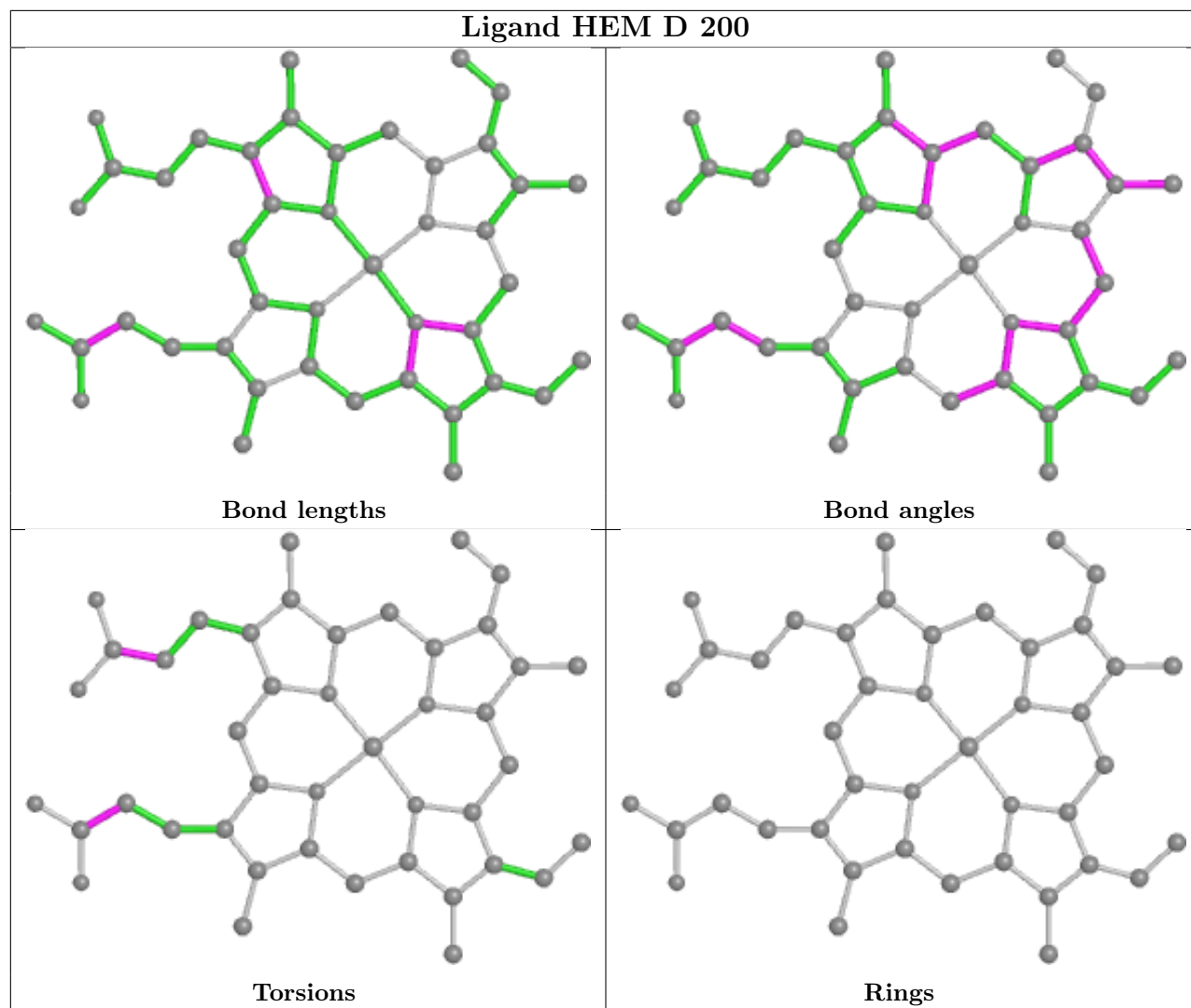
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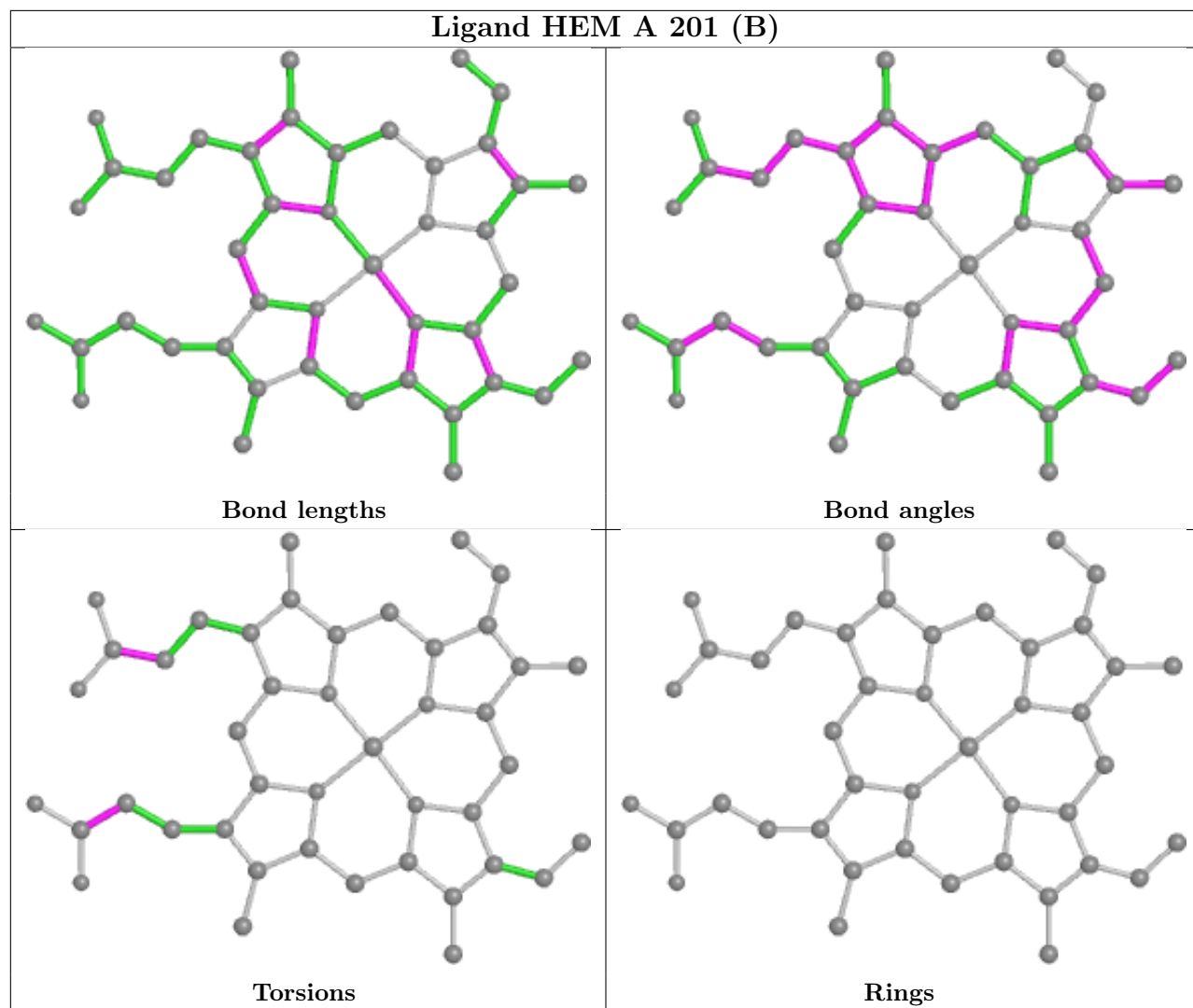
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	200	HEM	4	0
3	B	202	GOL	2	0
2	A	201[B]	HEM	1	0
3	A	202	GOL	2	0

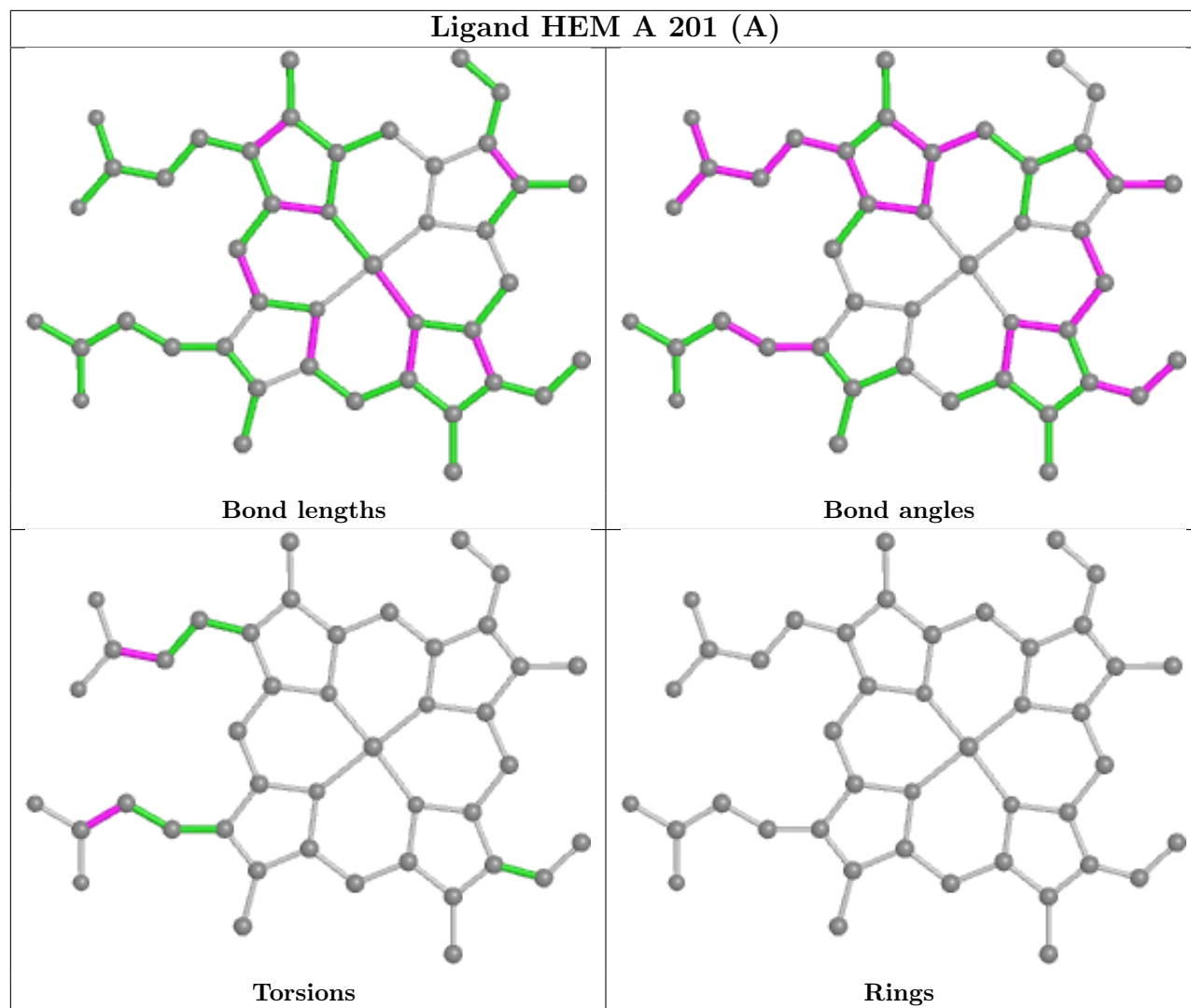
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

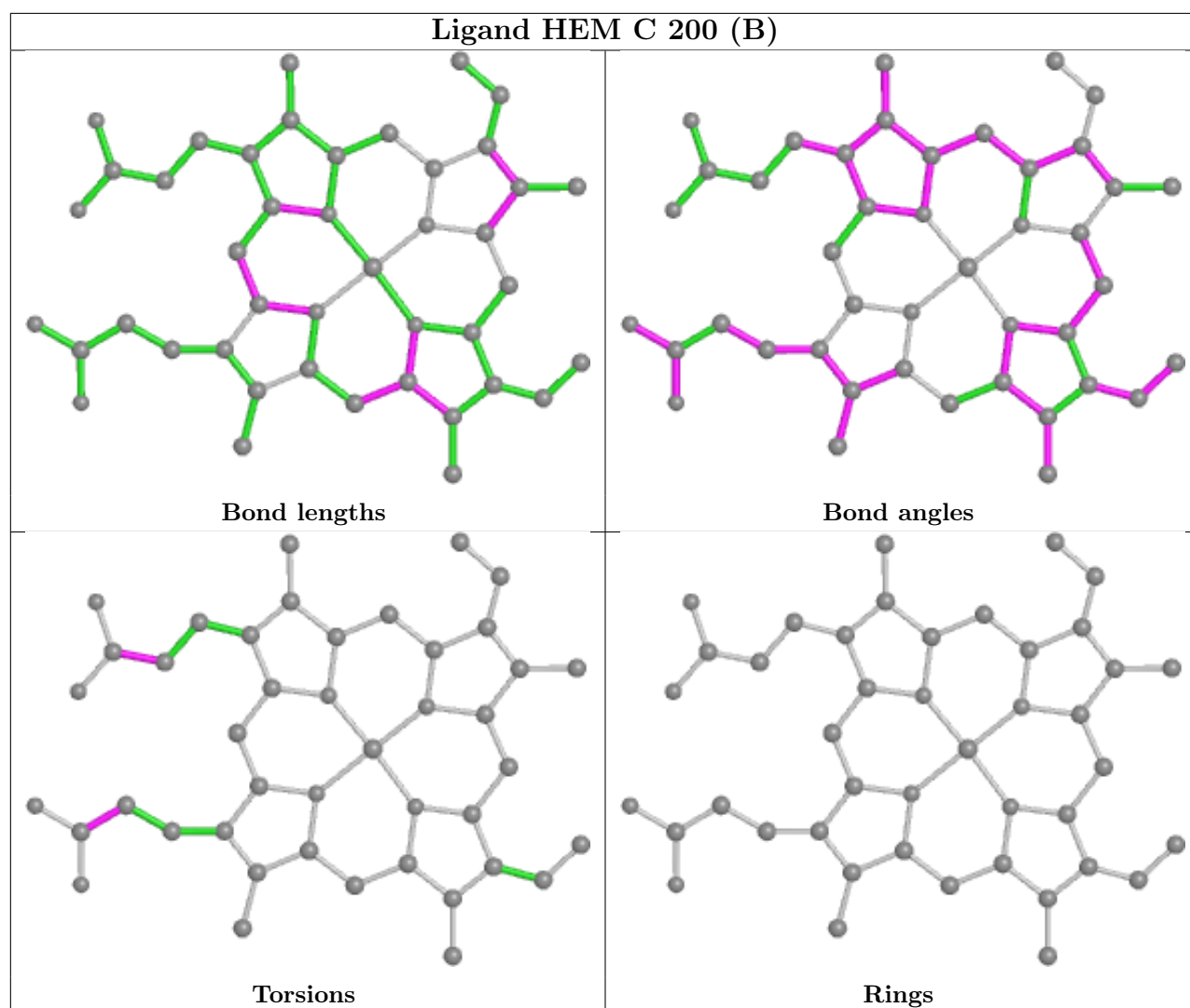












5.7 Other polymers [\(i\)](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	150/162 (92%)	-0.29	1 (0%) 87 90	9, 16, 41, 72	0
1	B	151/162 (93%)	-0.40	2 (1%) 77 81	7, 13, 26, 80	0
1	C	151/162 (93%)	-0.36	2 (1%) 77 81	10, 15, 33, 80	0
1	D	151/162 (93%)	-0.36	3 (1%) 65 69	9, 16, 33, 80	0
All	All	603/648 (93%)	-0.35	8 (1%) 77 81	7, 15, 33, 80	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	8	THR	13.0
1	A	8	THR	10.3
1	C	8	THR	6.9
1	D	8	THR	5.9
1	B	9[A]	LYS	5.3
1	D	158	LYS	2.4
1	C	56	ASN	2.3
1	D	157	GLN	2.3

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 monosaccharides in this entry.

6.4 Ligands

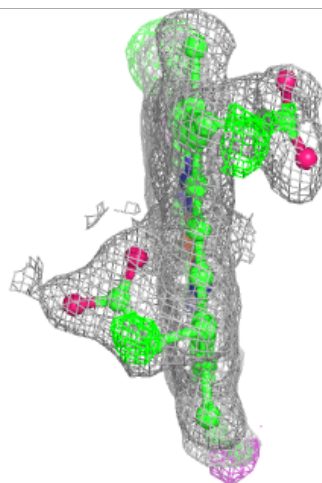
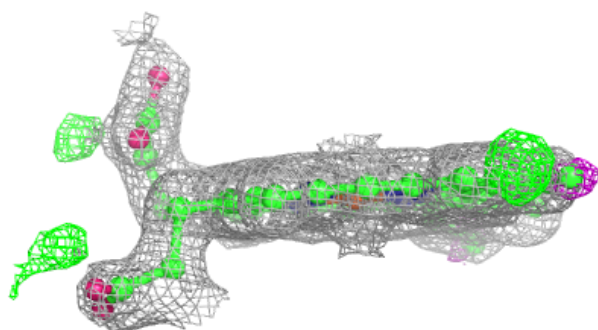
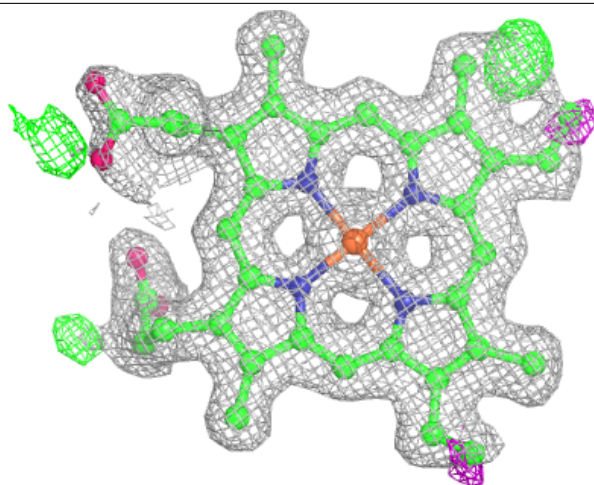
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	B	202	6/6	0.82	0.11	33,40,40,46	0
3	GOL	B	203	6/6	0.87	0.19	25,35,39,40	0
3	GOL	B	204	6/6	0.89	0.17	25,26,32,33	0
3	GOL	A	202	6/6	0.93	0.15	28,34,41,43	0
2	HEM	C	200[B]	43/43	0.98	0.09	11,14,24,29	5
2	HEM	D	200	43/43	0.98	0.07	11,13,22,34	0
2	HEM	A	201[A]	43/43	0.98	0.10	11,15,24,31	10
2	HEM	A	201[B]	43/43	0.98	0.10	11,15,22,24	10
2	HEM	B	201	43/43	0.98	0.09	9,13,25,36	0
2	HEM	C	200[A]	43/43	0.98	0.09	11,14,22,29	5

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.

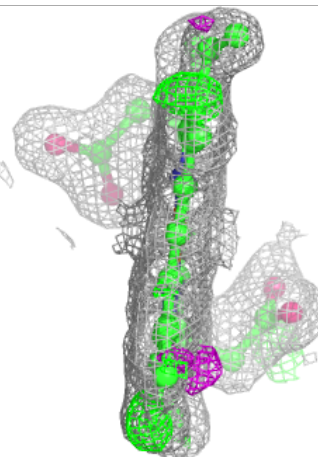
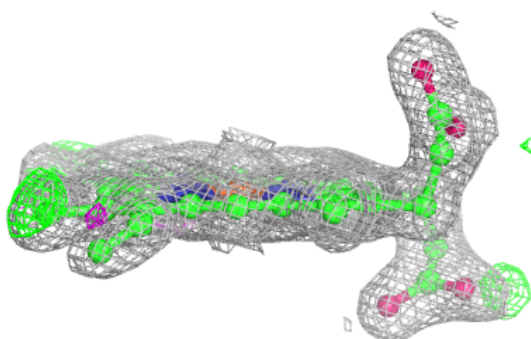
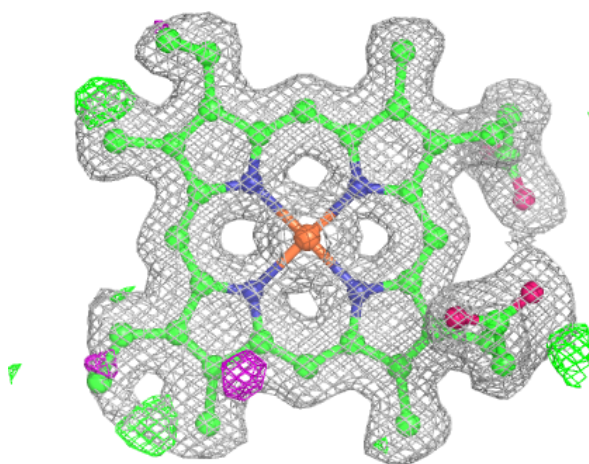
Electron density around HEM C 200 (B):

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



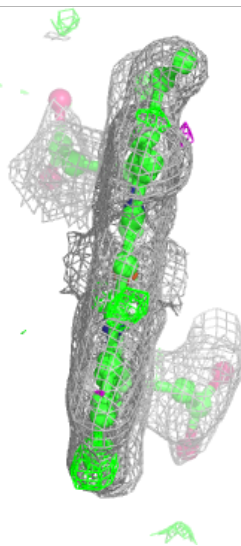
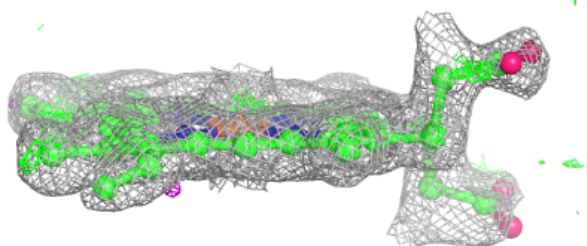
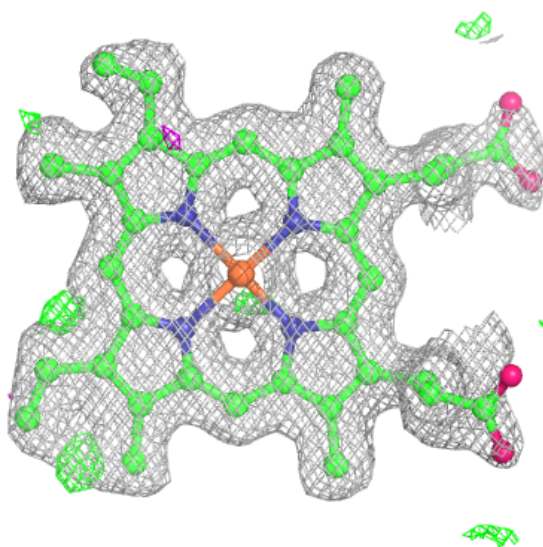
Electron density around HEM D 200:

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



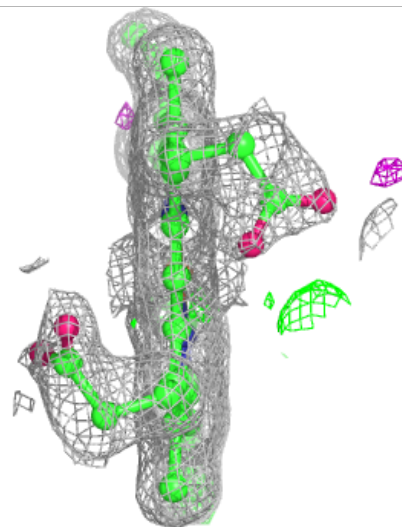
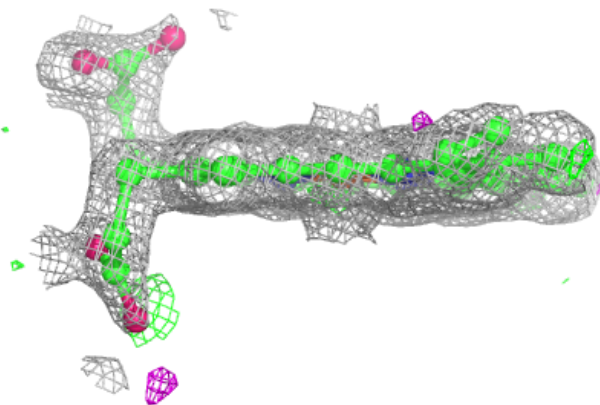
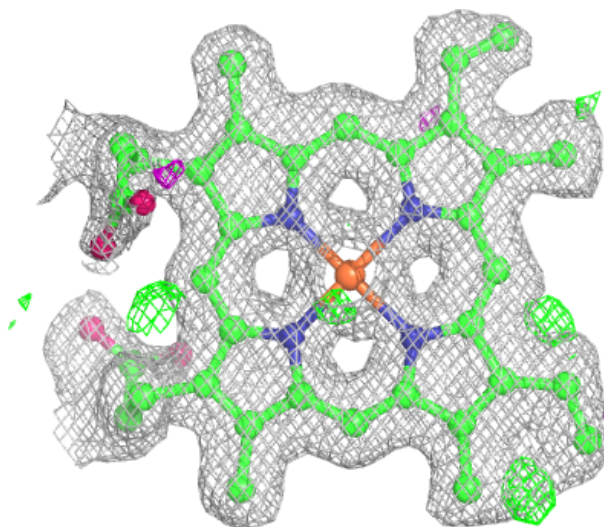
Electron density around HEM A 201 (A):

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



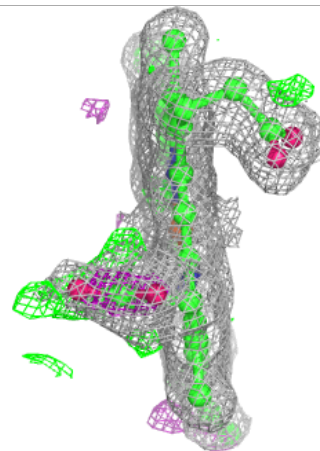
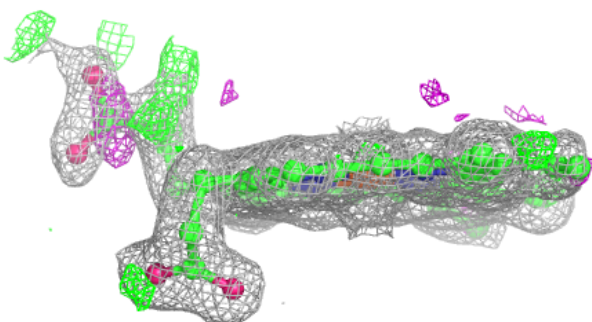
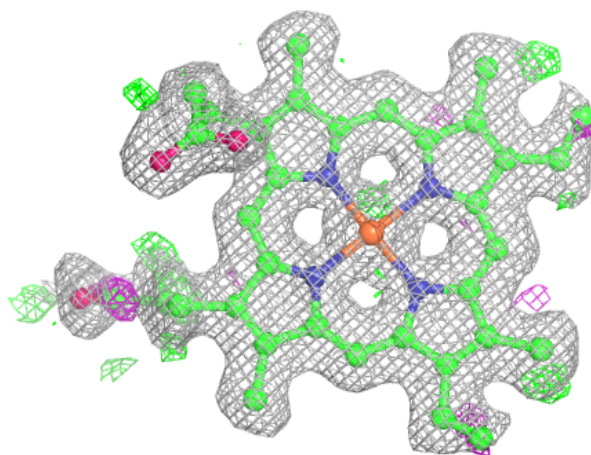
Electron density around HEM A 201 (B):

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



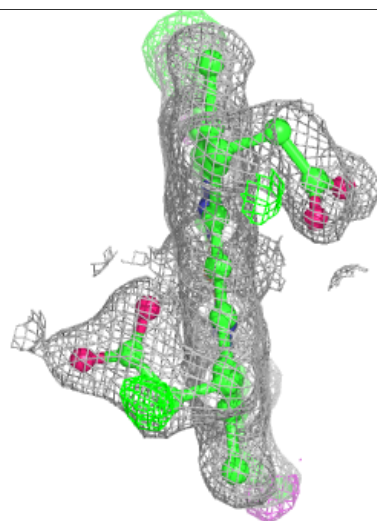
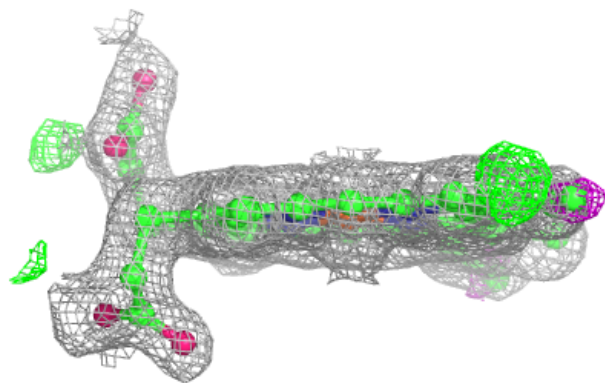
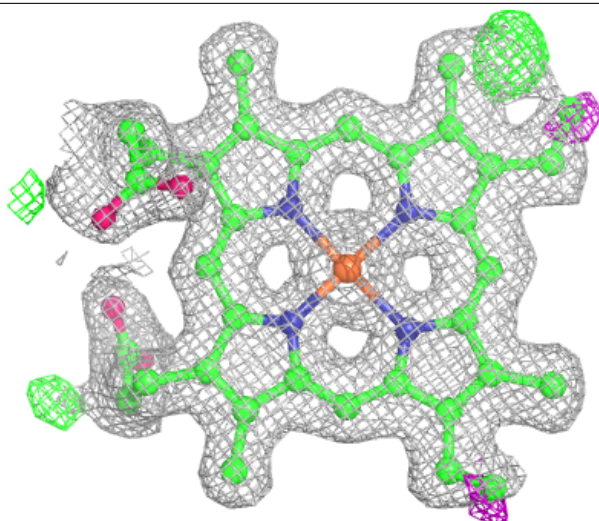
Electron density around HEM B 201:

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



Electron density around HEM C 200 (A):

$2mF_o-DF_c$ (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.