



Full wwPDB NMR Structure Validation Report ⓘ

Aug 5, 2026 – 12:34 AM EDT

PDB ID : 2MZ9 / pdb_00002mz9
BMRB ID : 25477
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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.50

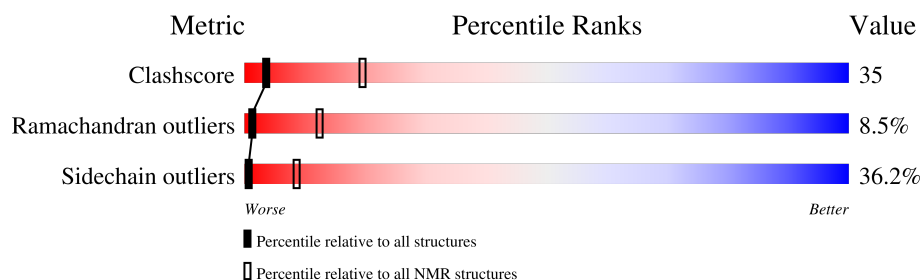
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 25%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA and RNA chains that are outliers for geometric criteria:

Mol	Chain	Compound	Res	Total models with violations	
				Chirality	Geometry
2	A	HEC	101	14	-
2	A	HEC	102	20	-
2	A	HEC	103	17	-

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)	0.54	10

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

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

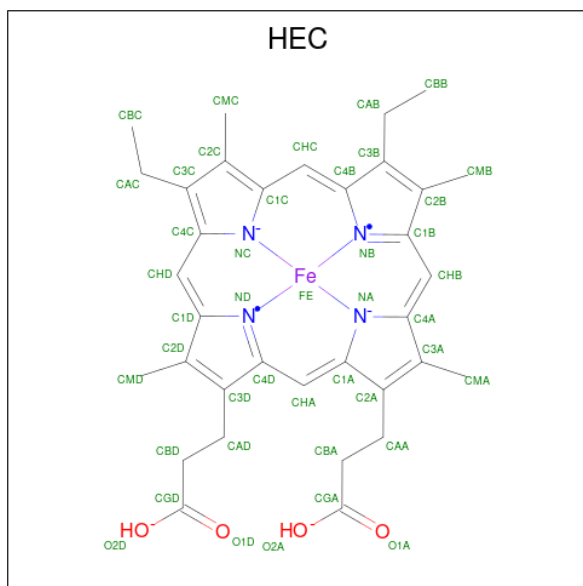
The models can be grouped into 2 clusters. No single-model clusters were found.

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

- Molecule 1 is a protein called PpcA.

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

- (CCD ID: HEC) (formula: $\text{C}_{34}\text{H}_{36}\text{FeN}_4\text{O}_4$).



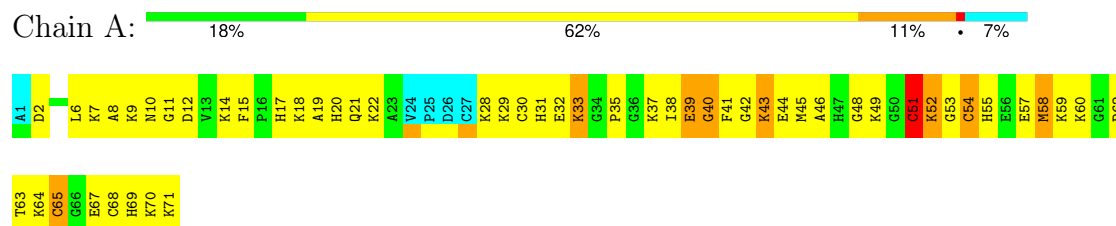
Mol	Chain	Residues	Atoms				
2	A	1	Total 43	C 34	Fe 1	N 4	O 4
2	A	1	Total 43	C 34	Fe 1	N 4	O 4
2	A	1	Total 43	C 34	Fe 1	N 4	O 4

4 Residue-property plots

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: PpcA

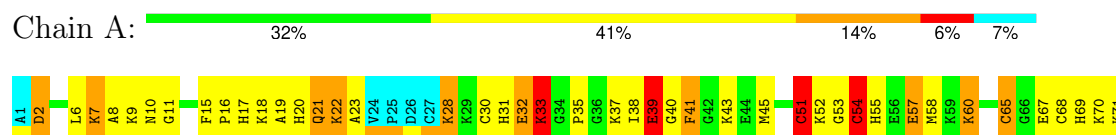


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

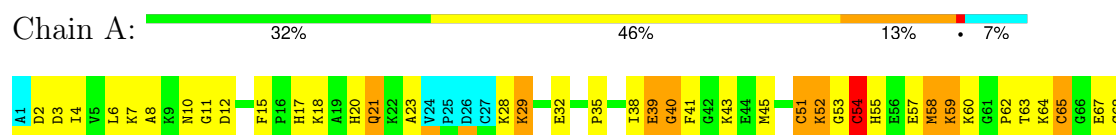
4.2.1 Score per residue for model 1

- Molecule 1: PpcA



4.2.2 Score per residue for model 2

- Molecule 1: PpcA



H69
K70
K71

4.2.3 Score per residue for model 3

- Molecule 1: PpcA

Chain A: 35% 45% 11% 7%



4.2.4 Score per residue for model 4

- Molecule 1: PpcA

Chain A: 28% 45% 17% 7%



C68
H69
K70
K71

4.2.5 Score per residue for model 5

- Molecule 1: PpcA

Chain A: 38% 42% 11% 7%



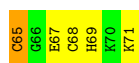
K70
K71

4.2.6 Score per residue for model 6

- Molecule 1: PpcA

Chain A: 23% 51% 17% 7%

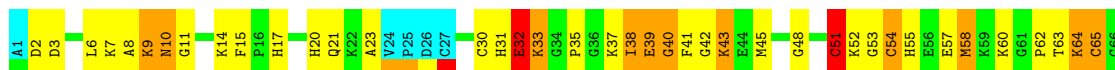




4.2.7 Score per residue for model 7

- Molecule 1: PpcA

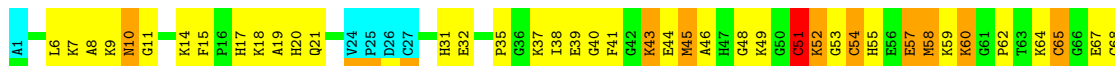
Chain A: 32% 42% 15% • 7%



4.2.8 Score per residue for model 8

- Molecule 1: PpcA

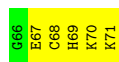
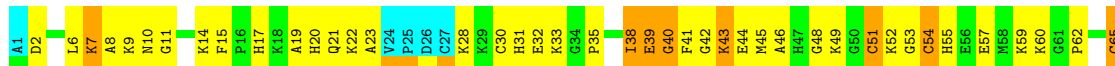
Chain A: 32% 46% 13% • 7%



4.2.9 Score per residue for model 9

- Molecule 1: PpcA

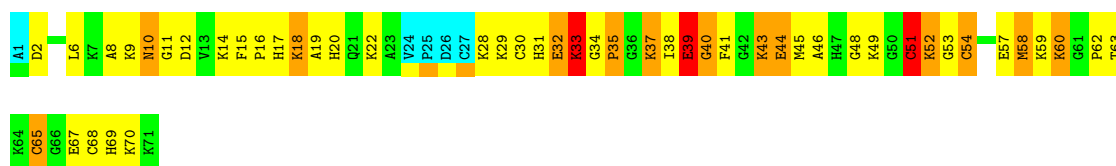
Chain A: 27% 55% 11% 7%



4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: PpcA

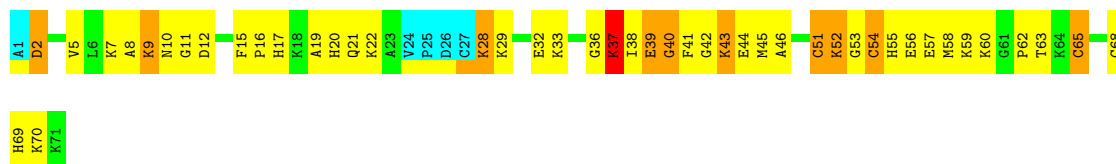
Chain A: 24% 46% 18% • 7%



4.2.11 Score per residue for model 11

- Molecule 1: PpcA

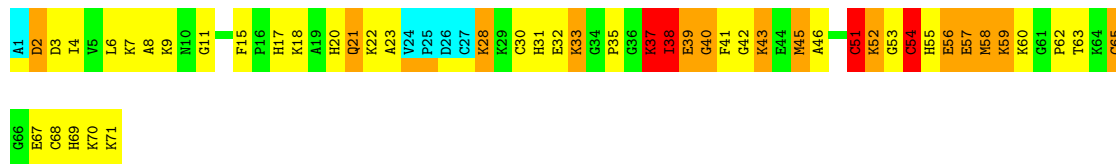
Chain A: 28% 49% 14% 7%



4.2.12 Score per residue for model 12

- Molecule 1: PpcA

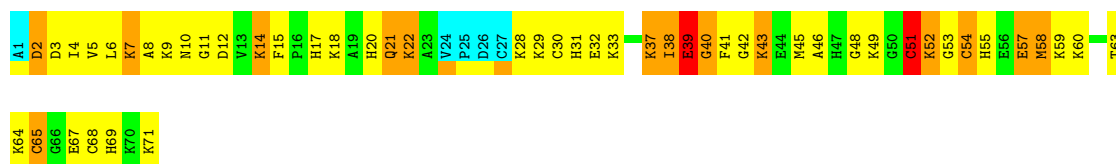
Chain A: 25% 42% 20% 6% 7%



4.2.13 Score per residue for model 13

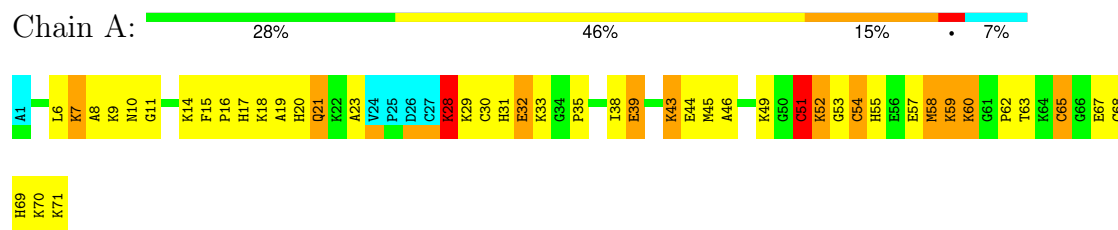
- Molecule 1: PpcA

Chain A: 21% 49% 20% 7%



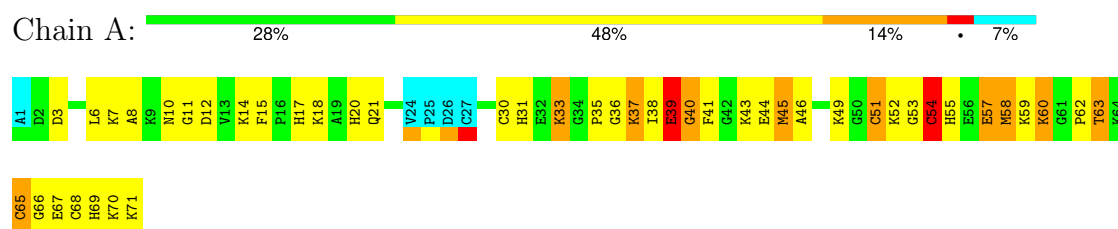
4.2.14 Score per residue for model 14

- Molecule 1: PpcA



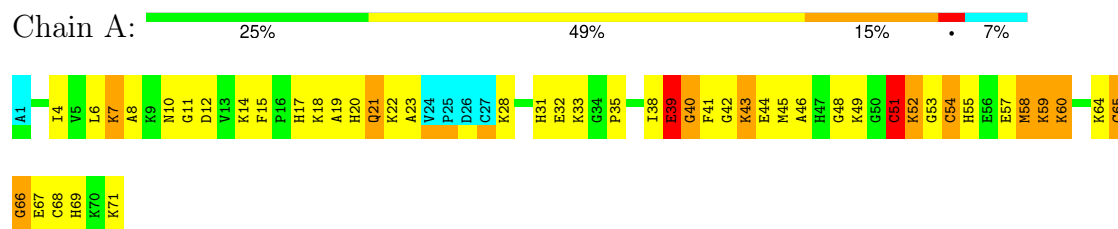
4.2.15 Score per residue for model 15

- Molecule 1: PpcA



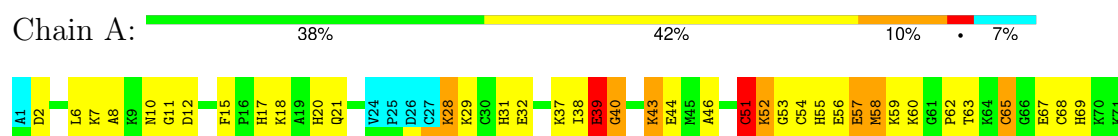
4.2.16 Score per residue for model 16

- Molecule 1: PpcA



4.2.17 Score per residue for model 17

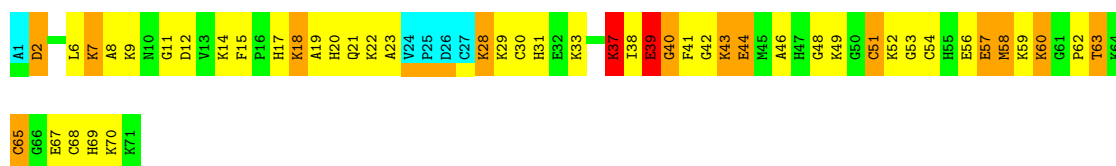
- Molecule 1: PpcA



4.2.18 Score per residue for model 18

- Molecule 1: PpcA

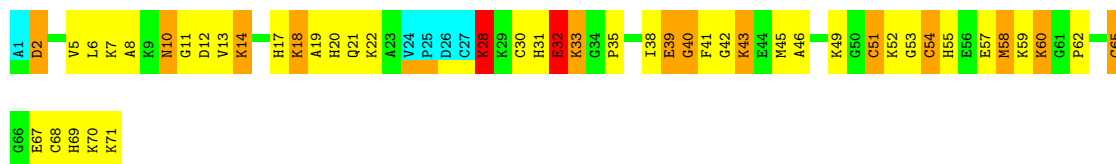




4.2.19 Score per residue for model 19

- Molecule 1: PpcA

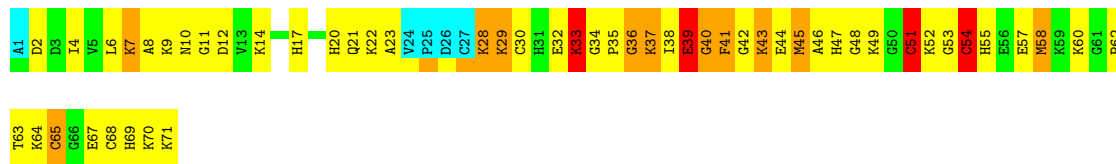
Chain A: 27% 45% 18% 7%



4.2.20 Score per residue for model 20

- Molecule 1: PpcA

Chain A: 18% 54% 15% 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)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	504
Number of shifts mapped to atoms	418
Number of unparsed shifts	0
Number of shifts with mapping errors	86
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	25%

6 Model quality

6.1 Standard geometry

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

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	38±8
2	A	129	0	90	17±6
All	All	12620	9520	12000	872

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:8:ALA:HB3	1:A:11:GLY:O	0.89	1.68	9	19
1:A:15:PHE:CE2	2:A:102:HEC:HBB2	0.83	2.09	8	6
1:A:52:LYS:CG	1:A:63:THR:HG22	0.79	2.07	15	1
1:A:15:PHE:CD2	2:A:102:HEC:HBB2	0.78	2.14	8	5
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
1:A:43:LYS:NZ	2:A:103:HEC:CAD	0.74	2.51	18	2
2:A:101:HEC:HMB1	2:A:101:HEC:HBB3	0.73	1.60	9	4
2:A:101:HEC:HBB2	2:A:101:HEC:HMB3	0.73	1.60	6	12
1:A:43:LYS:NZ	1:A:47:HIS:CE1	0.71	2.58	20	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:ILE:O	1:A:39:GLU:C	0.70	2.33	15	16
1:A:17:HIS:CE1	1:A:21:GLN:NE2	0.70	2.60	6	3
1:A:32:GLU:O	1:A:33:LYS:HB2	0.69	1.86	19	1
2:A:102:HEC:HMC3	2:A:102:HEC:HBC3	0.69	1.65	18	2
2:A:102:HEC:HMC3	2:A:102:HEC:CBC	0.67	2.19	17	2
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:23:ALA:HB1	2:A:102:HEC:HMD2	0.66	1.67	20	1
1:A:15:PHE:CE1	2:A:102:HEC:C1B	0.66	2.78	9	6
1:A:17:HIS:O	1:A:20:HIS:N	0.66	2.29	12	16
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
1:A:32:GLU:O	1:A:33:LYS:CG	0.64	2.46	14	2
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
1:A:33:LYS:CG	1:A:33:LYS:O	0.61	2.48	12	1
2:A:101:HEC:CGD	2:A:101:HEC:CHA	0.61	2.78	12	1
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:39:GLU:O	1:A:40:GLY:C	0.59	2.45	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
2:A:101:HEC:HMB1	2:A:101:HEC:CBB	0.58	2.28	9	4
1:A:52:LYS:O	1:A:53:GLY:C	0.58	2.45	5	20
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
1:A:60:LYS:CD	2:A:102:HEC:HMD2	0.58	2.28	4	3
1:A:4:ILE:HD13	2:A:101:HEC:O2D	0.58	1.97	13	1
1:A:60:LYS:HD3	2:A:102:HEC:HMD1	0.57	1.76	8	1
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:CGD	2:A:101:HEC:C4D	0.57	2.82	12	1
1:A:62:PRO:HG2	2:A:102:HEC:HMA3	0.57	1.76	7	2
1:A:3:ASP:CB	1:A:14:LYS:NZ	0.56	2.67	5	1
1:A:23:ALA:HB1	2:A:102:HEC:HMD3	0.56	1.78	1	2
1:A:31:HIS:O	1:A:32:GLU:C	0.56	2.49	9	3
2:A:101:HEC:C3D	2:A:101:HEC:O2D	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:101:HEC:CBB	2:A:101:HEC:CMB	0.55	2.85	9	9
1:A:43:LYS:HG2	2:A:103:HEC:CHA	0.55	2.31	6	3
2:A:101:HEC:HBC1	2:A:102:HEC:C2C	0.55	2.31	17	5
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:10:ASN:CG	1:A:10:ASN:O	0.55	2.46	15	10
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
1:A:60:LYS:CE	2:A:102:HEC:HMD2	0.54	2.32	9	4
1:A:28:LYS:O	1:A:32:GLU:N	0.54	2.41	17	4
1:A:62:PRO:HG3	2:A:102:HEC:HMA3	0.54	1.79	20	1
1:A:6:LEU:O	1:A:7:LYS:C	0.54	2.50	5	16
1:A:4:ILE:HD11	2:A:101:HEC:O1A	0.54	2.02	20	2
2:A:102:HEC:C1A	2:A:102:HEC:O1A	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:O1A	2:A:102:HEC:CHA	0.53	2.56	8	1
1:A:14:LYS:O	1:A:14:LYS:CG	0.53	2.57	4	3
2:A:102:HEC:HMB3	2:A:102:HEC:HBB3	0.53	1.79	20	1
1:A:15:PHE:CD1	2:A:102:HEC:C2B	0.53	2.92	6	13
1:A:23:ALA:CB	2:A:102:HEC:O2D	0.53	2.57	12	3
1:A:63:THR:O	2:A:103:HEC:CMC	0.53	2.56	6	11
1:A:3:ASP:CG	1:A:14:LYS:HZ1	0.53	2.12	15	1
1:A:62:PRO:HD3	2:A:102:HEC:C2A	0.53	2.34	20	13
1:A:40:GLY:O	1:A:41:PHE:C	0.52	2.53	5	5
1:A:39:GLU:O	1:A:39:GLU:CG	0.52	2.58	12	3
1:A:37:LYS:O	1:A:38:ILE:C	0.52	2.52	12	3
1:A:49:LYS:CG	1:A:49:LYS:O	0.52	2.57	18	2
1:A:36:GLY:O	1:A:37:LYS:C	0.52	2.51	20	5
1:A:41:PHE:CD1	1:A:41:PHE:C	0.52	2.88	11	9
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:8:ALA:HB3	1:A:11:GLY:C	0.52	2.30	8	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	2
1:A:2:ASP:OD1	1:A:3:ASP:N	0.52	2.42	12	1
1:A:48:GLY:O	1:A:53:GLY:N	0.52	2.42	20	8
1:A:43:LYS:HZ2	1:A:47:HIS:CE1	0.52	2.21	20	1
1:A:23:ALA:HB2	2:A:102:HEC:O1D	0.52	2.05	12	2
1:A:58:MET:SD	2:A:102:HEC:HMD2	0.51	2.45	7	1
2:A:101:HEC:HMB3	2:A:101:HEC:CBB	0.51	2.34	2	7

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:102:HEC:HBC3	2:A:102:HEC:CMC	0.51	2.36	17	2
1:A:54:CYS:O	1:A:57:GLU:N	0.51	2.43	20	15
1:A:3:ASP:CG	1:A:14:LYS:NZ	0.51	2.69	15	1
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
2:A:101:HEC:HBB2	2:A:101:HEC:CMB	0.51	2.36	11	9
1:A:58:MET:O	1:A:59:LYS:CB	0.51	2.58	14	1
1:A:2:ASP:CG	1:A:3:ASP:N	0.51	2.67	13	2
1:A:54:CYS:O	1:A:58:MET:N	0.51	2.43	16	13
2:A:101:HEC:CGD	2:A:101:HEC:HHA	0.51	2.36	12	1
1:A:21:GLN:CD	1:A:21:GLN:O	0.50	2.54	15	5
2:A:101:HEC:CMB	2:A:101:HEC:CBB	0.50	2.90	11	7
1:A:17:HIS:O	1:A:18:LYS:C	0.50	2.53	18	8
2:A:103:HEC:HMD3	2:A:103:HEC:O1D	0.50	2.06	10	1
1:A:58:MET:C	1:A:60:LYS:N	0.50	2.68	16	3
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
1:A:53:GLY:O	1:A:54:CYS:C	0.50	2.53	18	9
1:A:54:CYS:HB2	2:A:102:HEC:HMC2	0.50	1.84	13	12
2:A:103:HEC:CBA	2:A:103:HEC:HHA	0.50	2.36	4	3
1:A:3:ASP:HB2	1:A:14:LYS:HZ3	0.50	1.65	5	1
1:A:4:ILE:CD1	2:A:101:HEC:O1A	0.50	2.60	2	1
1:A:38:ILE:N	2:A:101:HEC:O1D	0.50	2.45	9	1
1:A:53:GLY:O	1:A:57:GLU:N	0.50	2.45	18	2
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
1:A:17:HIS:C	1:A:19:ALA:N	0.49	2.69	1	7
2:A:101:HEC:HBC1	2:A:102:HEC:CMC	0.49	2.37	17	2
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:29:LYS:CD	2:A:102:HEC:HBC1	0.49	2.37	17	3
1:A:43:LYS:N	1:A:43:LYS:CE	0.49	2.76	4	1
1:A:68:CYS:SG	2:A:102:HEC:HMB3	0.49	2.47	4	2
1:A:60:LYS:CD	2:A:102:HEC:HMD1	0.49	2.36	8	1
1:A:65:CYS:C	1:A:67:GLU:N	0.48	2.70	16	18
1:A:43:LYS:HZ3	2:A:103:HEC:CGD	0.48	2.21	4	1
1:A:23:ALA:CB	2:A:102:HEC:O1D	0.48	2.62	20	2
1:A:10:ASN:O	1:A:10:ASN:ND2	0.48	2.46	19	1
1:A:16:PRO:O	1:A:19:ALA:HB3	0.48	2.08	11	4
1:A:21:GLN:NE2	1:A:21:GLN:O	0.48	2.46	1	1
1:A:21:GLN:O	1:A:21:GLN:OE1	0.48	2.31	20	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:43:LYS:HG3	2:A:103:HEC:CHA	0.48	2.37	4	1
2:A:103:HEC:HMB1	2:A:103:HEC:HBB3	0.48	1.86	13	2
1:A:3:ASP:OD2	1:A:14:LYS:CE	0.48	2.62	7	1
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:9:LYS:N	2:A:103:HEC:O2A	0.48	2.47	11	1
1:A:32:GLU:O	1:A:33:LYS:CD	0.48	2.62	6	1
1:A:60:LYS:CE	2:A:102:HEC:CMD	0.47	2.92	1	2
1:A:55:HIS:O	1:A:59:LYS:N	0.47	2.47	11	6
1:A:38:ILE:HD13	2:A:101:HEC:HBD1	0.47	1.86	3	2
1:A:10:ASN:OD1	1:A:10:ASN:C	0.47	2.57	8	2
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:28:LYS:O	1:A:29:LYS:C	0.47	2.58	11	4
1:A:29:LYS:HD2	2:A:102:HEC:HBC1	0.47	1.87	6	1
1:A:44:GLU:OE1	1:A:44:GLU:N	0.47	2.47	15	3
1:A:41:PHE:C	1:A:41:PHE:CD1	0.47	2.92	10	2
1:A:15:PHE:CE1	2:A:102:HEC:C3B	0.47	2.97	12	4
1:A:32:GLU:C	1:A:33:LYS:CG	0.47	2.86	6	2
2:A:102:HEC:O2D	2:A:102:HEC:C3D	0.47	2.62	12	1
1:A:14:LYS:O	1:A:14:LYS:HG2	0.47	2.10	19	2
1:A:31:HIS:CE1	2:A:101:HEC:ND	0.47	2.82	13	3
1:A:6:LEU:HB3	2:A:103:HEC:CGD	0.47	2.40	10	3
1:A:4:ILE:HG21	2:A:101:HEC:O2D	0.47	2.10	13	1
1:A:43:LYS:NZ	2:A:103:HEC:CGD	0.47	2.78	14	1
1:A:52:LYS:HG2	1:A:63:THR:HG22	0.47	1.84	15	1
1:A:33:LYS:HG3	1:A:33:LYS:O	0.47	2.10	14	1
2:A:102:HEC:CBC	2:A:102:HEC:CMC	0.47	2.91	18	2
1:A:7:LYS:O	2:A:103:HEC:CGD	0.46	2.63	18	2
1:A:58:MET:O	1:A:59:LYS:C	0.46	2.59	16	1
1:A:28:LYS:O	1:A:31:HIS:C	0.46	2.58	6	2
1:A:10:ASN:ND2	2:A:103:HEC:O1A	0.46	2.49	1	1
1:A:43:LYS:NZ	1:A:47:HIS:NE2	0.46	2.63	20	1
1:A:58:MET:O	1:A:60:LYS:N	0.46	2.49	16	1
1:A:8:ALA:HB2	2:A:103:HEC:CBD	0.46	2.41	4	1
1:A:52:LYS:O	1:A:55:HIS:N	0.46	2.49	5	1
1:A:4:ILE:CD1	2:A:101:HEC:O2D	0.46	2.63	13	1
1:A:6:LEU:C	2:A:103:HEC:O1D	0.46	2.59	18	1
1:A:17:HIS:O	1:A:19:ALA:N	0.45	2.49	18	3
1:A:65:CYS:O	1:A:67:GLU:N	0.45	2.48	16	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:103:HEC:HBB3	2:A:103:HEC:CMB	0.45	2.41	13	4
2:A:102:HEC:C2A	2:A:102:HEC:O2A	0.45	2.64	14	2
1:A:43:LYS:O	1:A:44:GLU:C	0.45	2.58	20	10
1:A:43:LYS:CG	2:A:103:HEC:HHA	0.45	2.41	4	3
1:A:55:HIS:CE1	2:A:102:HEC:NB	0.45	2.84	15	5
1:A:46:ALA:O	1:A:51:CYS:HB3	0.45	2.11	15	3
1:A:52:LYS:O	1:A:54:CYS:N	0.45	2.49	5	1
1:A:39:GLU:O	1:A:39:GLU:CD	0.45	2.58	12	1
1:A:58:MET:SD	2:A:102:HEC:CMD	0.45	3.05	7	1
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:60:LYS:HE2	2:A:102:HEC:HMD2	0.45	1.88	9	1
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:64:LYS:O	2:A:103:HEC:HMC3	0.45	2.12	7	3
1:A:43:LYS:CE	2:A:103:HEC:HAD1	0.45	2.42	14	3
1:A:46:ALA:O	1:A:51:CYS:CB	0.45	2.65	4	6
1:A:2:ASP:OD1	1:A:2:ASP:C	0.45	2.59	12	1
1:A:56:GLU:OE1	1:A:57:GLU:N	0.45	2.50	12	1
1:A:9:LYS:C	2:A:103:HEC:O1A	0.44	2.59	7	1
2:A:102:HEC:CHA	2:A:102:HEC:HBD1	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:63:THR:O	2:A:103:HEC:HMC2	0.44	2.12	7	1
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:5:VAL:HG13	1:A:12:ASP:OD2	0.44	2.13	11	1
2:A:103:HEC:HMC1	2:A:103:HEC:HBC3	0.44	1.89	4	1
1:A:62:PRO:CD	2:A:102:HEC:C2A	0.44	2.96	15	4
1:A:32:GLU:O	1:A:33:LYS:HG2	0.44	2.12	14	1
2:A:103:HEC:HBC3	2:A:103:HEC:CMC	0.43	2.43	4	1
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:54:CYS:O	1:A:55:HIS:C	0.43	2.61	15	3
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:16:PRO:HG2	1:A:19:ALA:HB3	0.43	1.90	11	1
1:A:43:LYS:NZ	2:A:103:HEC:HAD1	0.43	2.26	18	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:ALA:O	2:A:102:HEC:HMD2	0.43	2.12	20	1
1:A:43:LYS:C	1:A:45:MET:N	0.43	2.76	8	1
1:A:2:ASP:CG	1:A:18:LYS:CB	0.43	2.92	10	1
1:A:15:PHE:CZ	2:A:102:HEC:C4B	0.43	3.02	8	2
1:A:5:VAL:HG13	1:A:12:ASP:CG	0.43	2.38	13	1
1:A:37:LYS:NZ	2:A:101:HEC:O2D	0.43	2.52	1	1
1:A:8:ALA:HB1	2:A:103:HEC:O1A	0.43	2.14	15	1
1:A:12:ASP:CG	1:A:13:VAL:N	0.43	2.77	19	1
2:A:103:HEC:CMB	2:A:103:HEC:HBB3	0.42	2.44	12	9
1:A:53:GLY:O	1:A:56:GLU:N	0.42	2.52	18	1
1:A:44:GLU:OE2	1:A:45:MET:SD	0.42	2.78	3	2
2:A:101:HEC:HHA	2:A:101:HEC:CGD	0.42	2.44	13	1
1:A:43:LYS:CE	1:A:43:LYS:HA	0.42	2.45	18	1
1:A:58:MET:HE3	1:A:58:MET:HA	0.42	1.90	3	1
1:A:38:ILE:HD13	2:A:101:HEC:CBD	0.42	2.45	6	1
1:A:38:ILE:HD12	2:A:101:HEC:HBD1	0.42	1.92	8	1
1:A:43:LYS:NZ	1:A:43:LYS:HA	0.42	2.29	18	1
1:A:39:GLU:OE2	1:A:45:MET:HE2	0.42	2.14	12	1
1:A:2:ASP:OD1	1:A:2:ASP:N	0.42	2.52	18	1
1:A:34:GLY:O	1:A:35:PRO:O	0.42	2.38	4	3
1:A:49:LYS:N	1:A:49:LYS:CD	0.42	2.83	5	1
1:A:37:LYS:O	1:A:37:LYS:CG	0.42	2.68	10	1
1:A:44:GLU:CG	1:A:45:MET:N	0.42	2.83	20	2
1:A:33:LYS:O	1:A:33:LYS:HG3	0.42	2.14	12	1
1:A:3:ASP:CB	1:A:14:LYS:HZ3	0.42	2.25	5	1
1:A:52:LYS:HG2	1:A:63:THR:CG2	0.42	2.44	15	1
1:A:65:CYS:O	1:A:66:GLY:C	0.42	2.62	16	2
1:A:22:LYS:O	1:A:22:LYS:CG	0.41	2.68	13	1
1:A:16:PRO:HB2	1:A:19:ALA:HB3	0.41	1.91	1	1
1:A:9:LYS:CB	2:A:103:HEC:O2A	0.41	2.68	14	1
1:A:32:GLU:C	1:A:33:LYS:HG2	0.41	2.40	14	1
1:A:44:GLU:CD	1:A:45:MET:N	0.41	2.78	3	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	3
1:A:31:HIS:O	1:A:32:GLU:O	0.41	2.38	19	1
1:A:32:GLU:C	1:A:33:LYS:HG3	0.41	2.40	19	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:38:ILE:HD12	2:A:101:HEC:O1D	0.41	2.14	7	1
1:A:51:CYS:O	1:A:55:HIS:ND1	0.41	2.53	17	1
1:A:43:LYS:CA	1:A:43:LYS:HE2	0.41	2.46	20	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:101:HEC:CMB	2:A:101:HEC:HBB2	0.41	2.46	7	1
2:A:102:HEC:O1A	2:A:102:HEC:C2A	0.41	2.69	8	1
2:A:103:HEC:HBB3	2:A:103:HEC:HMB1	0.41	1.91	12	2
1:A:43:LYS:CE	2:A:103:HEC:CAD	0.41	2.98	18	1
1:A:60:LYS:HE2	2:A:102:HEC:CMD	0.41	2.46	1	1
1:A:5:VAL:CG1	1:A:12:ASP:OD1	0.41	2.62	4	1
1:A:2:ASP:O	1:A:17:HIS:N	0.41	2.53	19	1
1:A:28:LYS:O	1:A:32:GLU:CA	0.41	2.69	20	1
1:A:32:GLU:O	1:A:33:LYS:HB3	0.40	2.15	6	1
1:A:21:GLN:OE1	1:A:21:GLN:CA	0.40	2.69	2	1
2:A:103:HEC:CBA	2:A:103:HEC:CHA	0.40	2.99	4	1
2:A:103:HEC:CHA	2:A:103:HEC:HBA2	0.40	2.47	4	1
1:A:17:HIS:CE1	1:A:21:GLN:HE22	0.40	2.32	6	1
2:A:103:HEC:O1A	2:A:103:HEC:O2D	0.40	2.40	18	1
1:A:60:LYS:HD2	2:A:102:HEC:HMD2	0.40	1.93	4	1
1:A:6:LEU:O	2:A:103:HEC:O1D	0.40	2.38	18	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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%)	1	12
All	All	1300/1420 (92%)	856 (66%)	334 (26%)	110 (8%)	1	12

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	2	ASP	5
1	A	41	PHE	5
1	A	54	CYS	5
1	A	28	LYS	3
1	A	48	GLY	3
1	A	37	LYS	3
1	A	10	ASN	2
1	A	59	LYS	2
1	A	53	GLY	1
1	A	38	ILE	1
1	A	66	GLY	1
1	A	34	GLY	1
1	A	36	GLY	1

6.3.2 Protein sidechains ⓘ

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%)	33±3 (64±6%)	19±3 (36±6%)	1	8
All	All	1040/1120 (93%)	664 (64%)	376 (36%)	1	8

All 35 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	43	LYS	20
1	A	65	CYS	20
1	A	45	MET	18
1	A	54	CYS	18
1	A	58	MET	17
1	A	60	LYS	16
1	A	9	LYS	14
1	A	30	CYS	13
1	A	51	CYS	13
1	A	70	LYS	13
1	A	71	LYS	13
1	A	22	LYS	12

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	33	LYS	12
1	A	39	GLU	12
1	A	57	GLU	12
1	A	59	LYS	12
1	A	49	LYS	12
1	A	37	LYS	12
1	A	7	LYS	11
1	A	18	LYS	11
1	A	52	LYS	11
1	A	21	GLN	10
1	A	2	ASP	10
1	A	14	LYS	10
1	A	28	LYS	9
1	A	64	LYS	9
1	A	12	ASP	8
1	A	32	GLU	6
1	A	29	LYS	4
1	A	56	GLU	4
1	A	38	ILE	4
1	A	4	ILE	3
1	A	63	THR	3
1	A	10	ASN	2
1	A	44	GLU	2

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 oligosaccharides 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	HEC	A	101	1	50,50,50	1.25±0.11	4±1 (8±1%)
2	HEC	A	103	1	50,50,50	1.03±0.06	3±1 (5±1%)
2	HEC	A	102	1	50,50,50	1.16±0.07	4±1 (8±1%)

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	68,82,82	0.65±0.02	0±0 (0±0%)
2	HEC	A	103	1	68,82,82	0.67±0.01	0±0 (0±0%)
2	HEC	A	102	1	68,82,82	0.65±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	1±0,1,3,7	0±0,14,54,54	-
2	HEC	A	103	1	1±0,1,3,7	0±0,14,54,54	-
2	HEC	A	102	1	1±0,1,3,7	0±0,14,54,54	-

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	101	HEC	FE-NA	6.04	2.15	1.95	13	20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	101	HEC	CHC-C1C	5.84	1.52	1.39	13	20
2	A	102	HEC	FE-NB	5.49	2.11	1.94	1	20
2	A	101	HEC	FE-ND	4.86	2.09	1.94	6	20
2	A	103	HEC	FE-NB	4.62	2.09	1.94	10	20
2	A	102	HEC	CHC-C1C	4.32	1.49	1.39	5	20
2	A	102	HEC	FE-NA	4.11	2.08	1.95	4	20
2	A	103	HEC	CHC-C1C	3.95	1.48	1.39	17	12
2	A	103	HEC	FE-NC	3.84	2.07	1.95	3	18
2	A	102	HEC	FE-NC	3.68	2.07	1.95	1	14
2	A	101	HEC	FE-NC	3.53	2.06	1.95	13	12
2	A	101	HEC	FE-NB	3.40	2.05	1.94	9	11
2	A	102	HEC	FE-ND	2.86	2.03	1.94	4	7
2	A	103	HEC	FE-ND	2.71	2.03	1.94	13	5
2	A	103	HEC	FE-NA	2.45	2.03	1.95	20	4

All 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(°)	Ideal(°)	Models	
								Worst	Total
2	A	101	HEC	CHC-C1C-NC	2.68	119.00	123.86	13	1
2	A	103	HEC	CHC-C1C-C2C	2.05	121.47	127.43	20	1

All unique chiral outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

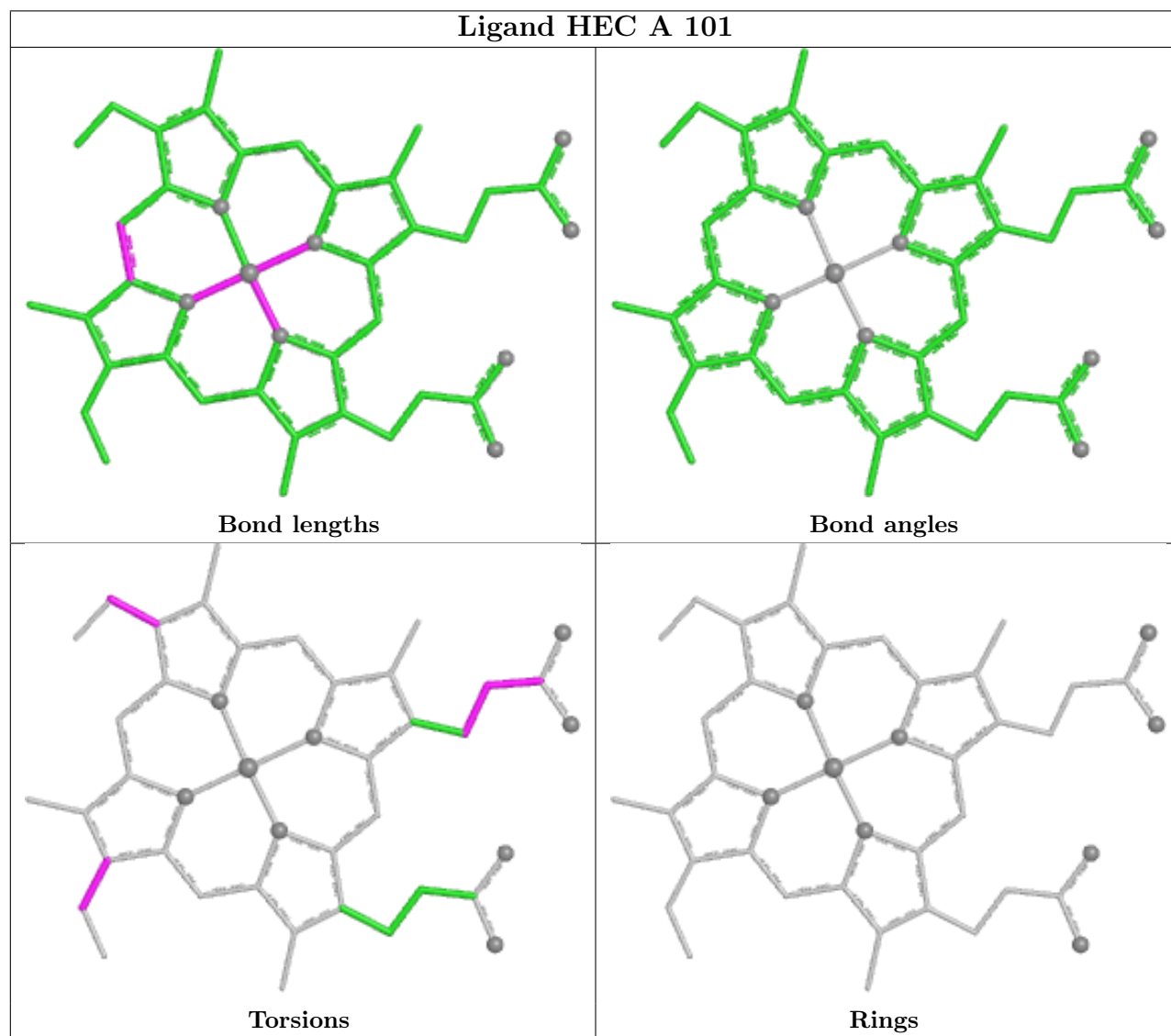
Mol	Chain	Res	Type	Atoms	Models (Total)
2	A	102	HEC	NA	20
2	A	103	HEC	NA	17
2	A	101	HEC	NA	14

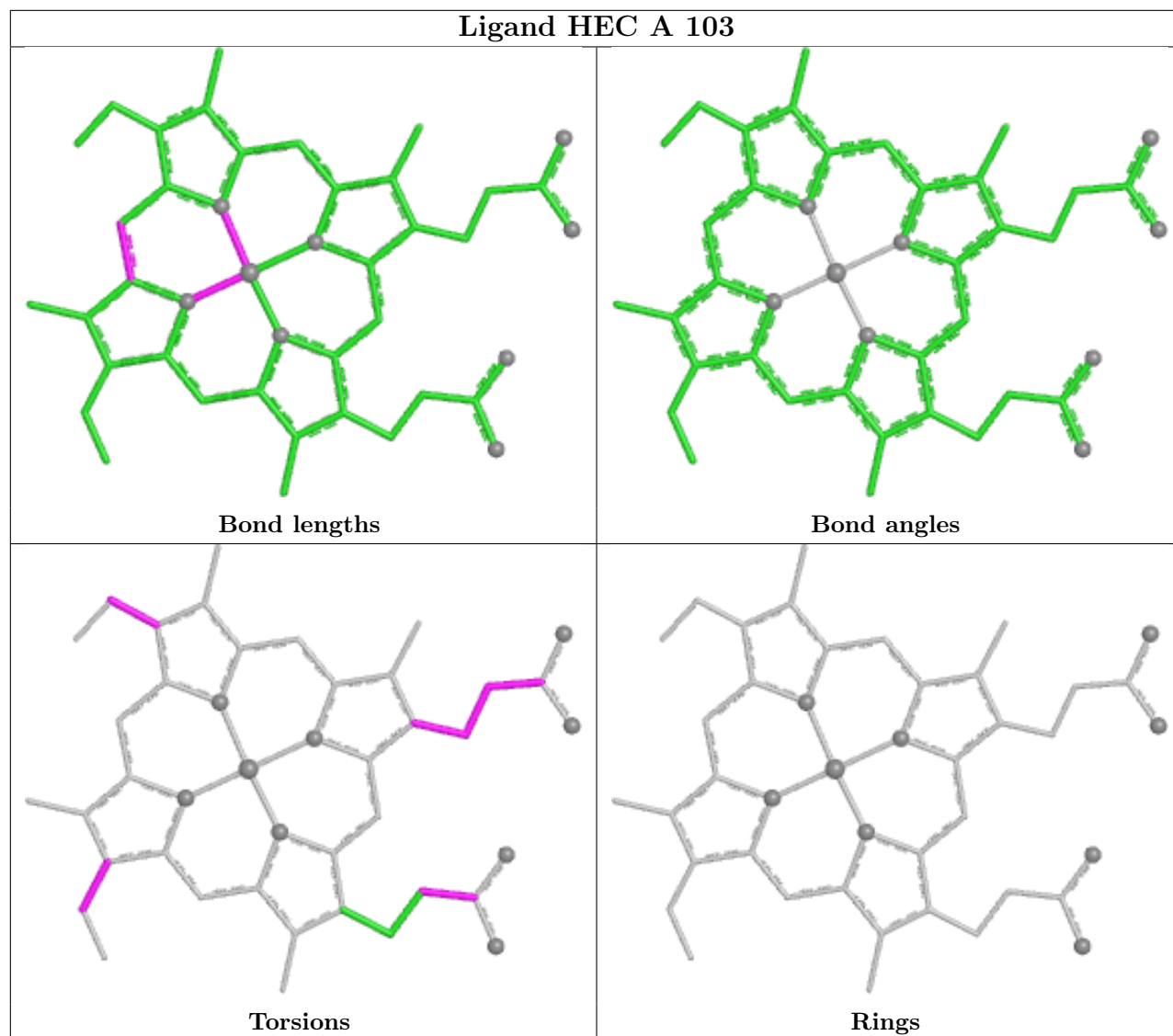
There are no torsion outliers.

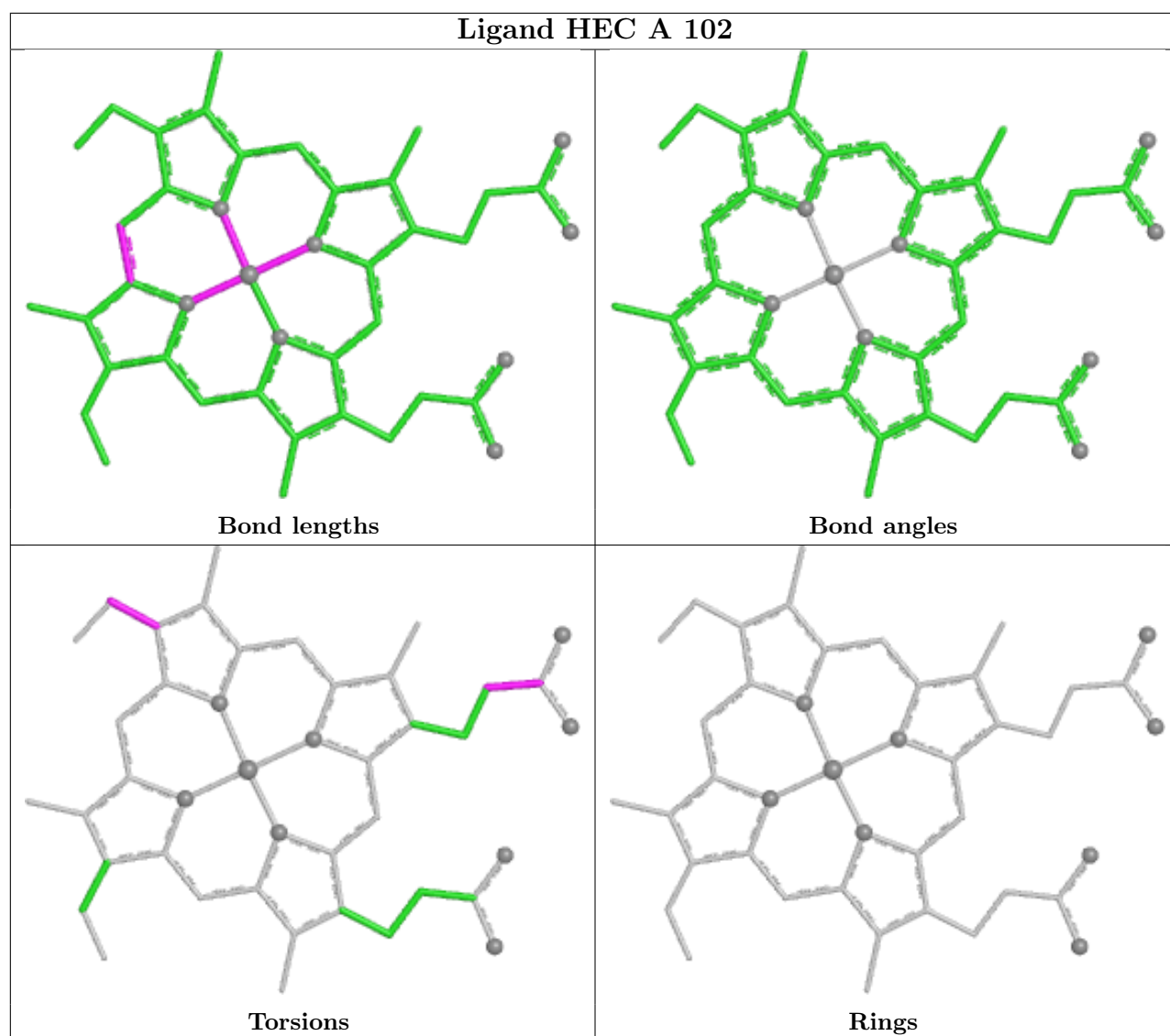
There are no ring outliers.

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 25% for the well-defined parts and 25% 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	504
Number of shifts mapped to atoms	418
Number of unparsed shifts	0
Number of shifts with mapping errors	86
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	40

- Can not parse the chemical shift value. All 219 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	2	ASP	HB2	4.032	0.003	.
1	A	2	ASP	HB3	4.489	0.005	.
1	A	3	ASP	HB2	3.448	0.006	.
1	A	3	ASP	HB3	3.486	0.008	.
1	A	4	ILE	HG12	2.409	0.009	.
1	A	4	ILE	HG13	4.077	0.010	.
1	A	5	VAL	HG11	1.355	0.007	.
1	A	5	VAL	HG12	1.355	0.007	.
1	A	5	VAL	HG13	1.355	0.007	.
1	A	5	VAL	HG21	1.485	0.004	.
1	A	5	VAL	HG22	1.485	0.004	.
1	A	5	VAL	HG23	1.485	0.004	.
1	A	6	LEU	HB2	1.957	0.007	.
1	A	6	LEU	HB3	0.840	0.010	.
1	A	6	LEU	HD11	-0.612	0.006	.
1	A	6	LEU	HD12	-0.612	0.006	.
1	A	6	LEU	HD13	-0.612	0.006	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	6	LEU	HD21	-0.156	0.005	.
1	A	6	LEU	HD22	-0.156	0.005	.
1	A	6	LEU	HD23	-0.156	0.005	.
1	A	7	LYS	HB2	1.768	0.008	.
1	A	7	LYS	HB3	1.871	0.008	.
1	A	7	LYS	HG2	1.674	0.005	.
1	A	7	LYS	HG3	1.644	0.002	.
1	A	9	LYS	HB2	1.525	0.009	.
1	A	9	LYS	HD2	1.262	0.007	.
1	A	9	LYS	HG2	0.974	0.005	.
1	A	9	LYS	HG3	1.118	0.004	.
1	A	10	ASN	HB2	1.655	0.008	.
1	A	10	ASN	HB3	2.802	0.007	.
1	A	11	GLY	HA2	5.349	0.008	.
1	A	11	GLY	HA3	6.962	0.006	.
1	A	12	ASP	HB2	3.543	0.008	.
1	A	12	ASP	HB3	3.836	0.008	.
1	A	13	VAL	HG11	1.095	0.008	.
1	A	13	VAL	HG12	1.095	0.008	.
1	A	13	VAL	HG13	1.095	0.008	.
1	A	13	VAL	HG21	6.495	0.007	.
1	A	13	VAL	HG22	6.495	0.007	.
1	A	13	VAL	HG23	6.495	0.007	.
1	A	14	LYS	HB2	2.362	0.006	.
1	A	14	LYS	HD2	2.181	0.007	.
1	A	14	LYS	HE2	3.427	0.005	.
1	A	14	LYS	HG2	1.812	0.007	.
1	A	14	LYS	HG3	2.067	0.008	.
1	A	15	PHE	HB2	2.722	0.010	.
1	A	15	PHE	HB3	3.687	0.009	.
1	A	16	PRO	HB2	3.260	0.006	.
1	A	16	PRO	HB3	4.343	0.007	.
1	A	16	PRO	HD2	4.518	0.009	.
1	A	16	PRO	HG2	2.136	0.009	.
1	A	17	HIS	HB2	11.352	0.012	.
1	A	17	HIS	HB3	15.704	0.016	.
1	A	18	LYS	HB2	4.154	0.003	.
1	A	18	LYS	HB3	4.587	0.007	.
1	A	18	LYS	HD2	3.156	0.015	.
1	A	18	LYS	HE2	4.069	0.007	.
1	A	18	LYS	HG2	3.064	0.019	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	18	LYS	HG3	3.153	0.015	.
1	A	20	HIS	HB2	6.070	0.011	.
1	A	20	HIS	HB3	9.634	0.011	.
1	A	21	GLN	HB2	2.127	0.004	.
1	A	21	GLN	HB3	3.464	0.010	.
1	A	21	GLN	HG2	0.671	0.006	.
1	A	21	GLN	HG3	4.373	0.002	.
1	A	22	LYS	HB2	2.379	0.004	.
1	A	22	LYS	HB3	2.462	0.003	.
1	A	22	LYS	HD2	2.021	0.006	.
1	A	22	LYS	HE2	3.296	0.012	.
1	A	22	LYS	HG2	1.797	0.015	.
1	A	24	VAL	HG11	-0.377	0.009	.
1	A	24	VAL	HG12	-0.377	0.009	.
1	A	24	VAL	HG13	-0.377	0.009	.
1	A	24	VAL	HG21	-0.150	0.007	.
1	A	24	VAL	HG22	-0.150	0.007	.
1	A	24	VAL	HG23	-0.150	0.007	.
1	A	25	PRO	HB2	1.778	0.008	.
1	A	25	PRO	HD2	3.128	0.008	.
1	A	25	PRO	HD3	3.340	0.006	.
1	A	25	PRO	HG2	1.708	0.005	.
1	A	26	ASP	HB2	2.280	0.012	.
1	A	26	ASP	HB3	2.473	0.005	.
1	A	27	CYS	HB2	3.230	0.008	.
1	A	28	LYS	HB2	2.270	0.008	.
1	A	28	LYS	HE2	3.362	0.001	.
1	A	28	LYS	HG2	2.014	0.010	.
1	A	28	LYS	HG3	2.145	0.009	.
1	A	29	LYS	HB2	0.682	0.006	.
1	A	29	LYS	HB3	1.115	0.006	.
1	A	29	LYS	HE2	2.338	0.000	.
1	A	29	LYS	HE3	2.455	0.008	.
1	A	29	LYS	HG2	0.495	0.012	.
1	A	30	CYS	HB2	0.468	0.013	.
1	A	30	CYS	HB3	1.790	0.024	.
1	A	31	HIS	HB2	10.292	0.013	.
1	A	31	HIS	HB3	12.897	0.011	.
1	A	32	GLU	HB2	2.805	0.018	.
1	A	32	GLU	HB3	2.864	0.007	.
1	A	33	LYS	HB2	2.784	0.027	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	33	LYS	HB3	2.830	0.031	.
1	A	33	LYS	HD2	2.197	0.000	.
1	A	33	LYS	HE2	3.383	0.002	.
1	A	33	LYS	HE3	4.014	0.000	.
1	A	33	LYS	HG2	2.021	0.007	.
1	A	33	LYS	HG3	2.165	0.006	.
1	A	34	GLY	HA2	4.982	0.010	.
1	A	34	GLY	HA3	5.238	0.007	.
1	A	35	PRO	HB2	-0.786	0.012	.
1	A	35	PRO	HB3	-0.268	0.007	.
1	A	35	PRO	HD2	3.735	0.003	.
1	A	35	PRO	HD3	4.167	0.006	.
1	A	35	PRO	HG2	1.374	0.006	.
1	A	36	GLY	HA2	1.010	0.004	.
1	A	36	GLY	HA3	3.934	0.009	.
1	A	37	LYS	HB2	1.242	0.011	.
1	A	37	LYS	HD2	0.970	0.005	.
1	A	37	LYS	HG2	0.535	0.003	.
1	A	37	LYS	HG3	0.766	0.005	.
1	A	38	ILE	HG12	4.296	0.005	.
1	A	39	GLU	HB2	2.164	0.009	.
1	A	39	GLU	HG2	2.351	0.006	.
1	A	39	GLU	HG3	2.388	0.005	.
1	A	40	GLY	HA2	3.579	0.007	.
1	A	40	GLY	HA3	4.038	0.006	.
1	A	41	PHE	HB2	2.174	0.007	.
1	A	41	PHE	HB3	2.535	0.005	.
1	A	41	PHE	HD1	6.033	0.001	.
1	A	41	PHE	HD2	6.031	0.006	.
1	A	41	PHE	HE1	5.013	0.003	.
1	A	41	PHE	HE2	5.004	0.011	.
1	A	42	GLY	HA2	2.380	0.005	.
1	A	42	GLY	HA3	3.075	0.003	.
1	A	43	LYS	HB2	-0.438	0.013	.
1	A	43	LYS	HB3	0.798	0.018	.
1	A	43	LYS	HE2	3.007	0.011	.
1	A	43	LYS	HE3	4.068	0.000	.
1	A	43	LYS	HG2	3.831	0.027	.
1	A	44	GLU	HB2	2.512	0.007	.
1	A	44	GLU	HB3	2.661	0.007	.
1	A	44	GLU	HG2	3.086	0.008	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	44	GLU	HG3	3.168	0.006	.
1	A	45	MET	HB2	0.813	0.009	.
1	A	45	MET	HB3	1.280	0.012	.
1	A	45	MET	HG2	1.814	0.013	.
1	A	45	MET	HG3	2.303	0.010	.
1	A	47	HIS	HB2	15.250	0.024	.
1	A	47	HIS	HB3	18.084	0.011	.
1	A	48	GLY	HA2	4.495	0.005	.
1	A	48	GLY	HA3	5.455	0.013	.
1	A	49	LYS	HB2	1.498	0.006	.
1	A	49	LYS	HD2	1.500	0.000	.
1	A	49	LYS	HG2	1.144	0.007	.
1	A	49	LYS	HG3	1.267	0.013	.
1	A	50	GLY	HA2	1.598	0.010	.
1	A	50	GLY	HA3	1.834	0.007	.
1	A	51	CYS	HB2	0.134	0.011	.
1	A	51	CYS	HB3	0.535	0.010	.
1	A	52	LYS	HB2	1.599	0.005	.
1	A	52	LYS	HB3	2.945	0.010	.
1	A	52	LYS	HD2	2.244	0.002	.
1	A	52	LYS	HD3	2.467	0.004	.
1	A	52	LYS	HE2	4.139	0.002	.
1	A	53	GLY	HA2	3.859	0.006	.
1	A	53	GLY	HA3	4.541	0.004	.
1	A	54	CYS	HB2	0.107	0.009	.
1	A	54	CYS	HB3	1.343	0.007	.
1	A	55	HIS	HB2	16.217	0.012	.
1	A	55	HIS	HB3	19.327	0.010	.
1	A	56	GLU	HB2	2.609	0.006	.
1	A	56	GLU	HB3	2.920	0.013	.
1	A	56	GLU	HG3	3.334	0.012	.
1	A	57	GLU	HB2	2.144	0.008	.
1	A	57	GLU	HB3	2.307	0.010	.
1	A	57	GLU	HG2	2.474	0.006	.
1	A	58	MET	HB2	2.201	0.012	.
1	A	58	MET	HB3	2.860	0.007	.
1	A	58	MET	HG2	2.444	0.004	.
1	A	59	LYS	HB2	1.994	0.000	.
1	A	59	LYS	HB3	1.502	0.002	.
1	A	59	LYS	HE2	3.140	0.003	.
1	A	60	LYS	HB2	0.535	0.008	.

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	60	LYS	HB3	0.863	0.008	.
1	A	60	LYS	HD2	1.109	0.008	.
1	A	60	LYS	HE2	2.542	0.000	.
1	A	60	LYS	HG2	0.870	0.013	.
1	A	60	LYS	HG3	0.921	0.006	.
1	A	61	GLY	HA2	-2.601	0.007	.
1	A	62	PRO	HB2	1.378	0.005	.
1	A	62	PRO	HB3	1.764	0.012	.
1	A	62	PRO	HD2	1.503	0.008	.
1	A	62	PRO	HG2	-0.233	0.008	.
1	A	64	LYS	HB2	1.094	0.009	.
1	A	64	LYS	HB3	1.465	0.014	.
1	A	64	LYS	HD2	1.334	0.033	.
1	A	64	LYS	HD3	1.386	0.022	.
1	A	64	LYS	HG2	1.141	0.003	.
1	A	64	LYS	HG3	1.249	0.005	.
1	A	65	CYS	HB2	-0.855	0.008	.
1	A	65	CYS	HB3	1.097	0.008	.
1	A	66	GLY	HA2	3.765	0.007	.
1	A	66	GLY	HA3	4.964	0.011	.
1	A	67	GLU	HB2	1.750	0.006	.
1	A	67	GLU	HB3	1.533	0.015	.
1	A	67	GLU	HG2	1.874	0.008	.
1	A	67	GLU	HG3	1.929	0.008	.
1	A	68	CYS	HB2	2.178	0.010	.
1	A	68	CYS	HB3	3.581	0.013	.
1	A	69	HIS	HB2	8.532	0.012	.
1	A	69	HIS	HB3	11.967	0.012	.
1	A	70	LYS	HB2	2.762	0.006	.
1	A	70	LYS	HB3	2.927	0.005	.
1	A	70	LYS	HD2	2.255	0.005	.
1	A	70	LYS	HE2	3.341	0.005	.
1	A	70	LYS	HG2	2.237	0.011	.
1	A	71	LYS	HB2	2.350	0.005	.
1	A	71	LYS	HB3	2.416	0.003	.
1	A	71	LYS	HD2	2.149	0.002	.
1	A	71	LYS	HE2	3.378	0.001	.
1	A	71	LYS	HG2	2.084	0.006	.

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

- No matching atom found in the structure. All 86 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	4	ILE	HD12	2.111	0.006	1
1	A	4	ILE	HD13	2.111	0.006	1
1	A	4	ILE	HG13	4.077	0.010	.
1	A	4	ILE	HG21	0.845	0.006	1
1	A	4	ILE	HG22	0.845	0.006	1
1	A	5	VAL	HG11	1.355	0.007	.
1	A	5	VAL	HG12	1.355	0.007	.
1	A	5	VAL	HG22	1.485	0.004	.
1	A	5	VAL	HG23	1.485	0.004	.
1	A	6	LEU	HD11	-0.612	0.006	.
1	A	6	LEU	HD12	-0.612	0.006	.
1	A	6	LEU	HD22	-0.156	0.005	.
1	A	6	LEU	HD23	-0.156	0.005	.
1	A	13	VAL	HG11	1.095	0.008	.
1	A	13	VAL	HG12	1.095	0.008	.
1	A	13	VAL	HG22	6.495	0.007	.
1	A	13	VAL	HG23	6.495	0.007	.
1	A	24	VAL	HG11	-0.377	0.009	.
1	A	24	VAL	HG12	-0.377	0.009	.
1	A	24	VAL	HG22	-0.15	0.007	.
1	A	24	VAL	HG23	-0.15	0.007	.
1	A	38	ILE	HD12	1.621	0.006	1
1	A	38	ILE	HD13	1.621	0.006	1
1	A	38	ILE	HG21	1.445	0.005	1
1	A	38	ILE	HG22	1.445	0.005	1
1	A	63	THR	HG22	2.302	0.006	1
1	A	63	THR	HG23	2.302	0.006	1
1	A	101	HEC	HAA1	0.862	0.024	.
1	A	101	HEC	HAA2	3.03	0.013	.
1	A	101	HEC	HAB	0.91	0.005	1
1	A	101	HEC	HAC	-4.323	0.009	1
1	A	101	HEC	HAD1	2.66	0.021	.
1	A	101	HEC	HAD2	6.713	0.029	.
1	A	101	HEC	HBA1	-0.871	0.016	.
1	A	101	HEC	HBA2	-0.414	0.012	.
1	A	101	HEC	HBB1	1.146	0.004	1
1	A	101	HEC	HBC1	-3.987	0.007	1
1	A	101	HEC	HBD1	-1.457	0.012	.
1	A	101	HEC	HBD2	-0.312	0.009	.
1	A	101	HEC	HHA	3.714	0.007	1
1	A	101	HEC	HHB	-0.713	0.005	1
1	A	101	HEC	HHH	-1.521	0.007	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	101	HEC	HMA1	15.723	0.011	1
1	A	101	HEC	HMB1	17.782	0.005	1
1	A	101	HEC	HMC1	10.407	0.007	1
1	A	101	HEC	HMD1	20.595	0.017	1
1	A	102	HEC	HAA1	3.685	0.010	.
1	A	102	HEC	HAA2	5.54	0.014	.
1	A	102	HEC	HAB	-2.546	0.012	1
1	A	102	HEC	HAC	-0.871	0.005	1
1	A	102	HEC	HAD1	16.042	0.029	.
1	A	102	HEC	HAD2	19.916	0.006	.
1	A	102	HEC	HBA1	-2.072	0.011	.
1	A	102	HEC	HBA2	-1.969	0.012	.
1	A	102	HEC	HBB1	-2.233	0.008	1
1	A	102	HEC	HBC1	-1.017	0.006	1
1	A	102	HEC	HBD1	-1.753	0.008	.
1	A	102	HEC	HBD2	-0.688	0.008	.
1	A	102	HEC	HHA	-1.675	0.005	1
1	A	102	HEC	HHB	8.078	0.005	1
1	A	102	HEC	HHC	-3.913	0.027	1
1	A	102	HEC	HHD	11.378	0.004	1
1	A	102	HEC	HMA1	0.654	0.008	1
1	A	102	HEC	HMB1	12.145	0.009	1
1	A	102	HEC	HMC1	18.001	0.006	1
1	A	102	HEC	HMD1	13.155	0.011	1
1	A	103	HEC	HAA1	2.877	0.013	.
1	A	103	HEC	HAA2	4.147	0.036	.
1	A	103	HEC	HAB	0.73	0.009	1
1	A	103	HEC	HAC	-0.062	0.016	1
1	A	103	HEC	HAD1	2.435	0.017	.
1	A	103	HEC	HAD2	6.471	0.011	.
1	A	103	HEC	HBA1	-0.853	0.007	.
1	A	103	HEC	HBA2	-0.257	0.009	.
1	A	103	HEC	HBB1	2.048	0.006	1
1	A	103	HEC	HBC1	1.623	0.015	1
1	A	103	HEC	HBD1	0.126	0.007	.
1	A	103	HEC	HBD2	0.466	0.009	.
1	A	103	HEC	HHA	0.769	0.006	1
1	A	103	HEC	HHB	-1.612	0.002	1
1	A	103	HEC	HHC	2.249	0.005	1
1	A	103	HEC	HHD	1.212	0.003	1
1	A	103	HEC	HMA1	14.578	0.032	1

Continued on next page...

Continued from previous page...

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	103	HEC	HMB1	14.484	0.022	1
1	A	103	HEC	HMC1	10.943	0.006	1
1	A	103	HEC	HMD1	17.414	0.011	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	-0.11 ± 0.59	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 25%, i.e. 211 atoms were assigned a chemical shift out of a possible 855. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	178/334 (53%)	118/139 (85%)	0/132 (0%)	60/63 (95%)
Sidechain	32/459 (7%)	32/291 (11%)	0/149 (0%)	0/19 (0%)
Aromatic	1/62 (2%)	1/34 (3%)	0/22 (0%)	0/6 (0%)
Overall	211/855 (25%)	151/464 (33%)	0/303 (0%)	60/88 (68%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 25%, i.e. 226 atoms were assigned a chemical shift out of a possible 908. 0 out of 4 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	189/357 (53%)	126/148 (85%)	0/142 (0%)	63/67 (94%)
Sidechain	36/489 (7%)	36/311 (12%)	0/159 (0%)	0/19 (0%)
Aromatic	1/62 (2%)	1/34 (3%)	0/22 (0%)	0/6 (0%)
Overall	226/908 (25%)	163/493 (33%)	0/323 (0%)	63/92 (68%)

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	46	ALA	HB1	-3.38	0.14 – 2.58	-19.4
1	A	46	ALA	HB2	-3.38	0.14 – 2.58	-19.4
1	A	46	ALA	HB3	-3.38	0.14 – 2.58	-19.4
1	A	69	HIS	HA	10.51	2.49 – 6.71	14.0
1	A	31	HIS	HA	10.23	2.49 – 6.71	13.3
1	A	51	CYS	HA	-1.92	1.97 – 7.35	-12.2
1	A	8	ALA	HB1	4.33	0.14 – 2.58	12.2
1	A	8	ALA	HB2	4.33	0.14 – 2.58	12.2
1	A	8	ALA	HB3	4.33	0.14 – 2.58	12.2
1	A	65	CYS	HA	-1.39	1.97 – 7.35	-11.2
1	A	43	LYS	HA	-0.12	2.15 – 6.37	-10.4
1	A	55	HIS	HA	8.56	2.49 – 6.71	9.4
1	A	16	PRO	HA	7.38	2.78 – 6.00	9.3
1	A	17	HIS	HA	8.38	2.49 – 6.71	8.9
1	A	3	ASP	HA	7.28	3.04 – 6.12	8.8
1	A	47	HIS	HA	8.27	2.49 – 6.71	8.7
1	A	2	ASP	HA	7.25	3.04 – 6.12	8.7
1	A	18	LYS	H	12.97	5.24 – 11.12	8.2
1	A	20	HIS	HA	7.92	2.49 – 6.71	7.9
1	A	12	ASP	HA	6.99	3.04 – 6.12	7.8
1	A	18	LYS	HA	7.45	2.15 – 6.37	7.6
1	A	19	ALA	HB1	3.02	0.14 – 2.58	6.8
1	A	19	ALA	HB2	3.02	0.14 – 2.58	6.8
1	A	19	ALA	HB3	3.02	0.14 – 2.58	6.8
1	A	41	PHE	HZ	4.35	4.94 – 9.06	-6.4
1	A	46	ALA	HA	1.73	2.13 – 6.34	-6.0
1	A	42	GLY	H	4.70	5.23 – 11.42	-5.9
1	A	20	HIS	H	12.11	4.92 – 11.57	5.8
1	A	35	PRO	HA	6.24	2.78 – 6.00	5.8
1	A	31	HIS	H	11.95	4.92 – 11.57	5.6
1	A	63	THR	HG21	2.30	0.08 – 2.19	5.5
1	A	63	THR	HG22	2.30	0.08 – 2.19	5.5
1	A	63	THR	HG23	2.30	0.08 – 2.19	5.5
1	A	47	HIS	H	11.69	4.92 – 11.57	5.2
1	A	4	ILE	HD11	2.11	-0.72 – 2.09	5.1
1	A	4	ILE	HD12	2.11	-0.72 – 2.09	5.1
1	A	4	ILE	HD13	2.11	-0.72 – 2.09	5.1
1	A	69	HIS	H	11.61	4.92 – 11.57	5.1

Continued on next page...

Continued from previous page...

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	17	HIS	H	11.61	4.92 – 11.57	5.1
1	A	51	CYS	H	4.99	5.02 – 11.74	-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. 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:

