



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:56 pm BST

PDB ID : 2LZZ
Title : Solution structure of a mutant of the triheme cytochrome PpcA from *Geobacter sulfurreducens* sheds light on the role of the conserved aromatic residue F15
Authors : Dantas, J.M.; Morgado, L.; Turner, D.L.; Salgueiro, C.A.
Deposited on : 2012-10-12

This is a Full wwPDB NMR 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/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
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)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

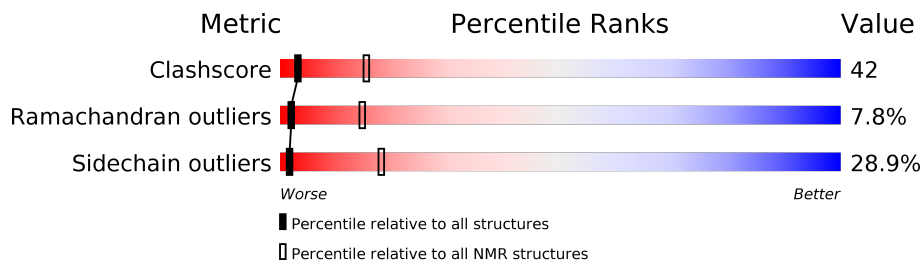
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 51%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	71	

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:3-A:41, A:45-A:71 (66)	0.13	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 3 clusters and 4 single-model clusters were found.

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

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1195 atoms, of which 534 are hydrogens and 0 are deuteriums.

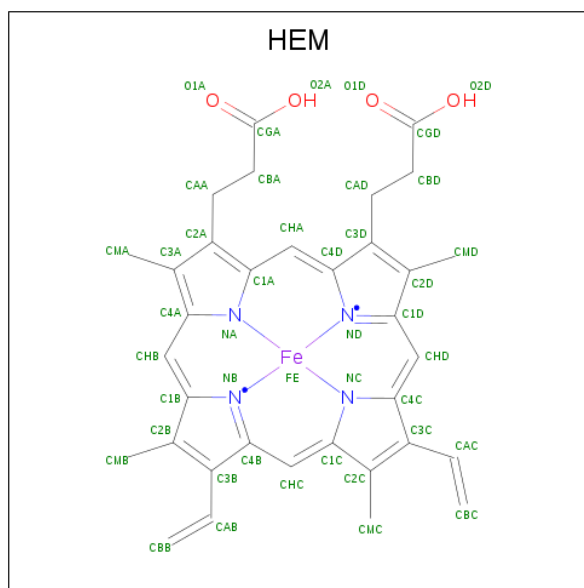
- Molecule 1 is a protein called Cytochrome c, 3 heme-binding sites.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	71	1066	328	534	102	94	8	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	LEU	PHE	ENGINEERED MUTATION	UNP D7AFU0

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



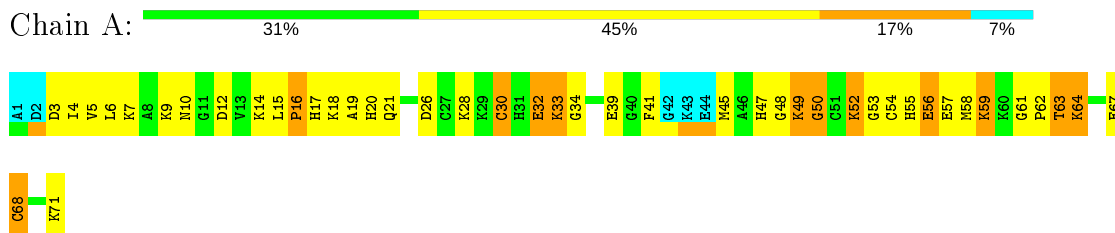
Mol	Chain	Residues	Atoms				
			Total	C	Fe	N	O
2	A	1	43	34	1	4	4
2	A	1	43	34	1	4	4
2	A	1	43	34	1	4	4

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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, 3 heme-binding sites

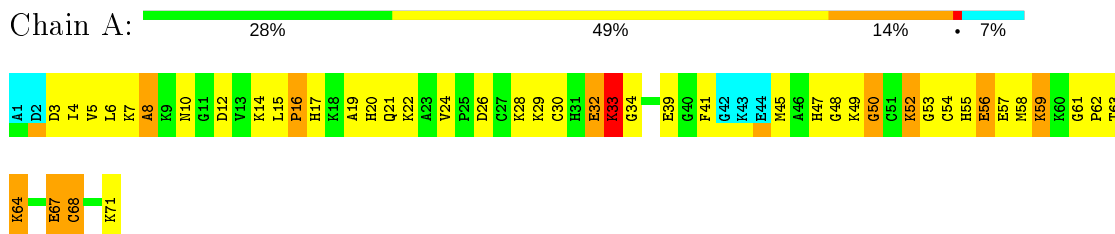


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

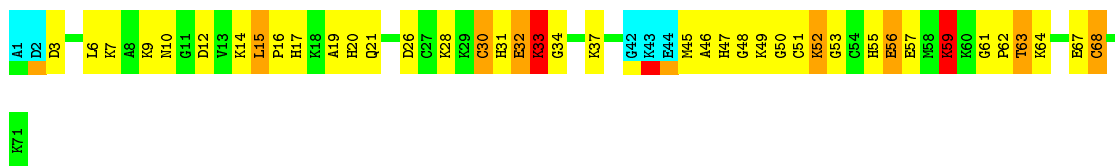
- Molecule 1: Cytochrome c, 3 heme-binding sites



4.2.2 Score per residue for model 2

- Molecule 1: Cytochrome c, 3 heme-binding sites

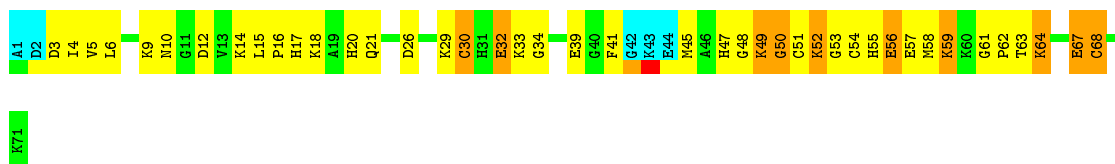




4.2.3 Score per residue for model 3

- Molecule 1: Cytochrome c, 3 heme-binding sites

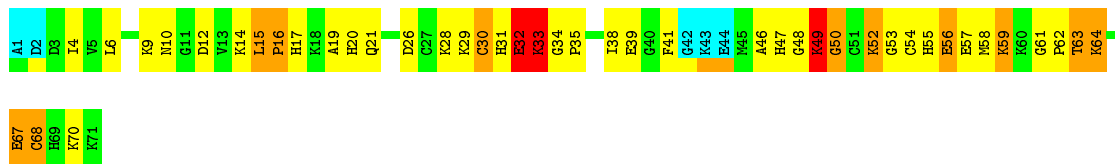
Chain A: 34% 45% 14% 7%



4.2.4 Score per residue for model 4

- Molecule 1: Cytochrome c, 3 heme-binding sites

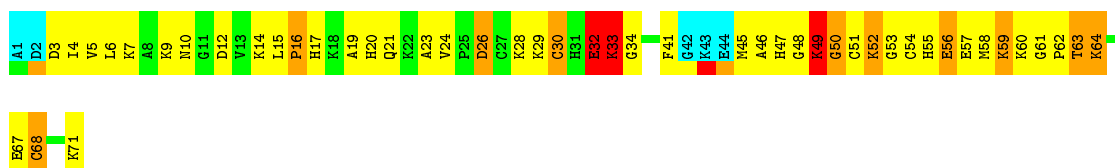
Chain A: 31% 42% 15% 7%



4.2.5 Score per residue for model 5 (medoid)

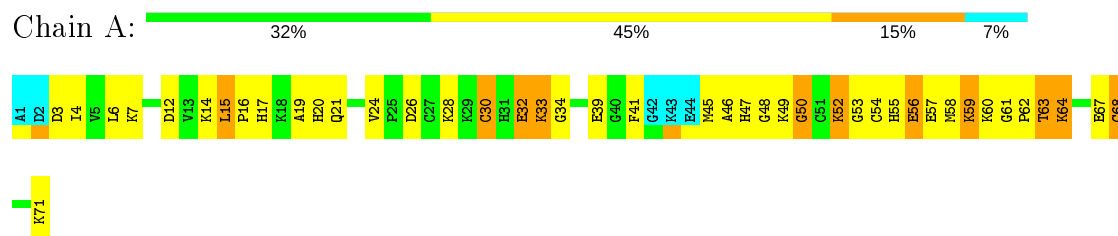
- Molecule 1: Cytochrome c, 3 heme-binding sites

Chain A: 25% 49% 14% 7%



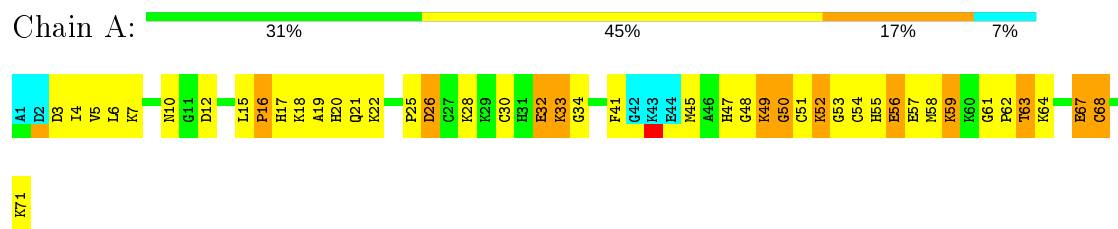
4.2.6 Score per residue for model 6

- Molecule 1: Cytochrome c, 3 heme-binding sites



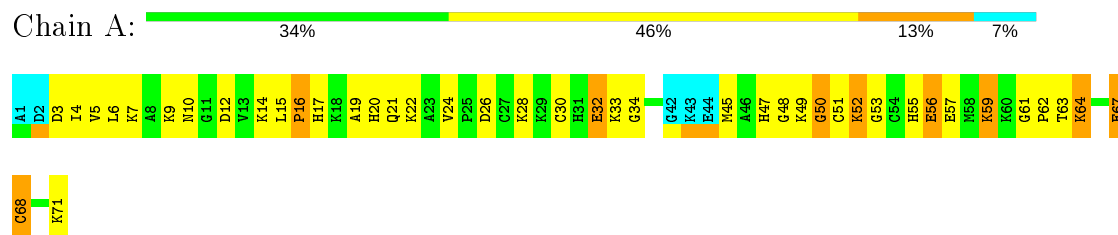
4.2.7 Score per residue for model 7

- Molecule 1: Cytochrome c, 3 heme-binding sites



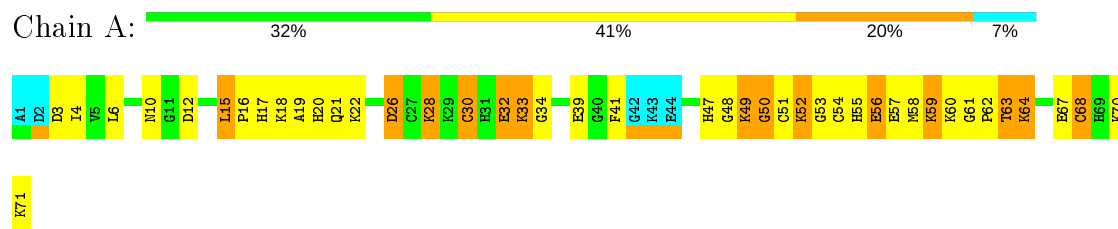
4.2.8 Score per residue for model 8

- Molecule 1: Cytochrome c, 3 heme-binding sites



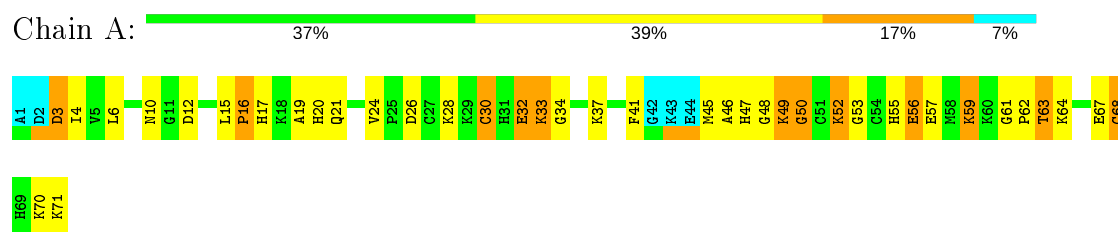
4.2.9 Score per residue for model 9

- Molecule 1: Cytochrome c, 3 heme-binding sites



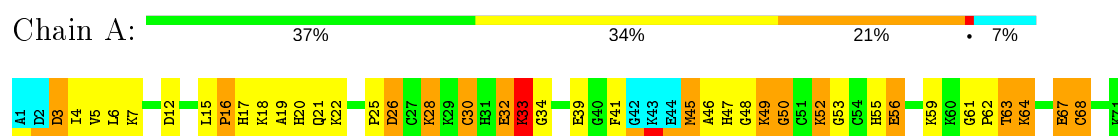
4.2.10 Score per residue for model 10

- Molecule 1: Cytochrome c, 3 heme-binding sites



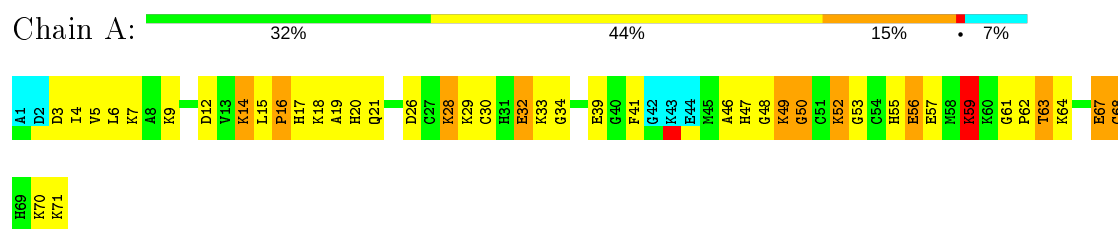
4.2.11 Score per residue for model 11

- Molecule 1: Cytochrome c, 3 heme-binding sites



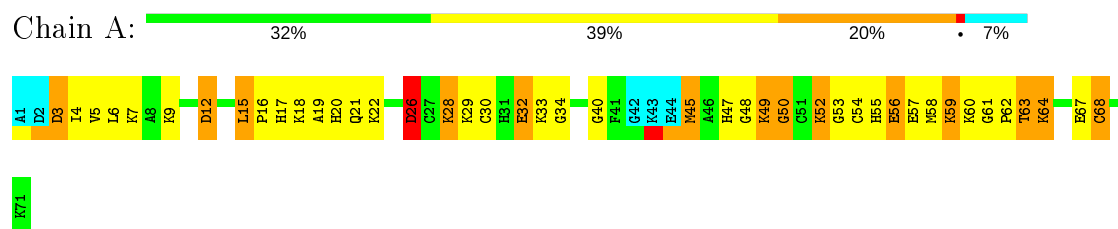
4.2.12 Score per residue for model 12

- Molecule 1: Cytochrome c, 3 heme-binding sites



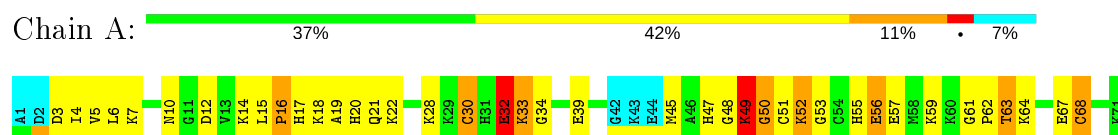
4.2.13 Score per residue for model 13

- Molecule 1: Cytochrome c, 3 heme-binding sites



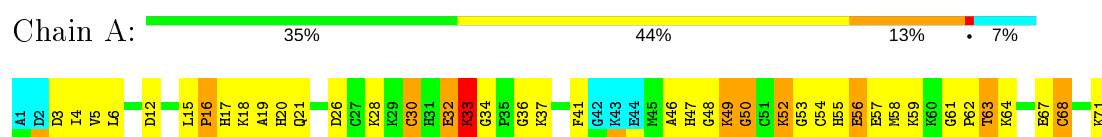
4.2.14 Score per residue for model 14

- Molecule 1: Cytochrome c, 3 heme-binding sites



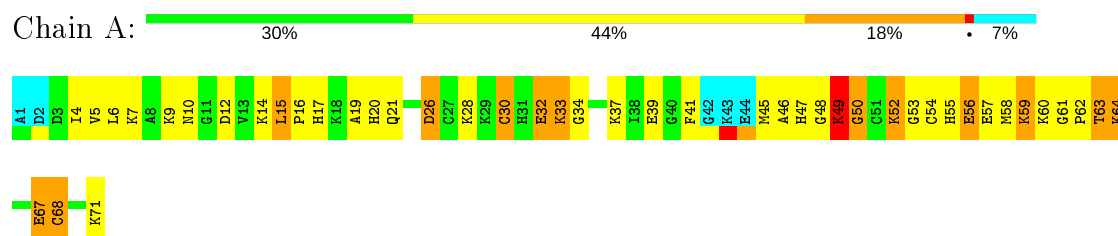
4.2.15 Score per residue for model 15

- Molecule 1: Cytochrome c, 3 heme-binding sites



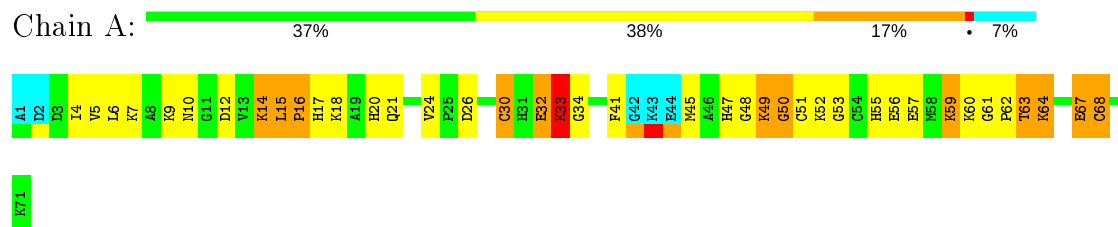
4.2.16 Score per residue for model 16

- Molecule 1: Cytochrome c, 3 heme-binding sites



4.2.17 Score per residue for model 17

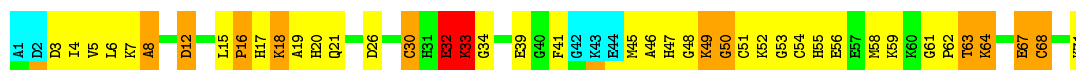
- Molecule 1: Cytochrome c, 3 heme-binding sites



4.2.18 Score per residue for model 18

- Molecule 1: Cytochrome c, 3 heme-binding sites

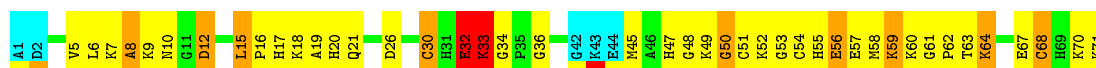
Chain A:  34% 41% 15% 7%



4.2.19 Score per residue for model 19


- Molecule 1: Cytochrome c, 3 heme-binding sites

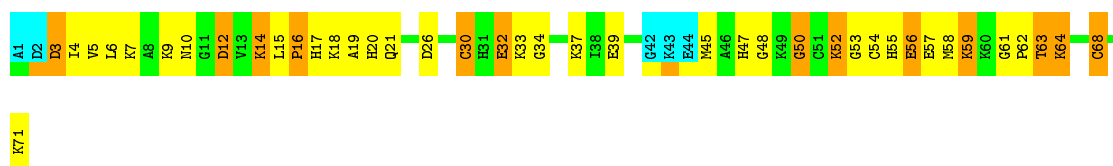
Chain A:  32% 45% 13% 7%



4.2.20 Score per residue for model 20

- Molecule 1: Cytochrome c, 3 heme-binding sites

Chain A:  35% 39% 18% 7%



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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	551
Number of shifts mapped to atoms	510
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	41
Assignment completeness (well-defined parts)	51%

No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality i

6.1 Standard geometry i

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 i

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	497	502	510	42±4
2	A	129	0	90	22±3
All	All	12520	10040	12000	1035

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 42.

All unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:102:HEM:HBC2	2:A:102:HEM:HMC1	1.00	1.32	9	9
2:A:102:HEM:HMC1	2:A:102:HEM:HBC2	0.99	1.35	3	7
2:A:103:HEM:O2D	2:A:103:HEM:HMD1	0.88	1.68	3	1
2:A:103:HEM:O1D	2:A:103:HEM:HMD1	0.87	1.68	19	3
1:A:16:PRO:HB2	1:A:19:ALA:HB3	0.78	1.55	15	18
1:A:15:LEU:HD13	2:A:102:HEM:C2B	0.77	2.15	9	20
1:A:32:GLU:OE2	1:A:38:ILE:HG23	0.75	1.81	4	1
1:A:6:LEU:HD13	2:A:103:HEM:O1D	0.71	1.85	20	4
1:A:6:LEU:HD22	2:A:103:HEM:O1D	0.71	1.85	3	1
1:A:52:LYS:CD	1:A:63:THR:HG22	0.70	2.17	13	12
1:A:6:LEU:HD21	2:A:101:HEM:O1D	0.69	1.87	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:LEU:HD13	2:A:102:HEM:C3B	0.68	2.24	5	20
1:A:3:ASP:OD1	1:A:5:VAL:HG23	0.67	1.90	20	1
2:A:102:HEM:CGD	2:A:102:HEM:HMD2	0.67	2.19	18	6
2:A:102:HEM:HBC2	2:A:102:HEM:CMC	0.67	2.19	14	10
1:A:4:ILE:HG22	1:A:4:ILE:O	0.67	1.89	8	10
1:A:30:CYS:SG	2:A:102:HEM:HMC3	0.67	2.30	17	4
2:A:102:HEM:CMC	2:A:102:HEM:HBC2	0.66	2.18	9	9
1:A:4:ILE:O	1:A:4:ILE:HG22	0.66	1.90	17	8
2:A:102:HEM:HMC1	2:A:102:HEM:CBC	0.66	2.19	4	7
2:A:102:HEM:CBC	2:A:102:HEM:HMC1	0.64	2.19	7	9
1:A:7:LYS:O	1:A:8:ALA:HB2	0.63	1.93	19	3
1:A:17:HIS:CE1	1:A:21:GLN:NE2	0.62	2.67	14	14
1:A:21:GLN:OE1	2:A:101:HEM:C2B	0.60	2.54	6	4
2:A:102:HEM:HMB1	2:A:102:HEM:HBB2	0.60	1.73	11	10
2:A:103:HEM:HMD1	2:A:103:HEM:O1D	0.60	1.97	20	1
1:A:52:LYS:HD3	1:A:63:THR:HG22	0.60	1.74	20	15
1:A:10:ASN:ND2	2:A:103:HEM:C3A	0.59	2.70	7	2
1:A:15:LEU:O	1:A:17:HIS:N	0.59	2.35	4	14
1:A:17:HIS:CE1	1:A:21:GLN:CD	0.59	2.76	6	14
1:A:6:LEU:HD21	2:A:101:HEM:O2D	0.59	1.98	13	3
1:A:64:LYS:O	2:A:103:HEM:HMC1	0.57	1.99	10	18
2:A:102:HEM:HBB2	2:A:102:HEM:HMB1	0.57	1.76	14	10
2:A:102:HEM:HMD2	2:A:102:HEM:CGD	0.57	2.28	14	3
1:A:6:LEU:HD22	2:A:103:HEM:O2D	0.56	2.00	19	1
1:A:30:CYS:SG	2:A:102:HEM:HMC2	0.56	2.41	6	10
2:A:102:HEM:HBC2	2:A:102:HEM:HMC2	0.56	1.76	14	3
1:A:24:VAL:HG12	1:A:24:VAL:O	0.56	2.00	1	2
1:A:24:VAL:O	1:A:24:VAL:HG12	0.56	2.00	17	3
1:A:53:GLY:O	1:A:57:GLU:CB	0.55	2.55	7	18
2:A:102:HEM:HMC2	2:A:102:HEM:HBC2	0.55	1.77	20	1
1:A:17:HIS:O	1:A:21:GLN:N	0.55	2.40	6	20
1:A:16:PRO:CB	1:A:19:ALA:HB3	0.55	2.30	18	9
2:A:101:HEM:CMC	2:A:101:HEM:HBC2	0.54	2.32	14	7
2:A:102:HEM:CMD	2:A:102:HEM:CGD	0.54	2.85	18	3
2:A:101:HEM:CGD	2:A:101:HEM:HMD2	0.54	2.32	17	2
1:A:20:HIS:CE1	2:A:102:HEM:NA	0.54	2.75	4	20
2:A:101:HEM:O1D	2:A:101:HEM:HMD2	0.54	2.03	18	1
2:A:102:HEM:CGD	2:A:102:HEM:CMD	0.54	2.85	2	2
1:A:20:HIS:HB3	2:A:101:HEM:HBC2	0.54	1.78	13	7
2:A:101:HEM:HBC2	2:A:101:HEM:CMC	0.53	2.33	19	2
1:A:62:PRO:HD3	2:A:102:HEM:C2A	0.53	2.39	9	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:101:HEM:O2D	2:A:101:HEM:HMD2	0.53	2.04	9	2
1:A:47:HIS:CE1	2:A:103:HEM:NA	0.52	2.78	13	20
1:A:4:ILE:CG2	1:A:4:ILE:O	0.52	2.58	13	9
1:A:41:PHE:CZ	1:A:46:ALA:HB2	0.52	2.40	12	9
1:A:5:VAL:CG1	1:A:12:ASP:CG	0.51	2.79	7	11
1:A:48:GLY:O	1:A:50:GLY:N	0.51	2.44	18	20
1:A:52:LYS:HD2	1:A:63:THR:HG22	0.51	1.81	13	2
1:A:5:VAL:CG1	1:A:12:ASP:OD1	0.51	2.59	19	6
2:A:101:HEM:HBC1	2:A:102:HEM:C2C	0.51	2.41	19	7
1:A:32:GLU:OE1	1:A:33:LYS:CD	0.51	2.59	8	1
1:A:55:HIS:CD2	1:A:61:GLY:HA3	0.50	2.41	4	20
2:A:102:HEM:HMB1	2:A:102:HEM:CBB	0.50	2.36	11	13
1:A:5:VAL:HG11	1:A:12:ASP:OD2	0.50	2.05	11	3
1:A:10:ASN:OD1	2:A:103:HEM:CGA	0.50	2.59	4	11
2:A:103:HEM:CMD	2:A:103:HEM:O1D	0.50	2.59	20	1
1:A:55:HIS:HB3	1:A:63:THR:HG23	0.50	1.82	19	18
1:A:49:LYS:CG	1:A:49:LYS:O	0.50	2.60	7	2
2:A:102:HEM:CBC	2:A:102:HEM:CMC	0.50	2.89	14	9
2:A:101:HEM:HBC1	2:A:102:HEM:C1C	0.50	2.42	17	4
1:A:4:ILE:O	1:A:4:ILE:CG2	0.50	2.59	14	3
1:A:62:PRO:CB	1:A:67:GLU:O	0.50	2.60	9	18
1:A:68:CYS:HB2	2:A:103:HEM:C2C	0.50	2.41	12	20
1:A:54:CYS:O	1:A:58:MET:N	0.50	2.43	15	13
1:A:5:VAL:HG11	1:A:12:ASP:OD1	0.49	2.07	3	4
1:A:49:LYS:O	1:A:49:LYS:CG	0.49	2.60	12	2
2:A:102:HEM:CBC	2:A:102:HEM:HMC2	0.49	2.38	14	3
1:A:16:PRO:HG2	1:A:20:HIS:ND1	0.49	2.23	9	6
1:A:5:VAL:CG1	1:A:12:ASP:OD2	0.49	2.60	11	5
1:A:41:PHE:CD2	1:A:45:MET:HB3	0.49	2.42	11	1
1:A:55:HIS:CE1	1:A:62:PRO:HD2	0.49	2.42	18	20
1:A:17:HIS:ND1	1:A:21:GLN:NE2	0.49	2.59	17	3
2:A:102:HEM:CBB	2:A:102:HEM:HMB1	0.49	2.38	14	7
2:A:101:HEM:O1D	2:A:101:HEM:CMD	0.49	2.61	18	1
1:A:56:GLU:HG2	1:A:63:THR:HG22	0.49	1.83	17	2
2:A:102:HEM:HMC2	2:A:102:HEM:CBC	0.49	2.38	20	1
1:A:55:HIS:O	1:A:59:LYS:N	0.49	2.45	9	19
2:A:102:HEM:CMC	2:A:102:HEM:CBC	0.49	2.89	9	8
1:A:6:LEU:HD13	2:A:103:HEM:O2D	0.49	2.07	12	1
1:A:21:GLN:OE1	2:A:101:HEM:C3B	0.48	2.65	17	4
1:A:61:GLY:HA2	2:A:102:HEM:CHA	0.48	2.39	8	8
1:A:52:LYS:O	1:A:55:HIS:N	0.48	2.46	6	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:LYS:O	1:A:56:GLU:N	0.48	2.34	10	17
1:A:52:LYS:O	1:A:56:GLU:CG	0.48	2.62	10	18
1:A:21:GLN:HG2	2:A:101:HEM:C4B	0.48	2.44	6	5
1:A:17:HIS:ND1	1:A:21:GLN:OE1	0.47	2.48	16	13
1:A:32:GLU:O	1:A:34:GLY:N	0.47	2.48	4	19
1:A:62:PRO:HD3	2:A:102:HEM:C1A	0.47	2.45	4	7
1:A:7:LYS:O	1:A:8:ALA:CB	0.47	2.59	19	1
1:A:52:LYS:HE3	1:A:63:THR:HG22	0.46	1.87	19	1
1:A:32:GLU:C	1:A:34:GLY:N	0.46	2.68	19	20
1:A:16:PRO:HG2	1:A:20:HIS:HD1	0.46	1.70	9	6
2:A:103:HEM:HMD1	2:A:103:HEM:CGD	0.46	2.40	20	1
1:A:51:CYS:O	1:A:55:HIS:CG	0.46	2.69	9	5
1:A:32:GLU:CD	1:A:33:LYS:N	0.46	2.69	8	1
1:A:17:HIS:ND1	1:A:21:GLN:CD	0.46	2.69	9	9
2:A:102:HEM:O1D	2:A:102:HEM:CMD	0.46	2.64	5	1
2:A:101:HEM:O1D	2:A:101:HEM:HMD1	0.46	2.11	8	1
1:A:15:LEU:CD1	2:A:102:HEM:C2B	0.45	2.96	6	10
1:A:26:ASP:O	1:A:28:LYS:N	0.45	2.49	12	5
1:A:18:LYS:O	1:A:21:GLN:N	0.45	2.50	9	5
1:A:48:GLY:O	1:A:53:GLY:N	0.45	2.48	18	2
1:A:10:ASN:ND2	2:A:103:HEM:C2A	0.45	2.85	7	2
2:A:101:HEM:HMD1	2:A:101:HEM:O2D	0.45	2.11	20	2
1:A:51:CYS:HA	2:A:102:HEM:CHC	0.44	2.43	2	8
1:A:28:LYS:O	1:A:31:HIS:N	0.44	2.50	2	1
2:A:101:HEM:HMD2	2:A:101:HEM:CGD	0.44	2.42	9	1
2:A:101:HEM:CMD	2:A:101:HEM:O2D	0.44	2.66	17	2
2:A:101:HEM:CBC	2:A:101:HEM:CMC	0.44	2.96	14	3
1:A:52:LYS:O	1:A:53:GLY:C	0.44	2.55	11	13
1:A:32:GLU:O	1:A:33:LYS:C	0.43	2.56	4	18
1:A:14:LYS:CE	1:A:16:PRO:HG3	0.43	2.44	20	3
1:A:32:GLU:CG	1:A:33:LYS:N	0.43	2.80	19	5
1:A:21:GLN:HG2	2:A:101:HEM:CHC	0.43	2.44	13	4
2:A:102:HEM:CHA	2:A:102:HEM:HBA1	0.43	2.44	14	4
1:A:16:PRO:O	1:A:17:HIS:C	0.43	2.57	13	9
1:A:32:GLU:OE2	1:A:38:ILE:CG2	0.43	2.61	4	1
2:A:102:HEM:CBA	2:A:102:HEM:HHA	0.42	2.45	11	13
1:A:62:PRO:HB3	1:A:67:GLU:O	0.42	2.15	7	7
1:A:19:ALA:O	1:A:23:ALA:N	0.42	2.53	5	1
1:A:6:LEU:O	1:A:12:ASP:OD1	0.42	2.38	9	13
1:A:28:LYS:C	1:A:30:CYS:N	0.42	2.72	2	2
2:A:101:HEM:CMC	2:A:101:HEM:CBC	0.42	2.98	17	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:102:HEM:HHA	2:A:102:HEM:CBA	0.42	2.45	13	6
2:A:102:HEM:HBA1	2:A:102:HEM:CHA	0.41	2.45	17	4
1:A:36:GLY:HA2	2:A:101:HEM:CBA	0.41	2.46	19	2
1:A:6:LEU:O	1:A:12:ASP:OD2	0.41	2.39	1	6
1:A:45:MET:SD	1:A:49:LYS:O	0.41	2.79	7	4
1:A:17:HIS:HD1	1:A:21:GLN:NE2	0.41	2.13	6	1
1:A:6:LEU:HD13	2:A:103:HEM:CGD	0.41	2.46	3	1
1:A:25:PRO:C	1:A:26:ASP:CG	0.41	2.80	7	1
1:A:25:PRO:O	1:A:26:ASP:CG	0.41	2.59	11	2
1:A:40:GLY:O	1:A:45:MET:SD	0.41	2.79	13	1
1:A:10:ASN:OD1	2:A:103:HEM:O1A	0.40	2.39	14	2
1:A:32:GLU:HG3	1:A:33:LYS:N	0.40	2.32	12	1
1:A:31:HIS:CG	1:A:35:PRO:HA	0.40	2.50	4	1
1:A:10:ASN:OD1	2:A:103:HEM:O2A	0.40	2.40	5	1
1:A:24:VAL:O	1:A:26:ASP:N	0.40	2.49	5	1

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	65/71 (92%)	45±2 (69±3%)	15±2 (23±3%)	5±1 (8±1%)	2	14
All	All	1300/1420 (92%)	897 (69%)	301 (23%)	102 (8%)	2	14

All 9 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	32	GLU	20
1	A	50	GLY	19
1	A	49	LYS	19
1	A	16	PRO	14
1	A	33	LYS	13
1	A	59	LYS	8
1	A	12	ASP	4

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Mol	Chain	Res	Type	Models (Total)
1	A	8	ALA	3
1	A	26	ASP	2

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	53/56 (95%)	38±2 (71±4%)	15±2 (29±4%)	2 18
All	All	1060/1120 (95%)	754 (71%)	306 (29%)	2 18

All 27 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	30	CYS	20
1	A	68	CYS	20
1	A	52	LYS	19
1	A	56	GLU	18
1	A	26	ASP	17
1	A	63	THR	16
1	A	64	LYS	16
1	A	33	LYS	13
1	A	71	LYS	13
1	A	14	LYS	12
1	A	28	LYS	12
1	A	7	LYS	12
1	A	49	LYS	11
1	A	9	LYS	11
1	A	45	MET	11
1	A	67	GLU	11
1	A	59	LYS	11
1	A	39	GLU	11
1	A	15	LEU	8
1	A	22	LYS	7
1	A	60	LYS	7
1	A	29	LYS	6
1	A	70	LYS	5

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Mol	Chain	Res	Type	Models (Total)
1	A	37	LYS	5
1	A	32	GLU	5
1	A	18	LYS	5
1	A	3	ASP	4

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.6 Ligand geometry [i](#)

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	102	1	27,50,50	1.60±0.00	0±0 (0±0%)
2	HEM	A	103	1	27,50,50	1.60±0.00	0±0 (0±0%)
2	HEM	A	101	1	27,50,50	1.60±0.00	0±0 (0±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	102	1	17,82,82	1.25±0.00	0±0 (0±0%)
2	HEM	A	103	1	17,82,82	1.25±0.00	0±0 (0±0%)
2	HEM	A	101	1	17,82,82	1.25±0.00	0±0 (0±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	101	1	-	0±0,6,54,54	-
2	HEM	A	103	1	-	0±0,6,54,54	-
2	HEM	A	102	1	-	0±0,6,54,54	-

There are no bond-length outliers.

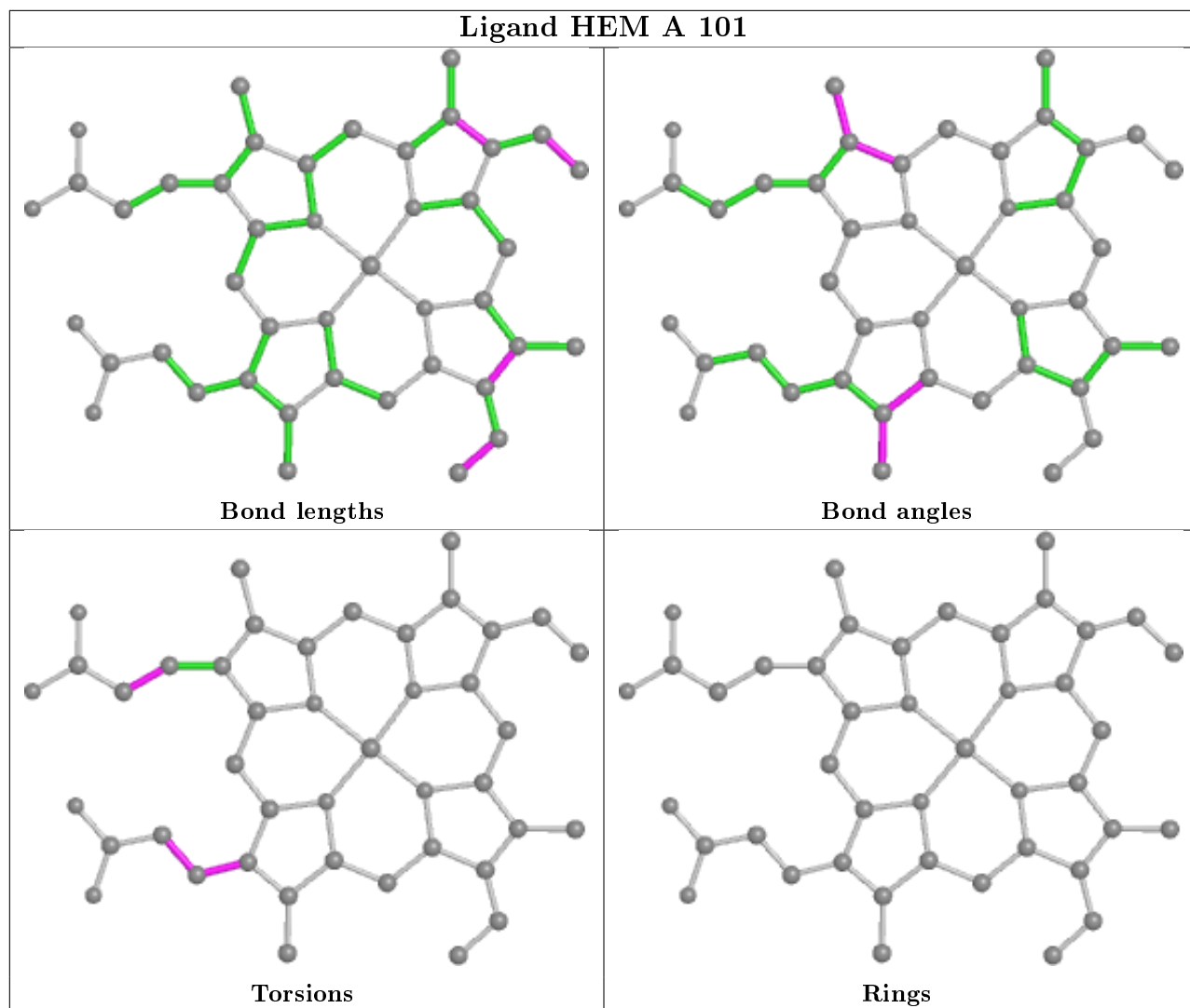
There are no bond-angle outliers.

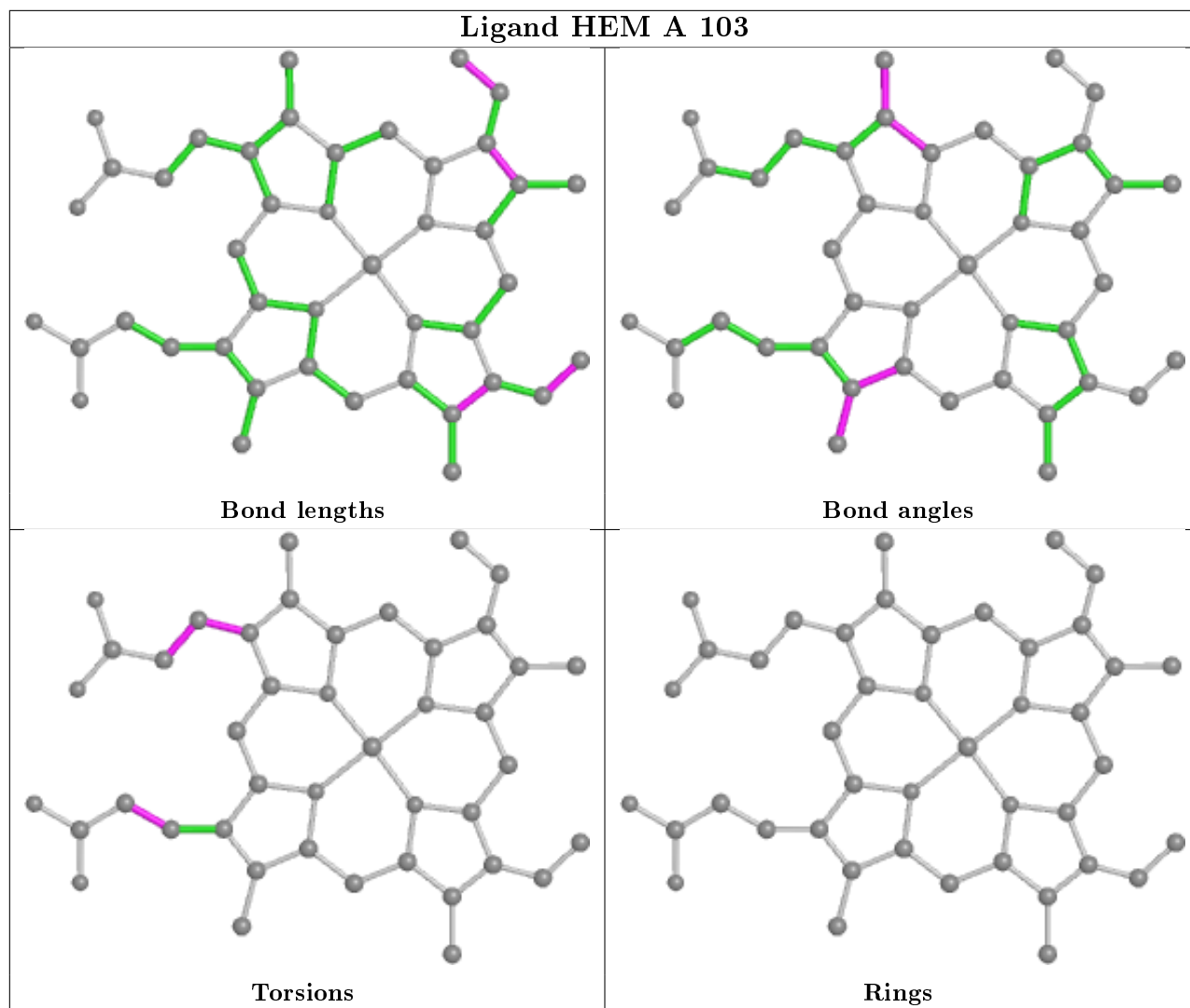
There are no chirality outliers.

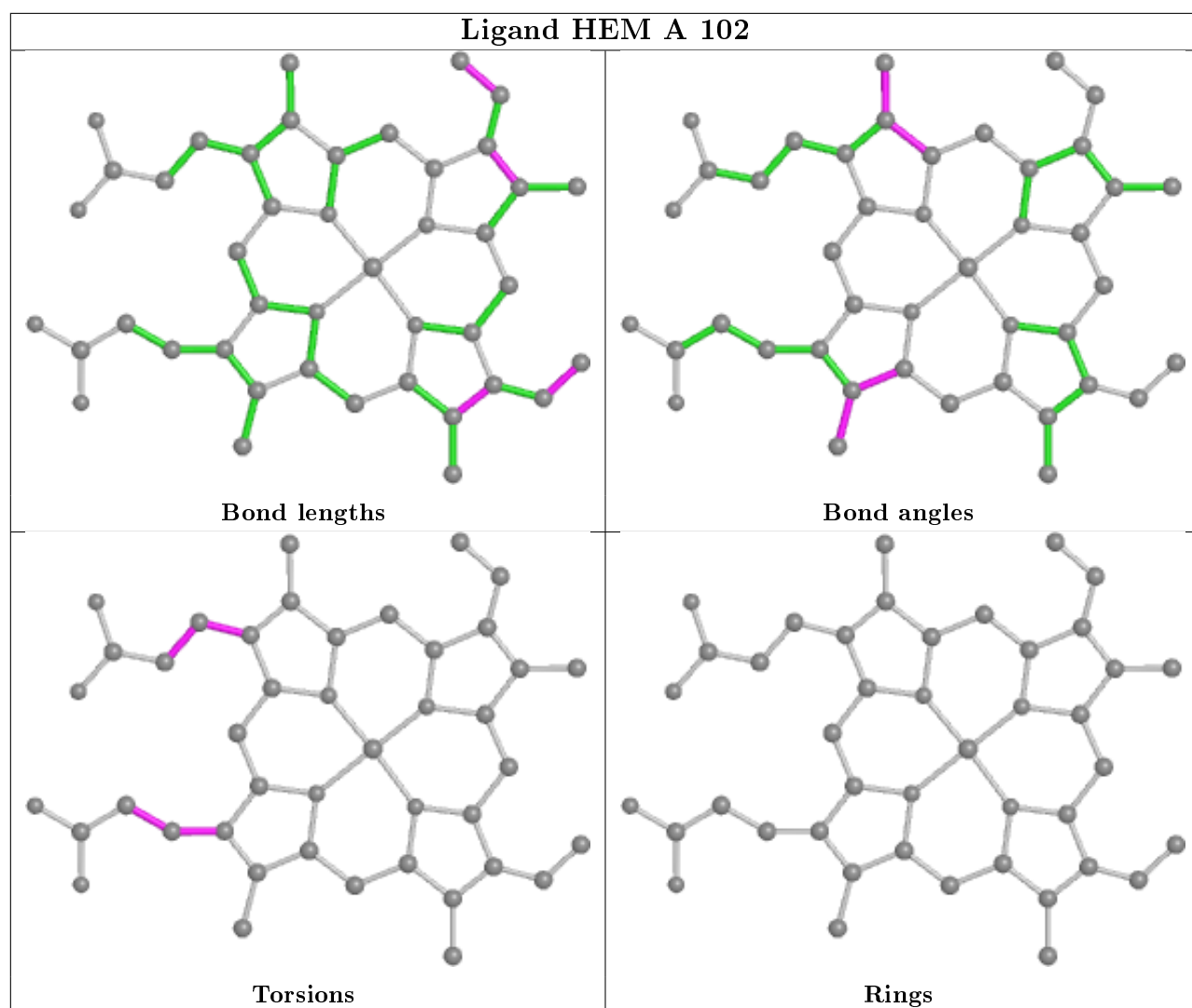
There are no torsion outliers.

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 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.







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 51% for the well-defined parts and 51% for the entire structure.

7.1 Chemical shift list 1

File name: input_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	551
Number of shifts mapped to atoms	510
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	41
Number of shift outliers (ShiftChecker)	38

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

- No matching atoms found in structure. All 41 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	103	HEM	HA72	4.444	0.002	1
A	103	HEM	HAM	8.987	0.002	1
A	103	HEM	HT4A	6.237	0.002	1
A	102	HEM	HB72	3.242	0.003	1
A	103	HEM	HB63	3.723	0.003	1
A	102	HEM	HDM	9.927	0.002	1
A	101	HEM	HA63	4.24	0.005	1
A	101	HEM	HGM	9.235	0.002	1
A	103	HEM	HA73	3.97	0.004	1
A	102	HEM	HT2A	7.292	0.003	1
A	102	HEM	HGM	9.42	0.001	1
A	101	HEM	HT4A	6.063	0.004	1
A	103	HEM	HB72	3.111	0.004	1
A	101	HEM	HBM	8.879	0.002	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	101	HEM	HA62	3.448	0.003	1
A	102	HEM	HT4A	6.518	0.002	1
A	103	HEM	HGM	9.466	0.005	1
A	102	HEM	HB63	2.977	0.002	1
A	102	HEM	HAM	10.583	0.001	1
A	102	HEM	HA73	4.153	0.005	1
A	103	HEM	HDM	9.363	0.002	1
A	102	HEM	HA72	4.117	0.0	1
A	101	HEM	HB62	2.474	0.004	1
A	103	HEM	HBM	9.322	0.002	1
A	103	HEM	HT2A	6.006	0.003	1
A	102	HEM	HB62	2.849	0.003	1
A	101	HEM	HAM	9.446	0.003	1
A	103	HEM	HA63	4.192	0.003	1
A	102	HEM	HA62	3.773	0.006	1
A	103	HEM	HB73	3.474	0.002	1
A	101	HEM	HB63	3.065	0.003	1
A	101	HEM	HA72	3.912	0.008	1
A	101	HEM	HB73	2.922	0.007	1
A	103	HEM	HA62	3.872	0.003	1
A	102	HEM	HBM	9.737	0.002	1
A	102	HEM	HA63	4.13	0.005	1
A	101	HEM	HDM	9.449	0.001	1
A	101	HEM	HT2A	6.119	0.003	1
A	101	HEM	HA73	3.927	0.003	1
A	103	HEM	HB62	3.119	0.003	1
A	101	HEM	HB72	2.809	0.001	1

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	0	—	None (insufficient data)
$^{13}\text{C}_\beta$	0	—	None (insufficient data)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	65	0.73 ± 0.43	None needed (imprecise)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 51%, i.e. 413 atoms were assigned a chemical shift out of a possible 802. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	190/322 (59%)	128/128 (100%)	0/132 (0%)	62/62 (100%)
Sidechain	197/429 (46%)	195/259 (75%)	0/152 (0%)	2/18 (11%)
Aromatic	26/51 (51%)	20/29 (69%)	0/16 (0%)	6/6 (100%)
Overall	413/802 (51%)	343/416 (82%)	0/300 (0%)	70/86 (81%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 51%, i.e. 439 atoms were assigned a chemical shift out of a possible 853. 0 out of 5 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	201/347 (58%)	136/138 (99%)	0/142 (0%)	65/67 (97%)
Sidechain	212/455 (47%)	210/274 (77%)	0/162 (0%)	2/19 (11%)
Aromatic	26/51 (51%)	20/29 (69%)	0/16 (0%)	6/6 (100%)
Overall	439/853 (51%)	366/441 (83%)	0/320 (0%)	73/92 (79%)

7.1.4 Statistically unusual chemical shifts [i](#)

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.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	31	HIS	HD2	0.45	9.28 – 4.78	-14.6
1	A	17	HIS	HD2	0.51	9.28 – 4.78	-14.5
1	A	47	HIS	HD2	0.72	9.28 – 4.78	-14.0
1	A	69	HIS	HD2	0.77	9.28 – 4.78	-13.9
1	A	69	HIS	HE1	0.94	10.53 – 5.43	-13.8
1	A	20	HIS	HE1	1.10	10.53 – 5.43	-13.5
1	A	55	HIS	HD2	0.98	9.28 – 4.78	-13.4
1	A	20	HIS	HD2	1.00	9.28 – 4.78	-13.4
1	A	17	HIS	HE1	1.17	10.53 – 5.43	-13.3
1	A	31	HIS	HE1	1.31	10.53 – 5.43	-13.1
1	A	10	ASN	HD21	1.13	9.74 – 4.94	-12.9
1	A	55	HIS	HE1	1.51	10.53 – 5.43	-12.7
1	A	62	PRO	HD2	-0.91	5.45 – 1.85	-12.7
1	A	21	GLN	HE21	2.04	9.53 – 4.93	-11.3

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	35	PRO	HA	0.77	6.05 – 2.75	-11.0
1	A	43	LYS	HG2	-1.29	2.67 – 0.07	-10.2
1	A	43	LYS	HD3	-0.52	2.75 – 0.45	-9.2
1	A	15	LEU	HD11	-1.31	2.16 – -0.64	-7.4
1	A	15	LEU	HD12	-1.31	2.16 – -0.64	-7.4
1	A	15	LEU	HD13	-1.31	2.16 – -0.64	-7.4
1	A	61	GLY	HA3	1.31	5.80 – 2.00	-6.8
1	A	17	HIS	HA	1.65	6.81 – 2.41	-6.7
1	A	21	GLN	HG2	0.54	3.67 – 0.97	-6.6
1	A	36	GLY	H	3.99	11.63 – 5.03	-6.6
1	A	17	HIS	HB2	0.79	4.91 – 1.31	-6.4
1	A	31	HIS	HB2	0.92	4.91 – 1.31	-6.1
1	A	13	VAL	HG23	-0.89	2.20 – -0.60	-6.0
1	A	13	VAL	HG22	-0.89	2.20 – -0.60	-6.0
1	A	13	VAL	HG21	-0.89	2.20 – -0.60	-6.0
1	A	20	HIS	HB2	1.05	4.91 – 1.31	-5.7
1	A	42	GLY	HA2	1.79	5.87 – 2.07	-5.7
1	A	15	LEU	HG	-0.36	3.16 – -0.14	-5.7
1	A	31	HIS	HB3	0.86	5.00 – 1.10	-5.6
1	A	4	ILE	HD12	-0.89	2.13 – -0.77	-5.4
1	A	4	ILE	HD13	-0.89	2.13 – -0.77	-5.4
1	A	4	ILE	HD11	-0.89	2.13 – -0.77	-5.4
1	A	69	HIS	HB3	1.03	5.00 – 1.10	-5.2
1	A	69	HIS	HB2	1.25	4.91 – 1.31	-5.2

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.

Random coil index (RCI) for chain A:

