



Full wwPDB NMR Structure Validation Report ⓘ

Mar 19, 2026 – 07:51 PM UTC

PDB ID : 2JRL / pdb_00002jrl
BMRB ID : 15334
Title : Solution structure of the beryllofluoride-activated NtrC4 receiver domain dimer
Authors : Lee, C.; Hong, E.; Doucleff, M.; Pelton, J.G.; Wemmer, D.E.; Berkeley Structural Genomics Center (BSGC)
Deposited on : 2007-06-27

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
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) : 2.49

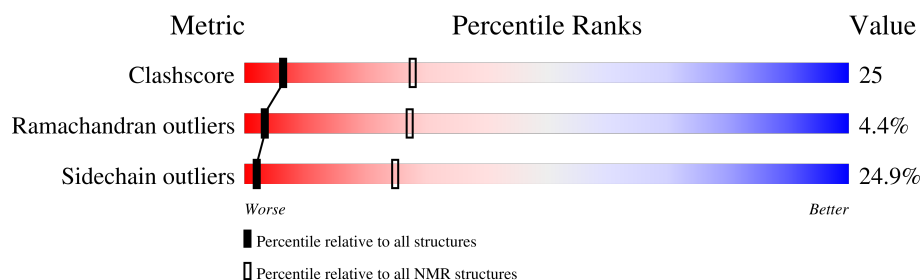
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 40%.

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	121	
1	B	121	

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:121, B:1-B:118 (237)	0.28	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 5 single-model clusters were found.

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

3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 3858 atoms, of which 1932 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcriptional regulator (NtrC family).

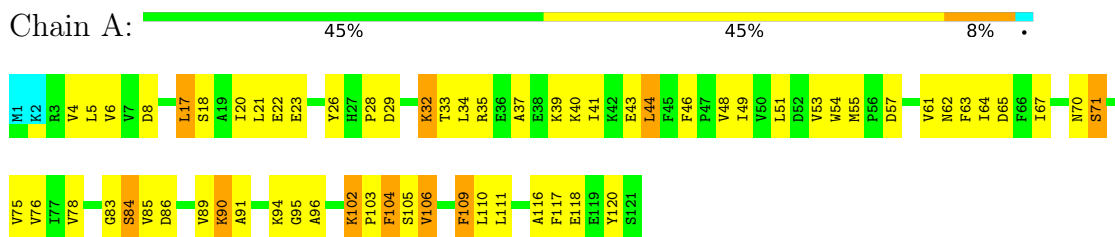
Mol	Chain	Residues	Atoms						Trace
1	A	121	Total	C	H	N	O	S	0
			1929	624	966	150	187	2	
1	B	121	Total	C	H	N	O	S	0
			1929	624	966	150	187	2	

4 Residue-property plots

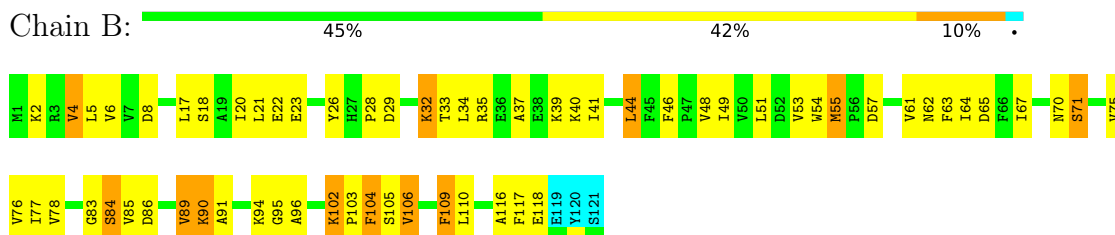
4.1 Average score per residue in the NMR ensemble

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: Transcriptional regulator (NtrC family)



- Molecule 1: Transcriptional regulator (NtrC family)

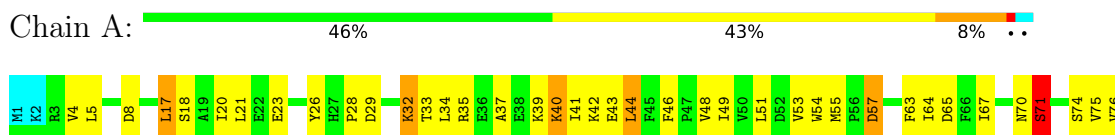


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

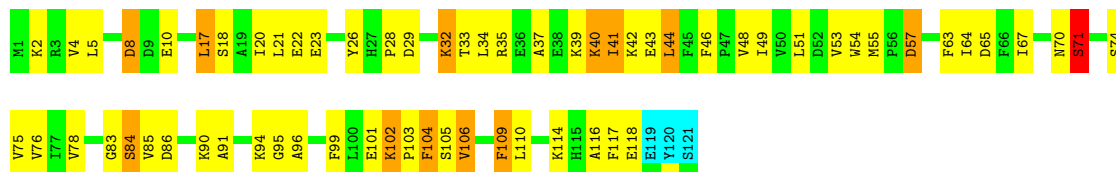
- Molecule 1: Transcriptional regulator (NtrC family)





- Molecule 1: Transcriptional regulator (NtrC family)

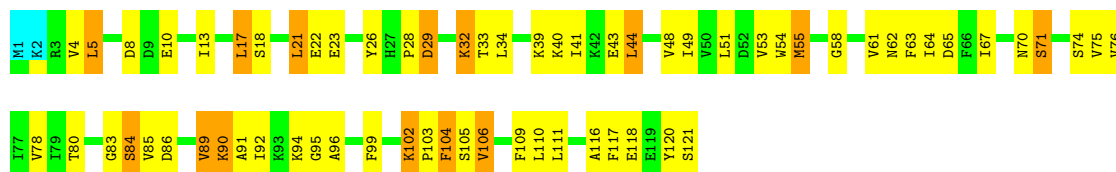
Chain B: 44% 43% 10% ..



4.2.2 Score per residue for model 2

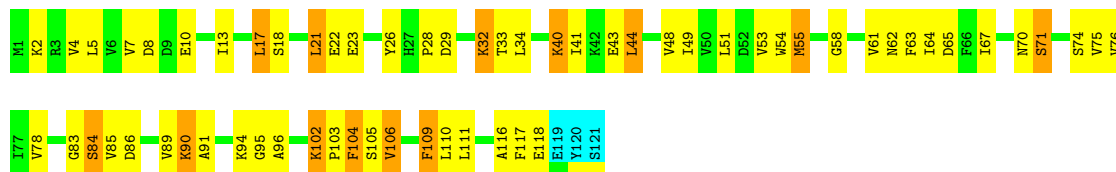
- Molecule 1: Transcriptional regulator (NtrC family)

Chain A: 44% 43% 12% .



- Molecule 1: Transcriptional regulator (NtrC family)

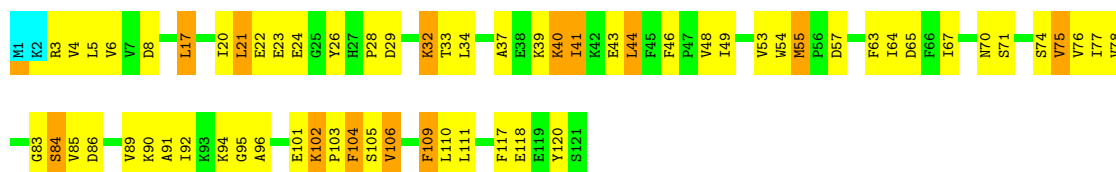
Chain B: 46% 40% 11% .



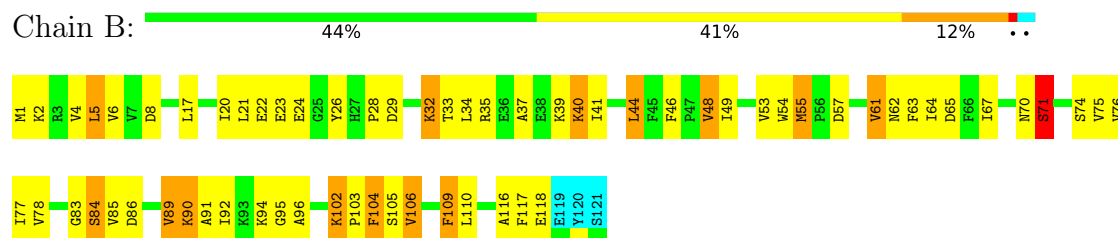
4.2.3 Score per residue for model 3

- Molecule 1: Transcriptional regulator (NtrC family)

Chain A: 45% 42% 11% .

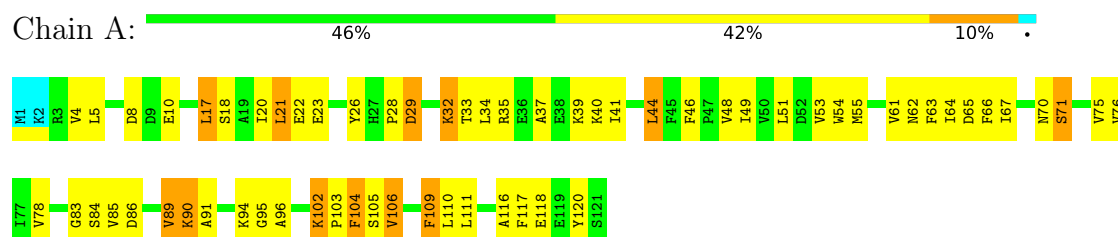


- Molecule 1: Transcriptional regulator (NtrC family)

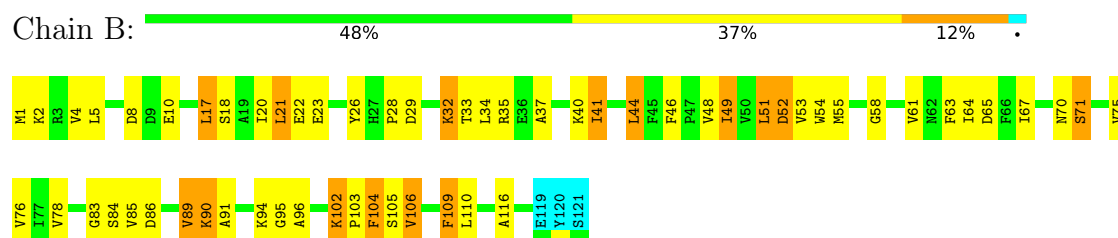


4.2.4 Score per residue for model 4

- Molecule 1: Transcriptional regulator (NtrC family)

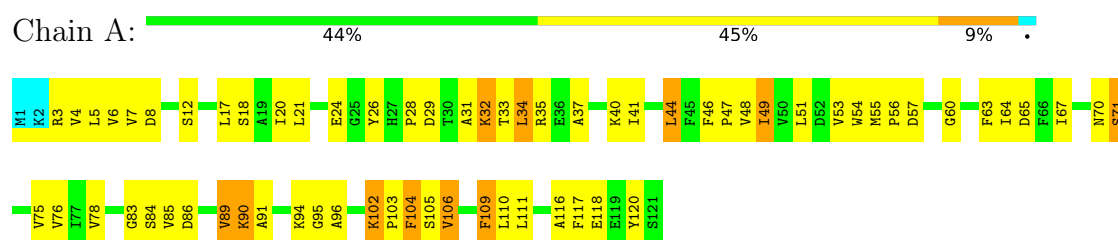


- Molecule 1: Transcriptional regulator (NtrC family)

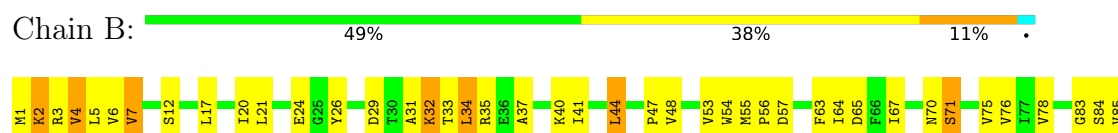


4.2.5 Score per residue for model 5 (medoid)

- Molecule 1: Transcriptional regulator (NtrC family)



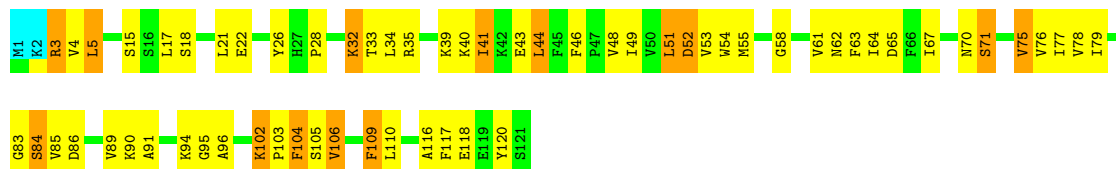
- Molecule 1: Transcriptional regulator (NtrC family)



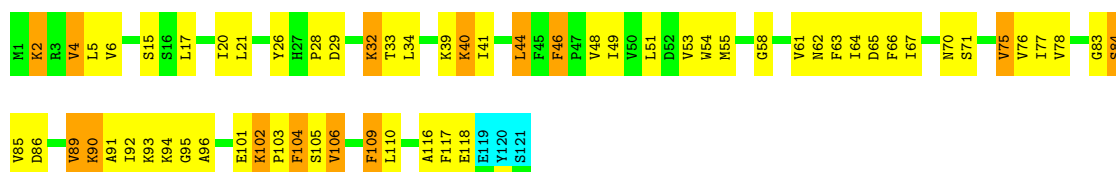


4.2.6 Score per residue for model 6

- Molecule 1: Transcriptional regulator (NtrC family)

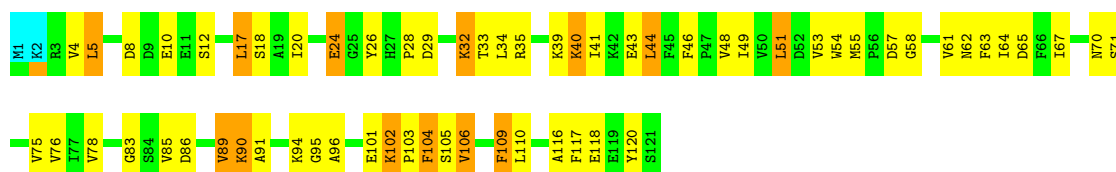


- Molecule 1: Transcriptional regulator (NtrC family)

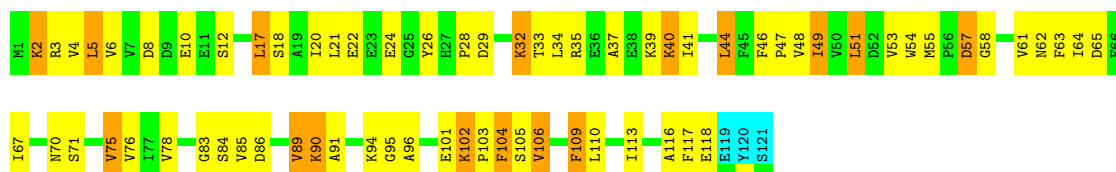


4.2.7 Score per residue for model 7

- Molecule 1: Transcriptional regulator (NtrC family)

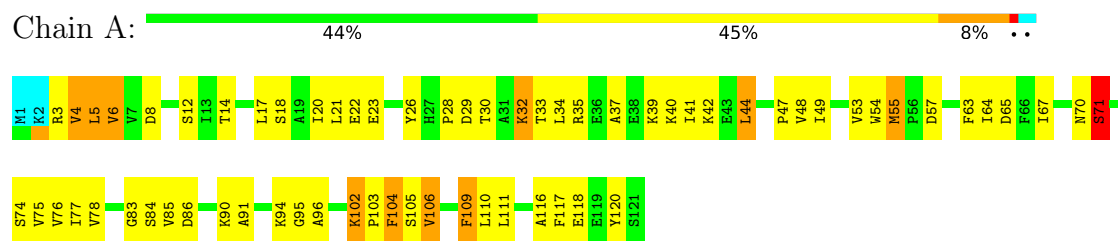


- Molecule 1: Transcriptional regulator (NtrC family)



4.2.8 Score per residue for model 8

- Molecule 1: Transcriptional regulator (NtrC family)

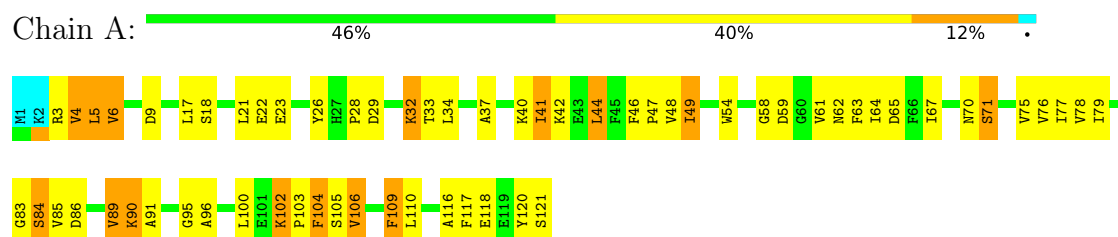


- Molecule 1: Transcriptional regulator (NtrC family)



4.2.9 Score per residue for model 9

- Molecule 1: Transcriptional regulator (NtrC family)

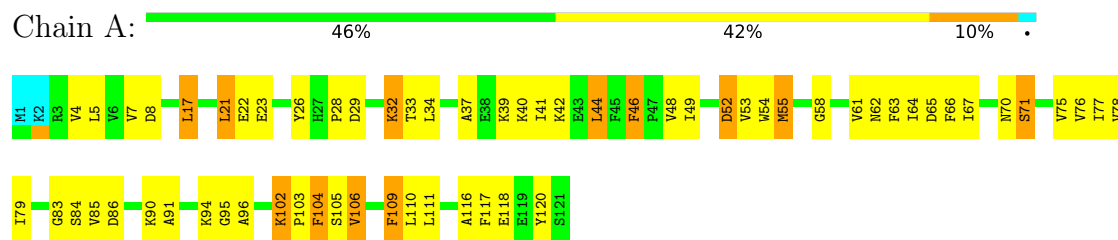


- Molecule 1: Transcriptional regulator (NtrC family)

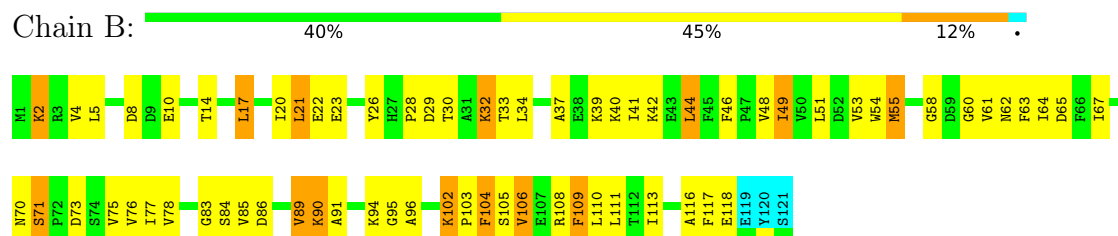


4.2.10 Score per residue for model 10

- Molecule 1: Transcriptional regulator (NtrC family)

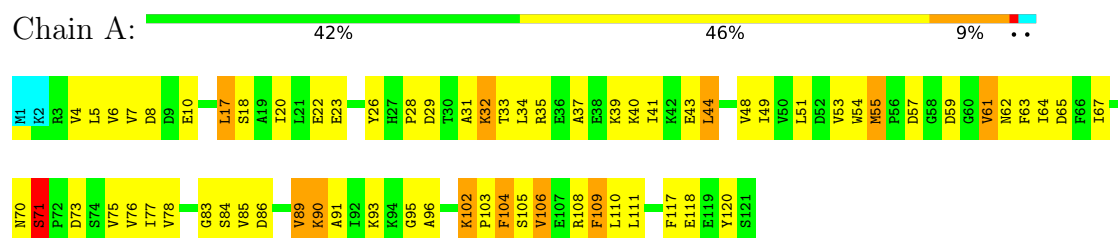


- Molecule 1: Transcriptional regulator (NtrC family)

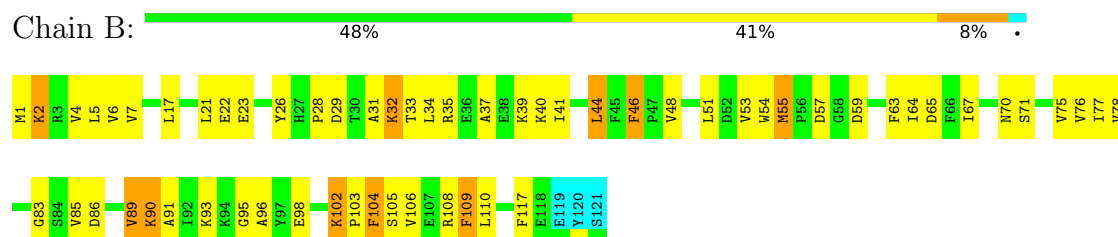


4.2.11 Score per residue for model 11

- Molecule 1: Transcriptional regulator (NtrC family)

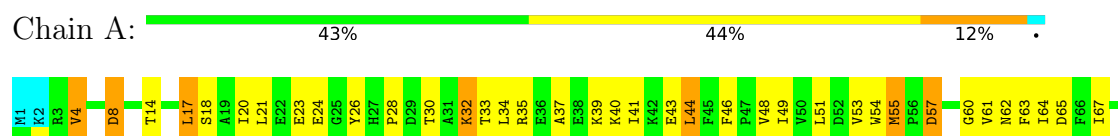


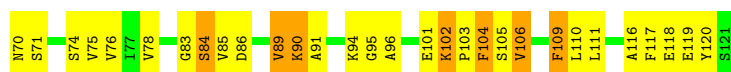
- Molecule 1: Transcriptional regulator (NtrC family)



4.2.12 Score per residue for model 12

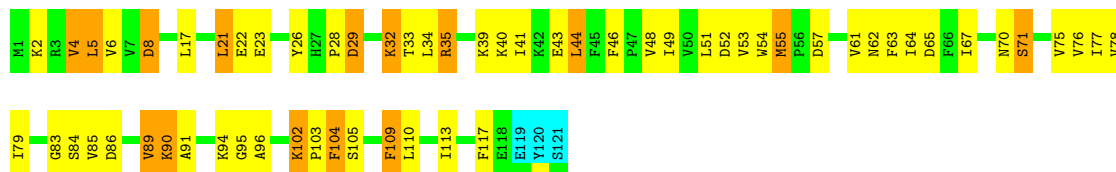
- Molecule 1: Transcriptional regulator (NtrC family)





- Molecule 1: Transcriptional regulator (NtrC family)

Chain B: 47% 38% 12% .



4.2.13 Score per residue for model 13

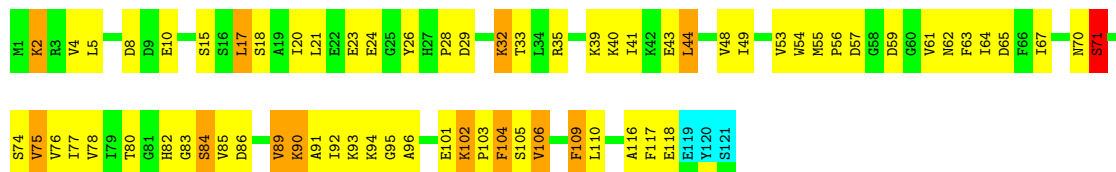
- Molecule 1: Transcriptional regulator (NtrC family)

Chain A: 41% 45% 12% .



- Molecule 1: Transcriptional regulator (NtrC family)

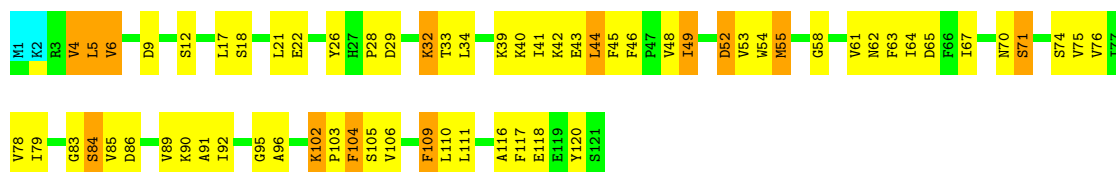
Chain B: 40% 46% 10% ..



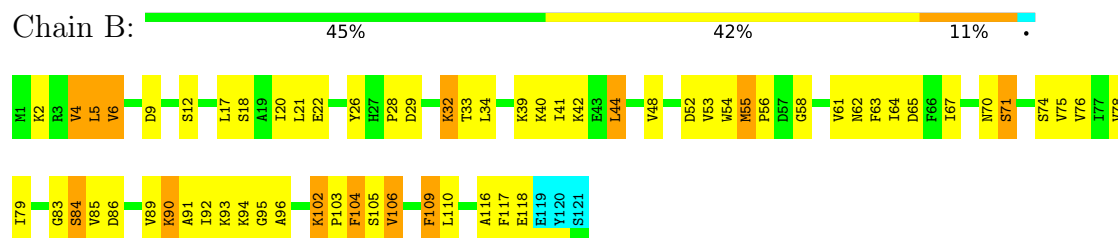
4.2.14 Score per residue for model 14

- Molecule 1: Transcriptional regulator (NtrC family)

Chain A: 45% 43% 11% .

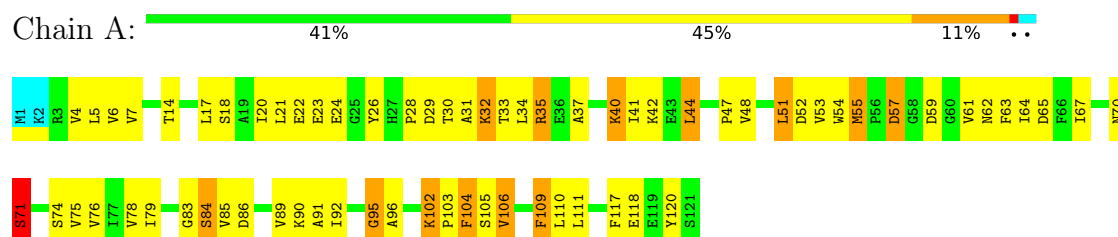


- Molecule 1: Transcriptional regulator (NtrC family)

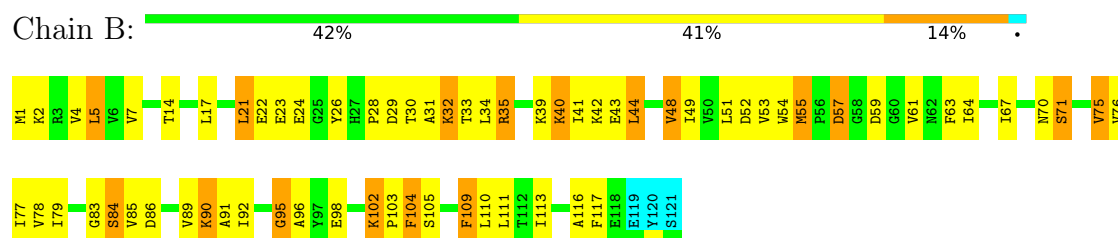


4.2.15 Score per residue for model 15

- Molecule 1: Transcriptional regulator (NtrC family)

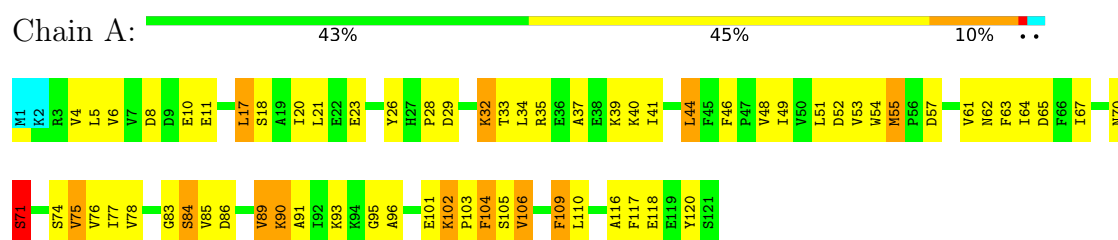


- Molecule 1: Transcriptional regulator (NtrC family)

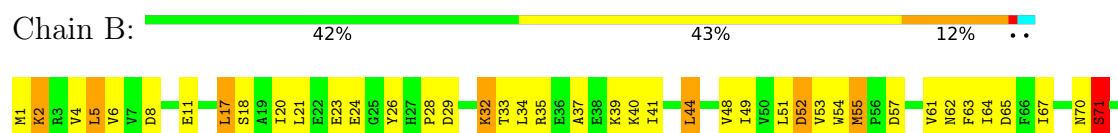


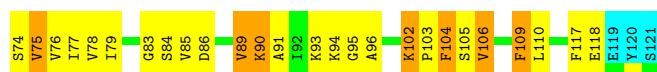
4.2.16 Score per residue for model 16

- Molecule 1: Transcriptional regulator (NtrC family)



- Molecule 1: Transcriptional regulator (NtrC family)

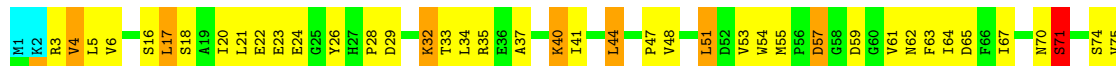




4.2.17 Score per residue for model 17

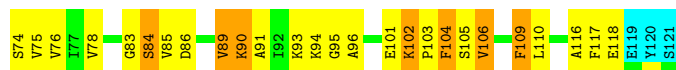
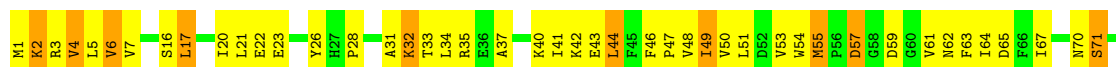
- Molecule 1: Transcriptional regulator (NtrC family)

Chain A: 45% 42% 11% ..



- Molecule 1: Transcriptional regulator (NtrC family)

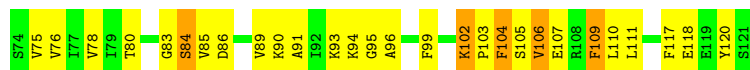
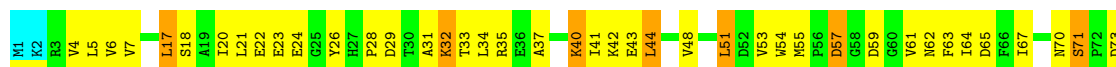
Chain B: 39% 45% 14% .



4.2.18 Score per residue for model 18

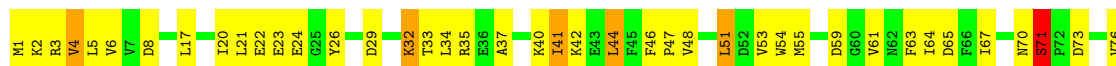
- Molecule 1: Transcriptional regulator (NtrC family)

Chain A: 41% 47% 10% .



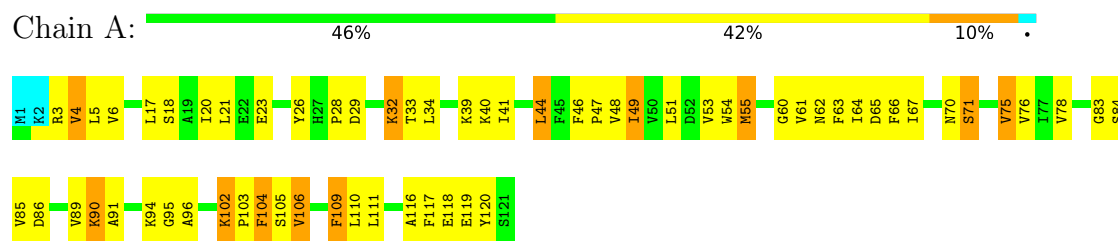
- Molecule 1: Transcriptional regulator (NtrC family)

Chain B: 45% 41% 10% ..

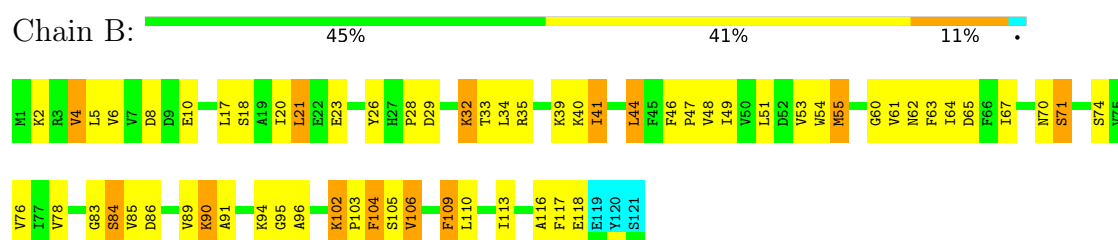


4.2.19 Score per residue for model 19

- Molecule 1: Transcriptional regulator (NtrC family)

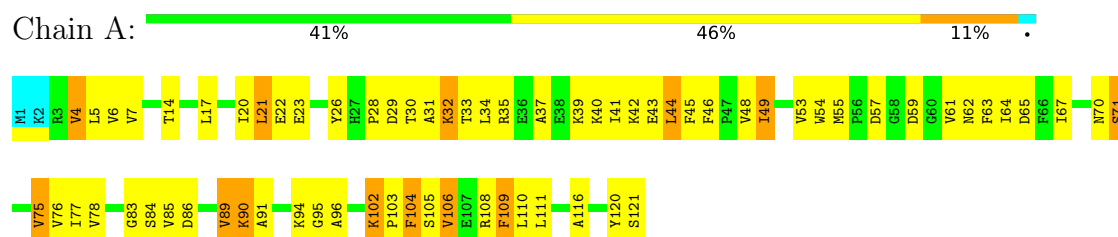


- Molecule 1: Transcriptional regulator (NtrC family)

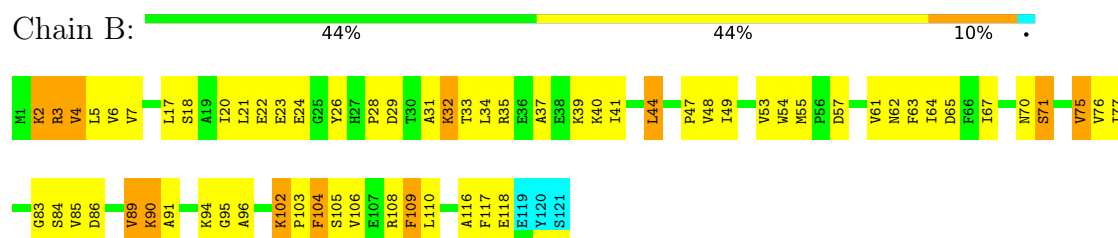


4.2.20 Score per residue for model 20

- Molecule 1: Transcriptional regulator (NtrC family)



- Molecule 1: Transcriptional regulator (NtrC family)



5 Refinement protocol and experimental data overview

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

Of the 50 calculated structures, 20 were deposited, based on the following criterion: *target function*.

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

Software name	Classification	Version
CYANA	structure solution	2.0
X-PLOR NIH	structure solution	2.1.2
X-PLOR NIH	refinement	2.1.2

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	1320
Number of shifts mapped to atoms	1320
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	40%

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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	946	942	941	47±4
1	B	936	945	945	49±5
All	All	37640	37740	37720	1913

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 25.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:40:LYS:O	1:A:44:LEU:HD12	0.88	1.69	14	2
1:B:34:LEU:HD12	1:B:51:LEU:HD11	0.86	1.45	12	6
1:A:34:LEU:HD12	1:A:51:LEU:HD11	0.84	1.48	16	5
1:A:44:LEU:HD13	1:A:44:LEU:O	0.84	1.72	20	2
1:B:40:LYS:O	1:B:44:LEU:HD23	0.84	1.73	3	12
1:A:40:LYS:O	1:A:44:LEU:HD23	0.82	1.74	11	13
1:B:21:LEU:HD13	1:B:26:TYR:HB2	0.80	1.51	19	1
1:A:48:VAL:HG11	1:A:116:ALA:HB1	0.80	1.54	9	16
1:B:48:VAL:HG11	1:B:116:ALA:HB1	0.78	1.55	3	17
1:A:44:LEU:HD13	1:A:44:LEU:C	0.77	2.04	20	2
1:B:17:LEU:HD21	1:B:104:PHE:CE1	0.74	2.17	14	8
1:A:48:VAL:HG12	1:A:75:VAL:HG13	0.74	1.58	19	5
1:B:7:VAL:HG13	1:B:31:ALA:HB3	0.73	1.60	5	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:ILE:HD13	1:A:76:VAL:HG21	0.73	1.59	16	19
1:B:40:LYS:O	1:B:44:LEU:HD22	0.73	1.84	20	8
1:B:48:VAL:HG12	1:B:75:VAL:HG13	0.72	1.59	13	4
1:B:67:ILE:HD13	1:B:76:VAL:HG21	0.72	1.62	12	18
1:A:17:LEU:HD21	1:A:104:PHE:CE1	0.72	2.19	19	13
1:A:91:ALA:O	1:A:96:ALA:HB3	0.71	1.85	15	20
1:B:44:LEU:HD11	1:B:46:PHE:CE1	0.71	2.21	11	2
1:A:40:LYS:O	1:A:44:LEU:HD22	0.71	1.86	10	5
1:B:91:ALA:O	1:B:96:ALA:HB3	0.70	1.85	3	20
1:A:5:LEU:HD12	1:A:29:ASP:HB3	0.70	1.61	4	3
1:B:34:LEU:HD22	1:B:51:LEU:HD11	0.70	1.64	7	1
1:B:89:VAL:HG12	1:B:90:LYS:N	0.70	2.02	13	16
1:A:89:VAL:HG12	1:A:90:LYS:N	0.69	2.03	11	11
1:B:5:LEU:HD12	1:B:29:ASP:HB3	0.69	1.64	12	1
1:B:44:LEU:HD21	1:B:46:PHE:CE2	0.69	2.23	3	1
1:B:4:VAL:HG12	1:B:48:VAL:HG23	0.68	1.65	15	1
1:A:44:LEU:HD22	1:A:45:PHE:N	0.68	2.04	14	2
1:A:34:LEU:HD22	1:A:51:LEU:HD11	0.68	1.64	7	1
1:A:17:LEU:HD21	1:A:104:PHE:CZ	0.66	2.25	1	13
1:A:44:LEU:HD11	1:A:46:PHE:CE1	0.66	2.25	10	1
1:B:44:LEU:HD11	1:B:46:PHE:CE2	0.66	2.25	12	1
1:B:21:LEU:HD12	1:B:109:PHE:CZ	0.66	2.25	10	2
1:B:34:LEU:HD21	1:B:55:MET:HG2	0.66	1.67	14	4
1:A:34:LEU:HD21	1:A:55:MET:HG2	0.66	1.67	2	5
1:B:17:LEU:HD21	1:B:104:PHE:CZ	0.65	2.27	7	13
1:A:17:LEU:HD11	1:A:104:PHE:CZ	0.65	2.26	5	5
1:B:17:LEU:HD11	1:B:104:PHE:CZ	0.65	2.26	9	3
1:A:89:VAL:HG13	1:B:92:ILE:HD12	0.65	1.69	18	3
1:A:7:VAL:HG13	1:A:31:ALA:HB3	0.64	1.69	20	5
1:B:34:LEU:CD1	1:B:51:LEU:HD11	0.63	2.22	12	6
1:A:48:VAL:HG12	1:A:75:VAL:CG1	0.63	2.23	11	4
1:B:17:LEU:HD11	1:B:104:PHE:CE1	0.63	2.28	15	6
1:A:4:VAL:HG22	1:A:48:VAL:HG23	0.63	1.69	2	13
1:A:21:LEU:HD12	1:A:109:PHE:CZ	0.62	2.28	3	3
1:A:44:LEU:HD21	1:A:46:PHE:CE2	0.62	2.29	7	4
1:B:4:VAL:HG22	1:B:48:VAL:HG23	0.62	1.71	13	8
1:A:34:LEU:CD1	1:A:55:MET:HE2	0.61	2.25	5	1
1:B:4:VAL:HG21	1:B:21:LEU:HD21	0.61	1.71	15	1
1:A:21:LEU:HD12	1:A:109:PHE:CE2	0.60	2.32	3	4
1:A:21:LEU:HD23	1:A:26:TYR:HB2	0.60	1.74	2	2
1:B:44:LEU:HD23	1:B:44:LEU:O	0.60	1.97	14	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:44:LEU:HD23	1:B:44:LEU:C	0.60	2.21	14	6
1:A:34:LEU:CD1	1:A:51:LEU:HD11	0.59	2.26	16	5
1:A:44:LEU:HD22	1:A:45:PHE:C	0.59	2.22	14	2
1:A:51:LEU:HD13	1:A:63:PHE:CD2	0.59	2.32	16	4
1:B:64:ILE:HA	1:B:67:ILE:HD12	0.58	1.75	2	20
1:A:34:LEU:CD2	1:A:51:LEU:HD11	0.58	2.27	7	1
1:A:48:VAL:HG12	1:A:75:VAL:HG23	0.58	1.74	6	4
1:B:3:ARG:NH1	1:B:44:LEU:HD12	0.58	2.12	17	1
1:A:78:VAL:HG23	1:A:96:ALA:HB2	0.58	1.75	11	20
1:B:89:VAL:CG1	1:B:90:LYS:N	0.58	2.65	13	3
1:A:32:LYS:HG2	1:A:33:THR:HG23	0.58	1.74	10	20
1:A:8:ASP:HA	1:A:55:MET:HE1	0.58	1.76	12	4
1:B:21:LEU:HD12	1:B:109:PHE:CE2	0.58	2.33	10	2
1:A:64:ILE:HA	1:A:67:ILE:HD12	0.58	1.75	2	20
1:B:51:LEU:HD13	1:B:63:PHE:CD2	0.58	2.33	12	7
1:A:85:VAL:O	1:A:89:VAL:HG23	0.57	1.99	6	2
1:B:44:LEU:HD11	1:B:46:PHE:CD1	0.57	2.34	11	1
1:A:3:ARG:CZ	1:A:44:LEU:HD11	0.57	2.30	6	2
1:A:6:VAL:HG12	1:A:14:THR:HG22	0.57	1.76	15	1
1:A:63:PHE:CE2	1:A:67:ILE:HD11	0.57	2.35	16	14
1:B:34:LEU:CD1	1:B:55:MET:HE2	0.57	2.28	5	1
1:B:51:LEU:HD12	1:B:63:PHE:CD2	0.57	2.35	18	2
1:A:44:LEU:HD11	1:A:46:PHE:CE2	0.57	2.34	16	4
1:B:63:PHE:CE2	1:B:67:ILE:HD11	0.56	2.34	12	17
1:B:102:LYS:CB	1:B:103:PRO:CD	0.56	2.83	11	20
1:B:4:VAL:HA	1:B:48:VAL:O	0.56	2.01	6	10
1:A:48:VAL:HG11	1:A:116:ALA:CB	0.56	2.29	9	7
1:B:61:VAL:HG21	1:B:90:LYS:HD2	0.56	1.77	9	11
1:B:4:VAL:CG2	1:B:21:LEU:HD21	0.56	2.31	15	4
1:B:76:VAL:O	1:B:96:ALA:HA	0.56	2.00	10	20
1:B:21:LEU:HD23	1:B:26:TYR:HB2	0.55	1.76	2	1
1:A:89:VAL:CG1	1:A:90:LYS:N	0.55	2.68	11	3
1:B:32:LYS:HG2	1:B:33:THR:HG23	0.55	1.78	1	20
1:B:61:VAL:HG21	1:B:90:LYS:HD3	0.55	1.77	18	4
1:A:17:LEU:HD11	1:A:104:PHE:CE1	0.55	2.36	6	3
1:B:26:TYR:CD1	1:B:26:TYR:N	0.55	2.74	12	20
1:B:91:ALA:O	1:B:96:ALA:CB	0.55	2.54	3	20
1:B:8:ASP:HA	1:B:55:MET:HE1	0.55	1.77	12	4
1:A:51:LEU:HD22	1:A:63:PHE:CD2	0.54	2.37	19	5
1:A:34:LEU:HD21	1:A:55:MET:CG	0.54	2.32	3	3
1:A:76:VAL:O	1:A:96:ALA:HA	0.54	2.02	6	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:LYS:CB	1:A:103:PRO:CD	0.54	2.85	5	20
1:B:7:VAL:HG11	1:B:34:LEU:CD1	0.54	2.33	8	1
1:B:41:ILE:HG23	1:B:46:PHE:CE1	0.54	2.37	4	5
1:A:21:LEU:HD23	1:A:26:TYR:CB	0.54	2.32	10	2
1:B:2:LYS:HD2	1:B:26:TYR:CE1	0.54	2.37	16	1
1:A:91:ALA:O	1:A:96:ALA:CB	0.54	2.55	19	20
1:A:44:LEU:C	1:A:44:LEU:CD1	0.54	2.77	20	1
1:B:51:LEU:HD22	1:B:63:PHE:CD2	0.54	2.38	6	5
1:B:78:VAL:HG23	1:B:96:ALA:HB2	0.54	1.80	15	19
1:A:4:VAL:HB	1:A:21:LEU:HD21	0.53	1.79	13	7
1:B:34:LEU:HD21	1:B:55:MET:CG	0.53	2.33	16	4
1:B:5:LEU:HD12	1:B:5:LEU:C	0.53	2.27	7	3
1:A:89:VAL:HG13	1:B:92:ILE:CD1	0.53	2.33	14	5
1:B:5:LEU:HD11	1:B:40:LYS:HD2	0.53	1.78	4	3
1:B:48:VAL:HG12	1:B:75:VAL:CG1	0.53	2.33	13	3
1:B:44:LEU:HD11	1:B:46:PHE:CD2	0.53	2.38	12	1
1:B:48:VAL:HG11	1:B:116:ALA:CB	0.53	2.30	9	9
1:A:34:LEU:HD13	1:A:55:MET:HE2	0.53	1.81	5	1
1:B:2:LYS:CG	1:B:26:TYR:CD1	0.53	2.92	7	2
1:B:9:ASP:N	1:B:55:MET:HE1	0.53	2.19	14	1
1:B:61:VAL:HG11	1:B:90:LYS:NZ	0.53	2.18	15	1
1:A:106:VAL:HG22	1:A:110:LEU:HD23	0.53	1.79	20	19
1:A:61:VAL:HG23	1:A:91:ALA:HA	0.53	1.81	10	7
1:A:109:PHE:CD1	1:A:110:LEU:N	0.52	2.78	8	19
1:B:61:VAL:HG23	1:B:91:ALA:HA	0.52	1.81	7	8
1:B:5:LEU:HD12	1:B:6:VAL:N	0.52	2.20	7	4
1:B:109:PHE:CD1	1:B:110:LEU:N	0.52	2.78	14	19
1:B:34:LEU:HD11	1:B:58:GLY:O	0.52	2.04	9	7
1:B:21:LEU:HD23	1:B:28:PRO:HB3	0.52	1.80	12	3
1:B:4:VAL:HB	1:B:21:LEU:HD21	0.52	1.80	11	5
1:A:92:ILE:CD1	1:B:89:VAL:HG13	0.52	2.35	14	2
1:B:4:VAL:CG1	1:B:21:LEU:HD21	0.52	2.34	9	5
1:B:20:ILE:HG21	1:B:106:VAL:HG23	0.52	1.82	4	13
1:A:20:ILE:HG21	1:A:106:VAL:HG23	0.52	1.81	11	14
1:A:4:VAL:CG1	1:A:21:LEU:HD21	0.52	2.34	9	5
1:A:9:ASP:N	1:A:55:MET:HE1	0.52	2.19	14	1
1:B:34:LEU:CD2	1:B:51:LEU:HD11	0.52	2.34	7	1
1:B:48:VAL:HG12	1:B:75:VAL:HG23	0.52	1.82	7	2
1:B:8:ASP:HA	1:B:55:MET:HE3	0.51	1.81	4	1
1:B:55:MET:HE3	1:B:56:PRO:HD2	0.51	1.81	5	4
1:A:6:VAL:CG1	1:A:14:THR:HG22	0.51	2.35	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:44:LEU:C	1:A:44:LEU:HD23	0.51	2.30	10	2
1:A:63:PHE:CE1	1:A:67:ILE:HD11	0.51	2.41	8	1
1:A:44:LEU:HD23	1:A:44:LEU:O	0.51	2.04	10	2
1:B:26:TYR:CE2	1:B:113:ILE:HG21	0.51	2.41	15	5
1:B:110:LEU:C	1:B:110:LEU:HD12	0.51	2.30	14	20
1:B:21:LEU:HD22	1:B:28:PRO:CA	0.51	2.36	2	3
1:B:34:LEU:HD23	1:B:57:ASP:HB3	0.51	1.82	15	4
1:A:34:LEU:HD23	1:A:57:ASP:HB3	0.51	1.81	18	6
1:A:34:LEU:HD11	1:A:58:GLY:O	0.51	2.06	9	6
1:B:78:VAL:CG2	1:B:96:ALA:HB2	0.51	2.35	13	13
1:A:78:VAL:CG2	1:A:96:ALA:HB2	0.51	2.35	11	14
1:A:92:ILE:HD12	1:B:89:VAL:HG13	0.50	1.82	2	2
1:B:85:VAL:O	1:B:89:VAL:HG23	0.50	2.06	2	2
1:B:3:ARG:O	1:B:47:PRO:HD2	0.50	2.07	17	7
1:A:92:ILE:CD1	1:B:89:VAL:HG22	0.50	2.35	15	1
1:A:21:LEU:HD22	1:A:28:PRO:CA	0.50	2.36	2	5
1:A:34:LEU:HD23	1:A:57:ASP:OD1	0.50	2.07	1	1
1:B:34:LEU:HD11	1:B:55:MET:HG2	0.50	1.84	16	3
1:B:61:VAL:HG21	1:B:90:LYS:CD	0.50	2.36	15	3
1:A:110:LEU:HD12	1:A:110:LEU:C	0.50	2.31	8	20
1:B:64:ILE:HG21	1:B:94:LYS:C	0.50	2.32	6	16
1:B:34:LEU:HD21	1:B:55:MET:HB3	0.50	1.83	17	4
1:A:63:PHE:CD2	1:A:67:ILE:HD11	0.50	2.42	16	19
1:B:106:VAL:HG22	1:B:110:LEU:HD23	0.50	1.84	20	16
1:A:61:VAL:CG1	1:A:62:ASN:N	0.50	2.75	11	13
1:A:48:VAL:CG1	1:A:116:ALA:HB1	0.50	2.34	9	2
1:A:5:LEU:HD11	1:A:40:LYS:HD2	0.50	1.84	11	1
1:B:5:LEU:HD23	1:B:49:ILE:HD13	0.50	1.83	15	2
1:B:44:LEU:HD11	1:B:46:PHE:CZ	0.49	2.43	3	1
1:A:64:ILE:HG21	1:A:94:LYS:C	0.49	2.33	4	14
1:B:55:MET:HE2	1:B:55:MET:HA	0.49	1.85	1	1
1:B:63:PHE:CD2	1:B:67:ILE:HD11	0.49	2.42	16	20
1:A:89:VAL:HG22	1:B:92:ILE:CD1	0.49	2.38	15	1
1:A:4:VAL:HA	1:A:48:VAL:O	0.49	2.08	12	9
1:B:7:VAL:HG11	1:B:34:LEU:HD13	0.49	1.85	8	1
1:A:26:TYR:CD1	1:A:26:TYR:N	0.49	2.80	16	20
1:A:5:LEU:O	1:A:49:ILE:HG23	0.48	2.08	16	4
1:B:21:LEU:HD23	1:B:26:TYR:CB	0.48	2.37	2	1
1:A:34:LEU:HD21	1:A:55:MET:HB3	0.48	1.86	11	3
1:B:34:LEU:O	1:B:37:ALA:N	0.48	2.47	17	13
1:B:61:VAL:CG1	1:B:62:ASN:N	0.48	2.77	9	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:4:VAL:HG22	1:A:48:VAL:CG2	0.48	2.39	15	2
1:A:92:ILE:HD11	1:B:89:VAL:HG22	0.47	1.86	15	2
1:A:7:VAL:HG11	1:A:34:LEU:CD1	0.47	2.39	13	1
1:B:3:ARG:CZ	1:B:44:LEU:HD11	0.47	2.39	20	1
1:A:85:VAL:HG13	1:A:86:ASP:N	0.47	2.25	8	20
1:B:46:PHE:O	1:B:46:PHE:CG	0.47	2.67	17	5
1:A:55:MET:HE3	1:A:56:PRO:HD2	0.47	1.84	5	2
1:A:89:VAL:HG11	1:B:98:GLU:CD	0.47	2.35	15	1
1:A:51:LEU:HD12	1:A:63:PHE:CD2	0.47	2.45	7	1
1:A:8:ASP:CA	1:A:55:MET:HE1	0.47	2.39	10	1
1:B:52:ASP:CG	1:B:53:VAL:N	0.47	2.72	16	1
1:B:85:VAL:HG13	1:B:86:ASP:N	0.47	2.25	5	20
1:A:5:LEU:HD23	1:A:49:ILE:HD13	0.47	1.85	6	3
1:B:64:ILE:HD13	1:B:94:LYS:HB3	0.47	1.87	14	6
1:A:3:ARG:O	1:A:47:PRO:HD2	0.47	2.10	8	5
1:A:46:PHE:CD2	1:A:49:ILE:HD12	0.47	2.45	14	6
1:B:17:LEU:HD11	1:B:104:PHE:HE1	0.47	1.68	15	2
1:B:7:VAL:HG13	1:B:31:ALA:CB	0.47	2.36	5	2
1:A:34:LEU:HD11	1:A:55:MET:HG2	0.47	1.85	16	1
1:B:2:LYS:HA	1:B:117:PHE:CZ	0.46	2.45	12	8
1:B:44:LEU:C	1:B:44:LEU:CD2	0.46	2.87	14	2
1:A:20:ILE:HG21	1:A:106:VAL:CG2	0.46	2.41	1	11
1:A:102:LYS:HB3	1:A:103:PRO:HD3	0.46	1.88	18	6
1:B:46:PHE:CD2	1:B:49:ILE:HD12	0.46	2.46	8	7
1:A:24:GLU:HB3	1:A:26:TYR:CZ	0.46	2.45	7	1
1:A:18:SER:O	1:A:28:PRO:HG3	0.46	2.11	18	16
1:B:102:LYS:HB3	1:B:103:PRO:HD3	0.46	1.87	19	7
1:A:4:VAL:CG2	1:A:21:LEU:HD21	0.46	2.41	19	2
1:A:104:PHE:CD1	1:A:104:PHE:N	0.46	2.84	7	14
1:B:104:PHE:CD1	1:B:104:PHE:N	0.46	2.84	17	13
1:B:2:LYS:HG3	1:B:26:TYR:CD1	0.46	2.46	7	2
1:B:102:LYS:HB3	1:B:103:PRO:CD	0.46	2.40	19	4
1:B:64:ILE:HD13	1:B:95:GLY:N	0.46	2.26	15	1
1:B:17:LEU:HD21	1:B:104:PHE:HZ	0.46	1.70	12	2
1:B:4:VAL:HG22	1:B:48:VAL:CG2	0.46	2.40	16	2
1:B:102:LYS:N	1:B:103:PRO:HD2	0.46	2.26	18	5
1:A:64:ILE:O	1:A:65:ASP:C	0.46	2.59	9	20
1:A:85:VAL:CG1	1:A:86:ASP:N	0.46	2.79	16	19
1:B:18:SER:O	1:B:28:PRO:HG3	0.46	2.11	1	11
1:B:48:VAL:CG1	1:B:116:ALA:HB1	0.46	2.40	4	4
1:A:44:LEU:C	1:A:44:LEU:HD22	0.46	2.36	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:21:LEU:HD12	1:B:28:PRO:N	0.46	2.26	19	1
1:A:55:MET:HA	1:A:55:MET:HE2	0.46	1.88	17	2
1:B:85:VAL:CG1	1:B:86:ASP:N	0.46	2.79	16	17
1:A:5:LEU:HD12	1:A:6:VAL:N	0.46	2.26	14	3
1:A:14:THR:HB	1:A:30:THR:HG22	0.46	1.88	20	4
1:A:61:VAL:HG21	1:A:90:LYS:HD3	0.45	1.85	9	1
1:A:21:LEU:HD22	1:A:28:PRO:HB3	0.45	1.88	20	1
1:A:34:LEU:HB3	1:A:63:PHE:CE1	0.45	2.46	1	2
1:A:64:ILE:HD13	1:A:94:LYS:HB3	0.45	1.88	4	3
1:B:20:ILE:HG21	1:B:106:VAL:CG2	0.45	2.41	1	5
1:B:21:LEU:HD22	1:B:28:PRO:HB3	0.45	1.88	4	2
1:B:52:ASP:OD1	1:B:52:ASP:N	0.45	2.50	4	2
1:B:14:THR:HB	1:B:30:THR:HG22	0.45	1.87	15	3
1:B:64:ILE:O	1:B:65:ASP:C	0.45	2.60	7	19
1:A:51:LEU:HD13	1:A:63:PHE:CE2	0.45	2.47	6	1
1:A:53:VAL:O	1:A:55:MET:N	0.45	2.50	12	19
1:B:21:LEU:HD23	1:B:28:PRO:CA	0.45	2.41	11	6
1:B:106:VAL:O	1:B:110:LEU:HD23	0.45	2.12	13	17
1:A:64:ILE:HD11	1:A:78:VAL:CG2	0.45	2.42	8	1
1:A:34:LEU:HD22	1:A:34:LEU:H	0.45	1.70	13	3
1:B:51:LEU:HD13	1:B:63:PHE:CE2	0.45	2.46	8	3
1:B:89:VAL:HG12	1:B:93:LYS:HD2	0.45	1.87	14	1
1:A:111:LEU:O	1:A:111:LEU:HD23	0.45	2.12	5	7
1:A:102:LYS:N	1:A:103:PRO:HD2	0.45	2.27	18	6
1:B:34:LEU:HD13	1:B:55:MET:HE2	0.45	1.89	5	1
1:B:53:VAL:O	1:B:55:MET:N	0.44	2.50	12	20
1:B:49:ILE:O	1:B:76:VAL:HG13	0.44	2.12	6	6
1:B:61:VAL:HG13	1:B:62:ASN:N	0.44	2.27	7	6
1:A:5:LEU:HD12	1:A:5:LEU:C	0.44	2.38	14	3
1:A:49:ILE:O	1:A:76:VAL:HA	0.44	2.13	12	5
1:B:5:LEU:O	1:B:49:ILE:HG23	0.44	2.13	3	2
1:B:61:VAL:HG11	1:B:90:LYS:HD2	0.44	1.89	8	1
1:A:34:LEU:O	1:A:37:ALA:N	0.44	2.50	8	14
1:B:102:LYS:CB	1:B:103:PRO:HD3	0.44	2.42	11	11
1:A:89:VAL:HG22	1:B:92:ILE:HG13	0.44	1.88	9	1
1:A:106:VAL:O	1:A:110:LEU:HD23	0.44	2.13	9	16
1:A:40:LYS:O	1:A:43:GLU:HG2	0.44	2.13	14	2
1:A:89:VAL:HG22	1:B:92:ILE:HD11	0.44	1.90	15	1
1:B:34:LEU:O	1:B:35:ARG:C	0.44	2.60	17	15
1:B:117:PHE:O	1:B:118:GLU:C	0.44	2.61	7	16
1:A:34:LEU:HD11	1:A:51:LEU:HD21	0.44	1.89	18	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:5:LEU:C	1:B:5:LEU:HD23	0.44	2.38	13	4
1:B:5:LEU:HD22	1:B:7:VAL:CG2	0.43	2.43	11	1
1:A:3:ARG:NH2	1:A:44:LEU:HD11	0.43	2.28	13	1
1:A:102:LYS:HB3	1:A:103:PRO:CD	0.43	2.42	13	3
1:B:24:GLU:HB3	1:B:26:TYR:CZ	0.43	2.48	16	1
1:A:34:LEU:O	1:A:35:ARG:C	0.43	2.61	18	12
1:A:49:ILE:O	1:A:76:VAL:HG13	0.43	2.13	3	6
1:B:8:ASP:CA	1:B:55:MET:HE1	0.43	2.42	10	1
1:A:102:LYS:CB	1:A:103:PRO:HD3	0.43	2.44	5	11
1:A:117:PHE:O	1:A:118:GLU:C	0.43	2.60	16	19
1:A:61:VAL:HG13	1:A:62:ASN:N	0.43	2.28	7	11
1:A:110:LEU:HD12	1:A:111:LEU:N	0.43	2.28	2	5
1:B:48:VAL:CG2	1:B:117:PHE:CE1	0.43	3.02	15	3
1:A:8:ASP:C	1:A:10:GLU:H	0.43	2.22	13	6
1:B:34:LEU:HD12	1:B:57:ASP:HB3	0.43	1.90	7	1
1:A:21:LEU:HD23	1:A:28:PRO:CA	0.43	2.44	13	4
1:A:89:VAL:HG21	1:B:99:PHE:H	0.43	1.74	1	1
1:B:21:LEU:HD23	1:B:28:PRO:HA	0.43	1.90	11	2
1:A:41:ILE:HG12	1:A:46:PHE:CE2	0.43	2.48	3	1
1:B:109:PHE:CD2	1:B:110:LEU:N	0.43	2.87	2	1
1:A:51:LEU:HD21	1:A:60:GLY:HA2	0.43	1.90	12	3
1:A:52:ASP:HA	1:A:79:ILE:O	0.42	2.14	14	4
1:B:52:ASP:HA	1:B:79:ILE:O	0.42	2.14	16	4
1:B:67:ILE:O	1:B:71:SER:N	0.42	2.52	3	6
1:A:67:ILE:O	1:A:71:SER:N	0.42	2.53	13	7
1:A:64:ILE:HD13	1:A:95:GLY:N	0.42	2.29	15	1
1:B:8:ASP:C	1:B:10:GLU:H	0.42	2.22	1	7
1:B:110:LEU:HD12	1:B:111:LEU:N	0.42	2.29	2	2
1:B:52:ASP:OD1	1:B:79:ILE:HD11	0.42	2.14	9	1
1:B:82:HIS:CD2	1:B:82:HIS:N	0.42	2.87	13	1
1:A:41:ILE:HG23	1:A:46:PHE:CE1	0.42	2.50	6	3
1:A:63:PHE:CD1	1:A:67:ILE:HD11	0.42	2.50	8	1
1:B:48:VAL:CG1	1:B:75:VAL:HG13	0.42	2.43	15	1
1:B:5:LEU:HD22	1:B:7:VAL:HG23	0.42	1.92	2	1
1:B:111:LEU:O	1:B:111:LEU:HD23	0.42	2.15	15	3
1:A:46:PHE:O	1:A:46:PHE:CG	0.42	2.72	9	2
1:A:44:LEU:HD11	1:A:46:PHE:CD1	0.42	2.50	10	1
1:B:34:LEU:HB3	1:B:63:PHE:CE1	0.41	2.49	5	2
1:A:21:LEU:HD23	1:A:28:PRO:HA	0.41	1.92	13	1
1:B:6:VAL:HG13	1:B:50:VAL:HB	0.41	1.92	17	1
1:A:48:VAL:HG12	1:A:75:VAL:CG2	0.41	2.44	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:LEU:HD23	1:A:28:PRO:HB3	0.41	1.91	12	1
1:A:34:LEU:H	1:A:34:LEU:HD22	0.41	1.74	16	1
1:B:21:LEU:HB3	1:B:28:PRO:HB3	0.41	1.92	19	1
1:A:21:LEU:HD22	1:A:28:PRO:CB	0.41	2.45	20	1
1:B:34:LEU:HD11	1:B:55:MET:HE2	0.41	1.93	5	1
1:B:61:VAL:HG11	1:B:90:LYS:HZ2	0.41	1.73	15	1
1:A:5:LEU:C	1:A:5:LEU:HD23	0.41	2.40	11	1
1:A:61:VAL:HG23	1:A:91:ALA:CB	0.41	2.46	11	1
1:B:20:ILE:HD13	1:B:20:ILE:N	0.41	2.31	19	1
1:B:49:ILE:O	1:B:76:VAL:HA	0.41	2.15	1	1
1:B:21:LEU:HD22	1:B:28:PRO:CB	0.41	2.45	4	1
1:B:34:LEU:HD11	1:B:55:MET:SD	0.41	2.56	11	1
1:B:52:ASP:OD2	1:B:55:MET:HE1	0.41	2.15	12	1
1:B:34:LEU:HD22	1:B:34:LEU:H	0.41	1.74	16	3
1:B:2:LYS:HD3	1:B:26:TYR:CE1	0.41	2.51	5	1
1:A:79:ILE:HG22	1:A:100:LEU:O	0.41	2.15	9	1
1:A:44:LEU:C	1:A:44:LEU:CD2	0.41	2.94	10	1
1:B:51:LEU:HD21	1:B:60:GLY:HA2	0.41	1.92	10	2
1:B:21:LEU:CB	1:B:28:PRO:HB3	0.41	2.46	19	2
1:A:51:LEU:HD23	1:A:52:ASP:O	0.41	2.15	16	1
1:A:80:THR:HG22	1:A:99:PHE:CZ	0.41	2.50	18	2
1:B:61:VAL:HG23	1:B:91:ALA:CB	0.41	2.46	6	2
1:A:7:VAL:HG12	1:A:55:MET:HE2	0.41	1.92	10	1
1:B:13:ILE:CG2	1:B:17:LEU:HD22	0.40	2.46	2	1
1:A:37:ALA:O	1:A:41:ILE:HD12	0.40	2.16	3	1
1:A:44:LEU:HD21	1:A:46:PHE:HE2	0.40	1.74	16	1
1:A:13:ILE:CG2	1:A:17:LEU:HD22	0.40	2.46	2	1
1:A:111:LEU:HD23	1:A:111:LEU:O	0.40	2.16	18	1
1:B:2:LYS:CB	1:B:26:TYR:CD1	0.40	3.05	16	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	118/121 (98%)	102±1 (86±1%)	11±2 (9±1%)	5±1 (4±1%)	3 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	117/121 (97%)	101±1 (86±1%)	11±2 (10±1%)	5±1 (4±1%)	3	27
All	All	4700/4840 (97%)	4051 (86%)	442 (9%)	207 (4%)	3	27

All 16 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	54	TRP	20
1	A	83	GLY	20
1	A	95	GLY	20
1	B	54	TRP	20
1	B	83	GLY	20
1	B	95	GLY	20
1	A	71	SER	16
1	B	71	SER	16
1	B	84	SER	15
1	A	84	SER	14
1	A	101	GLU	7
1	A	59	ASP	7
1	B	101	GLU	5
1	B	59	ASP	5
1	A	47	PRO	1
1	B	47	PRO	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	106/108 (98%)	80±2 (75±2%)	26±2 (25±2%)	2	25
1	B	105/108 (97%)	79±2 (75±2%)	26±2 (25±2%)	2	24
All	All	4220/4320 (98%)	3171 (75%)	1049 (25%)	2	25

All 112 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	32	LYS	20
1	A	41	ILE	20
1	A	44	LEU	20
1	A	70	ASN	20
1	A	71	SER	20
1	A	90	LYS	20
1	A	102	LYS	20
1	A	104	PHE	20
1	A	105	SER	20
1	A	109	PHE	20
1	A	120	TYR	20
1	B	32	LYS	20
1	B	44	LEU	20
1	B	70	ASN	20
1	B	71	SER	20
1	B	102	LYS	20
1	B	104	PHE	20
1	B	105	SER	20
1	B	109	PHE	20
1	A	106	VAL	19
1	B	29	ASP	19
1	B	90	LYS	19
1	A	29	ASP	18
1	B	41	ILE	18
1	B	75	VAL	18
1	A	75	VAL	17
1	B	2	LYS	17
1	A	23	GLU	16
1	A	84	SER	16
1	B	23	GLU	16
1	B	84	SER	16
1	B	106	VAL	16
1	A	39	LYS	15
1	B	22	GLU	15
1	B	5	LEU	15
1	B	89	VAL	15
1	B	39	LYS	14
1	A	5	LEU	14
1	A	22	GLU	13
1	B	6	VAL	13
1	A	17	LEU	12
1	A	57	ASP	12
1	B	57	ASP	11

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Mol	Chain	Res	Type	Models (Total)
1	B	55	MET	11
1	A	6	VAL	11
1	B	77	ILE	11
1	A	74	SER	10
1	A	55	MET	10
1	A	89	VAL	10
1	B	4	VAL	10
1	A	42	LYS	9
1	A	43	GLU	9
1	B	17	LEU	9
1	B	74	SER	9
1	A	77	ILE	9
1	B	1	MET	8
1	B	42	LYS	7
1	A	24	GLU	7
1	B	24	GLU	7
1	A	49	ILE	7
1	B	93	LYS	7
1	A	4	VAL	7
1	A	40	LYS	6
1	A	51	LEU	6
1	B	40	LYS	6
1	B	43	GLU	6
1	B	21	LEU	6
1	B	49	ILE	6
1	B	51	LEU	5
1	A	21	LEU	5
1	A	8	ASP	4
1	B	8	ASP	4
1	A	12	SER	4
1	B	12	SER	4
1	A	93	LYS	4
1	A	121	SER	3
1	A	66	PHE	3
1	A	52	ASP	3
1	B	108	ARG	3
1	A	35	ARG	3
1	B	35	ARG	3
1	B	114	LYS	2
1	B	48	VAL	2
1	B	52	ASP	2
1	A	15	SER	2

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Mol	Chain	Res	Type	Models (Total)
1	B	15	SER	2
1	B	46	PHE	2
1	B	66	PHE	2
1	B	73	ASP	2
1	A	73	ASP	2
1	A	108	ARG	2
1	A	119	GLU	2
1	A	111	LEU	2
1	A	114	LYS	1
1	B	61	VAL	1
1	A	34	LEU	1
1	B	7	VAL	1
1	B	34	LEU	1
1	A	3	ARG	1
1	A	9	ASP	1
1	B	9	ASP	1
1	B	86	ASP	1
1	A	46	PHE	1
1	A	61	VAL	1
1	B	98	GLU	1
1	B	80	THR	1
1	A	11	GLU	1
1	B	11	GLU	1
1	A	16	SER	1
1	B	16	SER	1
1	A	107	GLU	1
1	B	3	ARG	1

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

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 40% for the well-defined parts and 40% 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	1320
Number of shifts mapped to atoms	1320
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	120	-0.24 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	114	-0.02 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	112	0.08 ± 0.33	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 40%, i.e. 1299 atoms were assigned a chemical shift out of a possible 3258. 0 out of 44 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	468/1177 (40%)	238/476 (50%)	118/474 (25%)	112/227 (49%)
Sidechain	793/1810 (44%)	533/1181 (45%)	258/586 (44%)	2/43 (5%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	38/271 (14%)	37/136 (27%)	0/127 (0%)	1/8 (12%)
Overall	1299/3258 (40%)	808/1793 (45%)	376/1187 (32%)	115/278 (41%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 40%, i.e. 1320 atoms were assigned a chemical shift out of a possible 3328. 0 out of 44 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	472/1202 (39%)	240/486 (49%)	120/484 (25%)	112/232 (48%)
Sidechain	810/1846 (44%)	544/1204 (45%)	264/598 (44%)	2/44 (5%)
Aromatic	38/280 (14%)	37/140 (26%)	0/132 (0%)	1/8 (12%)
Overall	1320/3328 (40%)	821/1830 (45%)	384/1214 (32%)	115/284 (40%)

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.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	38	GLU	HG3	0.99	1.20 – 3.30	-6.0
1	A	5	LEU	HB3	-0.59	-0.26 – 3.31	-6.0
1	A	34	LEU	H	11.38	5.09 – 11.34	5.1

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:

