Full wwPDB NMR Structure Validation Report (i)

Feb 20, 2022 – 01:59 AM EST

PDB ID	:	1V2Y
Title	:	Solution Structure of Mouse Hypothetical Gene (RIKEN cDNA 3300001G02) Product Homologous to Ubiquitin Fold
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Deposited on	:	2003-10-17

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:

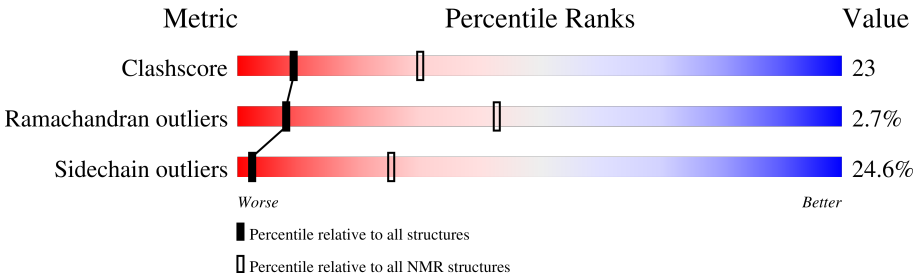
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	105	36% 34% • 27%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 8 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:7-A:14, A:19-A:46, A:55-A:95 (77)	0.29	8

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. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1667 atoms, of which 842 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called 3300001G02Rik protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	105	1667	513	842	153	155	4	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q8VIK1
A	2	SER	-	cloning artifact	UNP Q8VIK1
A	3	SER	-	cloning artifact	UNP Q8VIK1
A	4	GLY	-	cloning artifact	UNP Q8VIK1
A	5	SER	-	cloning artifact	UNP Q8VIK1
A	6	SER	-	cloning artifact	UNP Q8VIK1
A	7	GLY	-	cloning artifact	UNP Q8VIK1
A	100	SER	-	cloning artifact	UNP Q8VIK1
A	101	GLY	-	cloning artifact	UNP Q8VIK1
A	102	PRO	-	cloning artifact	UNP Q8VIK1
A	103	SER	-	cloning artifact	UNP Q8VIK1
A	104	SER	-	cloning artifact	UNP Q8VIK1
A	105	GLY	-	cloning artifact	UNP Q8VIK1

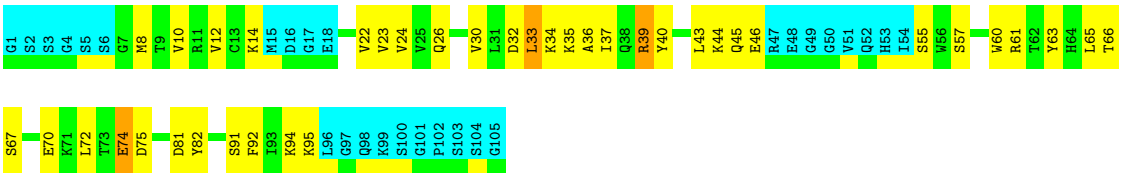
4 Residue-property plots (i)

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: 3300001G02Rik protein

Chain A: 36% 34% • 27%



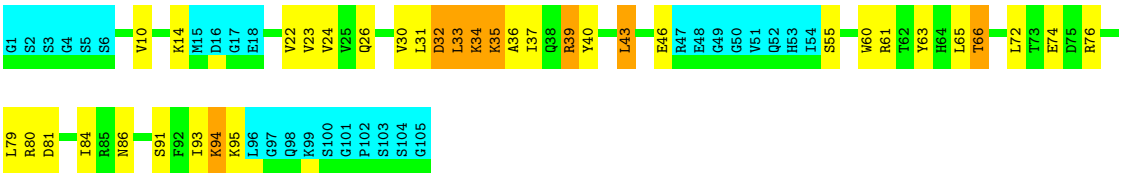
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: 3300001G02Rik protein

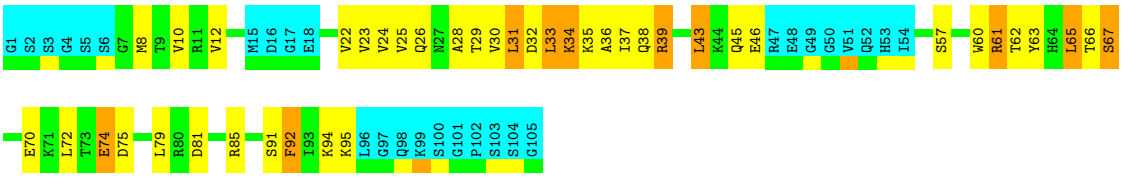
Chain A: 39% 27% 8% 27%



4.2.2 Score per residue for model 2

• Molecule 1: 3300001G02Rik protein

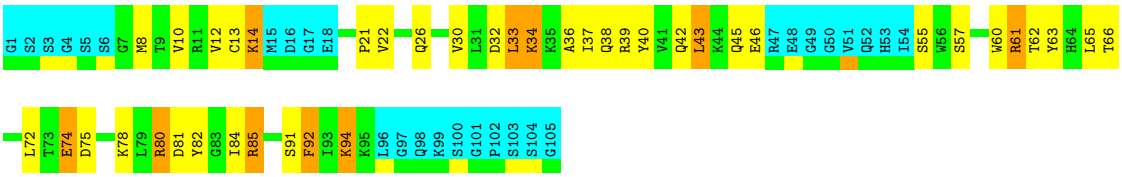
Chain A: 33% 30% 10% 27%



4.2.3 Score per residue for model 3

- Molecule 1: 3300001G02Rik protein

Chain A: 34% 30% 10% 27%



4.2.4 Score per residue for model 4

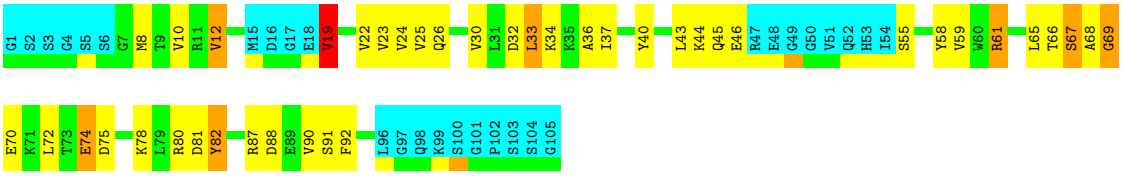
- Molecule 1: 3300001G02Rik protein

Chain A: 34% 32% 7% 27%

4.2.5 Score per residue for model 5

- Molecule 1: 3300001G02Rik protein

Chain A: 33% 32% 7% • 27%



4.2.6 Score per residue for model 6

- Molecule 1: 3300001G02Rik protein

Chain A: 36% 27% 10% 27%

G1 S2 S3 G4 S5 S6 G7 M8 T9 V10 R11 V12 C13 K14 M15 D16 G17 E18 P21 V22 V23 V24 V25 Q26 N27 V30 L31 D32 L33 K34 K35 A36 I37 Q38 R39 Y40 L43 K44 Q45 E46 R47 E48 G49 G50 V51 Q52 H53 I54 S55 W56 S57 W60 R61 T62 L65

T66 S67 E70 K71 L72 T73 E74 D75 L79 Y82 R87 S91 F92 L96 G97 Q98 K99 S100 G101 P102 S103 S104 G105

4.2.7 Score per residue for model 7

- Molecule 1: 3300001G02Rik protein

Chain A: 40% 24% 10% 27%

G1 S2 S3 G4 S5 S6 V10 R11 V12 M15 D16 G17 E18 V22 V23 V24 V25 A28 L31 D32 L33 K34 K35 A36 I37 Q38 R39 L43 K44 Q45 E46 R47 E48 G49 G50 V51 Q52 H53 I54 S55 W56 S57 R61 T62 Y63 H64 L65 T66 S67 A68 L72 T73

E74 D75 K78 R87 S91 F92 I93 K94 K95 L96 G97 Q98 K99 S100 G101 P102 S103 S104 G105

4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: 3300001G02Rik protein

Chain A: 34% 32% 7% 27%

G1 S2 S3 G4 S5 S6 G7 M8 T9 V10 C13 K14 M15 D16 G17 E18 V19 V22 V23 V24 V25 Q26 N27 V30 L31 D32 L33 K34 K35 A36 I37 Q38 R39 Y40 K44 Q45 E46 R47 E48 G49 G50 V51 Q52 H53 I54 R61 L65 T66 S67 A68 G69 E70 K71 L72

T73 E74 D75 R76 K77 K78 L79 R80 D81 Y82 G83 I84 R85 S91 F92 L96 G97 Q98 K99 S100 G101 P102 S103 S104 G105

4.2.9 Score per residue for model 9

- Molecule 1: 3300001G02Rik protein

Chain A: 35% 30% 8% 27%

G1 S2 S3 G4 S5 S6 G7 M8 T9 V10 R11 V12 C13 K14 M15 D16 G17 E18 V22 Q26 V30 L31 D32 L33 K34 K35 A36 I37 Q38 R39 Y40 L43 K44 Q45 E46 R47 E48 G49 G50 V51 Q52 H53 I54 W60 R61 T62 Y63 H64 L65 T66 S67 A68 L72 T73

E74 D75 K78 Y82 G83 I84 R85 N86 R87 D88 S91 F92 I93 K94 K95 L96 G97 Q98 K99 S100 G101 P102 S103 S104 G105

4.2.10 Score per residue for model 10

- Molecule 1: 3300001G02Rik protein

Chain A: 40% 26% 8% 27%

G1 S2 S3 G4 S5 S6 G7 M8 T9 V10 M15 D16 G17 E18 V22 V23 V24 V25 Q26 T29 V30 L33 K34 I37 Q38 R39 L43 E46 R47 E48 G49 G50 V51 Q52 H53 I54 S55 W56 S57 R61 T62 Y63 H64 L65 T66 S67 A68 G69 L72 T73 E74

D75 L79 R80 D81 Y82 S91 F92 I93 K94 K95 L96 G97 Q98 K99 S100 G101 P102 S103 S104 G105

4.2.11 Score per residue for model 11

- Molecule 1: 3300001G02Rik protein

Chain A: 34% 30% 10% 27%

G1 S2 S3 G4 S5 S6 G7 M8 T9 V10 K14 M15 D16 G17 E18 V22 V23 V24 V25 Q26 V30 L31 D32 L33 K34 K35 A36 I37 Q38 R39 Y40 V41 Q42 L43 K44 Q45 E46 R47 E48 G49 G50 V51 Q52 H53 I54 S57 W60 R61 L65 T66 S67 A68 G69 E70

K71 L72 T73 E74 D75 R76 K77 K78 N86 R87 D88 S91 F92 K95 L96 G97 Q98 K99 S100 G101 P102 S103 S104 G105

4.2.12 Score per residue for model 12

- Molecule 1: 3300001G02Rik protein

Chain A: 34% 29% 10% 27%

G1 S2 S3 G4 S5 S6 G7 M8 T9 V10 R11 V12 C13 K14 M15 D16 G17 E18 V19 V22 V23 V24 V30 L33 K34 K35 A36 I37 Q38 R39 L43 K44 Q45 E46 R47 E48 G49 G50 V51 Q52 H53 I54 S57 R61 T62 Y63 H64 L65 T66 S67 A68 G69 L72

T73 E74 D75 R76 K77 K78 D81 Y82 G83 I84 R85 D88 E89 V90 S91 F92 I93 K94 K95 L96 G97 Q98 K99 S100 G101 P102 S103 S104 G105

4.2.13 Score per residue for model 13

- Molecule 1: 3300001G02Rik protein

Chain A: 32% 32% 8% • 27%

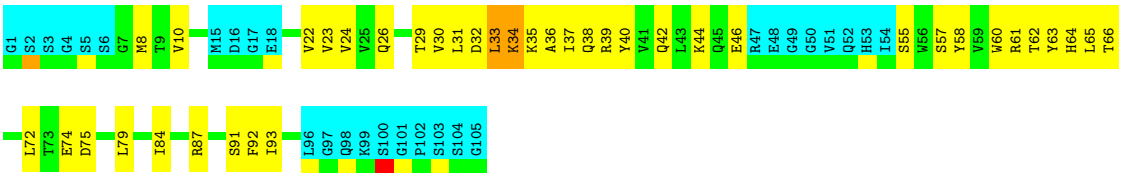
G1 S2 S3 G4 S5 S6 G7 M8 T9 V10 C13 K14 M15 D16 G17 E18 V22 V23 V24 V25 Q26 N27 A28 T29 V30 L33 K34 K35 A36 I37 Q38 R39 L43 K44 Q45 E46 R47 E48 G49 G50 V51 Q52 H53 I54 S55 W56 S57 Y58 V59 W60 R61 T62 Y63 H64 L65 T66

S67 A68 G69 E70 E74 K77 K78 L79 Y82 G83 I84 R87 D88 S91 F92 I93 K94 K95 L96 G97 Q98 K99 S100 G101 P102 S103 S104 G105

4.2.14 Score per residue for model 14

- Molecule 1: 3300001G02Rik protein

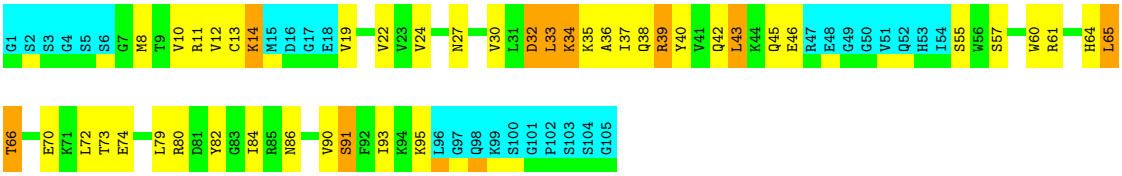
Chain A: 35% 36% • 27%



4.2.15 Score per residue for model 15

- Molecule 1: 3300001G02Rik protein

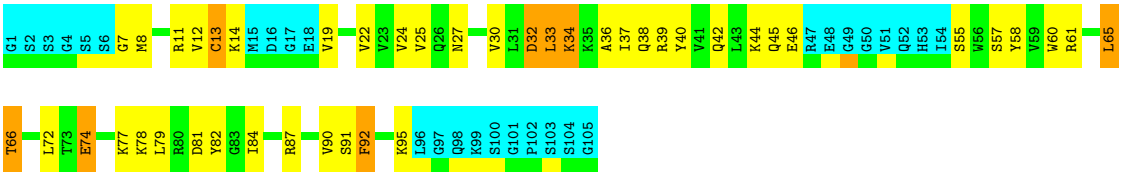
Chain A: 31% 33% 9% 27%



4.2.16 Score per residue for model 16

- Molecule 1: 3300001G02Rik protein

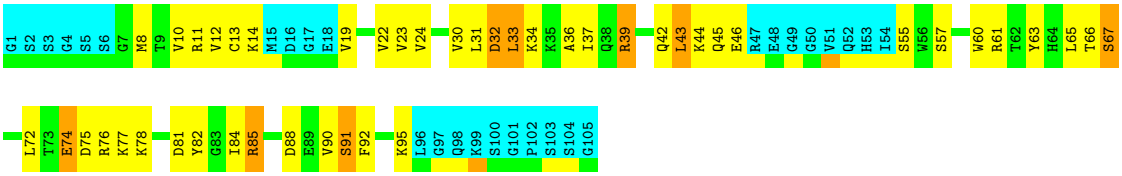
Chain A: 31% 34% 8% 27%



4.2.17 Score per residue for model 17

- Molecule 1: 3300001G02Rik protein

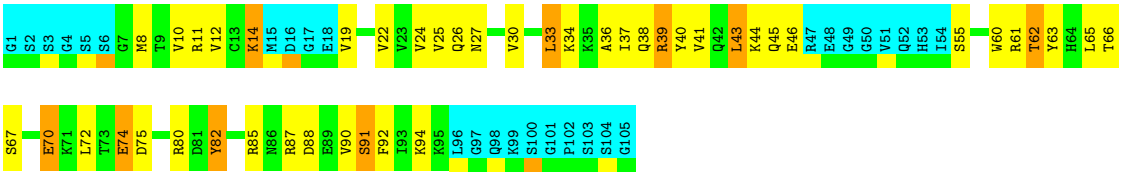
Chain A: 30% 36% 8% 27%



4.2.18 Score per residue for model 18

- Molecule 1: 3300001G02Rik protein

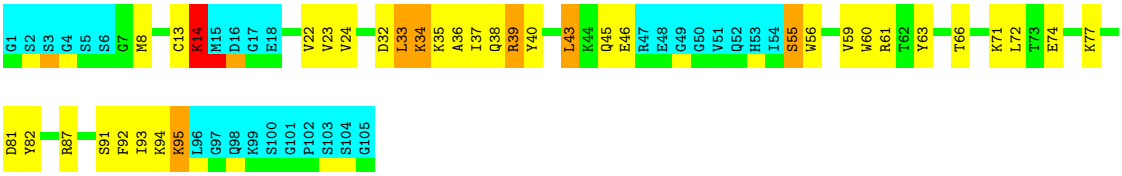
Chain A: 30% 34% 9% 27%



4.2.19 Score per residue for model 19

- Molecule 1: 3300001G02Rik protein

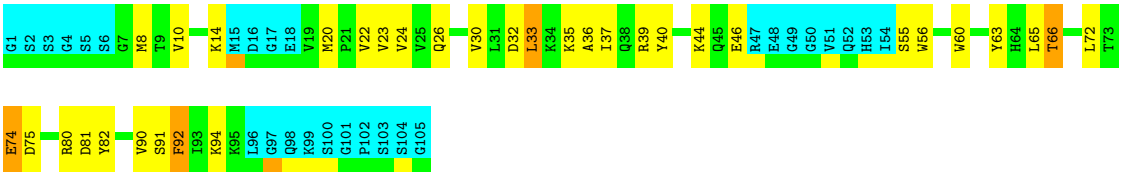
Chain A: 38% 29% 6% • 27%



4.2.20 Score per residue for model 20

- Molecule 1: 3300001G02Rik protein

Chain A: 41% 29% • 27%



5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the least restraint violations,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	639	671	671	30±4
All	All	12780	13420	13420	595

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 23.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ARG:O	1:A:43:LEU:HD23	0.88	1.69	17	14
1:A:72:LEU:HD23	1:A:82:TYR:CD1	0.85	2.05	20	8
1:A:71:LYS:HE3	1:A:93:ILE:HD13	0.83	1.51	19	1
1:A:67:SER:OG	1:A:72:LEU:HD21	0.82	1.73	8	2
1:A:22:VAL:HG21	1:A:37:ILE:HG12	0.77	1.55	12	20
1:A:33:LEU:HD12	1:A:65:LEU:HD13	0.77	1.56	8	10
1:A:71:LYS:CE	1:A:93:ILE:HD13	0.76	2.10	19	1
1:A:31:LEU:HD22	1:A:35:LYS:HE2	0.73	1.60	8	2
1:A:72:LEU:HD21	1:A:84:ILE:HD11	0.72	1.57	16	6
1:A:33:LEU:CD1	1:A:37:ILE:HD11	0.72	2.14	17	19
1:A:12:VAL:HG21	1:A:37:ILE:CD1	0.71	2.15	12	11
1:A:43:LEU:C	1:A:43:LEU:HD12	0.71	2.06	13	13
1:A:67:SER:HG	1:A:72:LEU:HD21	0.70	1.47	7	2
1:A:64:HIS:ND1	1:A:73:THR:HG22	0.69	2.01	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:LEU:HD21	1:A:92:PHE:CZ	0.69	2.23	7	13
1:A:72:LEU:HD23	1:A:82:TYR:CE1	0.69	2.23	12	9
1:A:67:SER:HB3	1:A:72:LEU:HD21	0.69	1.63	11	1
1:A:22:VAL:HG21	1:A:37:ILE:CG1	0.68	2.18	13	19
1:A:72:LEU:CD2	1:A:82:TYR:CD1	0.68	2.76	20	8
1:A:67:SER:OG	1:A:72:LEU:HD11	0.68	1.87	7	2
1:A:12:VAL:HG21	1:A:37:ILE:HD11	0.67	1.66	3	4
1:A:23:VAL:O	1:A:24:VAL:HG13	0.65	1.91	8	12
1:A:22:VAL:CG1	1:A:36:ALA:HB1	0.65	2.21	20	14
1:A:10:VAL:HG11	1:A:33:LEU:HD21	0.65	1.68	20	15
1:A:34:LYS:HG3	1:A:65:LEU:HD21	0.64	1.67	2	2
1:A:67:SER:O	1:A:68:ALA:HB3	0.64	1.92	13	3
1:A:24:VAL:HG12	1:A:32:ASP:OD1	0.64	1.92	14	1
1:A:71:LYS:NZ	1:A:93:ILE:HD13	0.61	2.09	19	1
1:A:65:LEU:HD22	1:A:92:PHE:CE1	0.60	2.32	6	1
1:A:30:VAL:HG12	1:A:34:LYS:HE2	0.60	1.74	17	1
1:A:33:LEU:HD23	1:A:79:LEU:CD1	0.60	2.27	16	2
1:A:84:ILE:HG23	1:A:88:ASP:OD2	0.59	1.97	17	1
1:A:64:HIS:CG	1:A:73:THR:HG22	0.58	2.33	15	1
1:A:31:LEU:HD22	1:A:35:LYS:HE3	0.58	1.75	1	2
1:A:31:LEU:HD12	1:A:75:ASP:CB	0.58	2.29	8	2
1:A:29:THR:C	1:A:79:LEU:HD21	0.58	2.19	10	4
1:A:65:LEU:CD2	1:A:92:PHE:CE1	0.57	2.88	6	9
1:A:67:SER:OG	1:A:84:ILE:HD11	0.57	1.99	8	1
1:A:33:LEU:HD12	1:A:65:LEU:CD1	0.56	2.30	8	2
1:A:33:LEU:HD12	1:A:37:ILE:HD11	0.56	1.74	17	1
1:A:33:LEU:CD1	1:A:37:ILE:CD1	0.56	2.83	6	13
1:A:65:LEU:HD13	1:A:65:LEU:N	0.56	2.15	15	3
1:A:66:THR:HG22	1:A:91:SER:O	0.56	1.99	15	4
1:A:21:PRO:O	1:A:40:TYR:CE2	0.56	2.59	6	2
1:A:62:THR:HG22	1:A:63:TYR:CD2	0.55	2.37	14	3
1:A:65:LEU:CD2	1:A:92:PHE:CZ	0.55	2.90	10	2
1:A:55:SER:O	1:A:59:VAL:HG23	0.54	2.03	19	3
1:A:10:VAL:CG1	1:A:33:LEU:HD21	0.54	2.32	9	5
1:A:58:TYR:CE1	1:A:62:THR:OG1	0.53	2.60	14	1
1:A:67:SER:HB2	1:A:90:VAL:HG22	0.53	1.79	12	2
1:A:33:LEU:HD13	1:A:37:ILE:HD11	0.53	1.80	8	1
1:A:34:LYS:HG3	1:A:65:LEU:HD11	0.53	1.81	10	2
1:A:22:VAL:CG1	1:A:36:ALA:CB	0.52	2.88	12	15
1:A:67:SER:HB3	1:A:72:LEU:HD11	0.52	1.80	17	1
1:A:33:LEU:HD12	1:A:65:LEU:HG	0.52	1.79	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:SER:O	1:A:68:ALA:CB	0.52	2.57	13	2
1:A:72:LEU:CD2	1:A:84:ILE:HD11	0.52	2.35	15	1
1:A:65:LEU:CD1	1:A:92:PHE:CE1	0.52	2.92	2	1
1:A:38:GLN:OE1	1:A:56:TRP:CG	0.52	2.63	19	1
1:A:20:MET:SD	1:A:40:TYR:CE1	0.52	3.03	20	1
1:A:12:VAL:CG1	1:A:12:VAL:O	0.51	2.58	5	1
1:A:12:VAL:CG1	1:A:92:PHE:CE1	0.51	2.93	16	1
1:A:65:LEU:HD21	1:A:92:PHE:CE1	0.51	2.40	9	2
1:A:84:ILE:CG2	1:A:88:ASP:CG	0.51	2.79	13	2
1:A:31:LEU:HD22	1:A:35:LYS:CE	0.51	2.36	7	3
1:A:11:ARG:HB3	1:A:19:VAL:HG13	0.51	1.82	18	1
1:A:31:LEU:HD12	1:A:75:ASP:HB3	0.51	1.81	8	1
1:A:34:LYS:CG	1:A:60:TRP:CZ3	0.50	2.94	11	2
1:A:30:VAL:CG2	1:A:74:GLU:O	0.50	2.60	12	14
1:A:65:LEU:CB	1:A:72:LEU:HD12	0.50	2.36	16	1
1:A:34:LYS:HG2	1:A:60:TRP:CZ3	0.49	2.42	17	7
1:A:80:ARG:CZ	1:A:81:ASP:OD1	0.49	2.60	3	1
1:A:23:VAL:O	1:A:24:VAL:CG1	0.49	2.60	20	6
1:A:66:THR:O	1:A:90:VAL:HG13	0.49	2.08	20	2
1:A:12:VAL:HG13	1:A:92:PHE:CD1	0.49	2.42	16	1
1:A:39:ARG:O	1:A:43:LEU:CD2	0.49	2.60	18	11
1:A:38:GLN:OE1	1:A:56:TRP:CD1	0.49	2.65	19	1
1:A:63:TYR:CE2	1:A:94:LYS:HB2	0.49	2.43	19	1
1:A:63:TYR:CE1	1:A:94:LYS:HG3	0.49	2.43	9	6
1:A:43:LEU:C	1:A:43:LEU:CD1	0.49	2.82	12	6
1:A:72:LEU:CD2	1:A:82:TYR:CG	0.48	2.97	15	2
1:A:34:LYS:HG2	1:A:60:TRP:CE3	0.48	2.44	1	7
1:A:12:VAL:HG13	1:A:92:PHE:CE1	0.48	2.43	16	1
1:A:85:ARG:N	1:A:85:ARG:CD	0.47	2.77	3	1
1:A:40:TYR:C	1:A:40:TYR:CD1	0.47	2.86	15	5
1:A:57:SER:O	1:A:61:ARG:CB	0.47	2.62	6	4
1:A:10:VAL:HG22	1:A:88:ASP:OD1	0.47	2.08	9	2
1:A:30:VAL:HG21	1:A:74:GLU:O	0.47	2.08	12	8
1:A:36:ALA:O	1:A:39:ARG:N	0.47	2.48	15	10
1:A:25:VAL:HG22	1:A:28:ALA:HB2	0.47	1.86	13	2
1:A:58:TYR:C	1:A:58:TYR:CD1	0.47	2.87	16	1
1:A:8:MET:SD	1:A:24:VAL:CG2	0.47	3.03	6	3
1:A:72:LEU:HD21	1:A:84:ILE:CD1	0.47	2.37	9	2
1:A:65:LEU:HD23	1:A:92:PHE:CE1	0.46	2.44	11	4
1:A:12:VAL:HG11	1:A:92:PHE:CE2	0.46	2.45	12	1
1:A:39:ARG:O	1:A:43:LEU:CG	0.46	2.63	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:THR:CG2	1:A:91:SER:O	0.46	2.64	15	1
1:A:8:MET:CG	1:A:24:VAL:HG23	0.46	2.41	2	3
1:A:10:VAL:N	1:A:22:VAL:O	0.46	2.49	15	7
1:A:30:VAL:N	1:A:79:LEU:HD21	0.46	2.26	10	3
1:A:63:TYR:CE1	1:A:94:LYS:HB2	0.46	2.46	10	2
1:A:71:LYS:HE3	1:A:93:ILE:HG21	0.46	1.87	19	1
1:A:61:ARG:O	1:A:61:ARG:CG	0.45	2.64	10	2
1:A:56:TRP:O	1:A:60:TRP:CD1	0.45	2.69	20	1
1:A:56:TRP:HB3	1:A:60:TRP:CD1	0.45	2.46	4	1
1:A:86:ASN:OD1	1:A:87:ARG:N	0.45	2.50	11	1
1:A:12:VAL:CG1	1:A:92:PHE:CD2	0.45	2.99	12	1
1:A:85:ARG:NH1	1:A:88:ASP:CG	0.45	2.70	17	1
1:A:45:GLN:N	1:A:45:GLN:CD	0.45	2.70	18	1
1:A:57:SER:O	1:A:61:ARG:N	0.45	2.50	11	5
1:A:36:ALA:O	1:A:40:TYR:N	0.45	2.50	6	7
1:A:63:TYR:CE2	1:A:94:LYS:HG3	0.45	2.46	7	2
1:A:41:VAL:O	1:A:45:GLN:NE2	0.44	2.50	18	1
1:A:66:THR:OG1	1:A:67:SER:N	0.44	2.51	4	4
1:A:33:LEU:HD13	1:A:37:ILE:CD1	0.44	2.42	5	4
1:A:67:SER:O	1:A:70:GLU:N	0.44	2.50	6	3
1:A:36:ALA:C	1:A:38:GLN:N	0.44	2.70	14	8
1:A:67:SER:O	1:A:69:GLY:N	0.44	2.49	8	5
1:A:25:VAL:HG23	1:A:27:ASN:C	0.44	2.32	18	4
1:A:12:VAL:HG12	1:A:12:VAL:O	0.44	2.12	3	1
1:A:62:THR:HG22	1:A:63:TYR:CD1	0.44	2.47	4	1
1:A:73:THR:OG1	1:A:74:GLU:N	0.44	2.50	9	1
1:A:90:VAL:CG1	1:A:91:SER:N	0.44	2.80	18	3
1:A:30:VAL:HA	1:A:79:LEU:HD21	0.43	1.87	8	2
1:A:32:ASP:O	1:A:36:ALA:N	0.43	2.50	14	1
1:A:32:ASP:O	1:A:33:LEU:C	0.43	2.57	16	12
1:A:65:LEU:O	1:A:72:LEU:CG	0.43	2.67	2	1
1:A:40:TYR:O	1:A:44:LYS:CB	0.43	2.66	8	4
1:A:40:TYR:HD2	1:A:41:VAL:HG23	0.43	1.73	4	1
1:A:77:LYS:HD3	1:A:82:TYR:CE2	0.43	2.49	19	1
1:A:66:THR:HG21	1:A:93:ILE:HB	0.43	1.89	1	3
1:A:13:CYS:O	1:A:14:LYS:C	0.43	2.56	8	7
1:A:72:LEU:CD2	1:A:82:TYR:CE1	0.43	2.98	12	1
1:A:24:VAL:CG1	1:A:32:ASP:OD1	0.43	2.65	14	1
1:A:25:VAL:C	1:A:27:ASN:N	0.43	2.73	16	1
1:A:65:LEU:O	1:A:72:LEU:N	0.42	2.49	7	1
1:A:13:CYS:O	1:A:14:LYS:O	0.42	2.37	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:38:GLN:OE1	1:A:60:TRP:NE1	0.42	2.53	2	2
1:A:58:TYR:O	1:A:61:ARG:N	0.42	2.52	5	1
1:A:34:LYS:CG	1:A:65:LEU:HD21	0.42	2.43	2	1
1:A:13:CYS:N	1:A:90:VAL:O	0.42	2.53	16	1
1:A:33:LEU:O	1:A:36:ALA:HB3	0.42	2.14	19	1
1:A:36:ALA:O	1:A:38:GLN:N	0.42	2.52	15	5
1:A:77:LYS:HG2	1:A:82:TYR:CD2	0.42	2.50	13	1
1:A:11:ARG:O	1:A:90:VAL:N	0.42	2.50	17	2
1:A:7:GLY:CA	1:A:24:VAL:O	0.42	2.68	16	1
1:A:65:LEU:HB2	1:A:72:LEU:HD12	0.42	1.92	16	1
1:A:10:VAL:CB	1:A:33:LEU:HD21	0.42	2.44	17	1
1:A:40:TYR:CD1	1:A:40:TYR:C	0.41	2.93	18	3
1:A:66:THR:O	1:A:67:SER:CB	0.41	2.68	2	1
1:A:86:ASN:OD1	1:A:86:ASN:C	0.41	2.59	1	2
1:A:86:ASN:O	1:A:87:ARG:C	0.41	2.58	9	1
1:A:71:LYS:NZ	1:A:93:ILE:CD1	0.41	2.83	19	1
1:A:72:LEU:HD22	1:A:82:TYR:CG	0.41	2.51	4	1
1:A:31:LEU:CD1	1:A:75:ASP:HB3	0.41	2.45	8	1
1:A:11:ARG:HB3	1:A:19:VAL:HG11	0.41	1.91	16	1
1:A:65:LEU:O	1:A:72:LEU:CB	0.41	2.69	6	1
1:A:36:ALA:O	1:A:37:ILE:C	0.41	2.59	13	9
1:A:45:GLN:O	1:A:46:GLU:C	0.40	2.60	9	1
1:A:34:LYS:HG3	1:A:60:TRP:CZ3	0.40	2.51	1	1
1:A:25:VAL:O	1:A:28:ALA:N	0.40	2.55	2	1
1:A:8:MET:SD	1:A:25:VAL:O	0.40	2.80	5	2
1:A:67:SER:O	1:A:68:ALA:C	0.40	2.59	11	1
1:A:40:TYR:CD2	1:A:41:VAL:HG23	0.40	2.50	4	1
1:A:25:VAL:CG2	1:A:28:ALA:HB2	0.40	2.45	7	1
1:A:64:HIS:HB2	1:A:93:ILE:HG23	0.40	1.92	14	1
1:A:34:LYS:HG2	1:A:65:LEU:HD11	0.40	1.93	17	1
1:A:43:LEU:O	1:A:44:LYS:C	0.40	2.59	5	1
1:A:77:LYS:HG2	1:A:82:TYR:CE2	0.40	2.51	16	1
1:A:10:VAL:HB	1:A:33:LEU:HD21	0.40	1.92	17	1
1:A:31:LEU:O	1:A:32:ASP:C	0.40	2.59	17	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	77/105 (73%)	60±3 (77±4%)	15±3 (20±4%)	2±1 (3±1%)	8 43
All	All	1540/2100 (73%)	1190 (77%)	309 (20%)	41 (3%)	8 43

All 8 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	LYS	13
1	A	95	LYS	9
1	A	67	SER	6
1	A	69	GLY	5
1	A	62	THR	4
1	A	19	VAL	2
1	A	68	ALA	1
1	A	86	ASN	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	71/91 (78%)	54±2 (75±3%)	18±2 (25±3%)	2 25
All	All	1420/1820 (78%)	1070 (75%)	350 (25%)	2 25

All 42 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	33	LEU	20
1	A	46	GLU	20
1	A	91	SER	20
1	A	61	ARG	19
1	A	74	GLU	18
1	A	75	ASP	15
1	A	34	LYS	14
1	A	39	ARG	14

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Mol	Chain	Res	Type	Models (Total)
1	A	43	LEU	14
1	A	66	THR	14
1	A	8	MET	14
1	A	26	GLN	13
1	A	55	SER	13
1	A	92	PHE	11
1	A	81	ASP	10
1	A	78	LYS	10
1	A	80	ARG	9
1	A	70	GLU	9
1	A	35	LYS	8
1	A	82	TYR	8
1	A	87	ARG	8
1	A	85	ARG	7
1	A	44	LYS	7
1	A	32	ASP	6
1	A	42	GLN	6
1	A	57	SER	6
1	A	76	ARG	5
1	A	67	SER	5
1	A	88	ASP	4
1	A	19	VAL	4
1	A	65	LEU	3
1	A	94	LYS	2
1	A	31	LEU	2
1	A	14	LYS	2
1	A	24	VAL	2
1	A	95	LYS	2
1	A	12	VAL	1
1	A	11	ARG	1
1	A	71	LYS	1
1	A	27	ASN	1
1	A	13	CYS	1
1	A	77	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 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