wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2N91
BMRB ID	:	25874
Title	:	A key amino acid in the control of different functional behavior within the triheme cytochrome family from Geobacter sulfurreducens
Authors	:	Dantas, J.M.; Simoes, T.; Bruix, M.; Salgueiro, C.A.
Deposited on	:	2015-11-02

This is a wwPDB NMR Structure Validation Summary 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/NMRValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

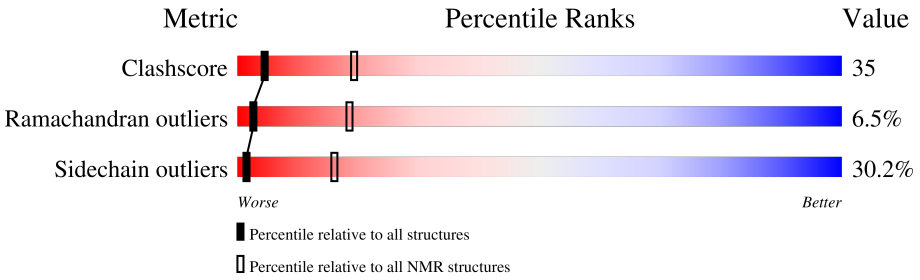
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 55%.

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)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	71	39% 51% 6% • •

2 Ensemble composition and analysis

This entry contains 20 models. Model 5 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:2-A:70 (69)	0.20	5

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters and 3 single-model clusters were found.

Cluster number	Models
1	2, 4, 5, 6, 11, 13, 16
2	8, 9, 10, 12, 15
3	3, 18, 19
4	1, 14
Single-model clusters	7; 17; 20

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1197 atoms, of which 530 are hydrogens and 0 are deuteriums.

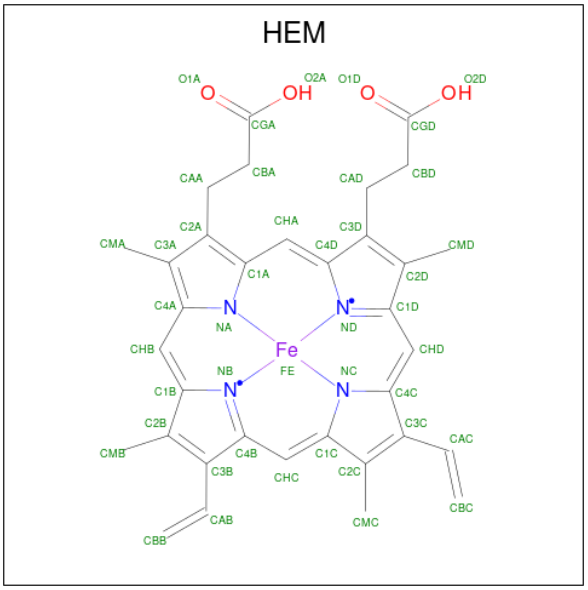
- Molecule 1 is a protein called Cytochrome C.

Mol	Chain	Residues	Atoms						Trace
1	A	71	Total	C	H	N	O	S	0
			1068	334	530	102	94	8	

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	PHE	LEU	engineered mutation	UNP Q8GGK7

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms				
2	A	1	Total	C	Fe	N	O
			43	34	1	4	4
2	A	1	Total	C	Fe	N	O
			43	34	1	4	4
2	A	1	Total	C	Fe	N	O
			43	34	1	4	4

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: Cytochrome C

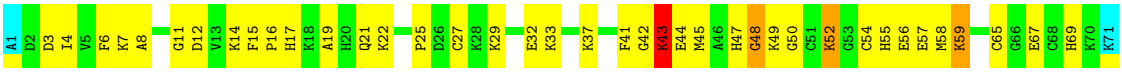
Chain A:

4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 5. Colouring as in section 4.1 above.

- Molecule 1: Cytochrome C

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing.*

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
PARADYANA	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	584
Number of shifts mapped to atoms	495
Number of unparsed shifts	0
Number of shifts with mapping errors	89
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	55%

6 Model quality

6.1 Standard geometry

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

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 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 each 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 averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	524	513	519	39±3
2	A	129	0	90	24±3
All	All	13060	10260	12180	878

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 35.

5 of 132 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ILE:HD12	2:A:101:HEM:O2D	0.88	1.68	17	2
1:A:8:ALA:HB3	1:A:11:GLY:O	0.80	1.77	12	20
2:A:101:HEM:HMB2	2:A:101:HEM:HBB2	0.79	1.55	20	1
1:A:15:PHE:CD1	2:A:102:HEM:C2B	0.73	2.76	9	20
1:A:15:PHE:CE1	2:A:102:HEM:C3B	0.73	2.77	9	18

6.3 Torsion angles (i)

6.3.1 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 PDB entries followed by that with respect to all NMR entries. 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	69/71 (97%)	48±1 (69±2%)	17±2 (24±3%)	4±1 (7±2%)	2 18
All	All	1380/1420 (97%)	956 (69%)	334 (24%)	90 (7%)	2 18

5 of 11 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	25	PRO	20
1	A	48	GLY	20
1	A	43	LYS	19
1	A	44	GLU	14
1	A	3	ASP	4

6.3.2 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 PDB entries followed by that with respect to all NMR entries. 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	55/56 (98%)	38±1 (70±3%)	17±1 (30±3%)	1 16
All	All	1100/1120 (98%)	768 (70%)	332 (30%)	1 16

5 of 29 unique residues with a non-rotameric sidechain are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	33	LYS	20
1	A	37	LYS	20
1	A	65	CYS	20
1	A	67	GLU	19
1	A	12	ASP	18

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

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

6.5 Carbohydrates

There are no monosaccharides in this entry.

6.6 Ligand geometry

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	HEM	A	103	1	41,50,50	1.44±0.00	5±0 (12±0%)
2	HEM	A	102	1	41,50,50	1.46±0.01	5±0 (12±0%)
2	HEM	A	101	1	41,50,50	1.44±0.01	5±0 (11±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	HEM	A	103	1	45,82,82	1.01±0.00	3±0 (6±0%)
2	HEM	A	102	1	45,82,82	0.98±0.01	2±0 (4±0%)
2	HEM	A	101	1	45,82,82	0.96±0.00	2±0 (4±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	103	1	-	0±0,12,54,54	-
2	HEM	A	101	1	-	0±0,12,54,54	-
2	HEM	A	102	1	-	0±0,12,54,54	-

5 of 15 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	101	HEM	CBB-CAB	4.61	1.53	1.30	18	20
2	A	102	HEM	CBB-CAB	4.61	1.53	1.30	18	20
2	A	103	HEM	CBB-CAB	4.61	1.53	1.30	13	20
2	A	102	HEM	C3C-C2C	3.65	1.35	1.40	16	20
2	A	101	HEM	C3C-C2C	3.62	1.35	1.40	8	20

5 of 8 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	101	HEM	CBB-CAB-C3B	2.75	113.95	127.62	1	20
2	A	102	HEM	CBB-CAB-C3B	2.75	113.94	127.62	7	20
2	A	103	HEM	CBB-CAB-C3B	2.75	113.95	127.62	6	20
2	A	102	HEM	C4B-CHC-C1C	2.60	125.99	122.56	17	1
2	A	103	HEM	CMA-C3A-C4A	2.36	124.84	128.46	17	20

There are no chirality outliers.

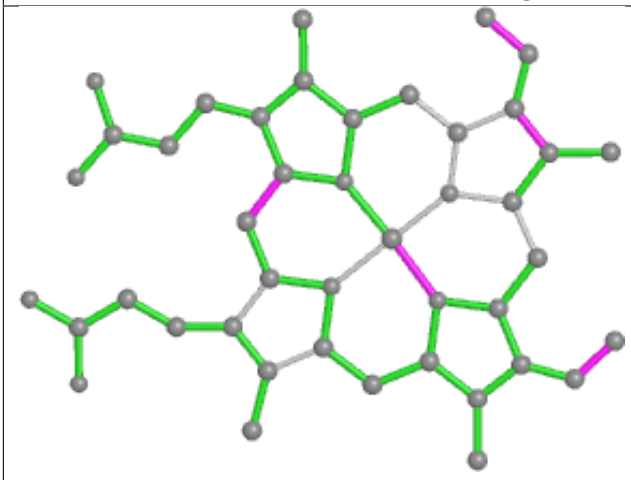
There are no torsion outliers.

There are no ring outliers.

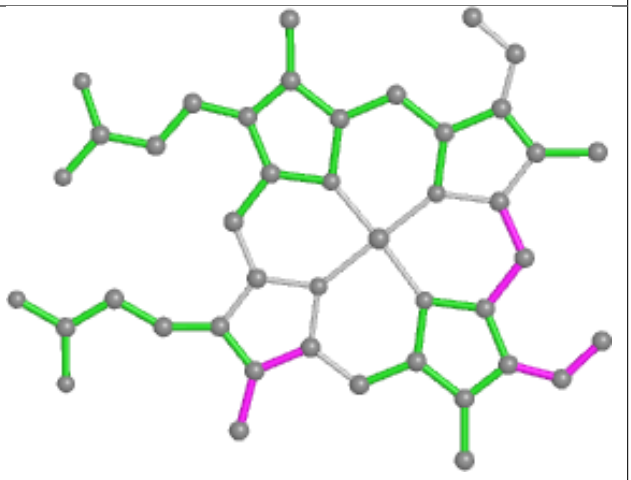
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

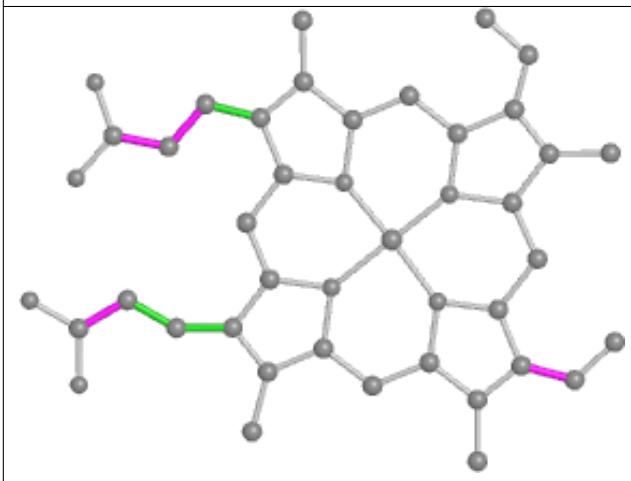
Ligand HEM A 103



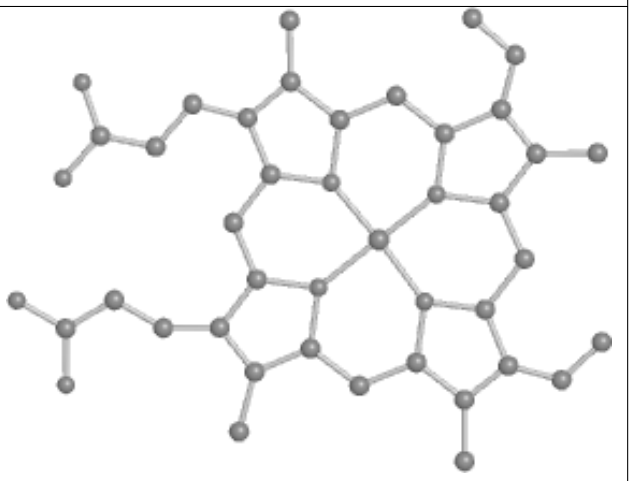
Bond lengths



Bond angles

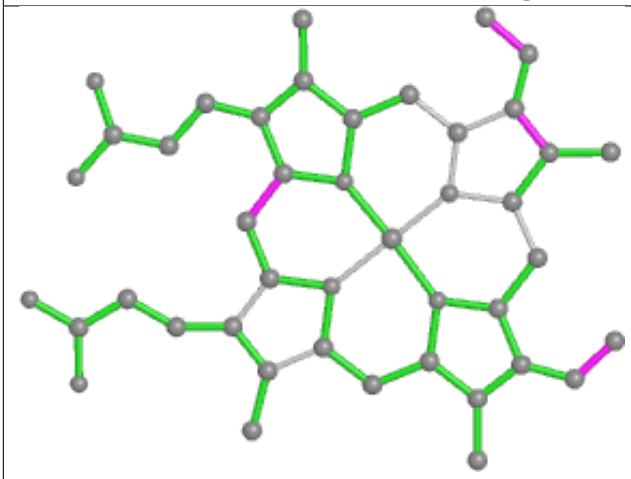


Torsions

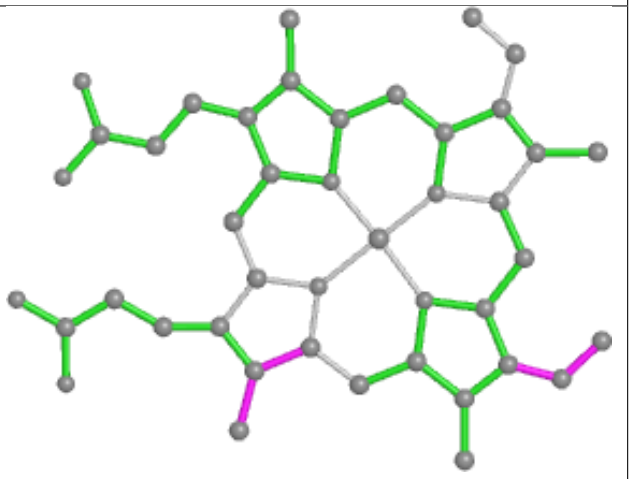


Rings

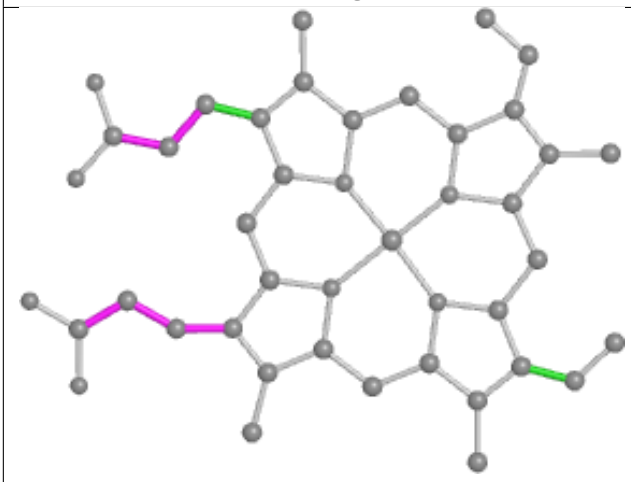
Ligand HEM A 101



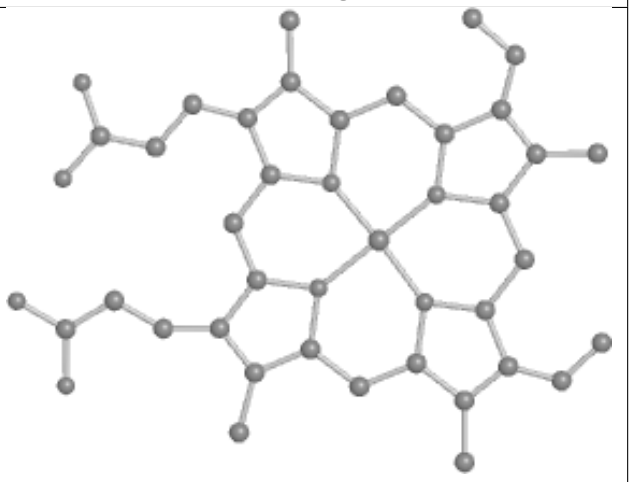
Bond lengths



Bond angles

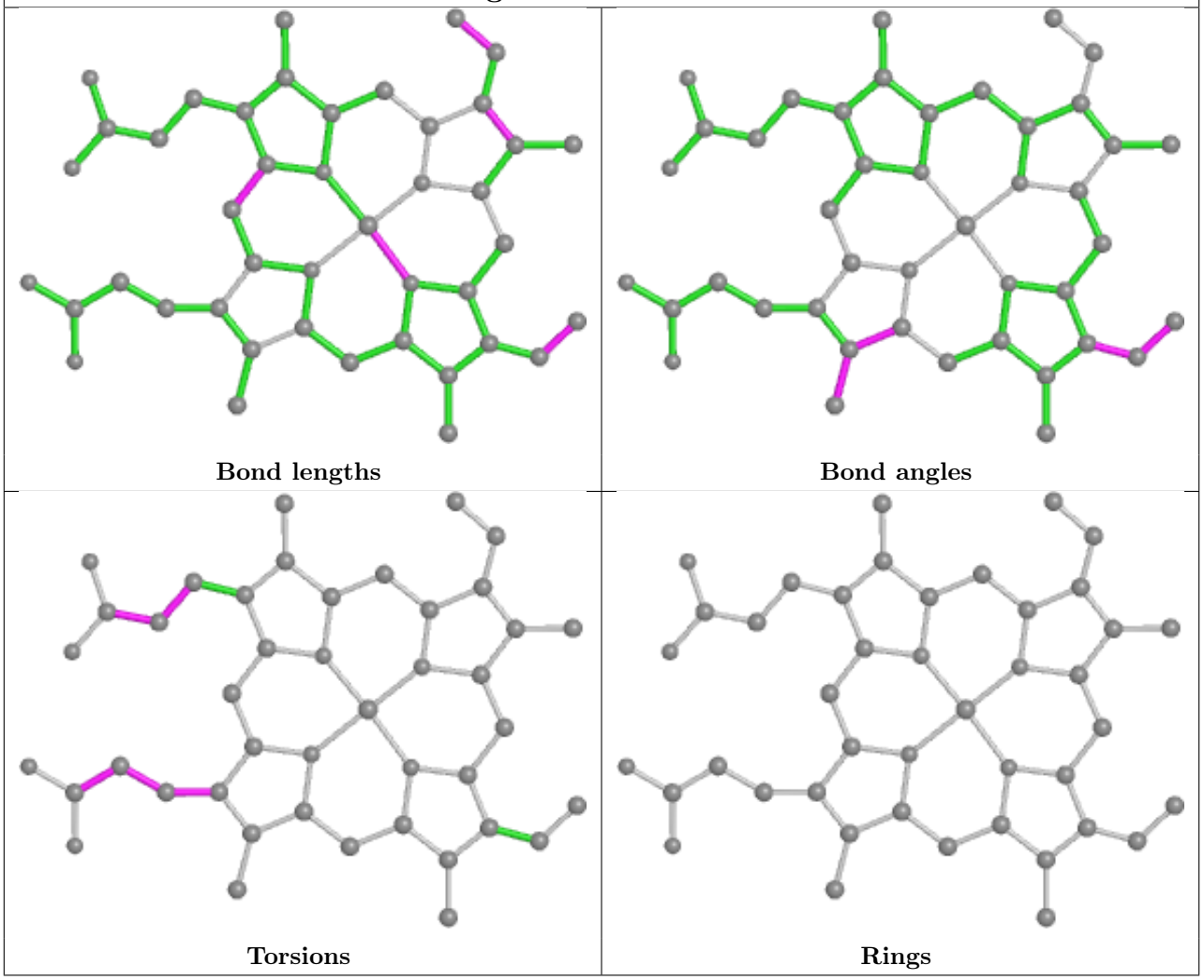


Torsions



Rings

Ligand HEM A 102



6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 55% for the well-defined parts and 55% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	584
Number of shifts mapped to atoms	495
Number of unparsed shifts	0
Number of shifts with mapping errors	89
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	34

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. First 5 (of 89) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	101	HEM	HAD	3.654	0.002	2
1	A	101	HEM	HADA	4.307	0.005	2
1	A	101	HEM	HAA	3.895	0.002	2
1	A	101	HEM	HAAA	3.935	0.003	2
1	A	101	HEM	HHC	9.603	0.002	1
1	A	101	HEM	HBD	2.577	0.003	2
1	A	101	HEM	HBDA	3.199	0.006	2
1	A	101	HEM	HBA	2.96	0.002	2
1	A	101	HEM	HBAA	2.924	0.003	2
1	A	101	HEM	HHD	9.176	0.001	1
1	A	101	HEM	HHB	9.427	0.000	1
1	A	101	HEM	HHA	9.229	0.001	1
1	A	101	HEM	HAB	6.272	0.003	1
1	A	101	HEM	HAC	6.271	0.028	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	101	HEM	HMB	3.493	0.001	1
1	A	101	HEM	HMBA	3.493	0.001	1
1	A	101	HEM	HMBB	3.493	0.001	1
1	A	101	HEM	HMC	3.518	0.002	1
1	A	101	HEM	HMCA	3.518	0.002	1
1	A	101	HEM	HMCB	3.518	0.002	1
1	A	101	HEM	HMD	2.735	0.001	1
1	A	101	HEM	HMDA	2.735	0.001	1
1	A	101	HEM	HMDB	2.735	0.001	1
1	A	101	HEM	HMA	3.284	0.002	1
1	A	101	HEM	HMAA	3.284	0.002	1
1	A	101	HEM	HMAB	3.284	0.002	1
1	A	101	HEM	HBB	2.069	0.010	1
1	A	101	HEM	HBBA	2.069	0.010	1
1	A	101	HEM	HBC	1.709	0.002	1
1	A	101	HEM	HBCA	1.709	0.002	1
1	A	102	HEM	HAD	3.76	0.003	2
1	A	102	HEM	HADA	4.13	0.007	2
1	A	102	HEM	HAA	4.112	0.000	2
1	A	102	HEM	HAAA	4.163	0.000	2
1	A	102	HEM	HHC	10.484	0.002	1
1	A	102	HEM	HBD	2.742	0.002	2
1	A	102	HEM	HBDA	2.913	0.002	2
1	A	102	HEM	HBA	3.196	0.002	2
1	A	102	HEM	HHD	9.796	0.001	1
1	A	102	HEM	HHB	10.159	0.002	1
1	A	102	HEM	HHA	9.393	0.002	1
1	A	102	HEM	HAB	6.75	0.002	1
1	A	102	HEM	HAC	6.537	0.001	1
1	A	102	HEM	HMB	4.326	0.003	1
1	A	102	HEM	HMBA	4.326	0.003	1
1	A	102	HEM	HMBB	4.326	0.003	1
1	A	102	HEM	HMC	4.085	0.003	1
1	A	102	HEM	HMCA	4.085	0.003	1
1	A	102	HEM	HMCB	4.085	0.003	1
1	A	102	HEM	HMD	3.448	0.002	1
1	A	102	HEM	HMDA	3.448	0.002	1
1	A	102	HEM	HMDB	3.448	0.002	1
1	A	102	HEM	HMA	3.829	0.002	1
1	A	102	HEM	HMAA	3.829	0.002	1
1	A	102	HEM	HMAB	3.829	0.002	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	102	HEM	HBB	1.609	0.002	1
1	A	102	HEM	HBBA	1.609	0.002	1
1	A	102	HEM	HBC	2.923	0.003	1
1	A	102	HEM	HBCA	2.923	0.003	1
1	A	103	HEM	HAD	3.807	0.002	2
1	A	103	HEM	HADA	4.167	0.000	2
1	A	103	HEM	HAA	4.448	0.001	2
1	A	103	HEM	HAAA	3.942	0.002	2
1	A	103	HEM	HHC	8.974	0.002	1
1	A	103	HEM	HBD	3.017	0.001	2
1	A	103	HEM	HBDA	3.27	0.002	2
1	A	103	HEM	HBA	3.063	0.002	2
1	A	103	HEM	HBAA	3.472	0.003	2
1	A	103	HEM	HHD	9.244	0.001	1
1	A	103	HEM	HHB	9.308	0.001	1
1	A	103	HEM	HHA	9.475	0.002	1
1	A	103	HEM	HAB	5.956	0.002	1
1	A	103	HEM	HAC	6.225	0.002	1
1	A	103	HEM	HMB	3.532	0.001	1
1	A	103	HEM	HMBA	3.532	0.001	1
1	A	103	HEM	HMBB	3.532	0.001	1
1	A	103	HEM	HMC	2.976	0.001	1
1	A	103	HEM	HMCA	2.976	0.001	1
1	A	103	HEM	HMCB	2.976	0.001	1
1	A	103	HEM	HMD	3.45	0.001	1
1	A	103	HEM	HMDA	3.45	0.001	1
1	A	103	HEM	HMDB	3.45	0.001	1
1	A	103	HEM	HMA	3.325	0.063	1
1	A	103	HEM	HMAA	3.325	0.063	1
1	A	103	HEM	HMAB	3.325	0.063	1
1	A	103	HEM	HBB	1.983	0.003	1
1	A	103	HEM	HBBA	1.983	0.003	1
1	A	103	HEM	HBC	1.501	0.001	1
1	A	103	HEM	HBCA	1.501	0.001	1

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	None (insufficient data)

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Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	65	0.70 ± 0.47	None needed (imprecise)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 55%, i.e. 484 atoms were assigned a chemical shift out of a possible 881. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	205/347 (59%)	141/144 (98%)	0/138 (0%)	64/65 (98%)
Sidechain	244/462 (53%)	242/293 (83%)	0/151 (0%)	2/18 (11%)
Aromatic	35/72 (49%)	29/39 (74%)	0/27 (0%)	6/6 (100%)
Overall	484/881 (55%)	412/476 (87%)	0/316 (0%)	72/89 (81%)

7.1.4 Statistically unusual chemical shifts

The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	15	PHE	HE1	0.72	5.56 – 8.62	-20.8
1	A	17	HIS	HD2	-0.38	4.65 – 9.35	-15.7
1	A	21	GLN	HE21	1.09	5.02 – 9.43	-13.9
1	A	31	HIS	HD2	0.54	4.65 – 9.35	-13.7
1	A	47	HIS	HD2	0.61	4.65 – 9.35	-13.6
1	A	69	HIS	HD2	0.73	4.65 – 9.35	-13.3
1	A	62	PRO	HD2	-0.74	1.93 – 5.38	-12.7
1	A	55	HIS	HD2	1.06	4.65 – 9.35	-12.6
1	A	10	ASN	HD21	1.32	4.94 – 9.72	-12.6
1	A	69	HIS	HE1	0.87	5.13 – 10.76	-12.6
1	A	20	HIS	HD2	1.11	4.65 – 9.35	-12.5
1	A	47	HIS	HE1	1.07	5.13 – 10.76	-12.2
1	A	17	HIS	HE1	1.16	5.13 – 10.76	-12.1
1	A	20	HIS	HE1	1.19	5.13 – 10.76	-12.0
1	A	35	PRO	HA	0.64	2.78 – 6.00	-11.7
1	A	31	HIS	HE1	1.40	5.13 – 10.76	-11.6
1	A	55	HIS	HE1	1.56	5.13 – 10.76	-11.3

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List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	43	LYS	HD3	-0.51	0.54 – 2.65	-10.0
1	A	43	LYS	HG2	-1.07	0.13 – 2.61	-9.8
1	A	17	HIS	HA	0.82	2.49 – 6.71	-9.0
1	A	61	GLY	HA2	1.06	2.15 – 5.77	-8.0
1	A	21	GLN	HG2	0.36	1.01 – 3.62	-7.5
1	A	17	HIS	HB2	0.49	1.36 – 4.85	-7.5
1	A	36	GLY	H	3.87	5.23 – 11.42	-7.2
1	A	13	VAL	HG21	-1.06	-0.58 – 2.19	-6.7
1	A	13	VAL	HG22	-1.06	-0.58 – 2.19	-6.7
1	A	13	VAL	HG23	-1.06	-0.58 – 2.19	-6.7
1	A	31	HIS	HB2	0.87	1.36 – 4.85	-6.4
1	A	69	HIS	HB2	0.97	1.36 – 4.85	-6.1
1	A	21	GLN	HE22	4.50	4.88 – 9.19	-5.9
1	A	31	HIS	HB3	0.85	1.18 – 4.91	-5.9
1	A	20	HIS	HB2	1.06	1.36 – 4.85	-5.8
1	A	17	HIS	HB3	1.10	1.18 – 4.91	-5.2
1	A	47	HIS	HB2	1.34	1.36 – 4.85	-5.0

7.1.5 Random Coil Index (RCI) plots

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A: