Full wwPDB NMR Structure Validation Report (i)

Feb 22, 2022 – 11:29 AM EST

PDB ID	:	1V60
Title	:	Solution structure of BolA1 protein from Mus musculus
Authors	:	Kasai, T.; Tomizawa, T.; Koshiba, S.; Inoue, M.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2003-11-26

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 (i) symbol.

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

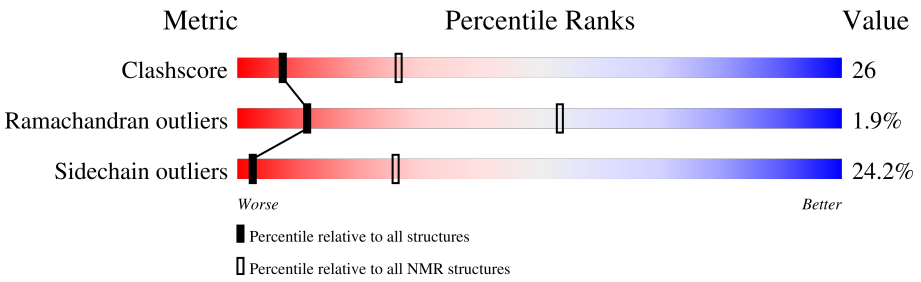
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

1 Overall quality at a glance (i)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	123	30% 28% • 38%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 15 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:32-A:52, A:66-A:120 (76)	0.18	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 4 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1773 atoms, of which 881 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called RIKEN cDNA 1810037G04.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	123	1773	545	881	170	173	4	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	GLY	-	cloning artifact	UNP Q9D8S9
A	7	SER	-	cloning artifact	UNP Q9D8S9
A	8	SER	-	cloning artifact	UNP Q9D8S9
A	9	GLY	-	cloning artifact	UNP Q9D8S9
A	10	SER	-	cloning artifact	UNP Q9D8S9
A	11	SER	-	cloning artifact	UNP Q9D8S9
A	12	GLY	-	cloning artifact	UNP Q9D8S9

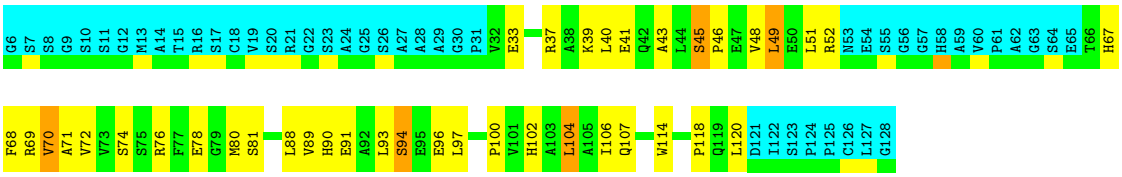
4 Residue-property plots (i)

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: RIKEN cDNA 1810037G04

Chain A: 30% 28% • 38%



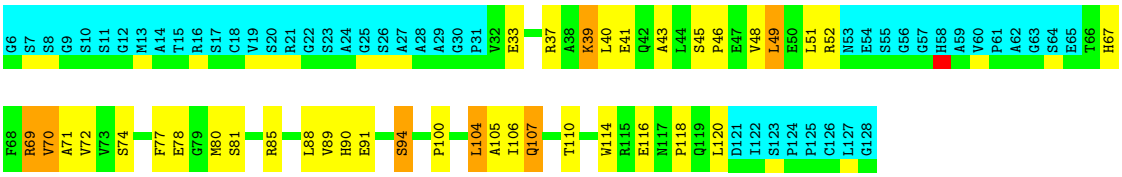
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: RIKEN cDNA 1810037G04

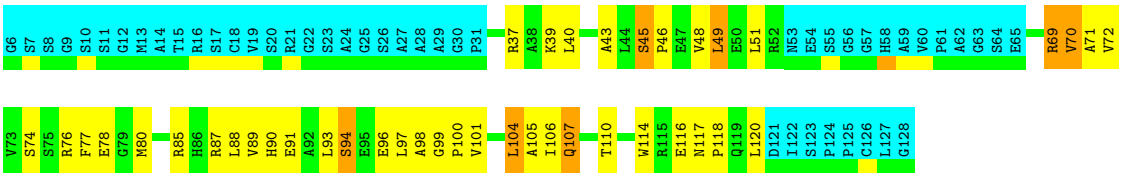
Chain A: 31% 25% 6% 38%



4.2.2 Score per residue for model 2

• Molecule 1: RIKEN cDNA 1810037G04

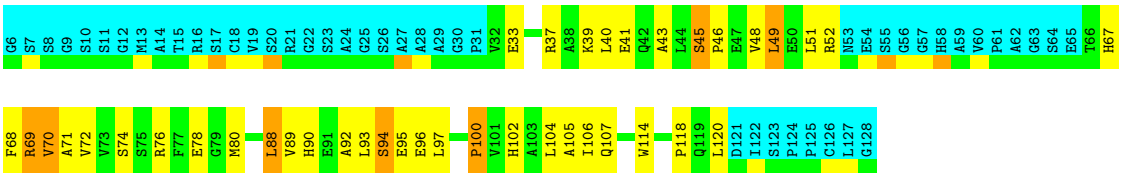
Chain A: 28% 28% 6% 38%



4.2.3 Score per residue for model 3

- Molecule 1: RIKEN cDNA 1810037G04

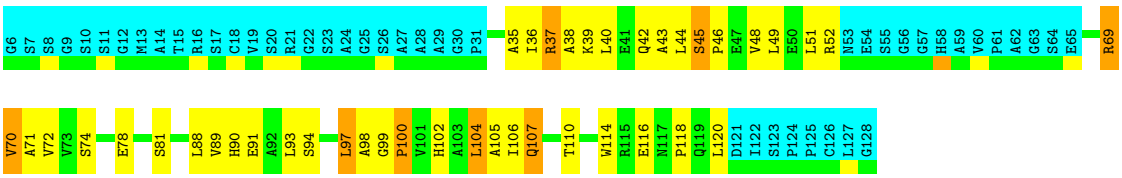
Chain A: 29% 27% 6% 38%



4.2.4 Score per residue for model 4

- Molecule 1: RIKEN cDNA 1810037G04

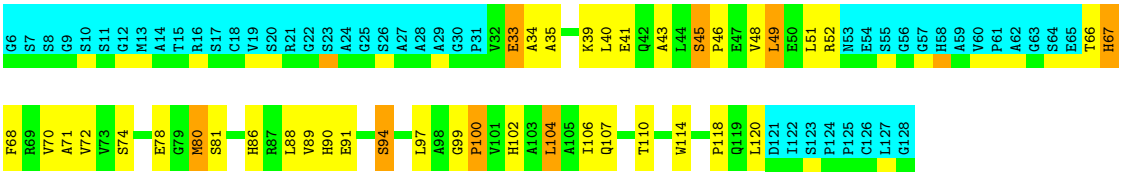
Chain A: 28% 28% 7% 38%



4.2.5 Score per residue for model 5

- Molecule 1: RIKEN cDNA 1810037G04

Chain A: 29% 26% 7% 38%



4.2.6 Score per residue for model 6

- Molecule 1: RIKEN cDNA 1810037G04

Chain A: 32% 25% 5% 38%

G6 S7 S8 G9 S10 S11 G12 M13 A14 T15 R16 S17 C18 V19 S20 R21 G22 S23 A24 G25 S26 A27 A28 A29 G30 P31 V32 E33 R37 A38 K39 L40 A43 L44 S45 P46 E47 V48 L49 E50 L51 R52 N53 E54 S55 G56 G57 H58 A59 V60 P61 A62 G63 S64 E65 T66 H67 F68

R69 V70 A71 V72 V73 S74 S75 R76 F77 E78 G79 M80 S81 L88 V89 H90 E91 A92 L93 S94 E95 E96 P100 L104 Q107 W114 P118 Q119 L120 D121 I122 S123 P124 P125 C126 L127 G128

4.2.7 Score per residue for model 7

- Molecule 1: RIKEN cDNA 1810037G04

Chain A: 22% 35% 5% 38%

G6 S7 S8 G9 S10 S11 G12 M13 A14 T15 R16 S17 C18 V19 S20 R21 G22 S23 A24 G25 S26 A27 A28 A29 G30 P31 V32 E33 R37 A38 K39 L40 E41 Q42 A43 L44 S45 P46 E47 V48 L49 E50 L51 R52 N53 E54 S55 G56 G57 H58 A59 V60 P61 A62 G63 S64 E65 T66 H67

F68 R69 V70 A71 V72 V73 S74 S75 R76 F77 E78 G79 M80 S81 L88 V89 H90 E91 A92 L93 S94 E95 E96 L97 P100 L104 A105 I106 Q107 A108 K109 Q113 W114 R115 E116 N117 P118 Q119 L120 D121 I122 S123 P124 P125 C126 L127 G128

4.2.8 Score per residue for model 8

- Molecule 1: RIKEN cDNA 1810037G04

Chain A: 28% 28% 6% 38%

G6 S7 S8 G9 S10 S11 G12 M13 A14 T15 R16 S17 C18 V19 S20 R21 G22 S23 A24 G25 S26 A27 A28 A29 G30 P31 K39 L40 E41 Q42 A43 L44 S45 P46 E47 V48 L49 E50 L51 R52 N53 E54 S55 G56 G57 H58 A59 V60 P61 A62 G63 S64 E65 T66 H67 F68 R69 V70 A71

V72 V73 S74 S75 R76 F77 E78 G79 M80 R85 L88 V89 H90 E91 A92 L93 S94 E95 E96 L97 A98 G99 P100 V101 L104 A105 I106 Q107 T110 W114 R115 P118 Q119 L120 D121 I122 S123 P124 P125 C126 L127 G128

4.2.9 Score per residue for model 9

- Molecule 1: RIKEN cDNA 1810037G04

Chain A: 27% 29% 6% 38%

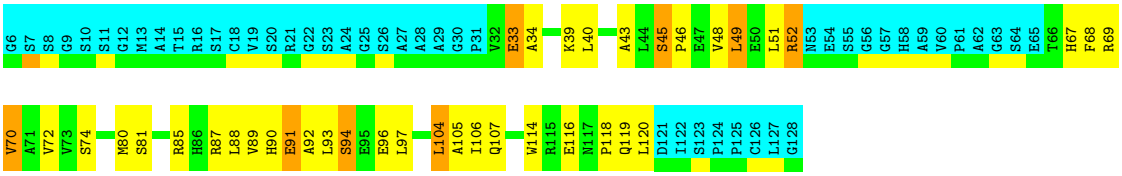
G6 S7 S8 G9 S10 S11 G12 M13 A14 T15 R16 S17 C18 V19 S20 R21 G22 S23 A24 G25 S26 A27 A28 A29 G30 P31 V32 E33 A34 R37 A38 K39 L40 E41 Q42 A43 L44 S45 P46 E47 V48 L49 E50 L51 R52 N53 E54 S55 G56 G57 H58 A59 V60 P61 A62 G63 S64 E65

F68 R69 V70 A71 V72 V73 S74 S75 R76 F77 E78 G79 M80 S81 P82 L83 Q84 R85 L88 V89 H90 E91 S94 E95 L104 A105 I106 Q107 T110 W114 R115 E116 N117 P118 Q119 L120 D121 I122 S123 P124 P125 C126 L127 G128

4.2.10 Score per residue for model 10

- Molecule 1: RIKEN cDNA 1810037G04

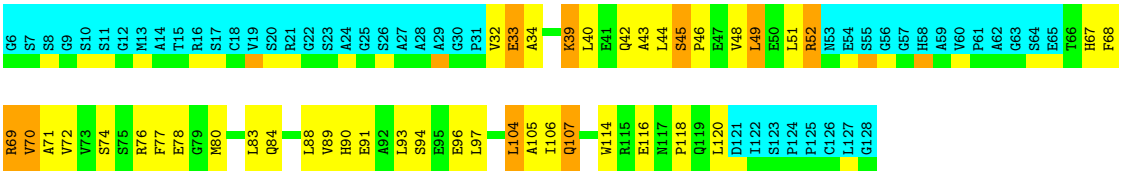
Chain A: 30% 25% 7% 38%



4.2.11 Score per residue for model 11

- Molecule 1: RIKEN cDNA 1810037G04

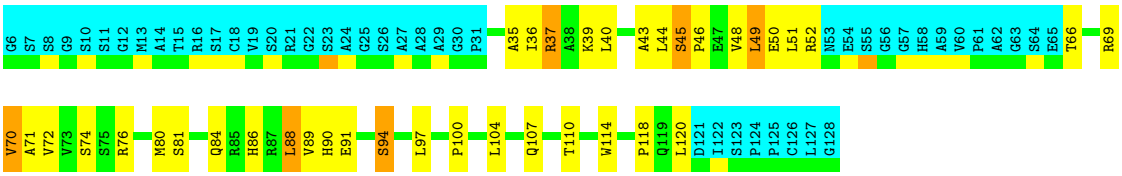
Chain A: 27% 28% 7% 38%



4.2.12 Score per residue for model 12

- Molecule 1: RIKEN cDNA 1810037G04

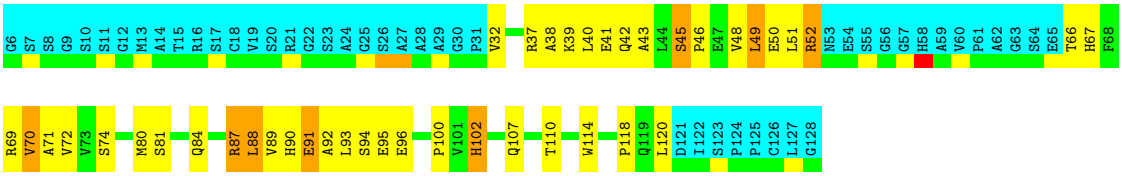
Chain A: 31% 26% 5% 38%



4.2.13 Score per residue for model 13

- Molecule 1: RIKEN cDNA 1810037G04

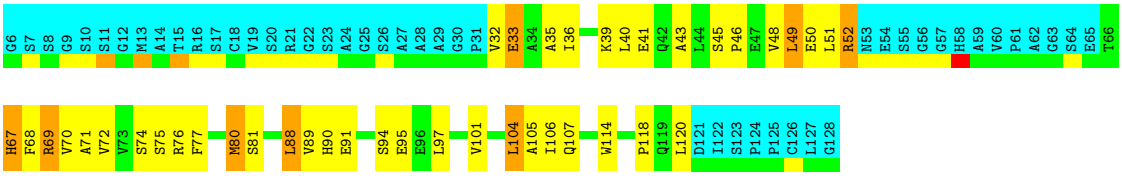
Chain A: 28% 28% 7% 38%



4.2.14 Score per residue for model 14

- Molecule 1: RIKEN cDNA 1810037G04

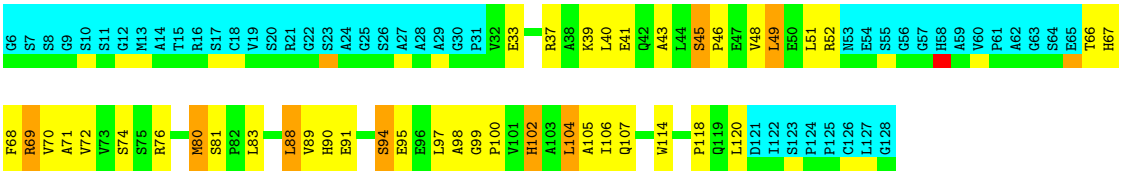
Chain A: 28% 28% 7% 38%



4.2.15 Score per residue for model 15 (medoid)

- Molecule 1: RIKEN cDNA 1810037G04

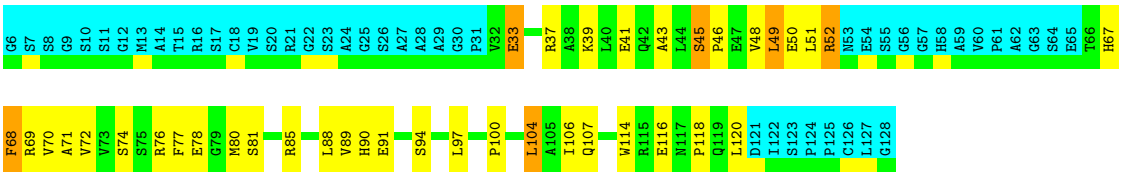
Chain A: 28% 28% 7% 38%



4.2.16 Score per residue for model 16

- Molecule 1: RIKEN cDNA 1810037G04

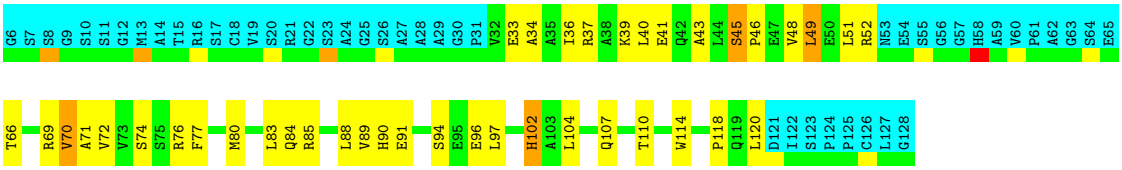
Chain A: 30% 27% 5% 38%



4.2.17 Score per residue for model 17

- Molecule 1: RIKEN cDNA 1810037G04

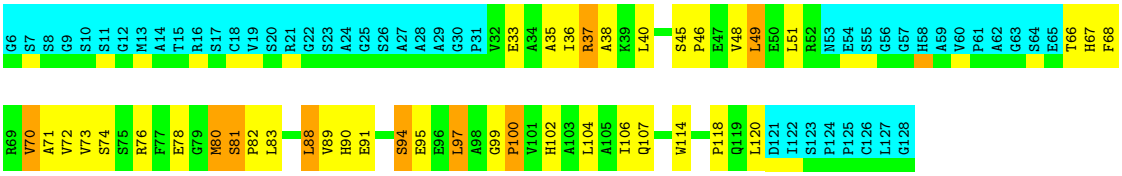
Chain A: 29% 29% • 38%



4.2.18 Score per residue for model 18

- Molecule 1: RIKEN cDNA 1810037G04

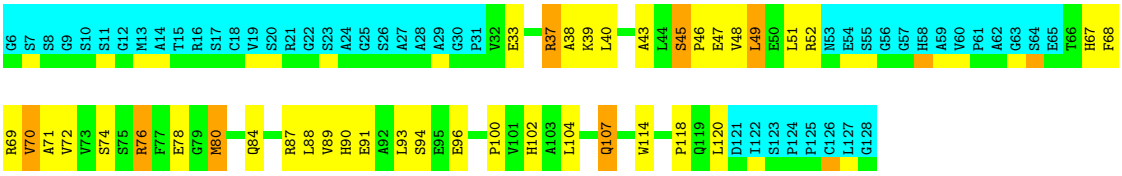
Chain A: 28% 26% 7% 38%



4.2.19 Score per residue for model 19

- Molecule 1: RIKEN cDNA 1810037G04

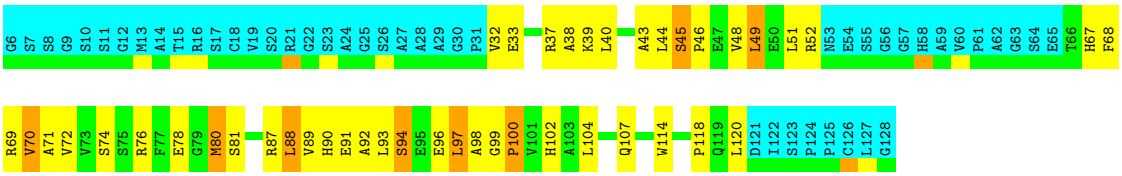
Chain A: 30% 26% 6% 38%



4.2.20 Score per residue for model 20

- Molecule 1: RIKEN cDNA 1810037G04

Chain A: 26% 29% 7% 38%



5 Refinement protocol and experimental data overview (i)

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

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	1.0.7
CYANA	refinement	1.0.7

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	600	612	612	31±6
All	All	12000	12240	12240	629

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 26.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:GLU:HG2	1:A:51:LEU:HD13	0.81	1.50	14	7
1:A:48:VAL:HG11	1:A:114:TRP:CZ2	0.80	2.11	17	20
1:A:40:LEU:HD11	1:A:89:VAL:HG13	0.79	1.53	19	13
1:A:40:LEU:HD12	1:A:44:LEU:HD12	0.75	1.59	11	1
1:A:68:PHE:HB3	1:A:104:LEU:HD13	0.74	1.60	16	9
1:A:93:LEU:HD12	1:A:96:GLU:HG3	0.72	1.60	7	4
1:A:40:LEU:HD12	1:A:44:LEU:CD1	0.72	2.14	11	1
1:A:70:VAL:CG1	1:A:106:ILE:HG23	0.71	2.14	14	13
1:A:89:VAL:HG11	1:A:106:ILE:HD13	0.69	1.64	9	6
1:A:40:LEU:HD22	1:A:44:LEU:CD1	0.69	2.17	20	3
1:A:51:LEU:HB2	1:A:70:VAL:HG23	0.69	1.65	18	11
1:A:46:PRO:CD	1:A:49:LEU:HD12	0.68	2.17	5	18
1:A:51:LEU:HD12	1:A:52:ARG:N	0.67	2.04	20	6
1:A:33:GLU:CG	1:A:51:LEU:HD13	0.67	2.20	14	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:92:ALA:C	1:A:93:LEU:HD22	0.67	2.10	10	6
1:A:40:LEU:HD21	1:A:93:LEU:CD2	0.67	2.20	8	1
1:A:33:GLU:HG3	1:A:51:LEU:HD22	0.66	1.65	9	5
1:A:40:LEU:HD21	1:A:89:VAL:HG13	0.66	1.68	17	10
1:A:46:PRO:HG3	1:A:72:VAL:HG23	0.66	1.66	8	20
1:A:40:LEU:HG	1:A:93:LEU:HD21	0.66	1.68	8	3
1:A:40:LEU:CD2	1:A:89:VAL:HG13	0.64	2.23	14	2
1:A:114:TRP:CZ2	1:A:118:PRO:O	0.63	2.51	10	9
1:A:46:PRO:CG	1:A:49:LEU:HD12	0.63	2.24	10	14
1:A:51:LEU:HD12	1:A:69:ARG:O	0.62	1.94	1	5
1:A:104:LEU:HD11	1:A:106:ILE:HG12	0.62	1.71	5	3
1:A:40:LEU:HD11	1:A:89:VAL:CG1	0.61	2.25	5	5
1:A:97:LEU:HD21	1:A:104:LEU:HD23	0.60	1.73	8	5
1:A:114:TRP:CH2	1:A:118:PRO:O	0.60	2.55	12	15
1:A:100:PRO:O	1:A:102:HIS:CD2	0.60	2.55	18	6
1:A:32:VAL:HG12	1:A:36:ILE:HD11	0.60	1.73	14	1
1:A:51:LEU:HD23	1:A:52:ARG:N	0.59	2.13	11	7
1:A:51:LEU:HG	1:A:70:VAL:HG23	0.59	1.74	10	6
1:A:69:ARG:CZ	1:A:105:ALA:CB	0.59	2.80	15	4
1:A:104:LEU:HD12	1:A:105:ALA:N	0.59	2.12	10	5
1:A:40:LEU:HD22	1:A:44:LEU:HD12	0.58	1.74	20	2
1:A:51:LEU:HD13	1:A:70:VAL:HG23	0.58	1.75	4	4
1:A:40:LEU:CD2	1:A:93:LEU:CD2	0.57	2.82	8	1
1:A:46:PRO:HD2	1:A:49:LEU:HD12	0.57	1.75	5	12
1:A:32:VAL:HG13	1:A:96:GLU:OE1	0.57	2.00	11	2
1:A:69:ARG:HG3	1:A:105:ALA:HB3	0.57	1.76	11	6
1:A:86:HIS:O	1:A:90:HIS:CD2	0.57	2.58	5	1
1:A:32:VAL:HG13	1:A:96:GLU:OE2	0.56	2.00	13	1
1:A:114:TRP:CZ3	1:A:120:LEU:HD21	0.56	2.36	10	3
1:A:71:ALA:CB	1:A:120:LEU:CD1	0.56	2.84	18	14
1:A:93:LEU:HD12	1:A:96:GLU:CG	0.55	2.31	7	2
1:A:48:VAL:HG11	1:A:114:TRP:CE2	0.55	2.36	15	1
1:A:86:HIS:O	1:A:90:HIS:CG	0.55	2.60	12	2
1:A:51:LEU:CG	1:A:70:VAL:HG23	0.55	2.31	10	6
1:A:72:VAL:HG13	1:A:77:PHE:CE2	0.54	2.36	7	3
1:A:51:LEU:HD23	1:A:52:ARG:H	0.54	1.63	10	4
1:A:114:TRP:CH2	1:A:120:LEU:HD21	0.53	2.39	10	3
1:A:71:ALA:CB	1:A:120:LEU:HD11	0.53	2.33	18	12
1:A:40:LEU:CD1	1:A:89:VAL:HG13	0.53	2.30	19	5
1:A:72:VAL:CG1	1:A:77:PHE:CE2	0.53	2.92	7	3
1:A:72:VAL:HG12	1:A:107:GLN:O	0.52	2.05	16	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:LEU:HD12	1:A:52:ARG:H	0.52	1.63	12	6
1:A:46:PRO:HG2	1:A:49:LEU:HD12	0.52	1.80	11	8
1:A:39:LYS:CB	1:A:93:LEU:HD21	0.52	2.34	13	4
1:A:107:GLN:NE2	1:A:120:LEU:HD23	0.51	2.20	6	1
1:A:89:VAL:CG1	1:A:106:ILE:HD13	0.51	2.35	9	1
1:A:94:SER:O	1:A:98:ALA:CB	0.51	2.59	20	5
1:A:90:HIS:O	1:A:94:SER:CA	0.51	2.59	20	8
1:A:93:LEU:HD12	1:A:96:GLU:HG2	0.50	1.84	10	1
1:A:32:VAL:HG12	1:A:36:ILE:CD1	0.50	2.36	14	1
1:A:80:MET:CE	1:A:88:LEU:CD1	0.50	2.89	14	3
1:A:46:PRO:CB	1:A:73:VAL:O	0.50	2.60	7	2
1:A:68:PHE:CB	1:A:104:LEU:HD13	0.49	2.37	20	4
1:A:104:LEU:HD12	1:A:104:LEU:C	0.49	2.28	7	2
1:A:40:LEU:CD2	1:A:93:LEU:HD23	0.49	2.38	11	1
1:A:66:THR:CB	1:A:102:HIS:CD2	0.49	2.95	13	2
1:A:39:LYS:HB2	1:A:93:LEU:HD21	0.49	1.83	11	1
1:A:66:THR:HB	1:A:102:HIS:CD2	0.49	2.43	15	3
1:A:104:LEU:C	1:A:104:LEU:HD12	0.48	2.29	16	3
1:A:45:SER:N	1:A:46:PRO:HD3	0.48	2.23	7	20
1:A:46:PRO:CG	1:A:49:LEU:CD1	0.48	2.91	11	9
1:A:69:ARG:NH2	1:A:105:ALA:CB	0.48	2.76	15	2
1:A:90:HIS:CD2	1:A:97:LEU:CD1	0.47	2.97	4	3
1:A:40:LEU:HD22	1:A:89:VAL:HG13	0.47	1.87	14	1
1:A:70:VAL:HG12	1:A:106:ILE:HG23	0.47	1.86	11	1
1:A:90:HIS:CD2	1:A:97:LEU:HD13	0.47	2.45	20	2
1:A:33:GLU:HB2	1:A:68:PHE:CE1	0.47	2.44	19	1
1:A:35:ALA:O	1:A:39:LYS:CG	0.47	2.62	14	2
1:A:77:PHE:CD1	1:A:85:ARG:HG2	0.47	2.45	17	6
1:A:40:LEU:HD22	1:A:44:LEU:HD11	0.47	1.86	20	1
1:A:94:SER:O	1:A:98:ALA:HB3	0.46	2.10	8	2
1:A:90:HIS:O	1:A:94:SER:N	0.46	2.49	3	18
1:A:51:LEU:HD13	1:A:70:VAL:CG2	0.46	2.40	4	2
1:A:40:LEU:CG	1:A:93:LEU:HD21	0.46	2.39	8	1
1:A:97:LEU:HD13	1:A:101:VAL:HG12	0.46	1.88	14	1
1:A:50:GLU:O	1:A:71:ALA:N	0.45	2.47	16	5
1:A:90:HIS:CE1	1:A:97:LEU:HG	0.45	2.46	11	4
1:A:114:TRP:CD1	1:A:118:PRO:HB3	0.45	2.46	20	7
1:A:39:LYS:O	1:A:43:ALA:N	0.45	2.48	11	19
1:A:90:HIS:O	1:A:93:LEU:N	0.45	2.50	19	1
1:A:96:GLU:O	1:A:101:VAL:N	0.45	2.50	2	2
1:A:47:GLU:N	1:A:73:VAL:O	0.45	2.44	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:84:GLN:O	1:A:87:ARG:N	0.45	2.50	19	1
1:A:114:TRP:O	1:A:118:PRO:N	0.45	2.50	11	6
1:A:96:GLU:N	1:A:96:GLU:CD	0.45	2.70	10	2
1:A:69:ARG:CZ	1:A:105:ALA:HB3	0.45	2.42	2	1
1:A:96:GLU:N	1:A:96:GLU:OE1	0.45	2.50	10	1
1:A:40:LEU:O	1:A:44:LEU:N	0.45	2.50	11	1
1:A:80:MET:O	1:A:85:ARG:NH2	0.44	2.50	10	2
1:A:80:MET:CE	1:A:88:LEU:HD13	0.44	2.42	7	4
1:A:83:LEU:O	1:A:84:GLN:C	0.44	2.56	17	2
1:A:39:LYS:HB3	1:A:93:LEU:HD21	0.44	1.88	13	1
1:A:33:GLU:HG3	1:A:51:LEU:HD21	0.44	1.89	20	1
1:A:97:LEU:HD11	1:A:104:LEU:HB3	0.44	1.90	16	1
1:A:107:GLN:CG	1:A:109:LYS:CE	0.44	2.95	7	1
1:A:113:GLN:O	1:A:116:GLU:N	0.44	2.51	7	1
1:A:87:ARG:O	1:A:91:GLU:N	0.44	2.49	10	2
1:A:46:PRO:HG2	1:A:49:LEU:CD1	0.44	2.43	7	6
1:A:37:ARG:O	1:A:41:GLU:N	0.44	2.49	7	3
1:A:50:GLU:OE2	1:A:52:ARG:NH1	0.43	2.51	13	1
1:A:51:LEU:HG	1:A:70:VAL:CG2	0.43	2.43	11	3
1:A:107:GLN:NE2	1:A:120:LEU:HD22	0.43	2.27	19	1
1:A:33:GLU:CG	1:A:51:LEU:HD22	0.43	2.38	5	1
1:A:40:LEU:HA	1:A:43:ALA:HB3	0.43	1.90	4	2
1:A:36:ILE:CG1	1:A:96:GLU:OE2	0.43	2.66	17	1
1:A:40:LEU:HD21	1:A:89:VAL:HA	0.43	1.91	19	1
1:A:66:THR:OG1	1:A:102:HIS:NE2	0.43	2.50	13	1
1:A:33:GLU:OE1	1:A:34:ALA:N	0.43	2.51	10	4
1:A:39:LYS:O	1:A:42:GLN:N	0.42	2.50	11	3
1:A:35:ALA:C	1:A:37:ARG:N	0.42	2.72	12	1
1:A:114:TRP:O	1:A:118:PRO:CB	0.42	2.67	9	2
1:A:84:GLN:O	1:A:88:LEU:N	0.42	2.50	12	1
1:A:40:LEU:HD11	1:A:89:VAL:HA	0.42	1.89	11	1
1:A:33:GLU:HG2	1:A:51:LEU:CD2	0.42	2.44	18	4
1:A:84:GLN:O	1:A:88:LEU:HD23	0.42	2.15	13	1
1:A:37:ARG:NE	1:A:41:GLU:CD	0.42	2.72	3	1
1:A:102:HIS:CD2	1:A:102:HIS:N	0.42	2.87	3	1
1:A:89:VAL:CG1	1:A:93:LEU:HD23	0.42	2.44	4	1
1:A:71:ALA:HB1	1:A:120:LEU:HD21	0.42	1.92	12	3
1:A:68:PHE:HB2	1:A:104:LEU:CD1	0.42	2.44	14	1
1:A:90:HIS:O	1:A:93:LEU:C	0.42	2.57	19	1
1:A:93:LEU:HD22	1:A:93:LEU:N	0.42	2.29	10	3
1:A:33:GLU:CG	1:A:51:LEU:HD21	0.42	2.44	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:LYS:C	1:A:41:GLU:N	0.42	2.73	13	8
1:A:114:TRP:O	1:A:118:PRO:CA	0.42	2.68	3	2
1:A:89:VAL:HG13	1:A:93:LEU:HD23	0.42	1.92	4	1
1:A:85:ARG:O	1:A:89:VAL:HG23	0.41	2.15	8	1
1:A:66:THR:OG1	1:A:67:HIS:N	0.41	2.53	5	4
1:A:37:ARG:C	1:A:39:LYS:N	0.41	2.73	20	2
1:A:37:ARG:O	1:A:38:ALA:C	0.41	2.59	4	6
1:A:47:GLU:C	1:A:48:VAL:CG2	0.41	2.89	19	1
1:A:35:ALA:O	1:A:36:ILE:C	0.41	2.59	18	3
1:A:33:GLU:O	1:A:34:ALA:C	0.41	2.59	17	1
1:A:76:ARG:O	1:A:80:MET:SD	0.41	2.79	8	3
1:A:51:LEU:HD13	1:A:70:VAL:CB	0.41	2.46	15	2
1:A:93:LEU:N	1:A:93:LEU:CD2	0.41	2.84	10	1
1:A:45:SER:N	1:A:46:PRO:CD	0.41	2.84	20	1
1:A:33:GLU:CG	1:A:51:LEU:CD2	0.40	2.99	17	2
1:A:81:SER:CB	1:A:82:PRO:CD	0.40	2.98	18	1
1:A:80:MET:HE1	1:A:88:LEU:HD13	0.40	1.91	7	1
1:A:35:ALA:O	1:A:37:ARG:N	0.40	2.55	12	1
1:A:33:GLU:HA	1:A:36:ILE:HD12	0.40	1.93	14	1
1:A:33:GLU:CG	1:A:51:LEU:HG	0.40	2.47	1	2

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	76/123 (62%)	60±2 (79±2%)	15±2 (19±3%)	1±1 (2±1%)	11	53
All	All	1520/2460 (62%)	1195 (79%)	296 (19%)	29 (2%)	11	53

All 4 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	PRO	14
1	A	99	GLY	7

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Mol	Chain	Res	Type	Models (Total)
1	A	80	MET	7
1	A	67	HIS	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	63/93 (68%)	48±2 (76±4%)	15±2 (24±4%)	2 26
All	All	1260/1860 (68%)	955 (76%)	305 (24%)	2 26

All 31 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	49	LEU	20
1	A	74	SER	20
1	A	88	LEU	20
1	A	91	GLU	19
1	A	107	GLN	18
1	A	45	SER	17
1	A	104	LEU	16
1	A	69	ARG	15
1	A	70	VAL	14
1	A	78	GLU	14
1	A	81	SER	14
1	A	76	ARG	14
1	A	94	SER	11
1	A	52	ARG	10
1	A	67	HIS	10
1	A	80	MET	10
1	A	37	ARG	9
1	A	110	THR	9
1	A	116	GLU	7
1	A	95	GLU	6
1	A	97	LEU	6
1	A	33	GLU	6
1	A	87	ARG	3

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Mol	Chain	Res	Type	Models (Total)
1	A	119	GLN	3
1	A	83	LEU	3
1	A	102	HIS	3
1	A	39	LYS	2
1	A	68	PHE	2
1	A	75	SER	2
1	A	117	ASN	1
1	A	115	ARG	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 monosaccharides 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 (i)

No chemical shift data were provided