



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 10:47 pm BST

PDB ID : 2KZ8
Title : Solution NMR structure of MqsA, a protein from E. coli, containing a Zinc finger, N-terminal and a Helix Turn-Helix C-terminal domain
Authors : Papadopoulos, E.; Vlamis-Gardikas, A.; Graslund, A.; Billeter, M.; Holmgren, A.; Collet, J.
Deposited on : 2010-06-14

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
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

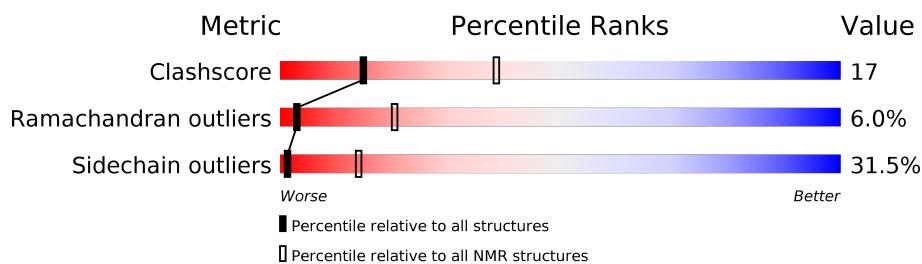
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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	131	

2 Ensemble composition and analysis i

This entry contains 20 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *fewest violations*.

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:1-A:65 (65)	0.17	18
2	A:69-A:131 (63)	0.14	15

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 1 single-model cluster was found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2082 atoms, of which 1053 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Uncharacterized HTH-type transcriptional regulator ygiT.

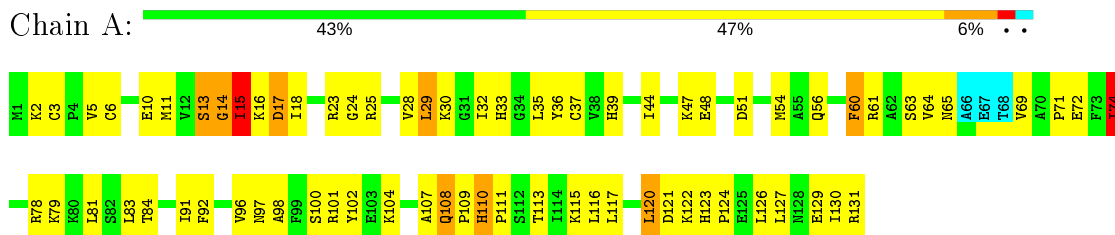
Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	131	2082	651	1053	184	186	8	0

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: Uncharacterized HTH-type transcriptional regulator ygiT

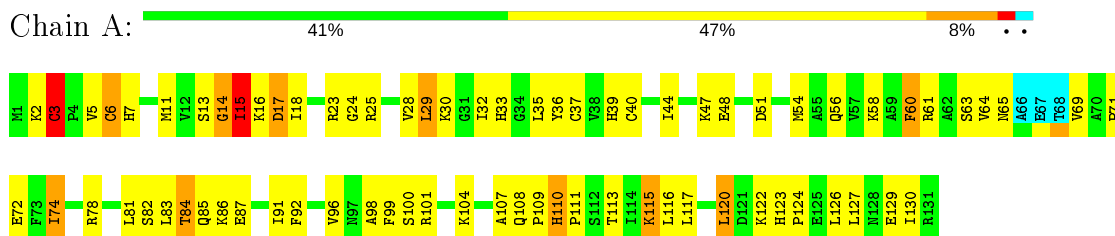


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

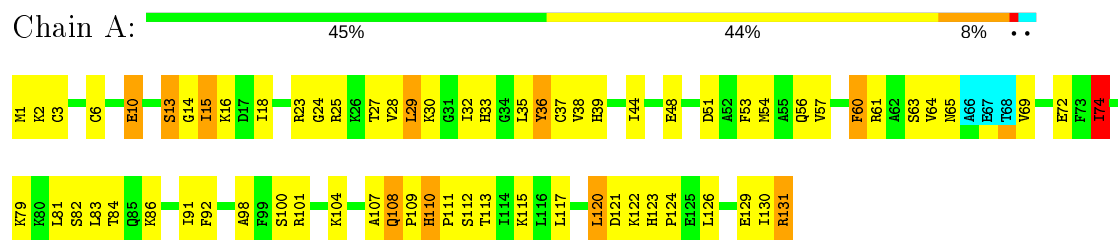
- Molecule 1: Uncharacterized HTH-type transcriptional regulator ygiT



4.2.2 Score per residue for model 2

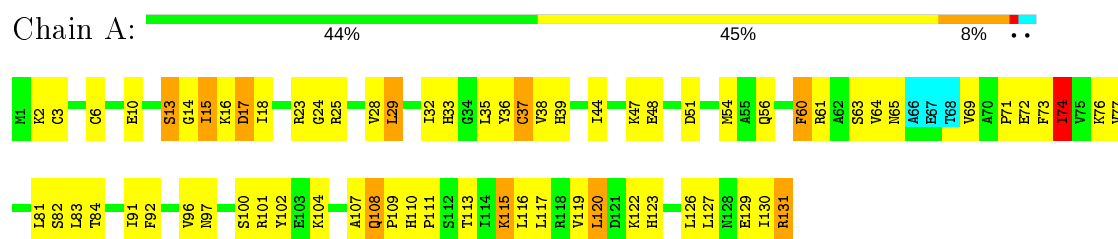
- Molecule 1: Uncharacterized HTH-type transcriptional regulator ygiT





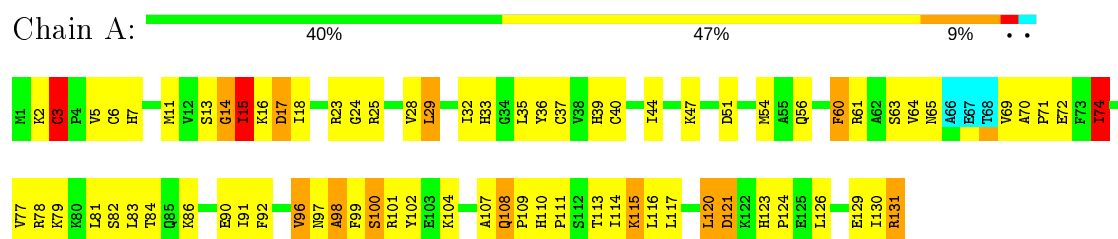
4.2.7 Score per residue for model 7

- Molecule 1: Uncharacterized HTH-type transcriptional regulator ygiT



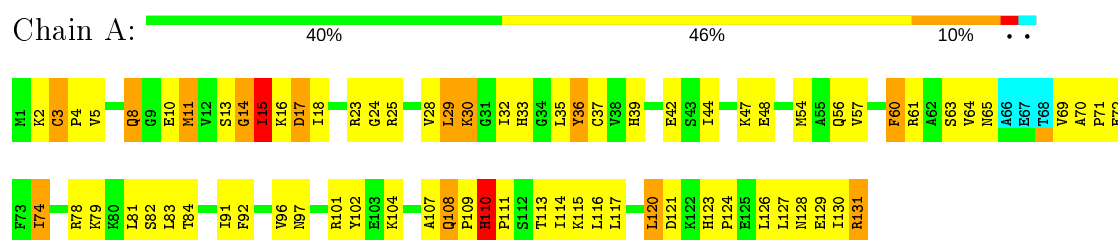
4.2.8 Score per residue for model 8

- Molecule 1: Uncharacterized HTH-type transcriptional regulator ygiT



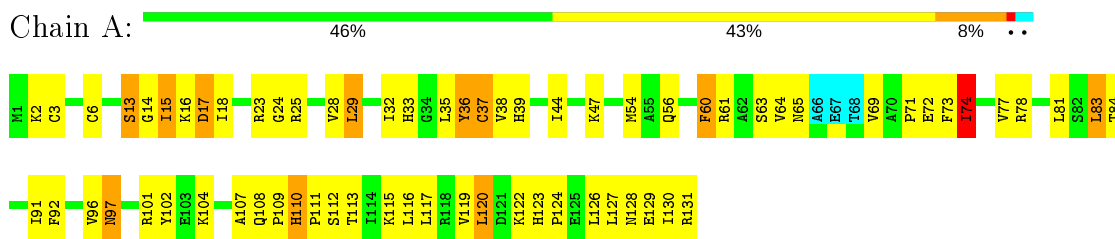
4.2.9 Score per residue for model 9

- Molecule 1: Uncharacterized HTH-type transcriptional regulator ygiT



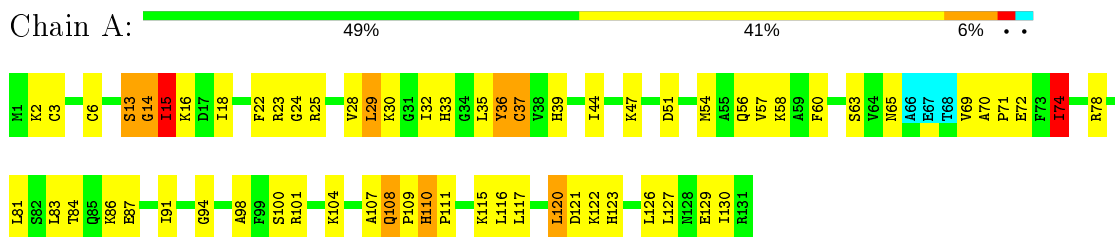
4.2.10 Score per residue for model 10

- Molecule 1: Uncharacterized HTH-type transcriptional regulator ygiT



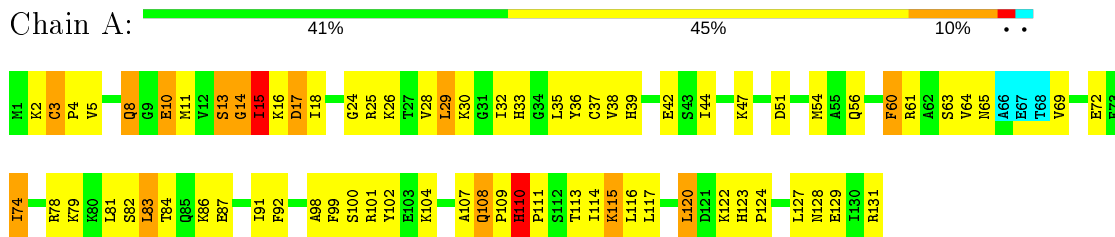
4.2.11 Score per residue for model 11

- Molecule 1: Uncharacterized HTH-type transcriptional regulator ygiT



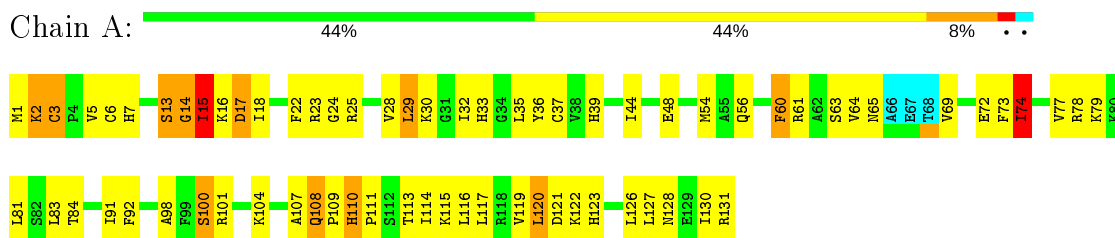
4.2.12 Score per residue for model 12

- Molecule 1: Uncharacterized HTH-type transcriptional regulator ygiT



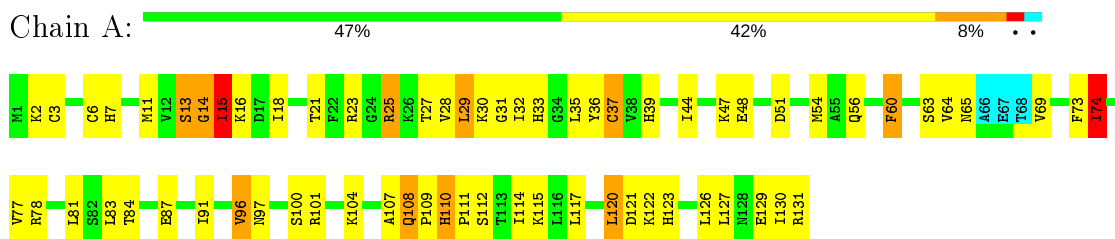
4.2.13 Score per residue for model 13

- Molecule 1: Uncharacterized HTH-type transcriptional regulator ygiT



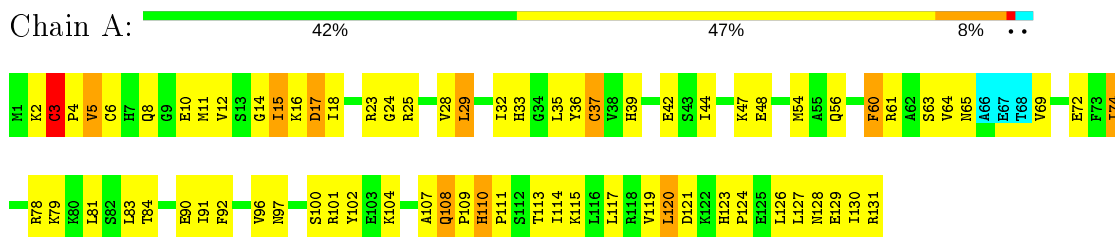
4.2.14 Score per residue for model 14

- Molecule 1: Uncharacterized HTH-type transcriptional regulator ygiT



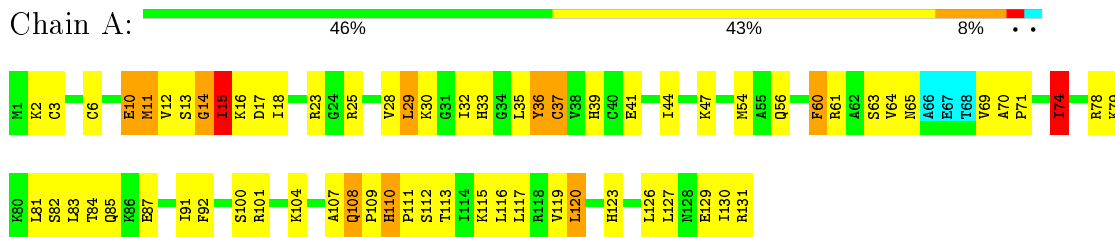
4.2.15 Score per residue for model 15

- Molecule 1: Uncharacterized HTH-type transcriptional regulator ygiT



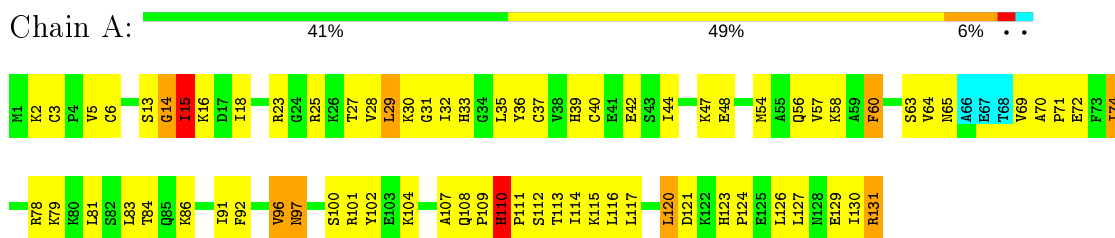
4.2.16 Score per residue for model 16

- Molecule 1: Uncharacterized HTH-type transcriptional regulator ygiT



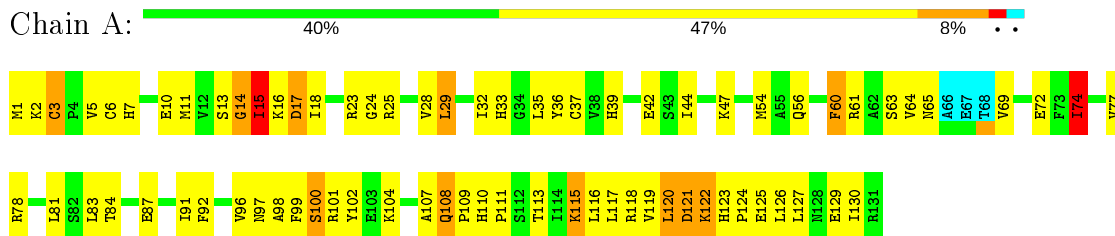
4.2.17 Score per residue for model 17

- Molecule 1: Uncharacterized HTH-type transcriptional regulator ygiT



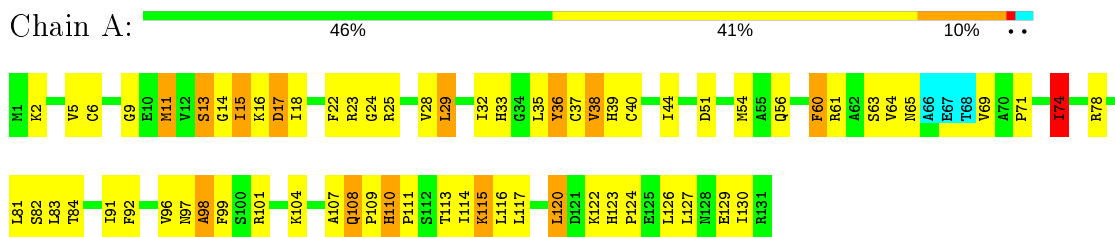
4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: Uncharacterized HTH-type transcriptional regulator ygiT



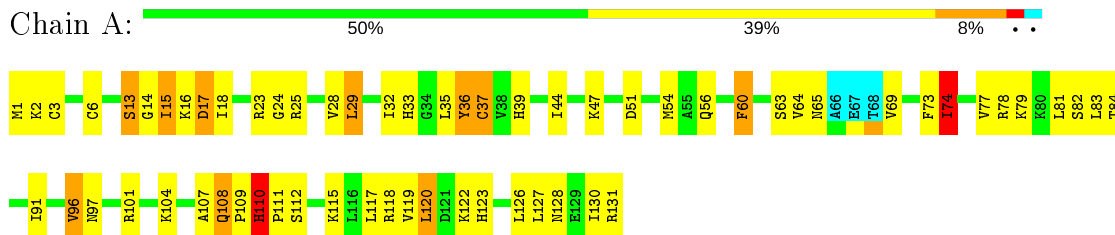
4.2.19 Score per residue for model 19

- Molecule 1: Uncharacterized HTH-type transcriptional regulator ygiT



4.2.20 Score per residue for model 20

- Molecule 1: Uncharacterized HTH-type transcriptional regulator ygiT



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with acceptable covalent geometry*.

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

Software name	Classification	Version
CYANA	refinement	3.1

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality

6.1 Standard geometry

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	1008	1035	1037	35±3
All	All	20160	20700	20740	691

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:HIS:N	1:A:111:PRO:CD	0.79	2.45	10	20
1:A:74:ILE:HG22	1:A:117:LEU:HD13	0.71	1.61	17	19
1:A:81:LEU:HD13	1:A:120:LEU:HD12	0.70	1.63	5	17
1:A:18:ILE:O	1:A:29:LEU:HD22	0.67	1.89	14	20
1:A:120:LEU:HD13	1:A:123:HIS:O	0.66	1.90	9	20
1:A:91:ILE:HD12	1:A:131:ARG:HB3	0.65	1.68	6	10
1:A:81:LEU:HB2	1:A:83:LEU:HD23	0.64	1.68	18	17
1:A:91:ILE:CD1	1:A:127:LEU:HD12	0.64	2.23	12	10
1:A:83:LEU:HD11	1:A:127:LEU:HD13	0.64	1.69	13	6
1:A:113:THR:HG22	1:A:117:LEU:CD1	0.63	2.22	17	8
1:A:91:ILE:HD12	1:A:131:ARG:CB	0.63	2.24	7	10
1:A:60:PHE:O	1:A:64:VAL:HG22	0.62	1.95	8	6
1:A:119:VAL:HG23	1:A:126:LEU:HD13	0.61	1.72	16	1
1:A:29:LEU:HD12	1:A:56:GLN:HB3	0.61	1.73	9	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:LEU:CD1	1:A:120:LEU:HD12	0.60	2.26	16	17
1:A:113:THR:HG22	1:A:117:LEU:HD11	0.60	1.73	17	3
1:A:83:LEU:HD22	1:A:92:PHE:CE2	0.60	2.32	12	3
1:A:126:LEU:O	1:A:130:ILE:HG23	0.60	1.97	13	19
1:A:35:LEU:HD12	1:A:44:ILE:HB	0.59	1.74	19	20
1:A:83:LEU:HD11	1:A:127:LEU:CD1	0.59	2.26	9	4
1:A:110:HIS:N	1:A:111:PRO:HD3	0.59	2.12	10	20
1:A:18:ILE:N	1:A:28:VAL:HG23	0.58	2.13	9	1
1:A:5:VAL:HG21	1:A:42:GLU:CD	0.57	2.20	9	5
1:A:83:LEU:HD21	1:A:127:LEU:HD13	0.57	1.77	10	3
1:A:71:PRO:HA	1:A:74:ILE:HD11	0.56	1.77	7	7
1:A:91:ILE:HG23	1:A:131:ARG:HB3	0.56	1.76	17	2
1:A:81:LEU:HD22	1:A:124:PRO:HB3	0.55	1.78	15	14
1:A:108:GLN:N	1:A:109:PRO:CD	0.55	2.69	19	15
1:A:60:PHE:O	1:A:64:VAL:HG23	0.55	2.01	12	10
1:A:17:ASP:HB2	1:A:28:VAL:HG11	0.55	1.78	13	15
1:A:27:THR:HG21	1:A:60:PHE:CD1	0.55	2.37	6	2
1:A:116:LEU:HG	1:A:130:ILE:HD12	0.55	1.79	16	1
1:A:29:LEU:CB	1:A:32:ILE:HD11	0.55	2.31	9	20
1:A:115:LYS:HD3	1:A:116:LEU:HD12	0.55	1.77	12	1
1:A:73:PHE:O	1:A:77:VAL:HG23	0.54	2.02	13	5
1:A:101:ARG:CB	1:A:107:ALA:HB2	0.54	2.32	2	20
1:A:13:SER:N	1:A:35:LEU:HD23	0.53	2.18	12	19
1:A:74:ILE:HG22	1:A:117:LEU:CD1	0.53	2.32	12	11
1:A:94:GLY:C	1:A:98:ALA:HB2	0.53	2.24	11	1
1:A:74:ILE:HD12	1:A:102:TYR:HB3	0.53	1.79	9	12
1:A:116:LEU:O	1:A:120:LEU:HD23	0.53	2.03	12	5
1:A:17:ASP:HB3	1:A:28:VAL:HG21	0.53	1.81	9	1
1:A:115:LYS:HG3	1:A:116:LEU:HD12	0.52	1.82	18	7
1:A:60:PHE:O	1:A:64:VAL:HG13	0.52	2.05	5	2
1:A:29:LEU:HD13	1:A:29:LEU:N	0.52	2.20	9	12
1:A:92:PHE:HB3	1:A:113:THR:HG23	0.52	1.82	13	17
1:A:5:VAL:HG21	1:A:42:GLU:OE1	0.51	2.05	3	1
1:A:91:ILE:HD13	1:A:127:LEU:HB2	0.50	1.84	16	8
1:A:8:GLN:HE21	1:A:8:GLN:N	0.50	2.05	12	2
1:A:5:VAL:HG12	1:A:6:CYS:N	0.50	2.21	4	2
1:A:101:ARG:HB3	1:A:107:ALA:HB2	0.50	1.83	20	13
1:A:8:GLN:N	1:A:8:GLN:HE21	0.50	2.05	5	1
1:A:27:THR:HG21	1:A:60:PHE:CD2	0.49	2.42	17	1
1:A:119:VAL:HG23	1:A:126:LEU:HD23	0.49	1.83	20	7
1:A:96:VAL:HG13	1:A:97:ASN:H	0.48	1.68	5	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:GLU:O	1:A:12:VAL:HG12	0.48	2.08	16	2
1:A:118:ARG:HG3	1:A:119:VAL:HG13	0.48	1.86	20	2
1:A:83:LEU:HD21	1:A:127:LEU:CD1	0.48	2.38	10	1
1:A:29:LEU:N	1:A:29:LEU:HD13	0.47	2.24	17	8
1:A:96:VAL:HG13	1:A:97:ASN:N	0.47	2.25	4	8
1:A:32:ILE:HG22	1:A:36:TYR:OH	0.47	2.10	19	6
1:A:9:GLY:HA3	1:A:38:VAL:HG13	0.47	1.86	19	1
1:A:36:TYR:CD1	1:A:36:TYR:N	0.47	2.83	2	5
1:A:116:LEU:CD2	1:A:130:ILE:HD12	0.46	2.40	17	10
1:A:29:LEU:HB2	1:A:32:ILE:HD11	0.46	1.87	9	5
1:A:91:ILE:HG21	1:A:127:LEU:HB2	0.46	1.87	13	1
1:A:18:ILE:C	1:A:28:VAL:HG23	0.46	2.31	9	1
1:A:29:LEU:HB3	1:A:32:ILE:HD11	0.46	1.88	4	15
1:A:108:GLN:HB2	1:A:114:ILE:HD11	0.46	1.87	9	4
1:A:36:TYR:N	1:A:36:TYR:CD1	0.45	2.84	20	2
1:A:70:ALA:HB1	1:A:71:PRO:HD2	0.45	1.88	16	8
1:A:3:CYS:O	1:A:7:HIS:N	0.45	2.50	8	5
1:A:119:VAL:CG2	1:A:126:LEU:HD13	0.45	2.39	16	1
1:A:109:PRO:N	1:A:111:PRO:HD3	0.44	2.27	10	10
1:A:1:MET:H2	1:A:10:GLU:HB2	0.44	1.72	6	1
1:A:29:LEU:HD12	1:A:56:GLN:CB	0.44	2.41	9	4
1:A:5:VAL:HG23	1:A:42:GLU:HG3	0.44	1.87	15	1
1:A:27:THR:HG21	1:A:60:PHE:CG	0.44	2.48	6	1
1:A:29:LEU:HD22	1:A:29:LEU:H	0.44	1.73	11	2
1:A:14:GLY:O	1:A:15:ILE:C	0.43	2.55	17	14
1:A:113:THR:HG22	1:A:117:LEU:HD12	0.43	1.88	9	5
1:A:29:LEU:H	1:A:29:LEU:HD22	0.43	1.73	6	2
1:A:98:ALA:O	1:A:99:PHE:C	0.42	2.57	8	5
1:A:77:VAL:HG22	1:A:121:ASP:HB2	0.42	1.91	8	2
1:A:2:LYS:O	1:A:3:CYS:HB2	0.42	2.14	13	1
1:A:10:GLU:HG2	1:A:38:VAL:HG12	0.42	1.91	12	1
1:A:96:VAL:HG22	1:A:97:ASN:N	0.42	2.29	8	2
1:A:84:THR:HG23	1:A:87:GLU:H	0.42	1.75	3	2
1:A:57:VAL:HG23	1:A:58:LYS:N	0.42	2.30	11	2
1:A:3:CYS:N	1:A:4:PRO:CD	0.42	2.83	5	4
1:A:119:VAL:HA	1:A:122:LYS:CD	0.42	2.45	18	1
1:A:29:LEU:O	1:A:30:LYS:C	0.41	2.59	12	9
1:A:69:VAL:HG22	1:A:108:GLN:HE22	0.41	1.74	20	1
1:A:31:GLY:O	1:A:32:ILE:HD13	0.41	2.15	14	2
1:A:11:MET:HB2	1:A:35:LEU:HB3	0.41	1.93	18	2
1:A:109:PRO:C	1:A:111:PRO:HD3	0.41	2.36	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:119:VAL:O	1:A:126:LEU:HD12	0.41	2.15	16	1
1:A:5:VAL:HG23	1:A:6:CYS:N	0.41	2.30	13	3
1:A:10:GLU:HG2	1:A:38:VAL:HG22	0.41	1.92	5	1
1:A:21:THR:HG21	1:A:25:ARG:HG2	0.41	1.93	14	1
1:A:53:PHE:O	1:A:57:VAL:HG13	0.40	2.16	3	2
1:A:108:GLN:N	1:A:109:PRO:HD3	0.40	2.31	19	1
1:A:119:VAL:HA	1:A:122:LYS:HD3	0.40	1.93	18	1
1:A:29:LEU:HD21	1:A:57:VAL:HG12	0.40	1.94	9	1
1:A:112:SER:O	1:A:116:LEU:HD13	0.40	2.17	16	1
1:A:123:HIS:HB2	1:A:126:LEU:HD12	0.40	1.93	16	1
1:A:115:LYS:CD	1:A:116:LEU:HD12	0.40	2.46	12	1
1:A:69:VAL:HG22	1:A:108:GLN:NE2	0.40	2.31	20	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	126/131 (96%)	90±2 (72±2%)	28±2 (22±2%)	8±1 (6±1%)	3	20
All	All	2520/2620 (96%)	1803 (72%)	566 (22%)	151 (6%)	3	20

All 13 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	14	GLY	20
1	A	37	CYS	20
1	A	15	ILE	20
1	A	24	GLY	17
1	A	3	CYS	16
1	A	110	HIS	14
1	A	74	ILE	13
1	A	100	SER	11
1	A	10	GLU	7
1	A	30	LYS	5

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Mol	Chain	Res	Type	Models (Total)
1	A	98	ALA	4
1	A	11	MET	3
1	A	38	VAL	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	111/113 (98%)	76±2 (69±2%)	35±2 (31±2%)	1 14
All	All	2220/2260 (98%)	1521 (69%)	699 (31%)	1 14

All 63 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	104	LYS	20
1	A	115	LYS	20
1	A	39	HIS	20
1	A	33	HIS	20
1	A	2	LYS	20
1	A	25	ARG	20
1	A	15	ILE	20
1	A	74	ILE	20
1	A	63	SER	20
1	A	120	LEU	20
1	A	36	TYR	20
1	A	60	PHE	20
1	A	54	MET	20
1	A	65	ASN	20
1	A	84	THR	20
1	A	29	LEU	20
1	A	16	LYS	20
1	A	23	ARG	19
1	A	129	GLU	18
1	A	78	ARG	18
1	A	47	LYS	17
1	A	108	GLN	17

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Mol	Chain	Res	Type	Models (Total)
1	A	61	ARG	15
1	A	72	GLU	15
1	A	17	ASP	15
1	A	122	LYS	15
1	A	6	CYS	13
1	A	121	ASP	12
1	A	79	LYS	12
1	A	13	SER	12
1	A	48	GLU	11
1	A	51	ASP	11
1	A	11	MET	11
1	A	131	ARG	10
1	A	82	SER	10
1	A	86	LYS	8
1	A	96	VAL	7
1	A	128	ASN	7
1	A	37	CYS	7
1	A	87	GLU	7
1	A	40	CYS	6
1	A	112	SER	6
1	A	100	SER	6
1	A	22	PHE	5
1	A	110	HIS	5
1	A	28	VAL	4
1	A	38	VAL	4
1	A	8	GLN	4
1	A	1	MET	4
1	A	97	ASN	4
1	A	69	VAL	3
1	A	3	CYS	3
1	A	85	GLN	3
1	A	83	LEU	3
1	A	127	LEU	2
1	A	90	GLU	2
1	A	26	LYS	2
1	A	5	VAL	1
1	A	125	GLU	1
1	A	58	LYS	1
1	A	41	GLU	1
1	A	80	LYS	1
1	A	76	LYS	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](#)

There are no ligands in this entry.

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

No chemical shift data were provided