



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 07:28 PM UTC

PDB ID : 1WHW / pdb_00001whw
Title : Solution structure of the N-terminal RNA binding domain from hypothetical protein BAB23448
Authors : Nagata, T.; Muto, Y.; Inoue, M.; Kigawa, T.; Terada, T.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2004-05-28

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

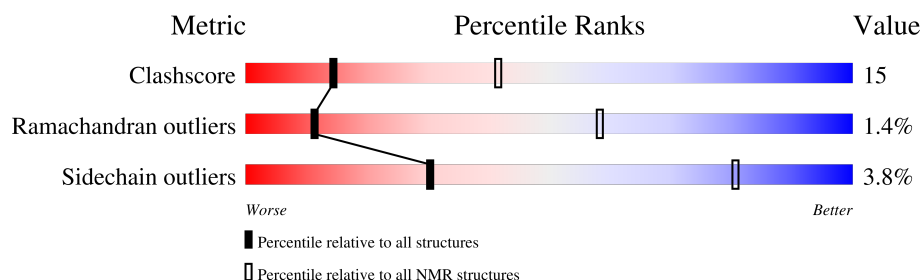
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment 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	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	99	

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 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:38-A:114 (77)	0.32	7

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 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1495 atoms, of which 740 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called hypothetical protein RIKEN CDNA 1200009A02.

Mol	Chain	Residues	Atoms						Trace
1	A	99	Total	C	H	N	O	S	0
			1495	481	740	125	147	2	

There are 13 discrepancies between the modelled and reference sequences:

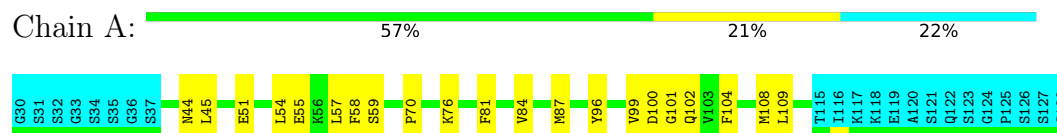
Chain	Residue	Modelled	Actual	Comment	Reference
A	30	GLY	-	cloning artifact	GB 12835985
A	31	SER	-	cloning artifact	GB 12835985
A	32	SER	-	cloning artifact	GB 12835985
A	33	GLY	-	cloning artifact	GB 12835985
A	34	SER	-	cloning artifact	GB 12835985
A	35	SER	-	cloning artifact	GB 12835985
A	36	GLY	-	cloning artifact	GB 12835985
A	123	SER	-	cloning artifact	GB 12835985
A	124	GLY	-	cloning artifact	GB 12835985
A	125	PRO	-	cloning artifact	GB 12835985
A	126	SER	-	cloning artifact	GB 12835985
A	127	SER	-	cloning artifact	GB 12835985
A	128	GLY	-	cloning artifact	GB 12835985

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: hypothetical protein RIKEN CDNA 1200009A02

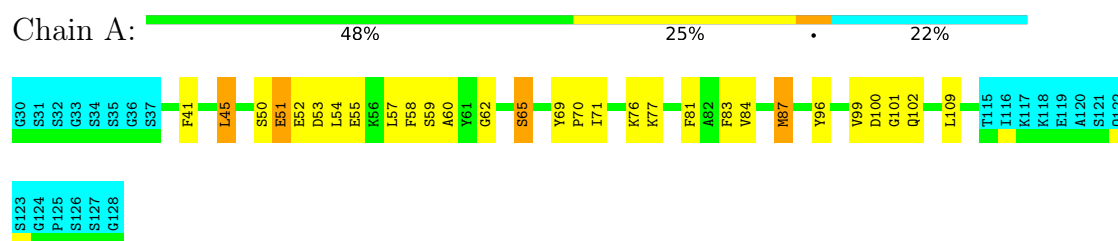


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

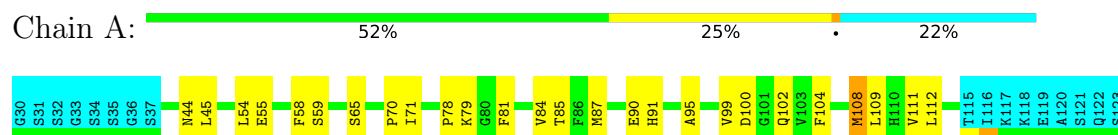
4.2.1 Score per residue for model 1

- Molecule 1: hypothetical protein RIKEN CDNA 1200009A02



4.2.2 Score per residue for model 2

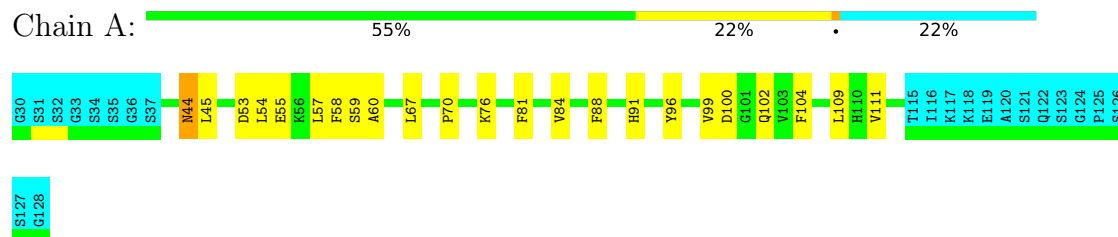
- Molecule 1: hypothetical protein RIKEN CDNA 1200009A02



G124
P125
S126
S127
G128

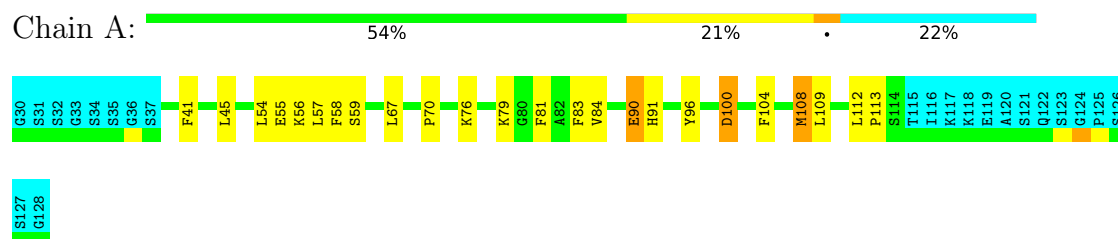
4.2.3 Score per residue for model 3

- Molecule 1: hypothetical protein RIKEN CDNA 1200009A02



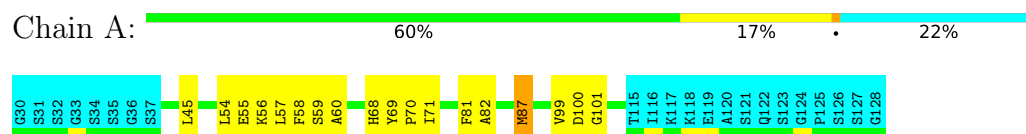
4.2.4 Score per residue for model 4

- Molecule 1: hypothetical protein RIKEN CDNA 1200009A02



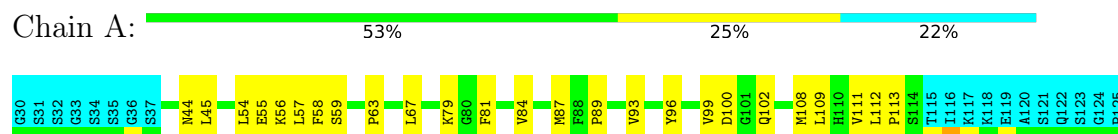
4.2.5 Score per residue for model 5

- Molecule 1: hypothetical protein RIKEN CDNA 1200009A02



4.2.6 Score per residue for model 6

- Molecule 1: hypothetical protein RIKEN CDNA 1200009A02



S126
S127
G128

4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: hypothetical protein RIKEN CDNA 1200009A02

Chain A: 

G30 S31 S32 S33 S34 S35 S36 S37 N44 L45 E51 L54 E55 K56 L57 F58 S59 A60 L67 E90 H91 V99 D100 G101 M108 T115 I116 K117 K118 E119 A120 S121 Q122 S123 G124 P125 S126 S127 G128

4.2.8 Score per residue for model 8

- Molecule 1: hypothetical protein RIKEN CDNA 1200009A02

Chain A: 

G30 S31 S32 S33 S34 S35 S36 S37 F41 L45 S50 E51 E52 D53 L54 E55 F58 S59 L67 H68 Y69 P70 K79 G80 F81 A82 F83 V84 M87 F88 P89 E90 H91 V93 V94 A95 Y96 V99 D100 G101 M108 T115 I116 K117 K118 E119 A120 S121 Q122

S123
G124
P125
S126
S127
G128

4.2.9 Score per residue for model 9

- Molecule 1: hypothetical protein RIKEN CDNA 1200009A02

Chain A: 

G30 S31 S32 S33 S34 S35 S36 S37 N44 L45 S46 V47 T48 L54 E55 E56 D53 L54 E55 F58 S59 H68 Y69 P70 L74 T75 K76 F81 E90 H91 Y96 V99 D100 G101 Q102 V103 F104 M108 L109 T115 I116 K117 K118 E119 A120 S121 Q122 S123 G124 P125 S126 S127

G128

4.2.10 Score per residue for model 10

- Molecule 1: hypothetical protein RIKEN CDNA 1200009A02

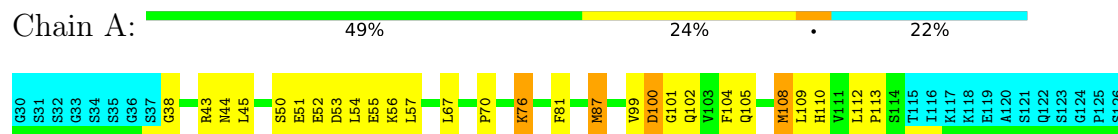
Chain A: 

G30 S31 S32 S33 S34 S35 S36 S37 L40 F41 N44 L45 S50 E51 E52 D53 L54 E55 K56 L57 F58 S59 L64 P70 F81 A82 F83 A92 A95 V99 D100 G101 Q102 V103 F104 M108 L109 H110 V111 L112 T115 I116 K117 K118 E119 A120 S121 Q122 S123

G124
P125
S126
S127
G128

4.2.11 Score per residue for model 11

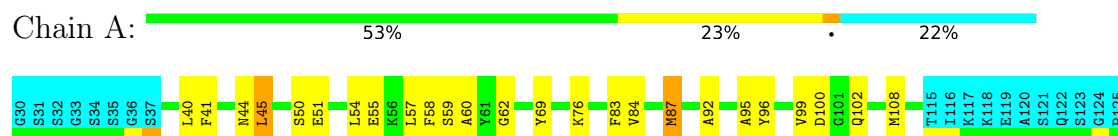
- Molecule 1: hypothetical protein RIKEN CDNA 1200009A02



S127
G128

4.2.12 Score per residue for model 12

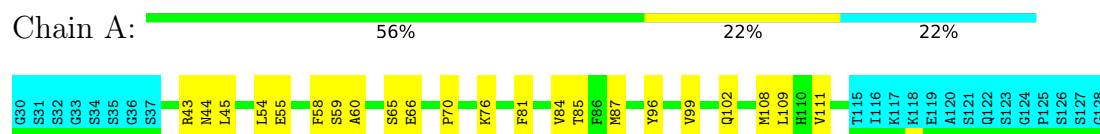
- Molecule 1: hypothetical protein RIKEN CDNA 1200009A02



S126
S127
G128

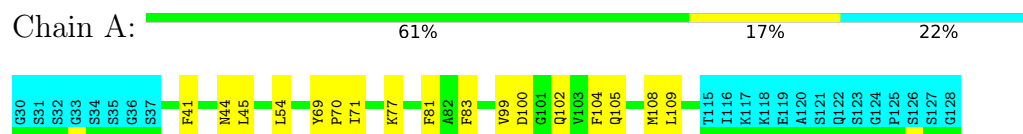
4.2.13 Score per residue for model 13

- Molecule 1: hypothetical protein RIKEN CDNA 1200009A02



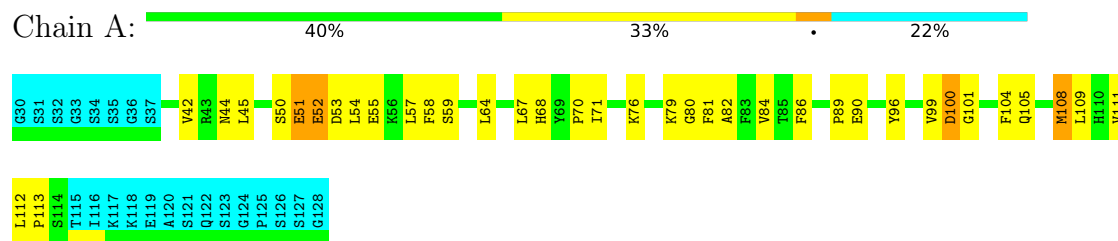
4.2.14 Score per residue for model 14

- Molecule 1: hypothetical protein RIKEN CDNA 1200009A02



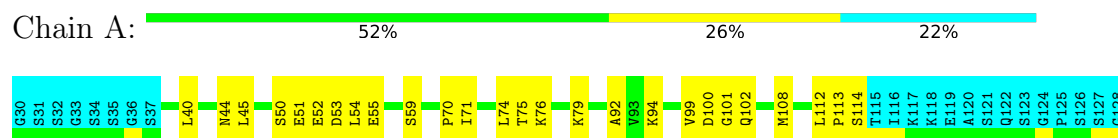
4.2.15 Score per residue for model 15

- Molecule 1: hypothetical protein RIKEN CDNA 1200009A02



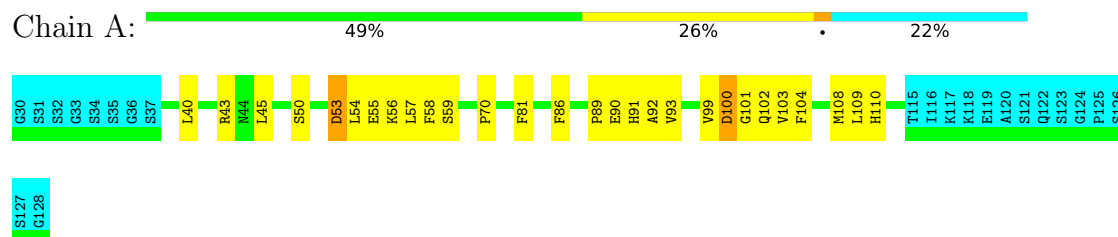
4.2.16 Score per residue for model 16

- Molecule 1: hypothetical protein RIKEN CDNA 1200009A02



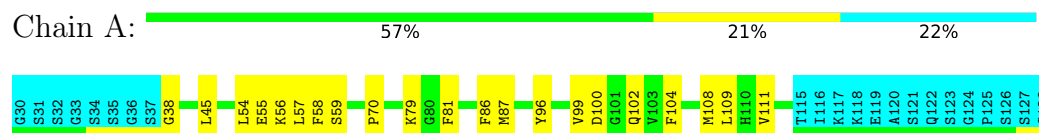
4.2.17 Score per residue for model 17

- Molecule 1: hypothetical protein RIKEN CDNA 1200009A02



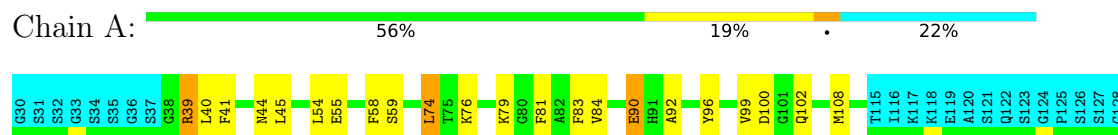
4.2.18 Score per residue for model 18

- Molecule 1: hypothetical protein RIKEN CDNA 1200009A02



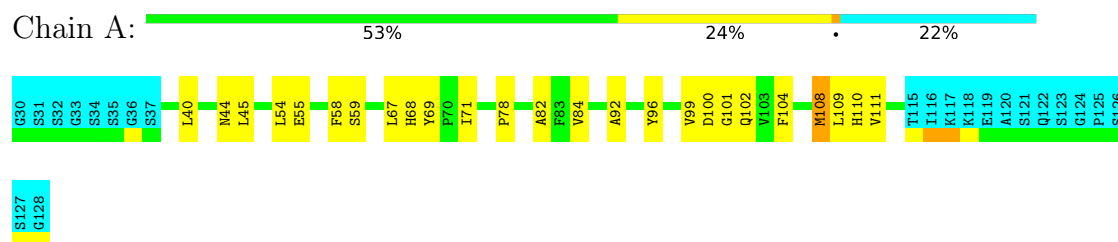
4.2.19 Score per residue for model 19

- Molecule 1: hypothetical protein RIKEN CDNA 1200009A02



4.2.20 Score per residue for model 20

- Molecule 1: hypothetical protein RIKEN CDNA 1200009A02



5 Refinement protocol and experimental data overview

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

Of the 100 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
CYANA	refinement	2.0

No chemical shift data was provided.

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	618	610	607	19±6
All	All	12360	12200	12140	377

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 15.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:45:LEU:HD11	1:A:54:LEU:HD21	0.93	1.40	11	13
1:A:99:VAL:HG13	1:A:102:GLN:NE2	0.87	1.85	19	9
1:A:45:LEU:CD1	1:A:54:LEU:HD21	0.81	2.05	11	14
1:A:68:HIS:O	1:A:82:ALA:HB1	0.79	1.77	15	3
1:A:58:PHE:CE2	1:A:84:VAL:HG21	0.79	2.11	1	9
1:A:74:LEU:N	1:A:74:LEU:HD13	0.74	1.97	19	1
1:A:45:LEU:HD21	1:A:54:LEU:HD21	0.74	1.58	20	1
1:A:99:VAL:HG13	1:A:102:GLN:HE21	0.74	1.41	12	3
1:A:41:PHE:CD1	1:A:83:PHE:CZ	0.68	2.82	10	6
1:A:90:GLU:CD	1:A:91:HIS:CD2	0.66	2.74	4	1
1:A:103:VAL:HG22	1:A:108:MET:SD	0.65	2.32	17	1
1:A:63:PRO:HB2	1:A:87:MET:HE3	0.61	1.71	6	1
1:A:99:VAL:HG13	1:A:102:GLN:OE1	0.61	1.96	14	1
1:A:44:ASN:ND2	1:A:108:MET:N	0.60	2.50	14	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:111:VAL:C	1:A:112:LEU:HD22	0.60	2.22	10	1
1:A:40:LEU:HD11	1:A:92:ALA:O	0.60	1.96	17	4
1:A:74:LEU:H	1:A:74:LEU:HD22	0.59	1.58	19	1
1:A:65:SER:HB3	1:A:85:THR:HG22	0.59	1.74	13	2
1:A:102:GLN:NE2	1:A:109:LEU:HD12	0.58	2.13	13	2
1:A:70:PRO:CG	1:A:81:PHE:CE1	0.57	2.86	11	2
1:A:76:LYS:N	1:A:76:LYS:CD	0.57	2.67	9	5
1:A:108:MET:SD	1:A:110:HIS:CD2	0.57	2.96	11	2
1:A:90:GLU:OE2	1:A:91:HIS:CD2	0.57	2.57	4	1
1:A:104:PHE:HB2	1:A:109:LEU:HD11	0.56	1.77	10	10
1:A:58:PHE:CD2	1:A:84:VAL:HG21	0.56	2.36	1	5
1:A:86:PHE:HB2	1:A:92:ALA:HB2	0.56	1.78	17	1
1:A:55:GLU:HG3	1:A:67:LEU:HD22	0.55	1.78	8	4
1:A:42:VAL:HG21	1:A:58:PHE:CZ	0.55	2.36	15	1
1:A:71:ILE:HD13	1:A:78:PRO:HB3	0.55	1.79	2	2
1:A:104:PHE:CB	1:A:109:LEU:HD11	0.54	2.32	4	2
1:A:74:LEU:N	1:A:74:LEU:CD1	0.54	2.69	19	1
1:A:57:LEU:HD22	1:A:104:PHE:CE1	0.54	2.37	15	1
1:A:44:ASN:O	1:A:109:LEU:HD23	0.54	2.02	3	2
1:A:55:GLU:OE1	1:A:64:LEU:HD12	0.54	2.03	10	1
1:A:96:TYR:O	1:A:96:TYR:CD1	0.54	2.60	3	6
1:A:81:PHE:C	1:A:81:PHE:CD1	0.53	2.86	15	2
1:A:101:GLY:C	1:A:108:MET:HE1	0.53	2.28	15	2
1:A:45:LEU:CD2	1:A:54:LEU:HD11	0.53	2.33	20	1
1:A:96:TYR:CD1	1:A:96:TYR:O	0.53	2.61	4	5
1:A:66:GLU:CD	1:A:66:GLU:C	0.53	2.76	13	1
1:A:58:PHE:CE2	1:A:84:VAL:CG2	0.53	2.90	1	1
1:A:55:GLU:CD	1:A:64:LEU:HD12	0.52	2.29	10	1
1:A:99:VAL:HG12	1:A:111:VAL:CG2	0.52	2.34	15	4
1:A:45:LEU:CD2	1:A:54:LEU:HD21	0.52	2.33	20	1
1:A:79:LYS:HB2	1:A:81:PHE:CE2	0.52	2.40	6	3
1:A:70:PRO:CG	1:A:81:PHE:CZ	0.52	2.93	11	1
1:A:45:LEU:HD11	1:A:54:LEU:CD2	0.52	2.27	11	3
1:A:67:LEU:HD12	1:A:84:VAL:HG22	0.51	1.81	6	3
1:A:70:PRO:HG2	1:A:81:PHE:CE1	0.51	2.39	11	1
1:A:54:LEU:HD11	1:A:69:TYR:CE1	0.51	2.41	12	4
1:A:99:VAL:O	1:A:101:GLY:N	0.50	2.44	16	10
1:A:44:ASN:CG	1:A:108:MET:O	0.50	2.55	20	3
1:A:50:SER:O	1:A:52:GLU:N	0.50	2.45	15	5
1:A:90:GLU:C	1:A:90:GLU:OE1	0.50	2.55	19	1
1:A:44:ASN:CB	1:A:108:MET:O	0.50	2.60	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:99:VAL:O	1:A:100:ASP:C	0.50	2.55	17	3
1:A:44:ASN:ND2	1:A:108:MET:O	0.50	2.45	16	6
1:A:55:GLU:O	1:A:59:SER:CB	0.50	2.60	3	16
1:A:58:PHE:O	1:A:59:SER:C	0.50	2.55	13	16
1:A:50:SER:O	1:A:51:GLU:C	0.49	2.55	1	7
1:A:100:ASP:O	1:A:100:ASP:CG	0.49	2.55	4	2
1:A:70:PRO:O	1:A:71:ILE:HD13	0.49	2.07	16	4
1:A:96:TYR:O	1:A:100:ASP:CG	0.49	2.56	4	2
1:A:41:PHE:CD1	1:A:83:PHE:CE1	0.48	3.01	10	2
1:A:45:LEU:HD22	1:A:54:LEU:HD11	0.48	1.84	20	1
1:A:99:VAL:HG12	1:A:111:VAL:HG21	0.48	1.84	15	2
1:A:52:GLU:O	1:A:53:ASP:C	0.48	2.56	8	2
1:A:90:GLU:OE1	1:A:90:GLU:C	0.48	2.55	4	1
1:A:69:TYR:CE2	1:A:71:ILE:HD11	0.48	2.43	20	1
1:A:70:PRO:HG3	1:A:81:PHE:CZ	0.48	2.43	10	10
1:A:99:VAL:CG1	1:A:111:VAL:HG21	0.48	2.39	13	7
1:A:89:PRO:O	1:A:93:VAL:HG23	0.47	2.08	17	3
1:A:50:SER:O	1:A:53:ASP:CG	0.47	2.58	17	1
1:A:79:LYS:HB2	1:A:81:PHE:CZ	0.47	2.45	6	1
1:A:40:LEU:HD11	1:A:92:ALA:HB1	0.47	1.87	16	2
1:A:50:SER:C	1:A:52:GLU:N	0.47	2.72	15	6
1:A:56:LYS:O	1:A:57:LEU:C	0.47	2.57	7	8
1:A:54:LEU:O	1:A:55:GLU:C	0.47	2.58	5	7
1:A:71:ILE:CG2	1:A:76:LYS:C	0.47	2.87	15	1
1:A:38:GLY:O	1:A:86:PHE:N	0.47	2.48	18	1
1:A:104:PHE:O	1:A:105:GLN:CG	0.47	2.62	15	1
1:A:99:VAL:O	1:A:102:GLN:N	0.47	2.48	9	2
1:A:102:GLN:HE21	1:A:109:LEU:HD12	0.46	1.67	13	2
1:A:90:GLU:HG3	1:A:91:HIS:CD2	0.46	2.45	17	4
1:A:68:HIS:CE1	1:A:70:PRO:HD3	0.46	2.45	8	2
1:A:67:LEU:CD1	1:A:84:VAL:HG22	0.46	2.41	6	2
1:A:70:PRO:HG3	1:A:81:PHE:CE2	0.46	2.46	10	1
1:A:50:SER:O	1:A:53:ASP:N	0.45	2.49	15	4
1:A:64:LEU:HD23	1:A:86:PHE:CE1	0.45	2.46	15	1
1:A:70:PRO:HG3	1:A:81:PHE:CE1	0.45	2.46	14	6
1:A:59:SER:O	1:A:62:GLY:N	0.45	2.49	12	2
1:A:55:GLU:O	1:A:59:SER:N	0.45	2.50	15	1
1:A:44:ASN:N	1:A:80:GLY:O	0.45	2.49	15	1
1:A:95:ALA:O	1:A:99:VAL:N	0.45	2.50	10	4
1:A:57:LEU:HD11	1:A:102:GLN:HE22	0.44	1.72	1	2
1:A:59:SER:O	1:A:60:ALA:C	0.44	2.60	12	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:GLN:CD	1:A:109:LEU:HD12	0.44	2.38	1	2
1:A:68:HIS:O	1:A:82:ALA:CB	0.44	2.60	15	1
1:A:57:LEU:HD21	1:A:102:GLN:NE2	0.44	2.28	3	1
1:A:65:SER:OG	1:A:87:MET:N	0.44	2.51	1	1
1:A:39:ARG:CB	1:A:39:ARG:CZ	0.44	2.96	19	1
1:A:51:GLU:HG2	1:A:67:LEU:HD23	0.43	1.90	7	1
1:A:41:PHE:CD1	1:A:83:PHE:CE2	0.43	3.06	8	1
1:A:89:PRO:O	1:A:90:GLU:C	0.43	2.60	15	1
1:A:81:PHE:CD1	1:A:81:PHE:C	0.43	2.96	18	3
1:A:90:GLU:OE2	1:A:91:HIS:NE2	0.43	2.50	4	1
1:A:112:LEU:HD12	1:A:113:PRO:HD2	0.43	1.90	6	5
1:A:65:SER:N	1:A:85:THR:O	0.43	2.52	2	1
1:A:88:PHE:CD2	1:A:91:HIS:CE1	0.43	3.07	3	1
1:A:54:LEU:HD22	1:A:58:PHE:HE1	0.43	1.74	10	1
1:A:57:LEU:HD21	1:A:102:GLN:HE22	0.42	1.73	3	1
1:A:54:LEU:HD22	1:A:58:PHE:HE2	0.42	1.73	6	1
1:A:74:LEU:O	1:A:76:LYS:CD	0.42	2.67	16	2
1:A:110:HIS:CD2	1:A:110:HIS:N	0.42	2.87	17	1
1:A:54:LEU:CD1	1:A:69:TYR:CE1	0.42	3.03	14	1
1:A:102:GLN:CG	1:A:109:LEU:HD12	0.42	2.44	17	1
1:A:87:MET:CE	1:A:87:MET:HA	0.42	2.45	5	2
1:A:58:PHE:O	1:A:60:ALA:N	0.41	2.53	5	2
1:A:45:LEU:HD21	1:A:54:LEU:CD2	0.41	2.39	20	1
1:A:87:MET:HA	1:A:87:MET:CE	0.41	2.46	11	1
1:A:71:ILE:HD12	1:A:78:PRO:HD3	0.41	1.93	2	1
1:A:53:ASP:OD2	1:A:104:PHE:CE2	0.41	2.73	3	1
1:A:71:ILE:HG23	1:A:77:LYS:C	0.41	2.40	14	2
1:A:46:SER:C	1:A:48:THR:N	0.41	2.78	9	1
1:A:75:THR:C	1:A:76:LYS:HD3	0.41	2.40	16	1
1:A:90:GLU:CG	1:A:91:HIS:N	0.41	2.83	8	1
1:A:55:GLU:CG	1:A:67:LEU:HD22	0.41	2.46	20	1
1:A:41:PHE:CE1	1:A:83:PHE:CZ	0.40	3.09	1	1
1:A:108:MET:HA	1:A:108:MET:CE	0.40	2.46	4	1
1:A:56:LYS:N	1:A:56:LYS:HD2	0.40	2.31	9	1
1:A:70:PRO:CB	1:A:81:PHE:CZ	0.40	3.04	11	1
1:A:90:GLU:OE1	1:A:90:GLU:O	0.40	2.40	19	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	77/99 (78%)	69±2 (90±3%)	7±2 (9±3%)	1±0 (1±1%)	11	58
All	All	1540/1980 (78%)	1383 (90%)	135 (9%)	22 (1%)	11	58

All 2 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	100	ASP	19
1	A	51	GLU	3

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	67/83 (81%)	64±1 (96±2%)	3±1 (4±2%)	30	81
All	All	1340/1660 (81%)	1289 (96%)	51 (4%)	30	81

All 17 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	108	MET	9
1	A	87	MET	8
1	A	45	LEU	6
1	A	76	LYS	6
1	A	79	LYS	6
1	A	43	ARG	3
1	A	90	GLU	2
1	A	105	GLN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	65	SER	1
1	A	112	LEU	1
1	A	44	ASN	1
1	A	56	LYS	1
1	A	52	GLU	1
1	A	94	LYS	1
1	A	53	ASP	1
1	A	39	ARG	1
1	A	74	LEU	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 oligosaccharides 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