



Full wwPDB NMR Structure Validation Report ⓘ

Jun 14, 2020 – 03:12 pm BST

PDB ID : 2MZ9
Title : Solution structure of oxidized triheme cytochrome PpcA from *Geobacter sulfurreducens*
Authors : Morgado, L.; Bruix, M.; Pokkuluri, R.; Salgueiro, C.A.; Turner, D.L.
Deposited on : 2015-02-08

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

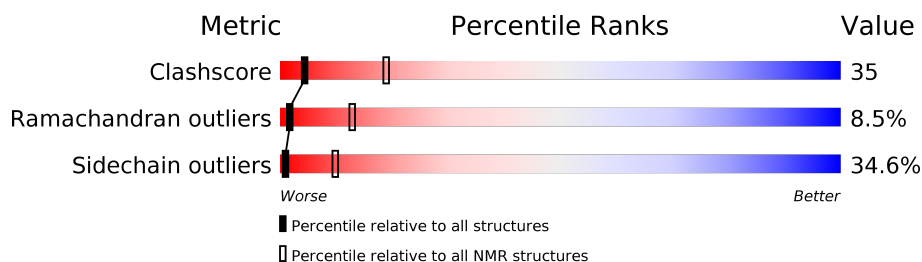
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 47%.

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 10 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:23, A:28-A:71 (66)	0.31	10

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 2 single-model clusters were found.

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

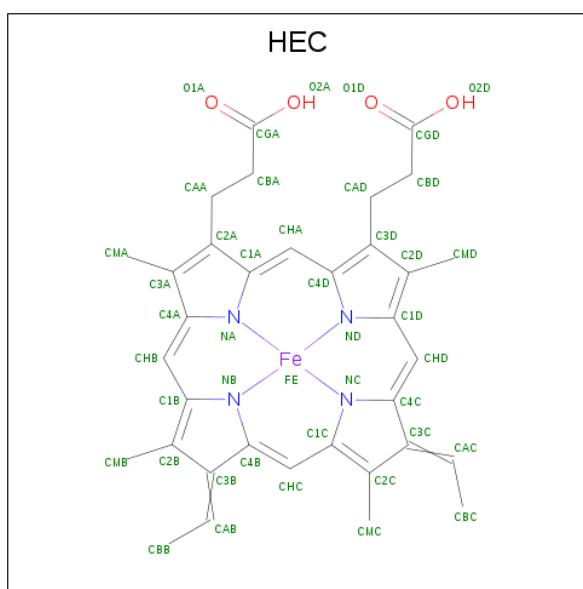
3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 1166 atoms, of which 502 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called PpcA.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	71	1037	331	502	102	94	8	0

- Molecule 2 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



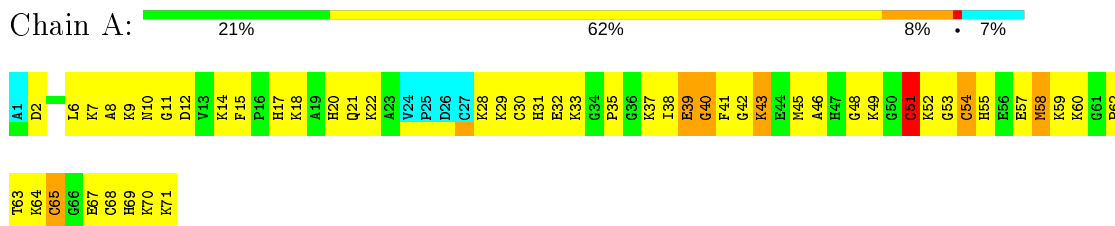
Mol	Chain	Residues	Atoms				
			Total	C	Fe	N	O
2	A	1	43	34	1	4	4
2	A	1	43	34	1	4	4
2	A	1	43	34	1	4	4

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: PpcA

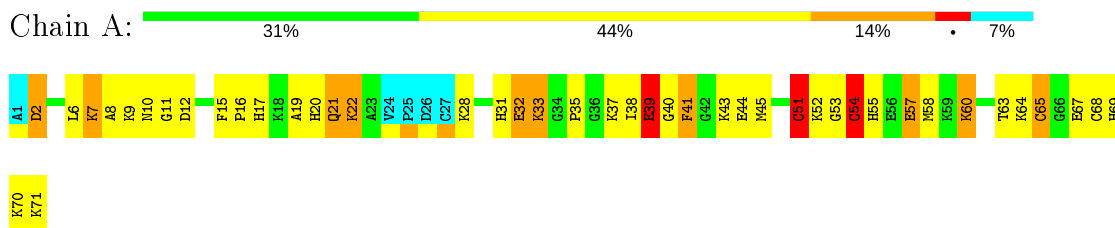


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

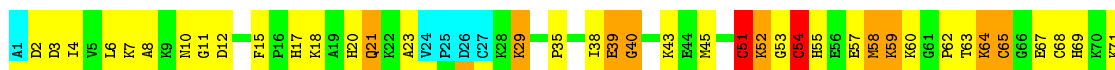
- Molecule 1: PpcA



4.2.2 Score per residue for model 2

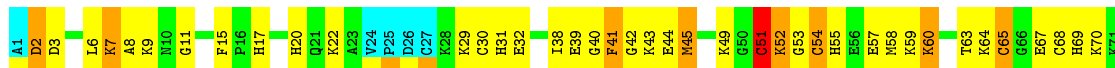
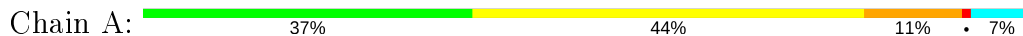
- Molecule 1: PpcA





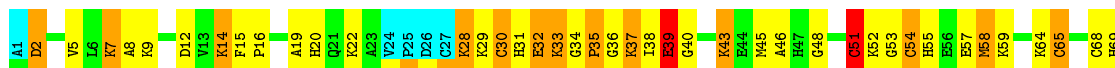
4.2.3 Score per residue for model 3

- Molecule 1: PpcA



4.2.4 Score per residue for model 4

- Molecule 1: PpcA



4.2.5 Score per residue for model 5

- Molecule 1: PpcA



4.2.6 Score per residue for model 6

- Molecule 1: PpcA





4.2.7 Score per residue for model 7

- Molecule 1: PpcA

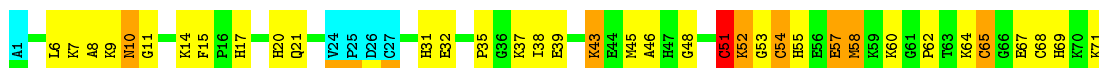
Chain A: 35% 45% 11% • 7%



4.2.8 Score per residue for model 8

- Molecule 1: PpcA

Chain A: 42% 39% 10% • 7%



4.2.9 Score per residue for model 9

- Molecule 1: PpcA

Chain A: 30% 54% 8% • 7%



4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: PpcA

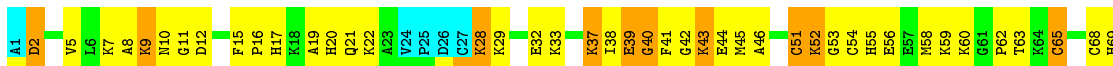
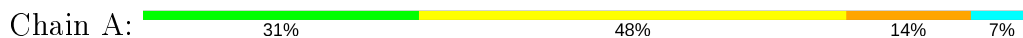
Chain A: 25% 48% 17% • 7%





