



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:57 AM UTC

PDB ID : 8OUP / pdb_00008oup
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 : 4-5-2 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

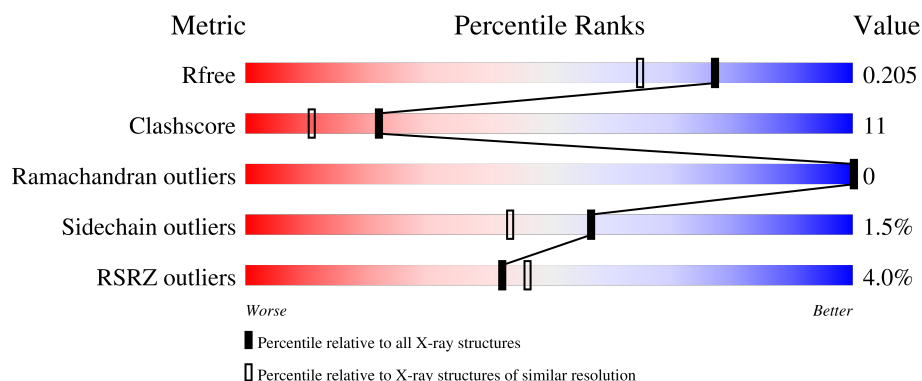
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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	6% 72% 17% • • 7%
1	B	162	2% 80% 10% • 7%
1	C	162	4% 84% 6% • 7%
1	D	162	2% 80% 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:

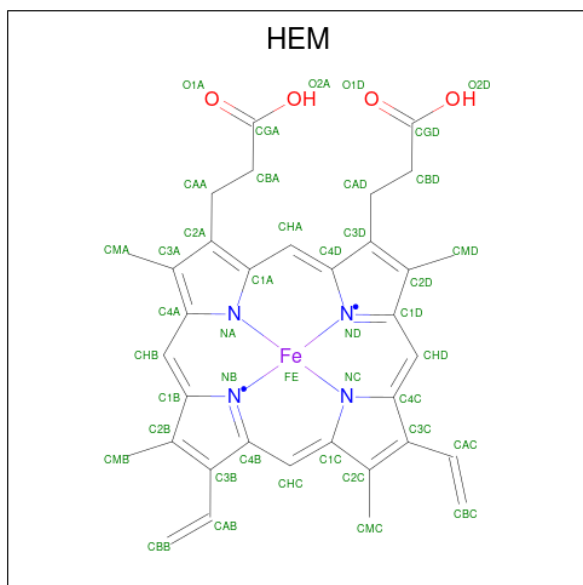
Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	B	204	-	-	X	-

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
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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).



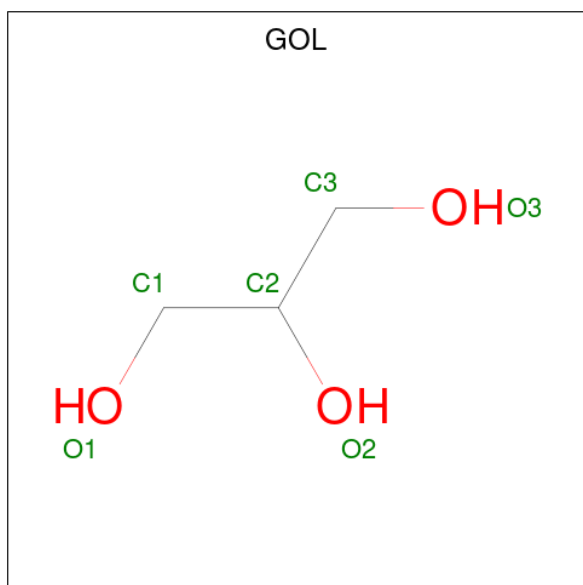
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 40	Fe 1	N 4	O 8	0	1
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

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

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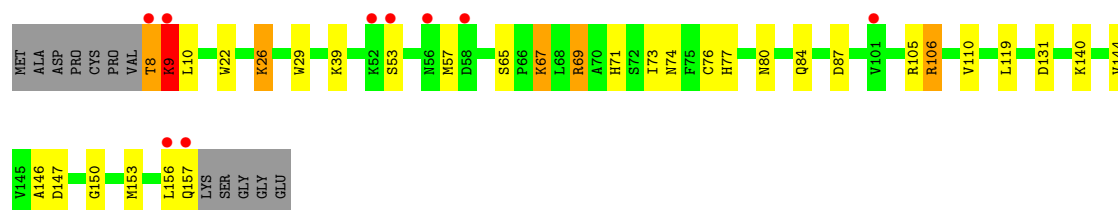
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	216	Total 225	O 225	0	9

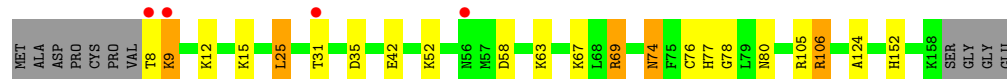
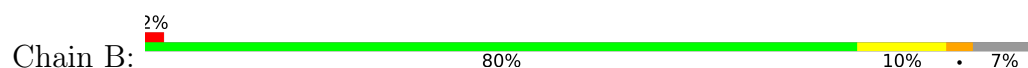
3 Residue-property plots [i](#)

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.

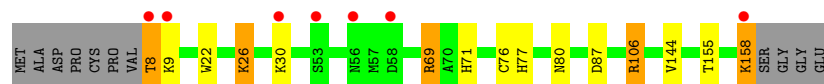
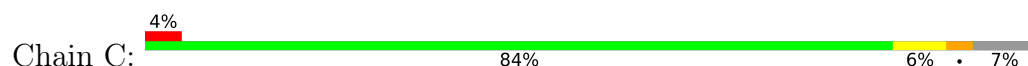
- Molecule 1: Nerve hemoglobin



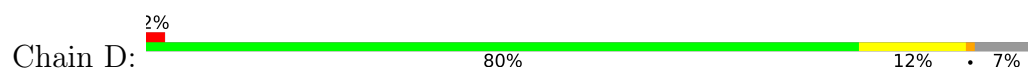
- Molecule 1: Nerve hemoglobin



- 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 49.01 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.0 (49.01-1.70) 95.0 (49.01-1.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.44 (at 1.70Å)	Xtriage
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 (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	14.4	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.66	1/1310 (0.1%)	1.11	4/1768 (0.2%)
1	B	0.73	2/1350 (0.1%)	1.09	3/1819 (0.2%)
1	C	0.71	1/1296 (0.1%)	1.06	2/1747 (0.1%)
1	D	0.69	0/1312	1.03	4/1769 (0.2%)
All	All	0.70	4/5268 (0.1%)	1.07	13/7103 (0.2%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	71	HIS	CE1-NE2	5.68	1.38	1.32
1	A	71	HIS	CE1-NE2	5.27	1.37	1.32
1	B	9[A]	LYS	N-CA	5.11	1.52	1.46
1	B	9[B]	LYS	N-CA	5.11	1.52	1.46

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	LYS	N-CA-C	-9.57	102.22	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	26	LYS	CB-CA-C	-8.51	96.67	110.79
1	A	26	LYS	CB-CA-C	-8.39	96.41	110.68
1	B	74	ASN	CA-CB-CG	5.93	118.53	112.60
1	C	9	LYS	N-CA-C	-5.92	102.69	111.81
1	D	74	ASN	CA-CB-CG	5.65	118.25	112.60
1	D	55	ASP	CA-C-N	-5.49	113.94	122.67
1	D	55	ASP	C-N-CA	-5.49	113.94	122.67
1	B	9[A]	LYS	CA-C-O	5.43	126.25	119.78
1	B	9[B]	LYS	CA-C-O	5.43	126.25	119.78
1	D	90	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	147	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	131	ASP	CA-CB-CG	5.08	117.68	112.60

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	42	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1288	0	1322	33	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
4	B	247	0	0	15	0
4	C	243	0	0	2	0
4	D	225	0	0	5	0
All	All	6204	0	5272	106	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 11.

All (106) 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:D:158:LYS:C	4:D:376:HOH:O	2.12	0.90
1:B:35[A]:ASP:OD1	1:B:63:LYS:NZ	2.05	0.90
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:76[A]:CYS:HG	3:B:202:GOL:HO3	1.49	0.60
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
1:A:146:ALA:C	3:A:202:GOL:H31	2.30	0.56
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:58[B]:ASP:OD2	1:D:60:SER:OG	2.13	0.54
1:A:8:THR:C	1:A:10:LEU:H	2.15	0.54
1:A:53:SER:O	1:A:57:MET:HE3	2.08	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: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:B:35[A]:ASP:CG	1:B:63:LYS:NZ	2.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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:A:9:LYS:HE2	1:A:140:LYS:HZ1	1.80	0.45
1:A:8:THR:HG22	1:A:144:VAL:HG21	1.99	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:8:THR:C	4:B:303:HOH:O	2.61	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:A:8:THR:C	1:A:10:LEU:N	2.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	45	29
1	B	142/138 (103%)	141 (99%)	1 (1%)	76	69
1	C	136/138 (99%)	133 (98%)	3 (2%)	45	29
1	D	138/138 (100%)	136 (99%)	2 (1%)	59	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	553/552 (100%)	544 (98%)	9 (2%)	57 41

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	9	LYS
1	A	67	LYS
1	B	25	LEU
1	C	8	THR
1	C	158[A]	LYS
1	C	158[B]	LYS
1	D	9	LYS
1	D	90	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	56	ASN
1	A	74	ASN
1	A	77	HIS
1	A	84	GLN
1	A	102	ASN
1	A	125	GLN
1	B	56	ASN
1	B	77	HIS
1	B	125	GLN
1	B	152	HIS
1	B	154	GLN
1	C	77	HIS
1	C	154	GLN
1	D	77	HIS
1	D	84	GLN
1	D	125	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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$
2	HEM	A	201[B]	-	50,50,50	1.69	12 (24%)	67,82,82	1.62	12 (17%)
3	GOL	B	203	-	5,5,5	0.13	0	5,5,5	0.27	0
2	HEM	D	200	1	50,50,50	1.38	7 (14%)	67,82,82	1.57	9 (13%)
2	HEM	B	201	1	50,50,50	1.50	10 (20%)	67,82,82	2.04	13 (19%)
3	GOL	A	202	-	5,5,5	0.14	0	5,5,5	0.60	0
2	HEM	C	200[A]	-	50,50,50	1.61	11 (22%)	67,82,82	1.75	22 (32%)
2	HEM	A	201[A]	-	50,50,50	1.70	12 (24%)	67,82,82	1.63	13 (19%)
2	HEM	C	200[B]	-	50,50,50	1.62	11 (22%)	67,82,82	1.72	21 (31%)
3	GOL	B	202	-	5,5,5	0.16	0	5,5,5	0.45	0
3	GOL	B	204	-	5,5,5	0.43	0	5,5,5	1.04	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
2	HEM	A	201[B]	-	-	4/14/54/54	-
3	GOL	B	203	-	-	2/4/4/4	-
2	HEM	D	200	1	-	4/14/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	201	1	-	4/14/54/54	-
3	GOL	A	202	-	-	2/4/4/4	-
2	HEM	C	200[A]	-	-	4/14/54/54	-
2	HEM	A	201[A]	-	-	4/14/54/54	-
2	HEM	C	200[B]	-	-	4/14/54/54	-
3	GOL	B	202	-	-	4/4/4/4	-
3	GOL	B	204	-	-	2/4/4/4	-

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201[A]	HEM	C1B-NB	-4.80	1.32	1.40
2	A	201[B]	HEM	C1B-NB	-4.80	1.32	1.40
2	A	201[A]	HEM	FE-NC	4.66	2.10	1.95
2	A	201[B]	HEM	FE-NC	4.66	2.10	1.95
2	C	200[A]	HEM	FE-NC	4.23	2.09	1.95
2	C	200[B]	HEM	FE-NC	4.23	2.09	1.95
2	A	201[A]	HEM	FE-NB	4.13	2.07	1.94
2	A	201[B]	HEM	FE-NB	4.13	2.07	1.94
2	D	200	HEM	FE-NC	4.10	2.08	1.95
2	D	200	HEM	FE-NB	3.55	2.05	1.94
2	C	200[A]	HEM	C1B-NB	-3.44	1.34	1.40
2	C	200[B]	HEM	C1B-NB	-3.44	1.34	1.40
2	C	200[A]	HEM	FE-NB	3.37	2.05	1.94
2	C	200[B]	HEM	FE-NB	3.37	2.05	1.94
2	B	201	HEM	FE-NB	3.35	2.05	1.94
2	B	201	HEM	C4D-ND	-3.34	1.34	1.40
2	B	201	HEM	C1B-NB	-3.33	1.34	1.40
2	A	201[A]	HEM	C1C-NC	-3.03	1.33	1.39
2	A	201[B]	HEM	C1C-NC	-3.03	1.33	1.39
2	A	201[A]	HEM	C4C-NC	-2.96	1.34	1.39
2	A	201[B]	HEM	C4C-NC	-2.96	1.34	1.39
2	D	200	HEM	C4C-NC	-2.91	1.34	1.39
2	C	200[A]	HEM	CHB-C1B	2.82	1.44	1.38
2	C	200[B]	HEM	CHB-C1B	2.82	1.44	1.38
2	B	201	HEM	C3C-C4C	-2.79	1.41	1.46
2	C	200[A]	HEM	C4D-ND	-2.76	1.35	1.40
2	C	200[B]	HEM	C4D-ND	-2.76	1.35	1.40
2	C	200[A]	HEM	C4A-NA	-2.74	1.34	1.39
2	C	200[B]	HEM	C4A-NA	-2.74	1.34	1.39
2	C	200[A]	HEM	C4C-NC	-2.74	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	200[B]	HEM	C4C-NC	-2.74	1.34	1.39
2	A	201[A]	HEM	C3B-C4B	2.65	1.50	1.44
2	A	201[B]	HEM	C3B-C4B	2.65	1.50	1.44
2	D	200	HEM	C4B-NB	-2.64	1.33	1.38
2	D	200	HEM	C1B-NB	-2.58	1.35	1.40
2	C	200[A]	HEM	FE-NA	2.37	2.03	1.95
2	C	200[B]	HEM	FE-NA	2.37	2.03	1.95
2	B	201	HEM	C1C-C2C	-2.37	1.40	1.45
2	A	201[A]	HEM	C3C-C4C	-2.33	1.41	1.46
2	A	201[B]	HEM	C3C-C4C	-2.33	1.41	1.46
2	B	201	HEM	FE-NC	2.29	2.02	1.95
2	D	200	HEM	C4D-C3D	2.22	1.48	1.45
2	B	201	HEM	CMC-C2C	2.21	1.55	1.50
2	B	201	HEM	CBD-CGD	2.20	1.55	1.50
2	B	201	HEM	CMD-C2D	2.20	1.55	1.50
2	C	200[A]	HEM	C1B-C2B	-2.19	1.40	1.44
2	C	200[B]	HEM	C1B-C2B	-2.19	1.40	1.44
2	A	201[A]	HEM	C1C-C2C	-2.19	1.41	1.45
2	A	201[B]	HEM	C1C-C2C	-2.19	1.41	1.45
2	A	201[A]	HEM	C4A-C3A	-2.13	1.38	1.43
2	A	201[B]	HEM	C4A-C3A	-2.13	1.38	1.43
2	C	200[A]	HEM	CMC-C2C	2.10	1.55	1.50
2	C	200[B]	HEM	CMC-C2C	2.10	1.55	1.50
2	D	200	HEM	CBA-CGA	-2.10	1.45	1.50
2	A	201[A]	HEM	C3D-C2D	-2.10	1.32	1.36
2	A	201[B]	HEM	C3D-C2D	-2.10	1.32	1.36
2	C	200[A]	HEM	CHA-C1A	-2.09	1.34	1.39
2	C	200[B]	HEM	CHA-C1A	-2.09	1.34	1.39
2	B	201	HEM	C4A-C3A	-2.08	1.38	1.43
2	A	201[A]	HEM	CHA-C1A	-2.01	1.34	1.39
2	A	201[B]	HEM	CHA-C1A	-2.01	1.34	1.39
2	A	201[A]	HEM	C1A-C2A	-2.00	1.40	1.44
2	A	201[B]	HEM	C1A-C2A	-2.00	1.40	1.44

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	HEM	CHC-C4B-NB	6.70	131.63	124.42
2	B	201	HEM	C3B-C4B-NB	-6.07	105.11	109.47
2	B	201	HEM	C1B-NB-C4B	5.46	111.67	105.21
2	B	201	HEM	C4C-C3C-C2C	4.72	110.91	106.81
2	A	201[A]	HEM	C3B-C4B-NB	-4.65	106.13	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201[B]	HEM	C3B-C4B-NB	-4.65	106.13	109.47
2	A	201[A]	HEM	C1B-NB-C4B	4.51	110.55	105.21
2	A	201[B]	HEM	C1B-NB-C4B	4.51	110.55	105.21
2	D	200	HEM	CAA-CBA-CGA	-3.85	103.44	113.67
2	D	200	HEM	CHB-C1B-NB	3.78	129.05	124.37
2	C	200[A]	HEM	CMD-C2D-C1D	3.75	130.89	125.03
2	C	200[B]	HEM	CMD-C2D-C1D	3.75	130.89	125.03
2	D	200	HEM	C2A-C1A-NA	-3.74	106.00	110.15
2	B	201	HEM	CHB-C1B-NB	3.73	128.98	124.37
2	B	201	HEM	CHD-C4C-NC	3.71	128.50	124.45
2	D	200	HEM	CHA-C1A-NA	3.67	130.51	123.86
2	B	201	HEM	CHA-C4D-ND	3.48	128.67	124.37
2	A	201[A]	HEM	CHC-C4B-NB	3.35	128.03	124.42
2	A	201[B]	HEM	CHC-C4B-NB	3.35	128.03	124.42
2	A	201[A]	HEM	CHD-C4C-NC	3.33	128.08	124.45
2	A	201[B]	HEM	CHD-C4C-NC	3.33	128.08	124.45
2	C	200[A]	HEM	C2D-C1D-ND	3.33	113.75	109.90
2	C	200[B]	HEM	C2D-C1D-ND	3.33	113.75	109.90
2	A	201[A]	HEM	CBA-CAA-C2A	-3.31	103.37	112.53
2	A	201[A]	HEM	CBD-CAD-C3D	-3.31	103.38	112.53
2	C	200[A]	HEM	CMB-C2B-C1B	-3.16	120.10	125.03
2	C	200[B]	HEM	CMB-C2B-C1B	-3.16	120.10	125.03
2	C	200[A]	HEM	C1D-C2D-C3D	-3.07	103.75	106.98
2	C	200[B]	HEM	C1D-C2D-C3D	-3.07	103.75	106.98
2	D	200	HEM	CHD-C1D-ND	3.03	127.68	124.42
2	A	201[B]	HEM	CAD-C3D-C4D	3.00	129.92	124.70
2	C	200[A]	HEM	CAA-CBA-CGA	-2.96	105.80	113.67
2	D	200	HEM	C1B-NB-C4B	2.95	108.69	105.21
2	B	201	HEM	CMD-C2D-C1D	-2.94	120.43	125.03
2	C	200[A]	HEM	CHD-C1D-C2D	-2.94	120.39	125.03
2	C	200[B]	HEM	CHD-C1D-C2D	-2.94	120.39	125.03
2	C	200[A]	HEM	C3B-C4B-NB	-2.88	107.40	109.47
2	C	200[B]	HEM	C3B-C4B-NB	-2.88	107.40	109.47
2	C	200[A]	HEM	C4C-NC-C1C	2.84	110.45	105.82
2	C	200[B]	HEM	C4C-NC-C1C	2.84	110.45	105.82
2	A	201[B]	HEM	CAA-CBA-CGA	-2.83	106.16	113.67
2	A	201[B]	HEM	CBD-CAD-C3D	-2.80	104.78	112.53
2	C	200[B]	HEM	CBA-CAA-C2A	-2.71	105.04	112.53
2	D	200	HEM	CHD-C1D-C2D	-2.68	120.80	125.03
2	B	201	HEM	CBD-CAD-C3D	-2.64	105.24	112.53
2	C	200[A]	HEM	CAC-C3C-C4C	-2.62	118.56	124.82
2	C	200[B]	HEM	CAC-C3C-C4C	-2.62	118.56	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	200[A]	HEM	O2A-CGA-CBA	2.59	122.19	114.00
2	A	201[A]	HEM	O2D-CGD-CBD	2.53	122.01	114.00
2	C	200[A]	HEM	CBB-CAB-C3B	-2.52	114.95	127.53
2	C	200[B]	HEM	CBB-CAB-C3B	-2.52	114.95	127.53
2	C	200[A]	HEM	CBC-CAC-C3C	-2.52	114.96	127.53
2	C	200[B]	HEM	CBC-CAC-C3C	-2.52	114.96	127.53
2	D	200	HEM	CBC-CAC-C3C	-2.50	115.02	127.53
2	A	201[A]	HEM	C2D-C1D-ND	2.50	112.79	109.90
2	A	201[B]	HEM	C2D-C1D-ND	2.50	112.79	109.90
2	C	200[A]	HEM	C4C-C3C-C2C	2.47	108.96	106.81
2	C	200[B]	HEM	C4C-C3C-C2C	2.47	108.96	106.81
2	B	201	HEM	CHA-C4D-C3D	-2.46	120.69	125.23
2	C	200[A]	HEM	CAD-C3D-C4D	2.45	128.97	124.70
2	C	200[B]	HEM	CAD-C3D-C4D	2.45	128.97	124.70
2	C	200[A]	HEM	CAD-C3D-C2D	-2.38	123.42	127.87
2	C	200[B]	HEM	CAD-C3D-C2D	-2.38	123.42	127.87
2	D	200	HEM	CHC-C4B-NB	2.36	126.96	124.42
2	A	201[A]	HEM	CAD-C3D-C4D	2.33	128.76	124.70
2	C	200[A]	HEM	O2A-CGA-O1A	-2.33	117.35	123.33
2	A	201[A]	HEM	CBB-CAB-C3B	-2.27	116.16	127.53
2	A	201[B]	HEM	CBB-CAB-C3B	-2.27	116.16	127.53
2	B	201	HEM	C4D-ND-C1D	2.27	107.89	105.21
2	C	200[A]	HEM	C2A-C1A-NA	-2.26	107.64	110.15
2	C	200[B]	HEM	C2A-C1A-NA	-2.26	107.64	110.15
2	C	200[A]	HEM	CAA-C2A-C1A	2.21	129.26	124.94
2	C	200[A]	HEM	C4A-C3A-C2A	2.19	109.33	106.82
2	C	200[B]	HEM	C4A-C3A-C2A	2.19	109.33	106.82
2	B	201	HEM	CHD-C1D-ND	2.18	126.77	124.42
2	A	201[A]	HEM	C4C-NC-C1C	2.17	109.36	105.82
2	A	201[B]	HEM	C4C-NC-C1C	2.17	109.36	105.82
2	C	200[B]	HEM	O2A-CGA-O1A	-2.12	117.89	123.33
2	A	201[A]	HEM	O2D-CGD-O1D	-2.11	117.90	123.33
2	A	201[A]	HEM	CHD-C1D-C2D	-2.10	121.70	125.03
2	A	201[B]	HEM	CHD-C1D-C2D	-2.10	121.70	125.03
2	A	201[B]	HEM	CAD-C3D-C2D	-2.10	123.93	127.87
2	C	200[A]	HEM	C4D-ND-C1D	-2.10	102.72	105.21
2	C	200[B]	HEM	C4D-ND-C1D	-2.10	102.72	105.21
2	B	201	HEM	C2D-C1D-ND	-2.04	107.55	109.90
2	C	200[A]	HEM	CHA-C1A-NA	2.03	127.55	123.86
2	C	200[B]	HEM	CHA-C1A-NA	2.03	127.55	123.86
2	C	200[B]	HEM	CAA-CBA-CGA	2.03	119.04	113.67
2	C	200[A]	HEM	CMA-C3A-C4A	-2.00	122.37	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	200[B]	HEM	CMA-C3A-C4A	-2.00	122.37	125.42

There are no chirality outliers.

All (34) torsion outliers are listed below:

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

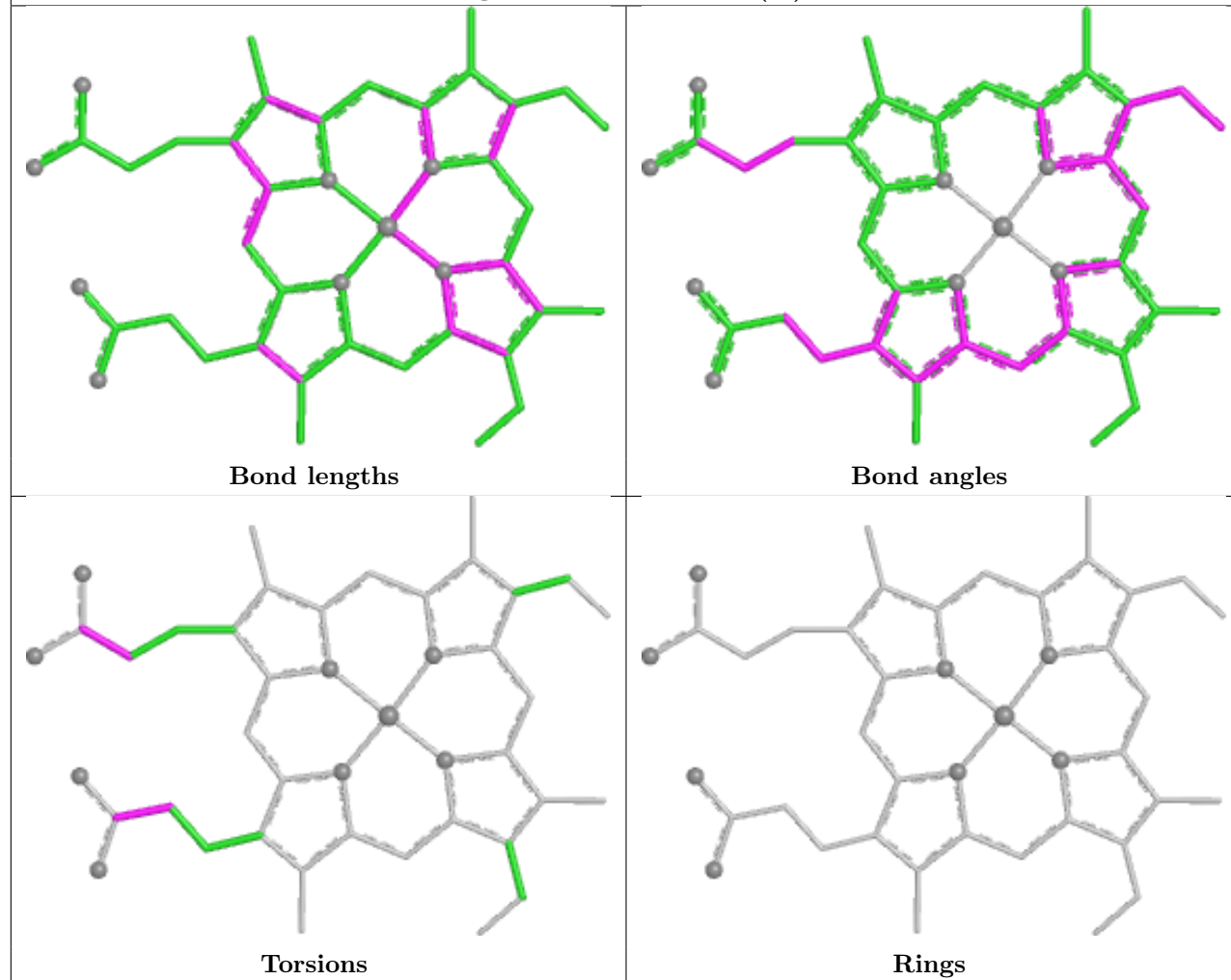
There are no ring outliers.

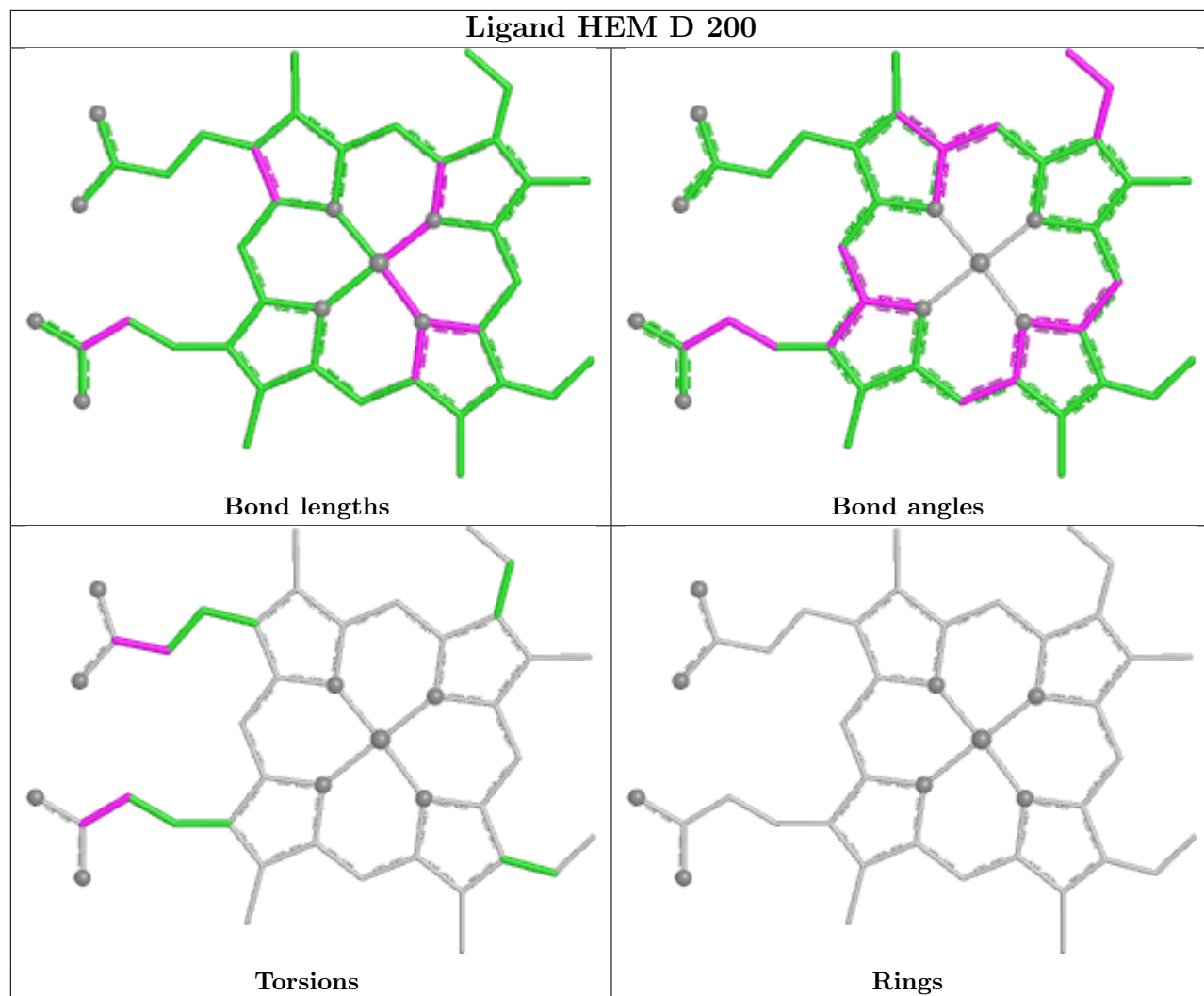
7 monomers are involved in 22 short contacts:

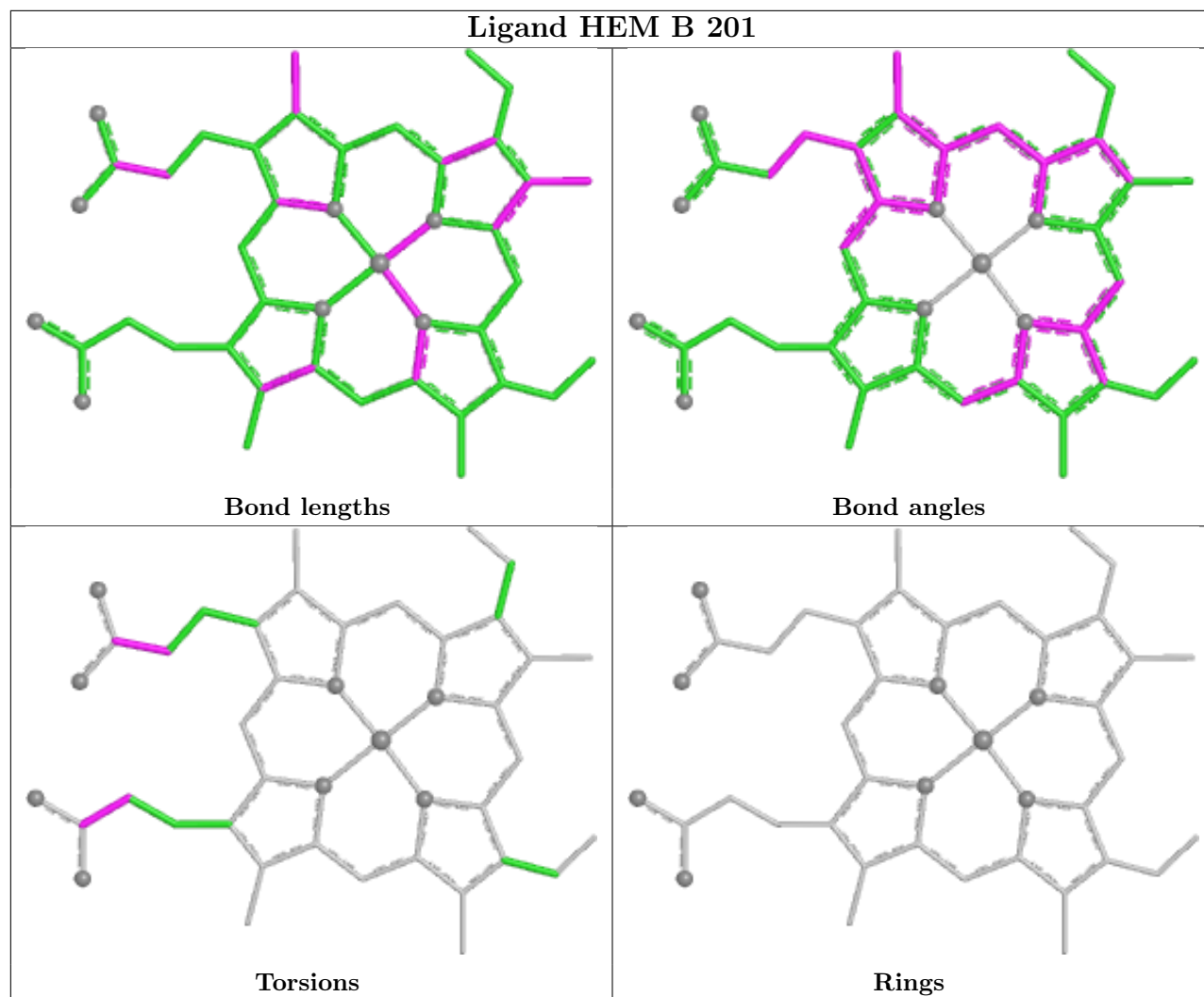
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201[B]	HEM	1	0
2	D	200	HEM	4	0
2	B	201	HEM	6	0
3	A	202	GOL	2	0
2	C	200[A]	HEM	1	0
3	B	202	GOL	2	0
3	B	204	GOL	6	0

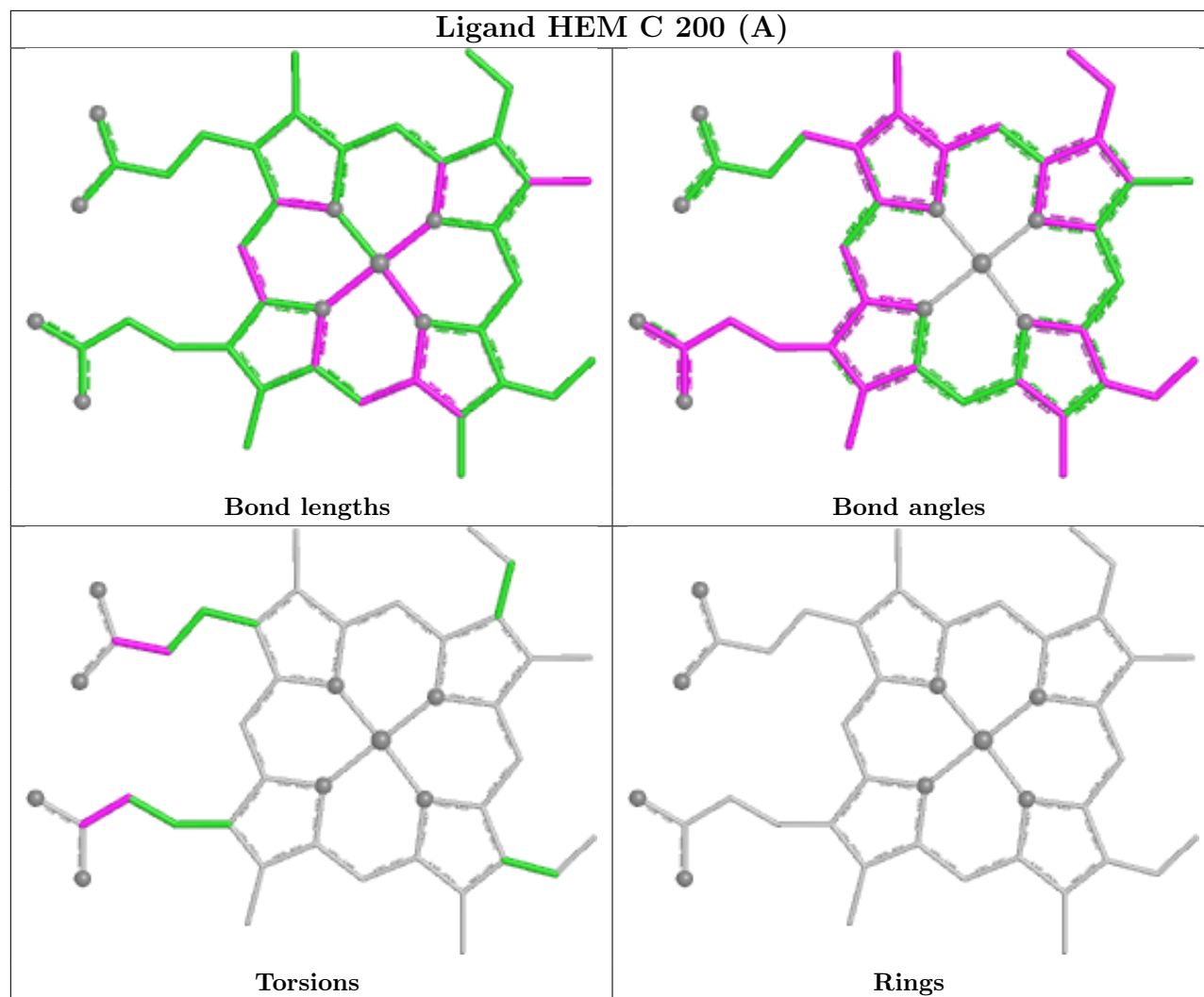
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand HEM A 201 (B)

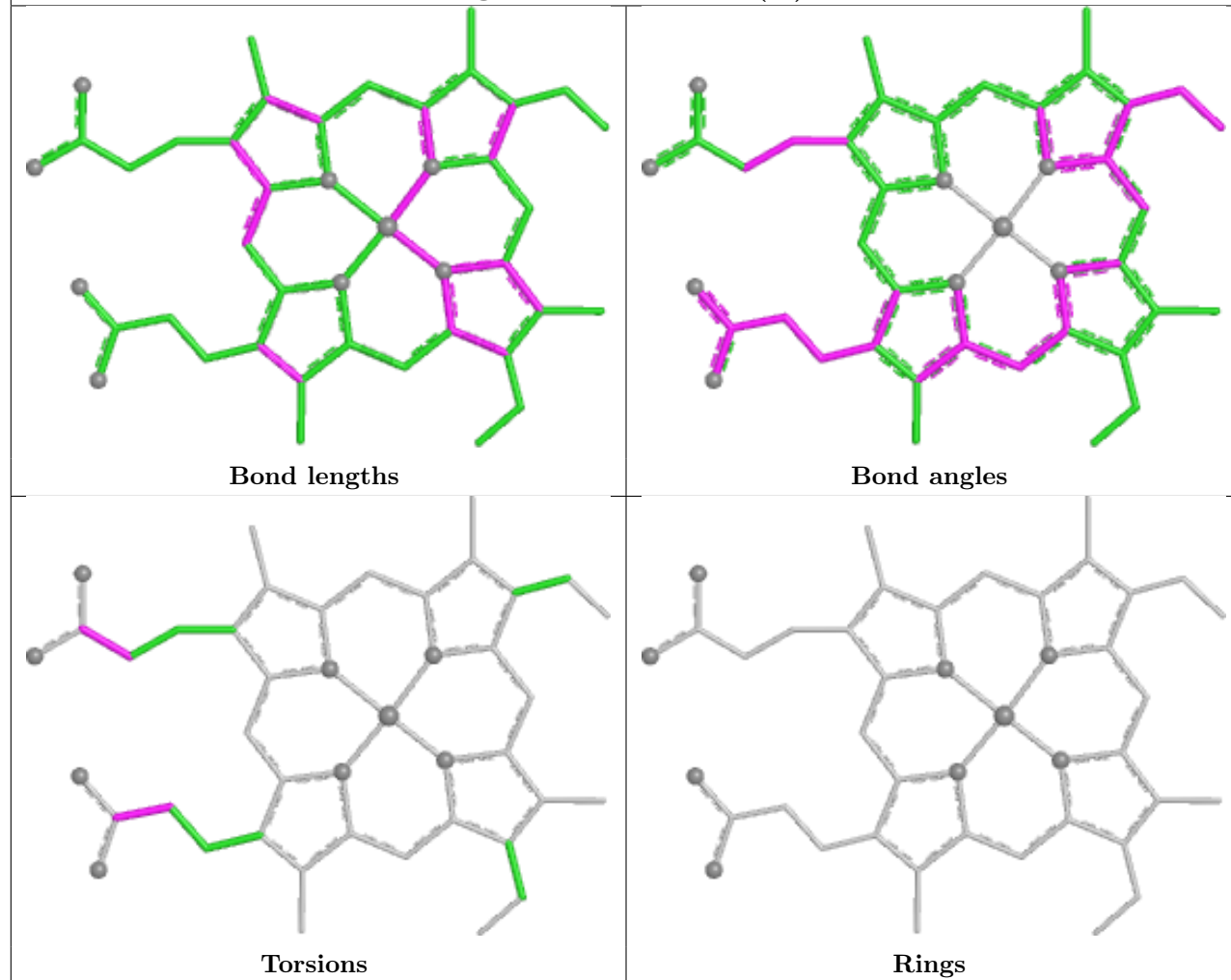


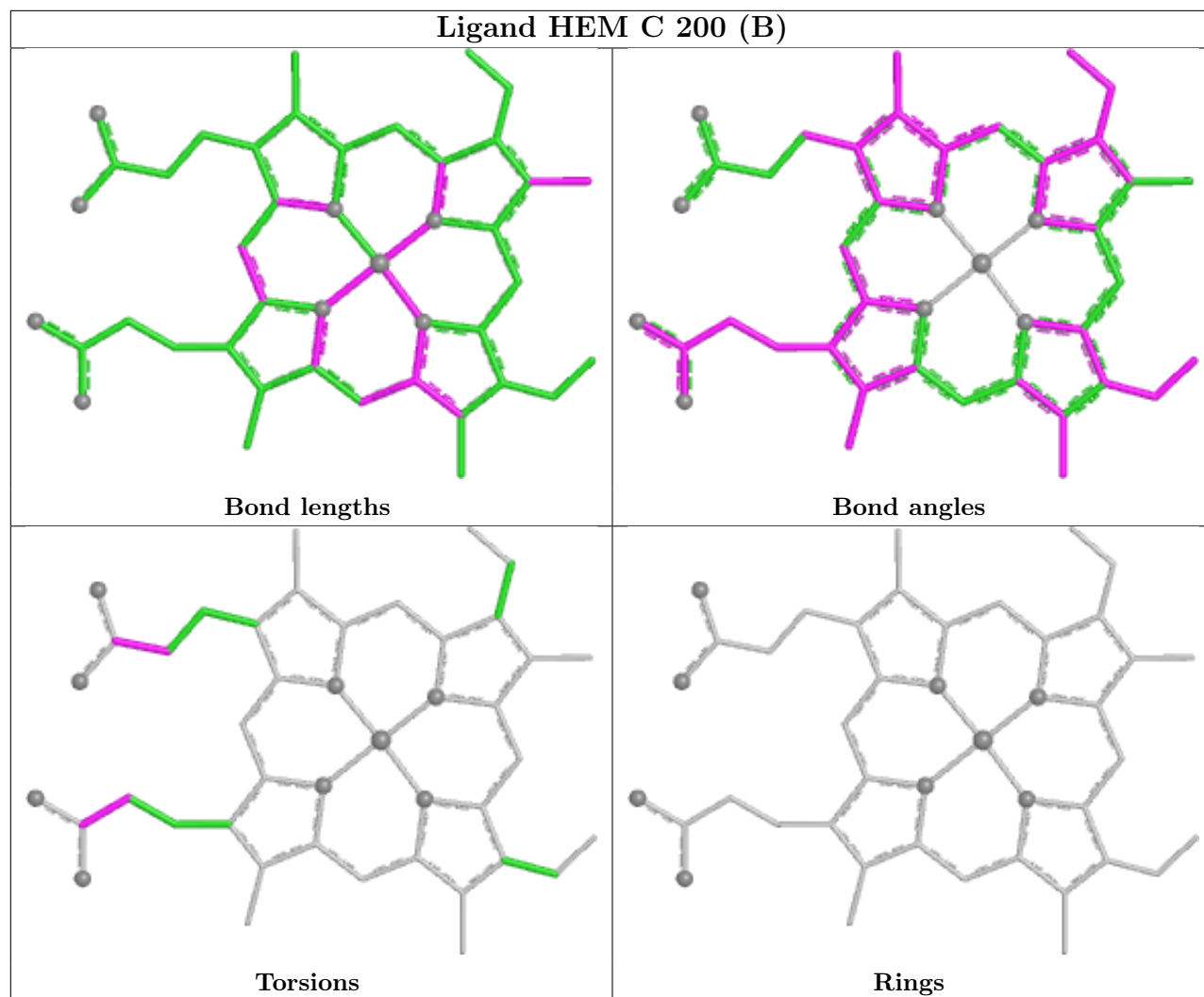






Ligand HEM A 201 (A)





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	150/162 (92%)	0.20	9 (6%)	27	30	6, 15, 41, 72	8 (5%)
1	B	151/162 (93%)	-0.06	4 (2%)	57	61	6, 12, 26, 80	12 (7%)
1	C	151/162 (93%)	0.08	7 (4%)	37	41	10, 14, 32, 80	6 (3%)
1	D	151/162 (93%)	0.11	4 (2%)	57	61	8, 16, 33, 80	8 (5%)
All	All	603/648 (93%)	0.08	24 (3%)	42	46	6, 14, 32, 80	34 (5%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	9[A]	LYS	9.3
1	B	8	THR	8.5
1	A	8	THR	6.7
1	C	8	THR	6.5
1	D	8	THR	6.0
1	A	53	SER	3.7
1	A	52	LYS	3.4
1	C	58	ASP	3.2
1	A	157	GLN	3.0
1	A	101	VAL	3.0
1	C	56	ASN	2.7
1	D	9	LYS	2.7
1	C	9	LYS	2.5
1	C	30	LYS	2.4
1	A	56	ASN	2.4
1	A	9	LYS	2.4
1	A	58	ASP	2.4
1	C	158[A]	LYS	2.3
1	B	56	ASN	2.2
1	D	157	GLN	2.2
1	D	158	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	53	SER	2.2
1	B	31	THR	2.1
1	A	156	LEU	2.1

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](#)

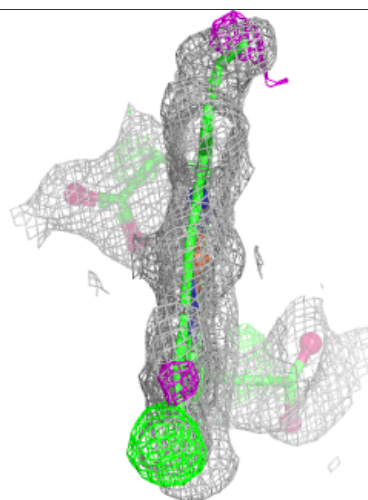
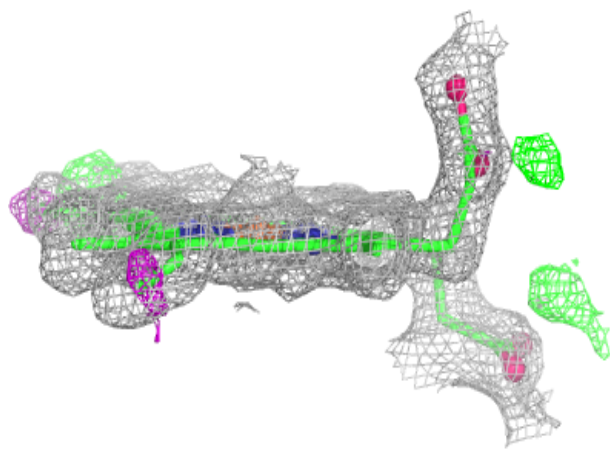
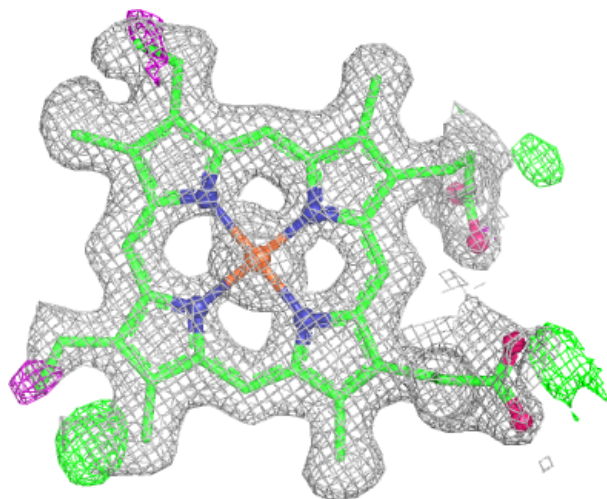
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	B	203	6/6	0.85	0.13	25,35,39,40	0
3	GOL	B	202	6/6	0.88	0.12	33,40,40,46	0
3	GOL	B	204	6/6	0.88	0.10	25,26,32,33	0
3	GOL	A	202	6/6	0.91	0.11	28,34,41,43	0
2	HEM	C	200[B]	43/43	0.98	0.07	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	0.07	11,15,24,31	10
2	HEM	A	201[B]	43/43	0.98	0.07	11,15,22,24	10
2	HEM	B	201	43/43	0.98	0.08	9,13,25,36	0
2	HEM	C	200[A]	43/43	0.98	0.07	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.

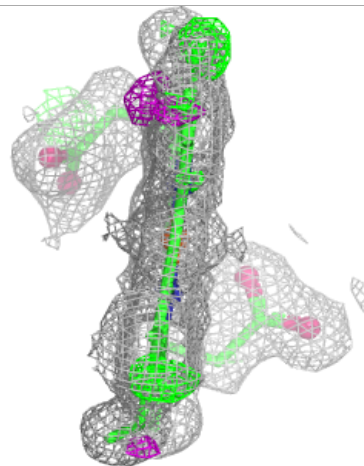
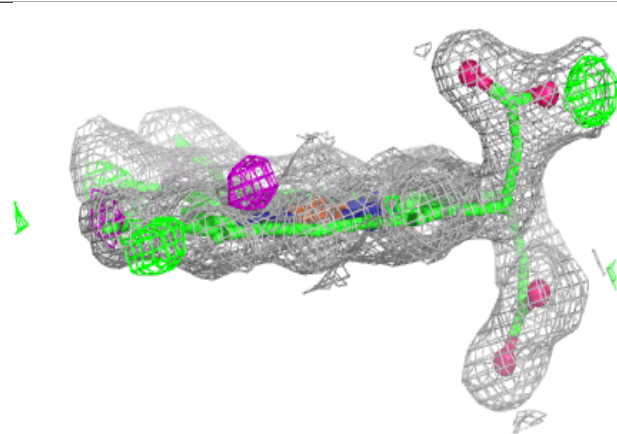
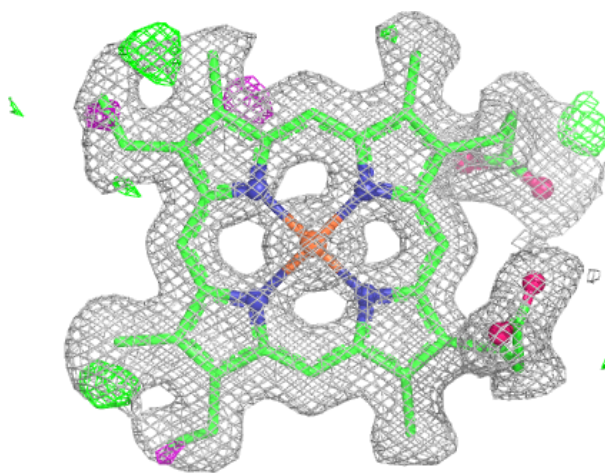
Electron density around HEM C 200 (B):

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



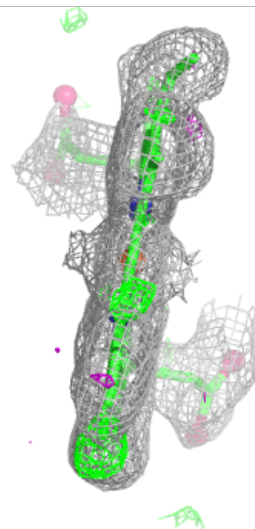
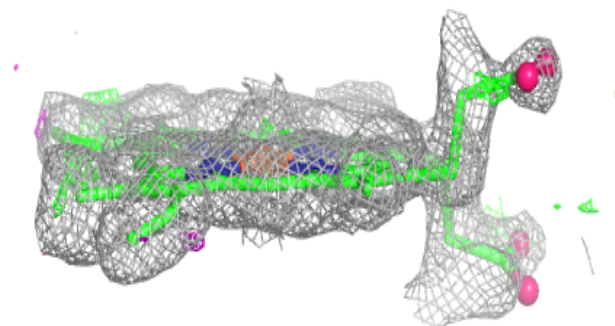
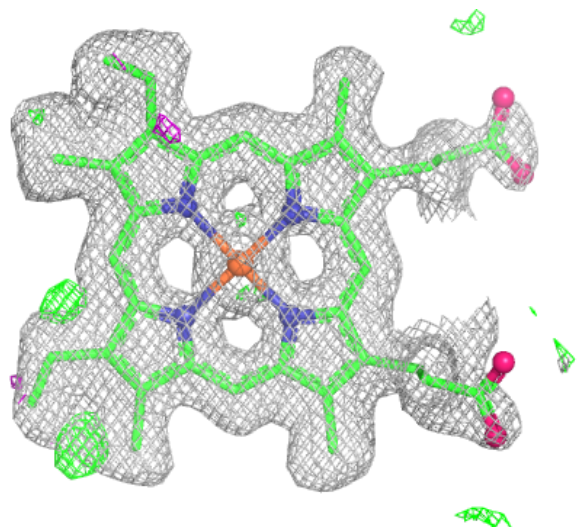
Electron density around HEM D 200:

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



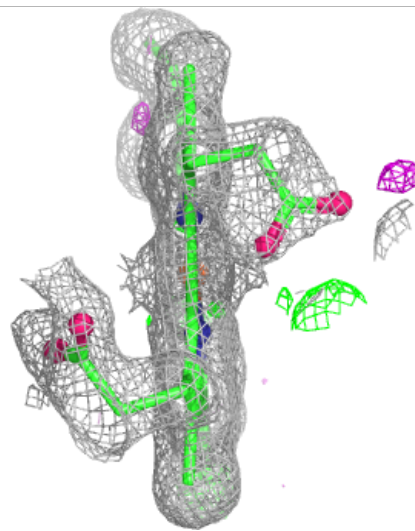
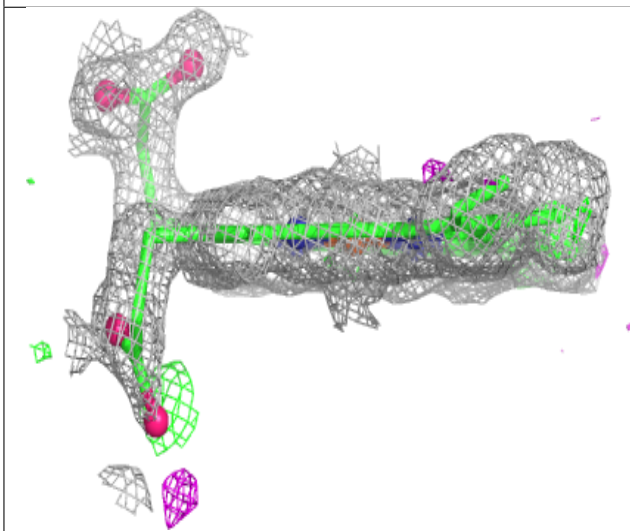
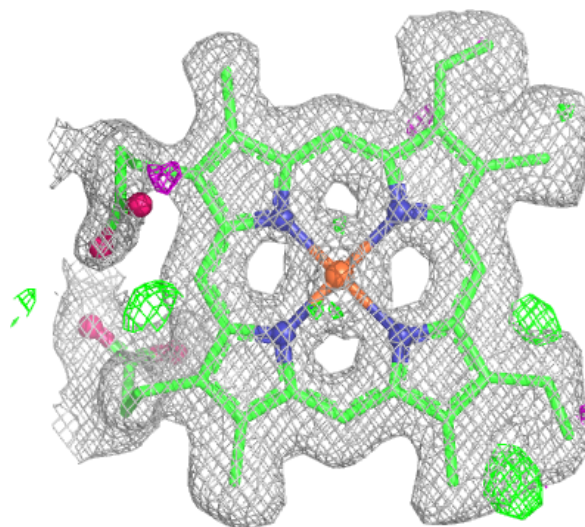
Electron density around HEM A 201 (A):

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



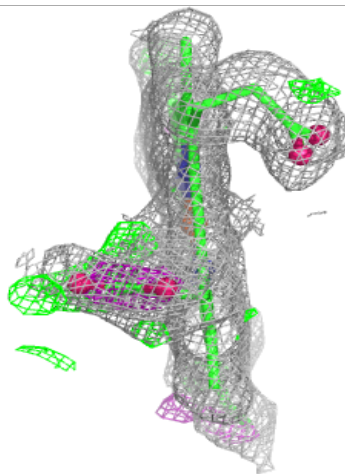
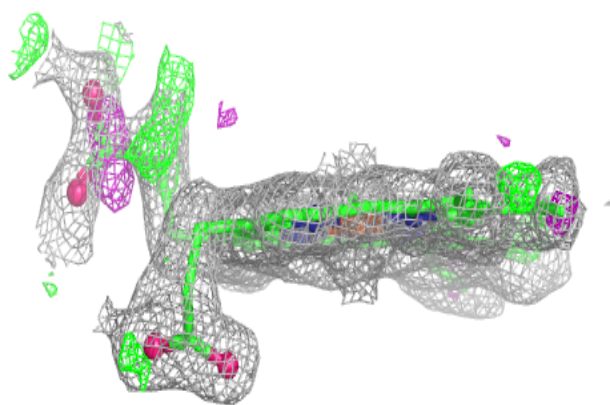
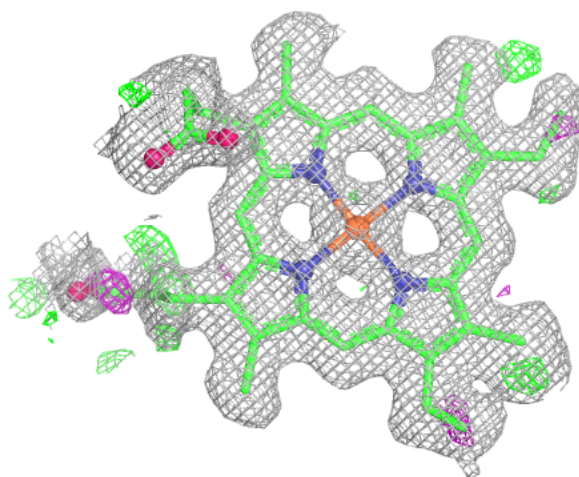
Electron density around HEM A 201 (B):

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



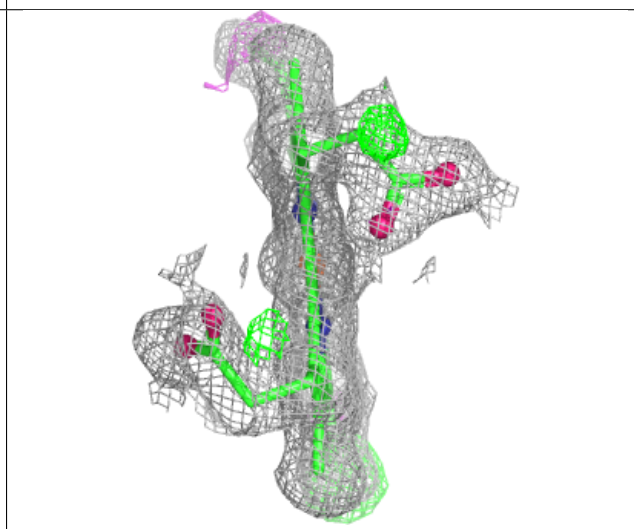
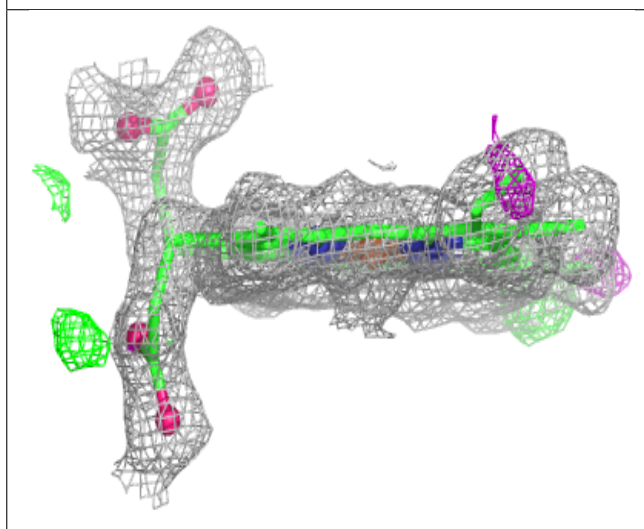
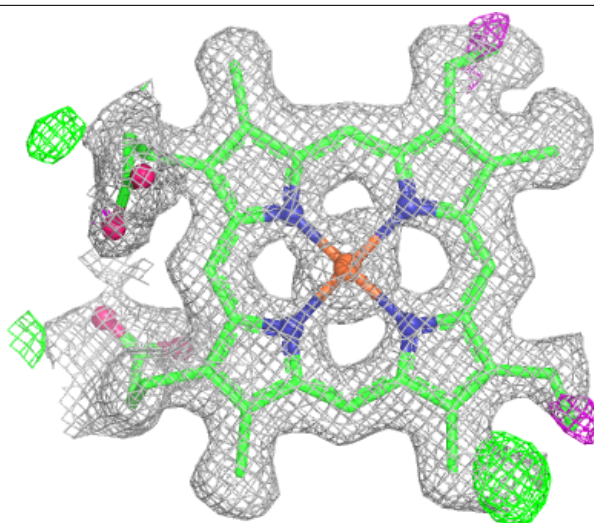
Electron density around HEM B 201:

$2mF_o-DF_c$ (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.