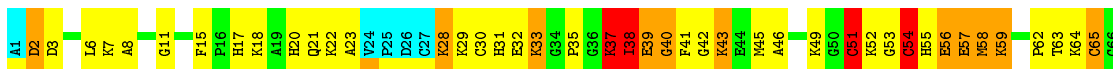
4.2.11 Score per residue for model 11

- Molecule 1: PpcA



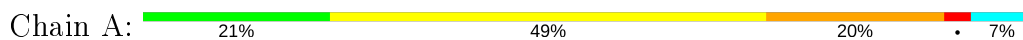
4.2.12 Score per residue for model 12

- Molecule 1: PpcA



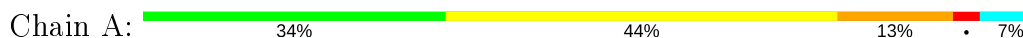
4.2.13 Score per residue for model 13

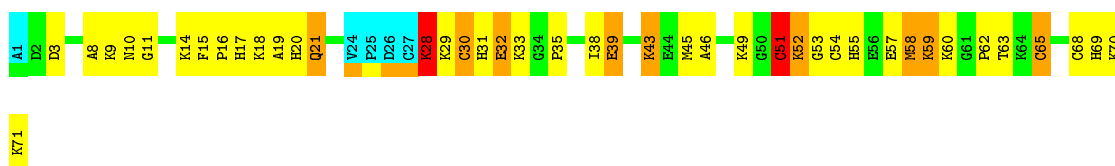
- Molecule 1: PpcA



4.2.14 Score per residue for model 14

- Molecule 1: PpcA

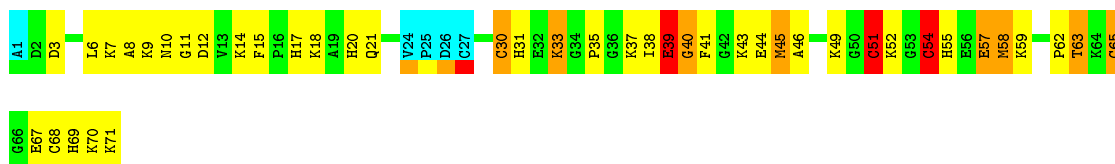




4.2.15 Score per residue for model 15

- Molecule 1: PpcA

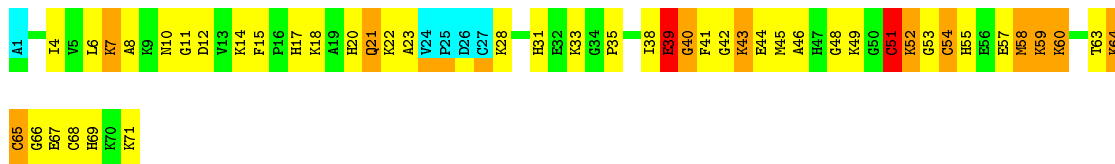
Chain A: 32% 45% 11% 7%



4.2.16 Score per residue for model 16

- Molecule 1: PpcA

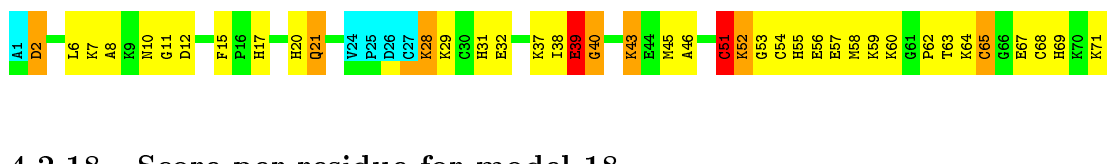
Chain A: 27% 48% 15% 7%



4.2.17 Score per residue for model 17

- Molecule 1: PpcA

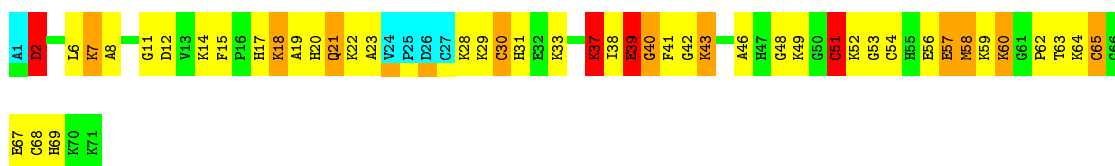
Chain A: 37% 44% 10% 7%



4.2.18 Score per residue for model 18

- Molecule 1: PpcA

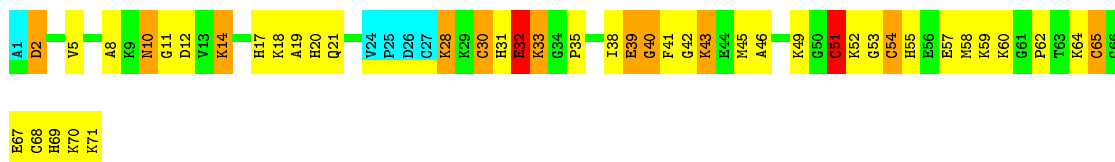
Chain A: 28% 45% 14% 6% 7%



4.2.19 Score per residue for model 19

- Molecule 1: PpcA

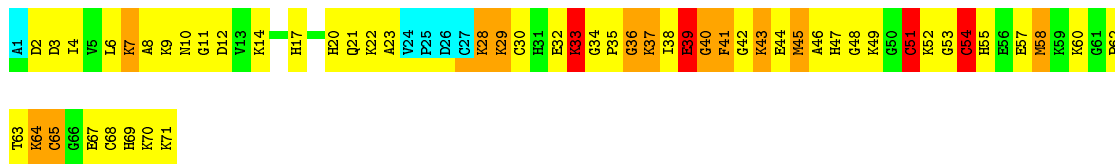
Chain A: 31% 44% 15% 7%



4.2.20 Score per residue for model 20

- Molecule 1: PpcA

Chain A: 17% 54% 17% 6% 7%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 500 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	structure solution	
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	504
Number of shifts mapped to atoms	445
Number of unparsed shifts	0
Number of shifts with mapping errors	59
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	47%

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: HEC

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	502	476	510	37±7
2	A	129	0	90	20±5
All	All	12620	9520	12000	869

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.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:62:PRO:HG2	2:A:102:HEC:HMA3	0.89	1.40	7	7
1:A:8:ALA:HB3	1:A:11:GLY:O	0.89	1.68	9	19
2:A:102:HEC:HMC1	2:A:102:HEC:HBC3	0.88	1.46	18	2
2:A:101:HEC:HMB1	2:A:101:HEC:HBB2	0.87	1.47	19	8
2:A:101:HEC:HBB2	2:A:101:HEC:HMB1	0.87	1.46	3	7
1:A:58:MET:SD	2:A:102:HEC:HMD3	0.83	2.14	7	2
1:A:15:PHE:CE2	2:A:102:HEC:HBB2	0.83	2.09	8	6
2:A:101:HEC:HBB3	2:A:101:HEC:HMB1	0.81	1.50	16	3
2:A:101:HEC:HMB1	2:A:101:HEC:HBB3	0.81	1.52	8	1
2:A:101:HEC:HMB1	2:A:101:HEC:CBB	0.80	2.07	4	12
1:A:52:LYS:CG	1:A:63:THR:HG22	0.79	2.07	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:15:PHE:CD2	2:A:102:HEC:HBB2	0.78	2.14	8	5
2:A:101:HEC:CBB	2:A:101:HEC:HMB1	0.77	2.08	16	5
2:A:103:HEC:HMB1	2:A:103:HEC:HBB3	0.77	1.56	13	10
1:A:32:GLU:O	1:A:33:LYS:CB	0.76	2.33	19	7
1:A:5:VAL:HG13	1:A:12:ASP:OD1	0.75	1.81	4	3
1:A:62:PRO:HG2	2:A:102:HEC:CMA	0.75	2.12	7	5
2:A:103:HEC:HMC1	2:A:103:HEC:HBC3	0.74	1.59	4	14
1:A:43:LYS:NZ	2:A:103:HEC:CAD	0.74	2.51	18	2
2:A:102:HEC:HMC1	2:A:102:HEC:CBC	0.72	2.13	17	2
2:A:103:HEC:HBB3	2:A:103:HEC:HMB1	0.72	1.60	12	10
1:A:43:LYS:NZ	1:A:47:HIS:CE1	0.71	2.58	20	1
1:A:62:PRO:HG3	2:A:102:HEC:HMA3	0.71	1.60	20	6
1:A:68:CYS:SG	2:A:102:HEC:HMB3	0.71	2.26	4	6
1:A:17:HIS:CE1	1:A:21:GLN:NE2	0.70	2.60	6	3
1:A:64:LYS:O	2:A:103:HEC:HMC3	0.69	1.86	3	16
1:A:32:GLU:O	1:A:33:LYS:HB2	0.69	1.86	19	1
1:A:43:LYS:HZ1	2:A:103:HEC:CAD	0.67	2.02	18	1
1:A:23:ALA:HB2	2:A:102:HEC:O2D	0.66	1.90	16	2
1:A:8:ALA:HB2	2:A:103:HEC:HBD2	0.66	1.67	18	4
1:A:15:PHE:CE1	2:A:102:HEC:C1B	0.66	2.78	9	6
2:A:103:HEC:O1D	2:A:103:HEC:HMD1	0.66	1.90	10	1
1:A:17:HIS:O	1:A:20:HIS:N	0.66	2.29	12	16
1:A:38:ILE:O	1:A:39:GLU:C	0.66	2.33	15	15
1:A:51:CYS:O	1:A:55:HIS:CE1	0.66	2.49	2	16
1:A:31:HIS:CE1	1:A:38:ILE:HD11	0.66	2.25	5	3
1:A:41:PHE:CD1	1:A:42:GLY:N	0.65	2.64	13	12
2:A:103:HEC:HBC3	2:A:103:HEC:HMC1	0.65	1.68	9	4
1:A:32:GLU:O	1:A:33:LYS:CG	0.64	2.46	14	2
1:A:60:LYS:CE	2:A:102:HEC:HMD1	0.62	2.24	1	3
1:A:23:ALA:HB2	2:A:102:HEC:CGD	0.62	2.23	16	1
1:A:31:HIS:O	1:A:32:GLU:CB	0.61	2.49	14	3
2:A:101:HEC:CHA	2:A:101:HEC:CGD	0.61	2.78	12	1
1:A:33:LYS:O	1:A:33:LYS:CG	0.61	2.48	12	1
1:A:30:CYS:SG	2:A:101:HEC:HMC1	0.60	2.35	14	6
1:A:41:PHE:CD1	2:A:101:HEC:O1D	0.60	2.54	15	1
1:A:17:HIS:CE1	1:A:21:GLN:OE1	0.60	2.55	11	2
1:A:63:THR:O	2:A:103:HEC:HMC2	0.59	1.97	7	14
1:A:46:ALA:HB1	2:A:103:HEC:C1D	0.59	2.26	15	1
1:A:41:PHE:CE1	1:A:42:GLY:O	0.59	2.55	20	5
1:A:43:LYS:HZ1	2:A:103:HEC:HAD2	0.58	1.56	18	1
1:A:52:LYS:HG3	1:A:63:THR:HG22	0.58	1.75	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ALA:O	2:A:102:HEC:HMD2	0.58	1.97	20	2
1:A:4:ILE:HD13	2:A:101:HEC:O2D	0.58	1.97	13	1
1:A:62:PRO:CG	2:A:102:HEC:HMA3	0.58	2.22	7	5
1:A:43:LYS:CG	2:A:103:HEC:CHA	0.57	2.82	6	3
1:A:14:LYS:CD	1:A:14:LYS:O	0.57	2.52	13	2
2:A:101:HEC:C4D	2:A:101:HEC:CGD	0.57	2.82	12	1
2:A:102:HEC:HMB1	2:A:102:HEC:HBB3	0.57	1.77	4	5
1:A:3:ASP:CB	1:A:14:LYS:NZ	0.56	2.67	5	1
2:A:101:HEC:O2D	2:A:101:HEC:C3D	0.56	2.52	12	1
1:A:43:LYS:CE	2:A:103:HEC:CHA	0.55	2.83	20	1
1:A:15:PHE:CE1	2:A:102:HEC:C2B	0.55	2.89	8	5
2:A:101:HEC:HBC1	2:A:102:HEC:C2C	0.55	2.31	17	5
1:A:43:LYS:HG2	2:A:103:HEC:CHA	0.55	2.31	6	3
1:A:43:LYS:NZ	2:A:103:HEC:C3D	0.55	2.70	18	1
1:A:43:LYS:O	1:A:46:ALA:N	0.55	2.39	20	13
1:A:60:LYS:HE3	2:A:102:HEC:HMD1	0.55	1.79	5	3
1:A:39:GLU:O	1:A:40:GLY:C	0.55	2.45	7	14
1:A:38:ILE:O	1:A:40:GLY:N	0.55	2.40	2	13
1:A:65:CYS:O	1:A:68:CYS:N	0.55	2.39	16	19
1:A:31:HIS:O	1:A:33:LYS:N	0.55	2.40	4	6
2:A:101:HEC:HBC1	2:A:102:HEC:HMC2	0.54	1.79	17	2
1:A:43:LYS:HZ2	1:A:47:HIS:CE1	0.54	2.19	20	1
1:A:28:LYS:O	1:A:32:GLU:N	0.54	2.41	17	4
1:A:4:ILE:HD11	2:A:101:HEC:O1A	0.54	2.02	20	2
1:A:52:LYS:O	1:A:53:GLY:C	0.54	2.45	5	19
2:A:102:HEC:O1A	2:A:102:HEC:C1A	0.53	2.57	8	1
1:A:43:LYS:HE3	2:A:103:HEC:C4D	0.53	2.33	20	1
2:A:102:HEC:CHA	2:A:102:HEC:O1A	0.53	2.56	8	1
1:A:14:LYS:O	1:A:14:LYS:CG	0.53	2.57	4	1
1:A:15:PHE:CD1	2:A:102:HEC:C2B	0.53	2.92	6	13
1:A:63:THR:O	2:A:103:HEC:CMC	0.53	2.56	6	11
1:A:23:ALA:CB	2:A:102:HEC:O2D	0.53	2.57	12	3
1:A:62:PRO:HD3	2:A:102:HEC:C2A	0.53	2.34	20	13
1:A:39:GLU:O	1:A:39:GLU:CG	0.52	2.58	12	2
1:A:49:LYS:O	1:A:49:LYS:CG	0.52	2.57	18	1
1:A:15:PHE:CE1	2:A:102:HEC:C4B	0.52	2.93	6	8
1:A:38:ILE:HD13	2:A:101:HEC:CGD	0.52	2.34	6	1
1:A:38:ILE:HD13	2:A:101:HEC:O1D	0.52	2.05	6	1
1:A:62:PRO:HG3	2:A:102:HEC:CMA	0.52	2.34	12	1
1:A:2:ASP:OD1	1:A:3:ASP:N	0.52	2.42	12	1
2:A:101:HEC:CMB	2:A:101:HEC:CBB	0.52	2.85	9	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:GLY:O	1:A:53:GLY:N	0.52	2.42	20	8
1:A:23:ALA:HB2	2:A:102:HEC:O1D	0.52	2.05	12	2
1:A:10:ASN:O	1:A:10:ASN:CG	0.51	2.46	15	3
1:A:54:CYS:O	1:A:57:GLU:N	0.51	2.43	20	15
1:A:31:HIS:O	1:A:32:GLU:C	0.51	2.49	9	2
1:A:23:ALA:CB	2:A:102:HEC:CGD	0.51	2.88	16	3
1:A:65:CYS:O	1:A:69:HIS:N	0.51	2.42	10	20
1:A:58:MET:O	1:A:59:LYS:CB	0.51	2.58	14	1
1:A:14:LYS:CG	1:A:14:LYS:O	0.51	2.59	13	2
1:A:54:CYS:O	1:A:58:MET:N	0.51	2.43	16	13
2:A:101:HEC:HHA	2:A:101:HEC:CGD	0.51	2.36	12	1
1:A:49:LYS:CG	1:A:49:LYS:O	0.50	2.59	16	1
1:A:37:LYS:CD	2:A:101:HEC:O2D	0.50	2.59	1	1
1:A:8:ALA:CB	1:A:11:GLY:O	0.50	2.59	5	8
2:A:103:HEC:CBA	2:A:103:HEC:HHA	0.50	2.36	4	2
1:A:10:ASN:CG	1:A:10:ASN:O	0.50	2.49	9	7
1:A:53:GLY:O	1:A:57:GLU:N	0.50	2.45	18	2
1:A:38:ILE:N	2:A:101:HEC:O1D	0.50	2.45	9	1
1:A:4:ILE:CD1	2:A:101:HEC:O1A	0.50	2.60	2	1
1:A:15:PHE:CE1	1:A:20:HIS:CD2	0.49	3.00	11	2
1:A:43:LYS:HE3	2:A:103:HEC:CHA	0.49	2.36	20	1
2:A:101:HEC:HBC1	2:A:102:HEC:CMC	0.49	2.37	17	2
2:A:101:HEC:HMA3	2:A:101:HEC:HBA2	0.49	1.84	6	1
1:A:58:MET:O	1:A:60:LYS:CD	0.49	2.61	2	1
1:A:32:GLU:O	1:A:33:LYS:HG3	0.49	2.06	14	1
1:A:6:LEU:O	1:A:7:LYS:C	0.49	2.50	5	13
1:A:54:CYS:SG	2:A:102:HEC:HMC1	0.49	2.48	5	4
1:A:29:LYS:CD	2:A:102:HEC:HBC1	0.49	2.37	17	3
2:A:101:HEC:CBB	2:A:101:HEC:CMB	0.49	2.85	8	4
1:A:43:LYS:N	1:A:43:LYS:CE	0.49	2.76	4	1
1:A:10:ASN:O	1:A:10:ASN:ND2	0.48	2.46	19	1
2:A:103:HEC:CBB	2:A:103:HEC:HMB1	0.48	2.36	13	1
1:A:23:ALA:CB	2:A:102:HEC:O1D	0.48	2.62	20	2
1:A:16:PRO:O	1:A:19:ALA:HB3	0.48	2.08	11	4
1:A:43:LYS:HG3	2:A:103:HEC:CHA	0.48	2.37	4	1
1:A:21:GLN:O	1:A:21:GLN:OE1	0.48	2.31	20	2
1:A:21:GLN:NE2	1:A:21:GLN:O	0.48	2.46	1	1
2:A:102:HEC:HBB3	2:A:102:HEC:HMB1	0.48	1.86	10	4
1:A:17:HIS:ND1	1:A:21:GLN:OE1	0.48	2.47	8	2
1:A:62:PRO:HG2	2:A:102:HEC:C3A	0.48	2.39	9	1
1:A:3:ASP:OD2	1:A:14:LYS:CE	0.48	2.62	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:9:LYS:N	2:A:103:HEC:O2A	0.48	2.47	11	1
1:A:37:LYS:O	1:A:38:ILE:C	0.48	2.52	12	3
1:A:40:GLY:O	1:A:41:PHE:C	0.48	2.53	5	4
1:A:32:GLU:O	1:A:33:LYS:CD	0.48	2.62	6	1
1:A:55:HIS:O	1:A:59:LYS:N	0.47	2.47	11	6
1:A:41:PHE:CD1	1:A:41:PHE:C	0.47	2.88	11	6
1:A:60:LYS:CE	2:A:102:HEC:CMD	0.47	2.92	1	2
1:A:36:GLY:O	1:A:37:LYS:C	0.47	2.51	20	3
1:A:38:ILE:HD13	2:A:101:HEC:HBD1	0.47	1.86	3	2
1:A:8:ALA:HB3	1:A:11:GLY:C	0.47	2.30	8	1
1:A:31:HIS:HE1	1:A:38:ILE:HD11	0.47	1.66	6	3
1:A:29:LYS:HD3	2:A:102:HEC:HBC1	0.47	1.84	17	2
1:A:15:PHE:CZ	1:A:20:HIS:CD2	0.47	3.03	4	2
1:A:44:GLU:N	1:A:44:GLU:OE1	0.47	2.47	15	3
1:A:29:LYS:HD2	2:A:102:HEC:HBC1	0.47	1.87	6	1
1:A:15:PHE:CE1	2:A:102:HEC:C3B	0.47	2.97	12	4
2:A:102:HEC:O2D	2:A:102:HEC:C3D	0.47	2.62	12	1
1:A:43:LYS:NZ	2:A:103:HEC:CGD	0.47	2.78	14	1
1:A:14:LYS:HG2	1:A:14:LYS:O	0.47	2.10	19	1
1:A:6:LEU:HB3	2:A:103:HEC:CGD	0.47	2.40	10	3
1:A:31:HIS:CE1	2:A:101:HEC:ND	0.47	2.82	13	3
1:A:4:ILE:HG21	2:A:101:HEC:O2D	0.47	2.10	13	1
1:A:60:LYS:HE2	2:A:102:HEC:HMD1	0.47	1.87	1	2
1:A:52:LYS:HG2	1:A:63:THR:HG22	0.47	1.84	15	1
1:A:33:LYS:O	1:A:33:LYS:HG3	0.47	2.10	14	2
2:A:103:HEC:HMB1	2:A:103:HEC:CBB	0.47	2.37	5	1
1:A:41:PHE:C	1:A:41:PHE:CD1	0.46	2.88	19	3
2:A:103:HEC:HHA	2:A:103:HEC:CBA	0.46	2.41	8	1
1:A:7:LYS:O	2:A:103:HEC:CGD	0.46	2.63	18	2
1:A:43:LYS:NZ	1:A:47:HIS:NE2	0.46	2.63	20	1
1:A:10:ASN:ND2	2:A:103:HEC:O1A	0.46	2.49	1	1
1:A:2:ASP:CG	1:A:3:ASP:N	0.46	2.67	13	2
1:A:21:GLN:O	1:A:21:GLN:CD	0.46	2.54	15	3
1:A:58:MET:O	1:A:60:LYS:N	0.46	2.49	16	1
1:A:3:ASP:CG	1:A:14:LYS:NZ	0.46	2.69	15	1
1:A:52:LYS:O	1:A:55:HIS:N	0.46	2.49	5	1
1:A:8:ALA:HB2	2:A:103:HEC:CBD	0.46	2.41	4	1
1:A:17:HIS:O	1:A:18:LYS:C	0.46	2.53	18	3
1:A:4:ILE:CD1	2:A:101:HEC:O2D	0.46	2.63	13	1
2:A:102:HEC:O2A	2:A:102:HEC:C2A	0.45	2.64	14	1
1:A:65:CYS:O	1:A:67:GLU:N	0.45	2.48	16	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:HIS:O	1:A:19:ALA:N	0.45	2.49	18	3
1:A:46:ALA:O	1:A:51:CYS:HB3	0.45	2.11	15	3
1:A:55:HIS:CE1	2:A:102:HEC:NB	0.45	2.84	15	5
1:A:43:LYS:CG	2:A:103:HEC:HHA	0.45	2.41	4	3
1:A:58:MET:C	1:A:60:LYS:N	0.45	2.68	16	1
1:A:52:LYS:O	1:A:54:CYS:N	0.45	2.49	5	1
1:A:53:GLY:O	1:A:54:CYS:C	0.45	2.53	18	4
1:A:41:PHE:CG	2:A:101:HEC:O1D	0.45	2.70	15	1
1:A:5:VAL:CG1	1:A:12:ASP:OD2	0.45	2.65	13	2
1:A:39:GLU:O	1:A:40:GLY:O	0.45	2.35	20	3
1:A:10:ASN:N	2:A:103:HEC:O2A	0.45	2.50	11	1
1:A:43:LYS:CE	2:A:103:HEC:HAD1	0.45	2.42	14	3
1:A:17:HIS:C	1:A:19:ALA:N	0.45	2.69	1	4
1:A:46:ALA:O	1:A:51:CYS:CB	0.45	2.65	4	6
1:A:56:GLU:OE1	1:A:57:GLU:N	0.45	2.50	12	1
2:A:102:HEC:HBD1	2:A:102:HEC:CHA	0.44	2.43	14	1
1:A:43:LYS:CD	2:A:103:HEC:HAD1	0.44	2.43	19	3
1:A:55:HIS:CD2	2:A:102:HEC:ND	0.44	2.86	1	4
1:A:35:PRO:O	1:A:36:GLY:O	0.44	2.34	20	1
1:A:44:GLU:HG2	1:A:45:MET:N	0.44	2.27	15	2
1:A:58:MET:HB3	1:A:60:LYS:CG	0.44	2.43	18	1
1:A:39:GLU:CG	1:A:39:GLU:O	0.44	2.66	4	1
1:A:5:VAL:HG13	1:A:12:ASP:OD2	0.44	2.13	11	1
1:A:65:CYS:C	1:A:67:GLU:N	0.44	2.70	15	13
1:A:32:GLU:O	1:A:33:LYS:HG2	0.44	2.12	14	1
1:A:62:PRO:CD	2:A:102:HEC:C2A	0.44	2.96	15	4
1:A:51:CYS:HA	2:A:102:HEC:CHC	0.43	2.43	14	3
1:A:46:ALA:HB1	2:A:103:HEC:C2D	0.43	2.42	15	1
1:A:10:ASN:O	1:A:10:ASN:OD1	0.43	2.36	14	1
1:A:52:LYS:CG	1:A:63:THR:CG2	0.43	2.90	15	1
1:A:7:LYS:O	2:A:103:HEC:O2D	0.43	2.37	8	2
1:A:69:HIS:CE1	2:A:103:HEC:ND	0.43	2.86	20	3
1:A:43:LYS:NZ	2:A:103:HEC:HAD1	0.43	2.26	18	1
1:A:16:PRO:HG2	1:A:19:ALA:HB3	0.43	1.90	11	1
1:A:15:PHE:CZ	2:A:102:HEC:C4B	0.43	3.02	8	2
1:A:14:LYS:O	1:A:14:LYS:HG2	0.43	2.14	4	1
1:A:10:ASN:OD1	1:A:10:ASN:C	0.43	2.57	8	1
1:A:2:ASP:OD1	1:A:2:ASP:N	0.43	2.52	18	1
1:A:8:ALA:HB1	2:A:103:HEC:O1A	0.43	2.14	15	1
1:A:37:LYS:NZ	2:A:101:HEC:O2D	0.43	2.52	1	1
1:A:53:GLY:O	1:A:56:GLU:N	0.42	2.52	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:LYS:O	1:A:29:LYS:C	0.42	2.58	11	2
1:A:32:GLU:C	1:A:33:LYS:CG	0.42	2.86	6	2
2:A:101:HEC:CGD	2:A:101:HEC:HHA	0.42	2.44	13	1
1:A:44:GLU:OE2	1:A:45:MET:SD	0.42	2.78	3	2
1:A:43:LYS:CE	1:A:43:LYS:HA	0.42	2.45	18	1
1:A:38:ILE:HD12	2:A:101:HEC:HBD1	0.42	1.92	8	1
1:A:38:ILE:HD13	2:A:101:HEC:CBD	0.42	2.45	6	1
1:A:43:LYS:NZ	1:A:43:LYS:HA	0.42	2.29	18	1
1:A:3:ASP:HB2	1:A:14:LYS:HZ3	0.42	1.74	5	1
1:A:37:LYS:O	1:A:37:LYS:CG	0.42	2.68	10	1
1:A:34:GLY:O	1:A:35:PRO:O	0.42	2.38	4	3
1:A:21:GLN:OE1	1:A:21:GLN:O	0.42	2.38	13	1
1:A:49:LYS:N	1:A:49:LYS:CD	0.42	2.83	5	1
1:A:44:GLU:CG	1:A:45:MET:N	0.42	2.83	20	2
1:A:58:MET:O	1:A:59:LYS:C	0.42	2.59	16	1
1:A:52:LYS:HG2	1:A:63:THR:CG2	0.42	2.44	15	1
1:A:28:LYS:O	1:A:31:HIS:C	0.41	2.58	6	2
1:A:22:LYS:CG	1:A:22:LYS:O	0.41	2.68	13	1
1:A:3:ASP:CG	1:A:14:LYS:HZ1	0.41	2.17	15	1
1:A:9:LYS:CB	2:A:103:HEC:O2A	0.41	2.68	14	1
1:A:21:GLN:CD	1:A:21:GLN:O	0.41	2.59	18	1
1:A:16:PRO:HB2	1:A:19:ALA:HB3	0.41	1.91	1	1
1:A:31:HIS:O	1:A:32:GLU:O	0.41	2.38	19	1
2:A:101:HEC:HMA2	2:A:101:HEC:HBA1	0.41	1.91	8	1
1:A:7:LYS:O	2:A:103:HEC:O1D	0.41	2.38	16	2
1:A:43:LYS:N	1:A:43:LYS:HE3	0.41	2.30	12	2
1:A:39:GLU:O	1:A:39:GLU:CD	0.41	2.58	12	1
1:A:10:ASN:OD1	1:A:10:ASN:O	0.41	2.38	8	1
1:A:43:LYS:HZ1	2:A:103:HEC:C3D	0.41	2.27	18	1
1:A:51:CYS:O	1:A:55:HIS:ND1	0.41	2.53	17	1
1:A:38:ILE:HD12	2:A:101:HEC:O1D	0.41	2.14	7	1
1:A:43:LYS:CA	1:A:43:LYS:HE2	0.41	2.46	20	1
2:A:102:HEC:C2A	2:A:102:HEC:O1A	0.41	2.69	8	1
1:A:3:ASP:CB	1:A:14:LYS:HZ1	0.41	2.28	5	1
1:A:43:LYS:CE	2:A:103:HEC:CAD	0.41	2.98	18	1
1:A:6:LEU:C	2:A:103:HEC:O1D	0.41	2.59	18	1
2:A:102:HEC:C2A	2:A:102:HEC:O2A	0.41	2.69	11	1
1:A:43:LYS:O	1:A:44:GLU:C	0.41	2.58	20	1
1:A:2:ASP:O	1:A:17:HIS:N	0.41	2.53	19	1
1:A:5:VAL:CG1	1:A:12:ASP:OD1	0.41	2.62	4	1
1:A:28:LYS:O	1:A:32:GLU:CA	0.41	2.69	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:60:LYS:HE2	2:A:102:HEC:CMD	0.41	2.46	1	1
1:A:32:GLU:O	1:A:33:LYS:HB3	0.40	2.15	6	1
1:A:43:LYS:HE3	1:A:43:LYS:N	0.40	2.31	11	1
1:A:10:ASN:C	1:A:10:ASN:OD1	0.40	2.60	13	1
1:A:17:HIS:CE1	1:A:21:GLN:HE22	0.40	2.32	6	1
2:A:103:HEC:CBA	2:A:103:HEC:CHA	0.40	2.99	4	1
2:A:103:HEC:HBA2	2:A:103:HEC:CHA	0.40	2.47	4	1
1:A:21:GLN:CA	1:A:21:GLN:OE1	0.40	2.69	2	1
2:A:103:HEC:O1A	2:A:103:HEC:O2D	0.40	2.40	18	1
1:A:6:LEU:O	2:A:103:HEC:O1D	0.40	2.38	18	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%)	43±3 (66±5%)	17±3 (26±5%)	6±2 (8±3%)	2	13
All	All	1300/1420 (92%)	856 (66%)	334 (26%)	110 (8%)	2	13

All 19 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	51	CYS	19
1	A	39	GLU	17
1	A	35	PRO	14
1	A	40	GLY	13
1	A	33	LYS	8
1	A	32	GLU	6
1	A	2	ASP	5
1	A	41	PHE	5
1	A	54	CYS	5
1	A	48	GLY	3
1	A	37	LYS	3
1	A	28	LYS	3

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Mol	Chain	Res	Type	Models (Total)
1	A	10	ASN	2
1	A	59	LYS	2
1	A	36	GLY	1
1	A	34	GLY	1
1	A	66	GLY	1
1	A	38	ILE	1
1	A	53	GLY	1

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	52/56 (93%)	34±3 (65±6%)	18±3 (35±6%)	1 10
All	All	1040/1120 (93%)	680 (65%)	360 (35%)	1 10

All 36 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	65	CYS	20
1	A	43	LYS	20
1	A	51	CYS	19
1	A	45	MET	19
1	A	54	CYS	18
1	A	60	LYS	15
1	A	58	MET	15
1	A	71	LYS	14
1	A	37	LYS	14
1	A	21	GLN	13
1	A	9	LYS	12
1	A	2	ASP	12
1	A	70	LYS	11
1	A	12	ASP	11
1	A	14	LYS	11
1	A	59	LYS	11
1	A	39	GLU	11
1	A	33	LYS	10

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Mol	Chain	Res	Type	Models (Total)
1	A	49	LYS	10
1	A	22	LYS	10
1	A	7	LYS	10
1	A	52	LYS	9
1	A	18	LYS	9
1	A	30	CYS	9
1	A	57	GLU	8
1	A	28	LYS	7
1	A	64	LYS	7
1	A	29	LYS	5
1	A	32	GLU	4
1	A	3	ASP	3
1	A	44	GLU	3
1	A	56	GLU	3
1	A	10	ASN	2
1	A	38	ILE	2
1	A	63	THR	2
1	A	4	ILE	1

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	HEC	A	101	1	26,50,50	1.71±0.04	2±0 (6±1%)
2	HEC	A	103	1	26,50,50	1.65±0.02	2±0 (7±1%)
2	HEC	A	102	1	26,50,50	1.69±0.03	2±0 (7±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	HEC	A	101	1	18,82,82	1.35±0.01	0±0 (0±0%)
2	HEC	A	103	1	18,82,82	1.35±0.01	0±0 (0±0%)
2	HEC	A	102	1	18,82,82	1.35±0.01	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	HEC	A	101	1	-	0±0,6,54,54	-
2	HEC	A	103	1	-	0±0,6,54,54	-
2	HEC	A	102	1	-	0±0,6,54,54	-

All 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	102	HEC	C3B-C2B	5.23	1.35	1.40	6	20
2	A	101	HEC	C3C-C2C	5.22	1.35	1.40	19	18
2	A	103	HEC	C3C-C2C	5.21	1.35	1.40	4	19
2	A	103	HEC	C3B-C2B	5.20	1.35	1.40	6	19
2	A	102	HEC	C3C-C2C	5.18	1.35	1.40	12	20
2	A	101	HEC	C3B-C2B	5.16	1.35	1.40	14	18

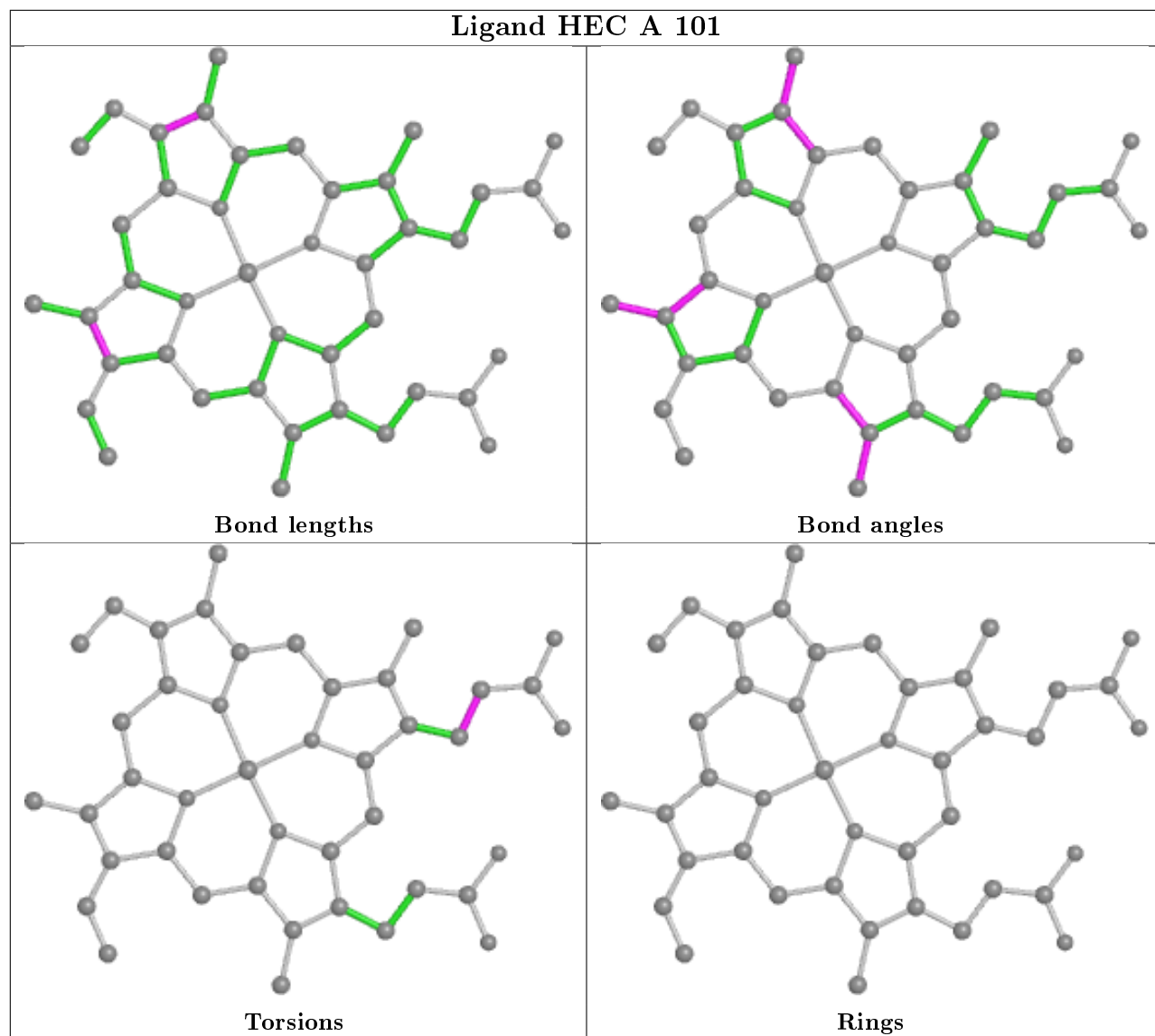
There are no bond-angle outliers.

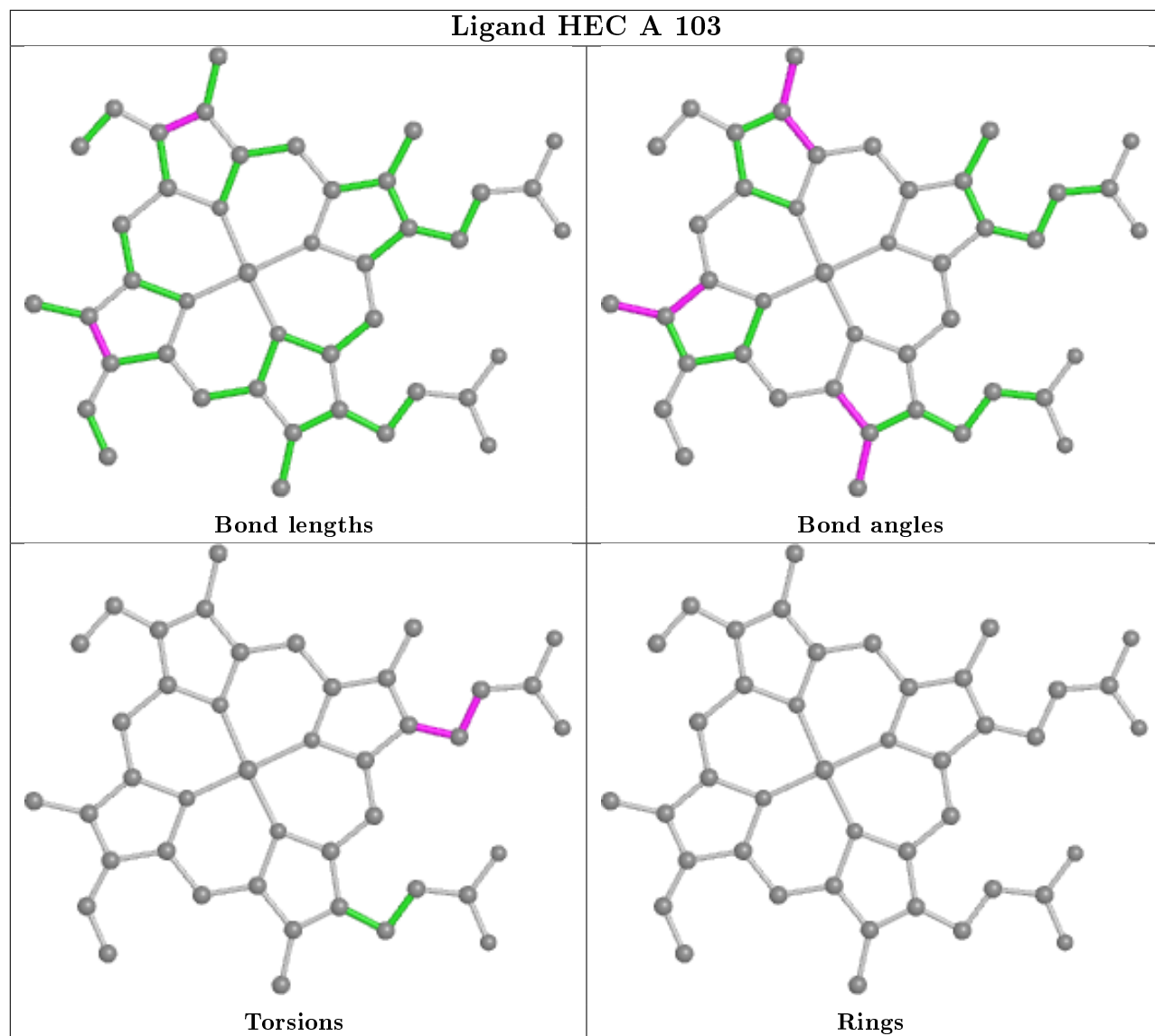
There are no chirality outliers.

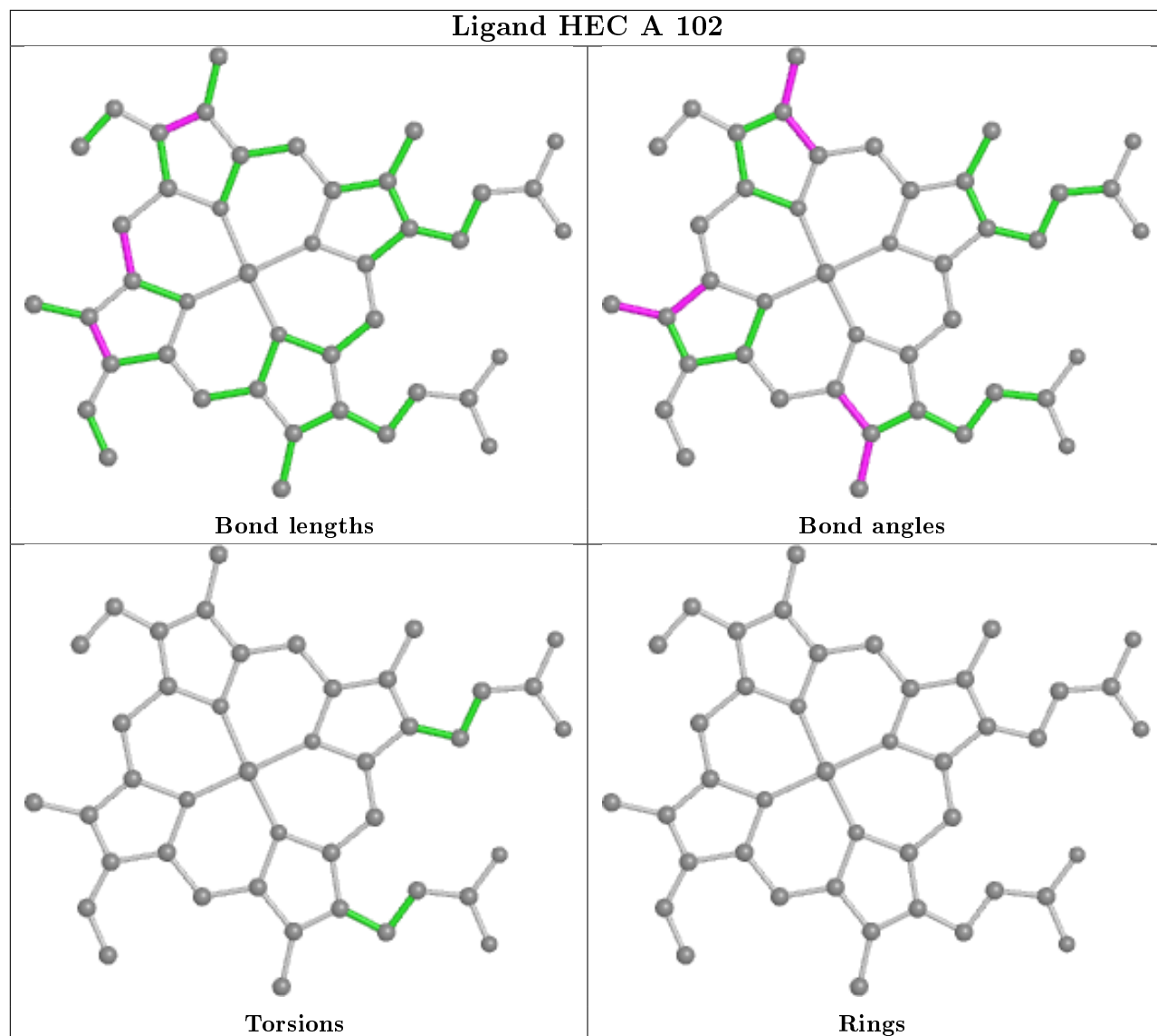
There are no torsion outliers.

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 i

The completeness of assignment taking into account all chemical shift lists is 47% for the well-defined parts and 47% 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 i

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	504
Number of shifts mapped to atoms	445
Number of unparsed shifts	0
Number of shifts with mapping errors	59
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	85

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

- Residue not found in structure. All 59 occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	168	HEC	HHD	1.212	0.003	1
A	130	HEC	HAB	0.91	0.005	1
A	154	HEC	HAA1	3.685	0.01	1
A	168	HEC	HBA1	-0.853	0.007	1
A	130	HEC	HBA2	-0.414	0.012	1
A	130	HEC	HMC1	10.407	0.007	1
A	154	HEC	HHC	-3.913	0.027	1
A	168	HEC	HAC	-0.062	0.016	1
A	168	HEC	HAB	0.73	0.009	1
A	154	HEC	HBA2	-1.969	0.012	1
A	154	HEC	HMC1	18.001	0.006	1
A	130	HEC	HAA2	3.03	0.013	1
A	130	HEC	HAC	-4.323	0.009	1
A	154	HEC	HAA2	5.54	0.014	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	130	HEC	HMA1	15.723	0.011	1
A	154	HEC	HBC1	-1.017	0.006	1
A	168	HEC	HMC1	10.943	0.006	1
A	154	HEC	HBB1	-2.233	0.008	1
A	168	HEC	HMA1	14.578	0.032	1
A	168	HEC	HAA1	2.877	0.013	1
A	130	HEC	HBC1	-3.987	0.007	1
A	154	HEC	HBA1	-2.072	0.011	1
A	168	HEC	HHB	-1.612	0.002	1
A	154	HEC	HAB	-2.546	0.012	1
A	154	HEC	HBD1	-1.753	0.008	1
A	168	HEC	HAD1	2.435	0.017	1
A	168	HEC	HMB1	14.484	0.022	1
A	168	HEC	HBD1	0.126	0.007	1
A	130	HEC	HBA1	-0.871	0.016	1
A	130	HEC	HMB1	17.782	0.005	1
A	154	HEC	HMD1	13.155	0.011	1
A	130	HEC	HAD1	2.66	0.021	1
A	130	HEC	HBD2	-0.312	0.009	1
A	154	HEC	HAC	-0.871	0.005	1
A	168	HEC	HBA2	-0.257	0.009	1
A	154	HEC	HBD2	-0.688	0.008	1
A	130	HEC	HHD	-1.521	0.007	1
A	154	HEC	HHD	11.378	0.004	1
A	154	HEC	HMB1	12.145	0.009	1
A	154	HEC	HHA	-1.675	0.005	1
A	130	HEC	HBB1	1.146	0.004	1
A	130	HEC	HAA1	0.862	0.024	1
A	130	HEC	HHB	-0.713	0.005	1
A	154	HEC	HHB	8.078	0.005	1
A	168	HEC	HBB1	2.048	0.006	1
A	130	HEC	HHA	3.714	0.007	1
A	168	HEC	HMD1	17.414	0.011	1
A	130	HEC	HBD1	-1.457	0.012	1
A	154	HEC	HMA1	0.654	0.008	1
A	168	HEC	HHA	0.769	0.006	1
A	168	HEC	HAA2	4.147	0.036	1
A	130	HEC	HMD1	20.595	0.017	1
A	154	HEC	HAD2	19.916	0.006	1
A	168	HEC	HBC1	1.623	0.015	1
A	168	HEC	HAD2	6.471	0.011	1

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Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
A	168	HEC	HHC	2.249	0.005	1
A	168	HEC	HBD2	0.466	0.009	1
A	154	HEC	HAD1	16.042	0.029	1
A	130	HEC	HAD2	6.713	0.029	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	63	-0.08 ± 0.71	None needed (< 0.5 ppm)

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 47%, i.e. 377 atoms were assigned a chemical shift out of a possible 809. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	187/324 (58%)	127/129 (98%)	0/132 (0%)	60/63 (95%)
Sidechain	185/425 (44%)	185/257 (72%)	0/149 (0%)	0/19 (0%)
Aromatic	5/60 (8%)	5/34 (15%)	0/20 (0%)	0/6 (0%)
Overall	377/809 (47%)	317/420 (75%)	0/301 (0%)	60/88 (68%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 47%, i.e. 399 atoms were assigned a chemical shift out of a possible 856. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	198/347 (57%)	135/138 (98%)	0/142 (0%)	63/67 (94%)
Sidechain	196/449 (44%)	196/271 (72%)	0/159 (0%)	0/19 (0%)
Aromatic	5/60 (8%)	5/34 (15%)	0/20 (0%)	0/6 (0%)
Overall	399/856 (47%)	336/443 (76%)	0/321 (0%)	63/92 (68%)

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	55	HIS	HB3	19.33	5.00 – 1.10	41.7
1	A	47	HIS	HB3	18.08	5.00 – 1.10	38.5
1	A	55	HIS	HB2	16.22	4.91 – 1.31	36.4
1	A	47	HIS	HB2	15.25	4.91 – 1.31	33.7
1	A	17	HIS	HB3	15.70	5.00 – 1.10	32.4
1	A	31	HIS	HB3	12.90	5.00 – 1.10	25.2
1	A	17	HIS	HB2	11.35	4.91 – 1.31	22.9
1	A	69	HIS	HB3	11.97	5.00 – 1.10	22.9
1	A	13	VAL	HG23	6.50	2.20 – -0.60	20.3
1	A	13	VAL	HG22	6.50	2.20 – -0.60	20.3
1	A	13	VAL	HG21	6.50	2.20 – -0.60	20.3
1	A	31	HIS	HB2	10.29	4.91 – 1.31	19.9
1	A	46	ALA	HB2	-3.38	2.61 – 0.11	-19.0
1	A	46	ALA	HB3	-3.38	2.61 – 0.11	-19.0
1	A	46	ALA	HB1	-3.38	2.61 – 0.11	-19.0
1	A	61	GLY	HA2	-2.60	5.87 – 2.07	-17.3
1	A	20	HIS	HB3	9.63	5.00 – 1.10	16.9
1	A	69	HIS	HB2	8.53	4.91 – 1.31	15.1
1	A	69	HIS	HA	10.51	6.81 – 2.41	13.4
1	A	31	HIS	HA	10.23	6.81 – 2.41	12.8
1	A	8	ALA	HB3	4.33	2.61 – 0.11	11.9
1	A	8	ALA	HB1	4.33	2.61 – 0.11	11.9
1	A	8	ALA	HB2	4.33	2.61 – 0.11	11.9
1	A	51	CYS	HA	-1.92	7.47 – 1.87	-11.8
1	A	65	CYS	HA	-1.39	7.47 – 1.87	-10.8
1	A	18	LYS	HB3	4.59	3.10 – 0.40	10.5
1	A	43	LYS	HA	-0.12	6.46 – 2.06	-9.9
1	A	18	LYS	HB2	4.15	3.03 – 0.53	9.5
1	A	43	LYS	HG2	3.83	2.67 – 0.07	9.5
1	A	16	PRO	HA	7.38	6.05 – 2.75	9.0
1	A	55	HIS	HA	8.56	6.81 – 2.41	9.0
1	A	43	LYS	HB2	-0.44	3.03 – 0.53	-8.9
1	A	3	ASP	HA	7.28	6.15 – 3.05	8.6
1	A	17	HIS	HA	8.38	6.81 – 2.41	8.6
1	A	2	ASP	HA	7.25	6.15 – 3.05	8.5
1	A	65	CYS	HB2	-0.85	5.20 – 0.70	-8.5
1	A	47	HIS	HA	8.27	6.81 – 2.41	8.3
1	A	20	HIS	HB2	6.07	4.91 – 1.31	8.2

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	35	PRO	HB2	-0.79	3.82 – 0.32	-8.2
1	A	11	GLY	HA3	6.96	5.80 – 2.00	8.1
1	A	18	LYS	H	12.97	11.24 – 5.14	7.8
1	A	36	GLY	HA2	1.01	5.87 – 2.07	-7.8
1	A	12	ASP	HA	6.99	6.15 – 3.05	7.7
1	A	38	ILE	HG12	4.30	3.27 – -0.73	7.6
1	A	20	HIS	HA	7.92	6.81 – 2.41	7.5
1	A	18	LYS	HA	7.45	6.46 – 2.06	7.2
1	A	21	GLN	HG3	4.37	3.75 – 0.85	7.1
1	A	4	ILE	HG13	4.08	3.26 – -0.84	7.0
1	A	62	PRO	HG2	-0.23	3.48 – 0.38	-7.0
1	A	18	LYS	HD2	3.16	2.76 – 0.46	6.7
1	A	19	ALA	HB1	3.02	2.61 – 0.11	6.6
1	A	19	ALA	HB3	3.02	2.61 – 0.11	6.6
1	A	19	ALA	HB2	3.02	2.61 – 0.11	6.6
1	A	41	PHE	HE2	5.00	8.69 – 5.49	-6.5
1	A	18	LYS	HG2	3.06	2.67 – 0.07	6.5
1	A	2	ASP	HB3	4.49	4.07 – 1.27	6.5
1	A	41	PHE	HE1	5.01	8.69 – 5.49	-6.5
1	A	16	PRO	HB3	4.34	3.81 – 0.21	6.5
1	A	52	LYS	HE2	4.14	3.87 – 1.97	6.4
1	A	18	LYS	HG3	3.15	2.76 – -0.04	6.4
1	A	41	PHE	HZ	4.35	9.11 – 4.91	-6.3
1	A	35	PRO	HB3	-0.27	3.81 – 0.21	-6.3
1	A	54	CYS	HB2	0.11	5.20 – 0.70	-6.3
1	A	51	CYS	HB2	0.13	5.20 – 0.70	-6.3
1	A	50	GLY	HA2	1.60	5.87 – 2.07	-6.2
1	A	21	GLN	HG2	0.67	3.67 – 0.97	-6.1
1	A	43	LYS	HE3	4.07	3.86 – 1.96	6.1
1	A	18	LYS	HE2	4.07	3.87 – 1.97	6.0
1	A	62	PRO	HD2	1.50	5.45 – 1.85	-6.0
1	A	33	LYS	HE3	4.01	3.86 – 1.96	5.8
1	A	46	ALA	HA	1.73	6.46 – 2.06	-5.8
1	A	20	HIS	H	12.11	11.68 – 4.78	5.6
1	A	35	PRO	HA	6.24	6.05 – 2.75	5.6
1	A	30	CYS	HB2	0.47	5.20 – 0.70	-5.5
1	A	42	GLY	H	4.70	11.63 – 5.03	-5.5
1	A	50	GLY	HA3	1.83	5.80 – 2.00	-5.4
1	A	31	HIS	H	11.95	11.68 – 4.78	5.4
1	A	21	GLN	HB3	3.46	3.37 – 0.67	5.3
1	A	56	GLU	HG3	3.33	3.31 – 1.21	5.1
1	A	51	CYS	H	4.99	11.75 – 5.05	-5.1

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Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	63	THR	HG21	2.30	2.29 – -0.01	5.1
1	A	63	THR	HG23	2.30	2.29 – -0.01	5.1
1	A	63	THR	HG22	2.30	2.29 – -0.01	5.1
1	A	51	CYS	HB3	0.54	5.25 – 0.55	-5.0
1	A	47	HIS	H	11.69	11.68 – 4.78	5.0

7.1.5 Random Coil Index (RCI) plots [i](#)

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:

