Full wwPDB NMR Structure Validation Report (i)

Feb 27, 2022 – 09:29 PM EST

PDB ID	:	2DGY
Title	:	Solution structure of the eukaryotic initiation factor 1A in MGC11102 protein
Authors	:	Abe, C.; Muto, Y.; Inoue, M.; Kigawa, T.; Terada, T.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2006-03-16

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:

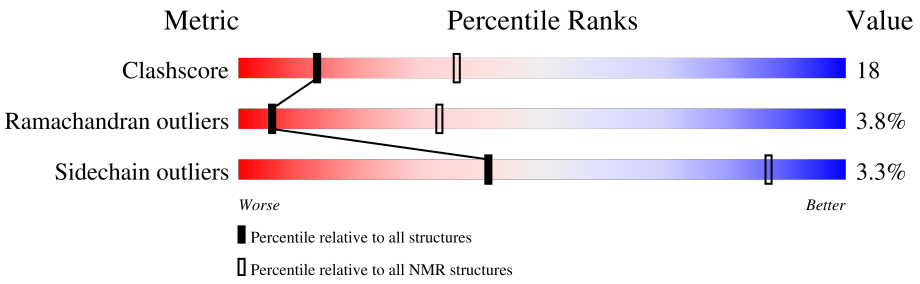
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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	111	50% 31% 19%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 11 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:19-A:108 (90)	0.20	11

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 5 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1734 atoms, of which 862 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called MGC11102 protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	111	1734	546	862	158	166	2	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	GLY	-	cloning artifact	UNP Q9BSC1
A	11	SER	-	cloning artifact	UNP Q9BSC1
A	12	SER	-	cloning artifact	UNP Q9BSC1
A	13	GLY	-	cloning artifact	UNP Q9BSC1
A	14	SER	-	cloning artifact	UNP Q9BSC1
A	15	SER	-	cloning artifact	UNP Q9BSC1
A	16	GLY	-	cloning artifact	UNP Q9BSC1
A	115	SER	-	cloning artifact	UNP Q9BSC1
A	116	GLY	-	cloning artifact	UNP Q9BSC1
A	117	PRO	-	cloning artifact	UNP Q9BSC1
A	118	SER	-	cloning artifact	UNP Q9BSC1
A	119	SER	-	cloning artifact	UNP Q9BSC1
A	120	GLY	-	cloning artifact	UNP Q9BSC1

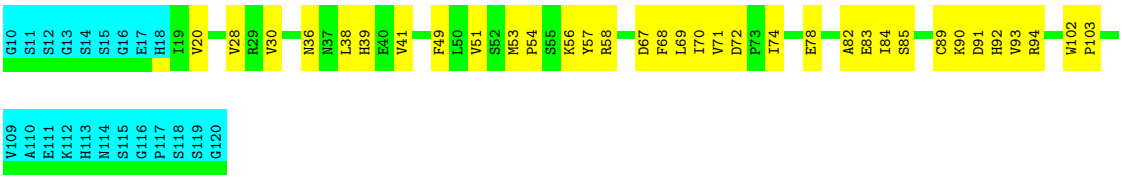
4 Residue-property plots (i)

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: MGC11102 protein

Chain A: 50% 31% 19%



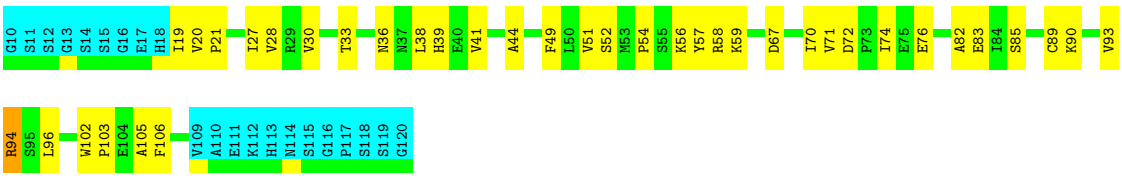
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: MGC11102 protein

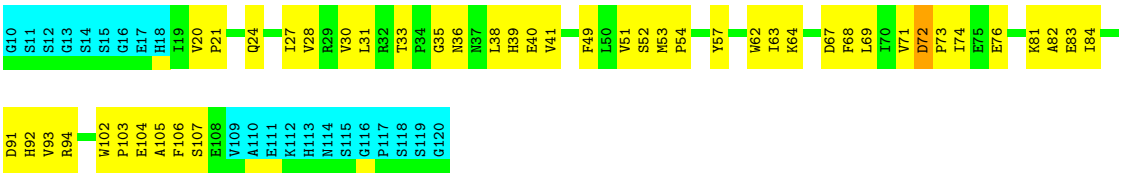
Chain A: 47% 33% • 19%



4.2.2 Score per residue for model 2

• Molecule 1: MGC11102 protein

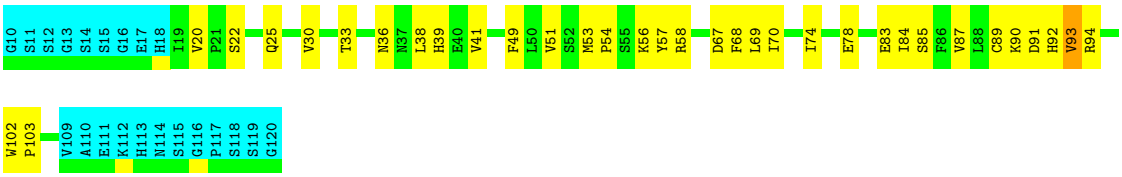
Chain A: 41% 40% • 19%



4.2.3 Score per residue for model 3

- Molecule 1: MGC11102 protein

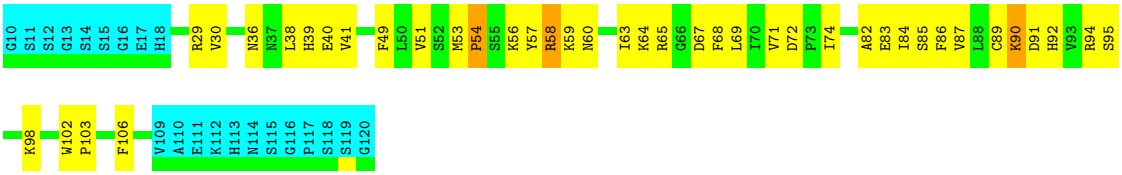
Chain A: 50% 30% • 19%



4.2.4 Score per residue for model 4

- Molecule 1: MGC11102 protein

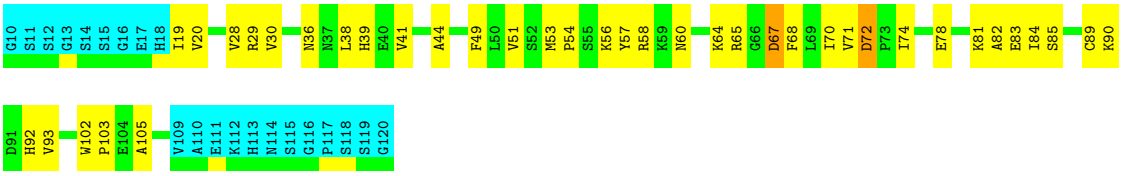
Chain A: 44% 34% • 19%



4.2.5 Score per residue for model 5

- Molecule 1: MGC11102 protein

Chain A: 46% 33% • 19%



4.2.6 Score per residue for model 6

- Molecule 1: MGC11102 protein

Chain A: 51% 29% • 19%

G10 S11 S12 G13 S14 S15 G16 E17 H18 V28 R29 V30 T33 N36 N37 L38 H39 E40 V41 E42 F49 L50 V51 S52 M53 P54 S55 K56 Y57 D67 F68 L69 D72 P73 I74 E78 K79 V80 K81 A82 E83 I84 L88 C89 K90 D91 H92 V93 W102 P103

V109 A110 E111 K112 H113 N114 S115 G116 P117 S118 S119 G120

4.2.7 Score per residue for model 7

- Molecule 1: MGC11102 protein

Chain A: 46% 33% • 19%

G10 S11 S12 G13 S14 S15 G16 E17 H18 I19 V20 V30 L31 R32 T33 N36 N37 L38 H39 E40 V41 E42 R48 F49 L50 V51 S52 M53 P54 S55 K56 Y57 R58 K59 R65 G66 D67 F68 L69 I70 V71 D72 P73 I74 K79 A82 E83 I84 S85 F86 D91 H92 V93

R94 W102 P103 V109 A110 E111 K112 H113 N114 S115 G116 P117 S118 S119 G120

4.2.8 Score per residue for model 8

- Molecule 1: MGC11102 protein

Chain A: 46% 35% 19%

G10 S11 S12 G13 S14 S15 G16 E17 H18 I19 V20 P21 S22 N23 Q24 I27 V28 R29 V30 L31 R32 T33 P34 G35 N36 N37 L38 H39 E40 V41 M53 P54 S55 K56 Y57 R58 K59 N60 I63 K64 F68 L69 I70 V71 D72 P73 I74 E78 A82 E83 I84 S85 F86 V87

V93 F101 W102 P103 V109 A110 E111 K112 H113 N114 S115 G116 P117 S118 S119 G120

4.2.9 Score per residue for model 9

- Molecule 1: MGC11102 protein

Chain A: 41% 39% • 19%

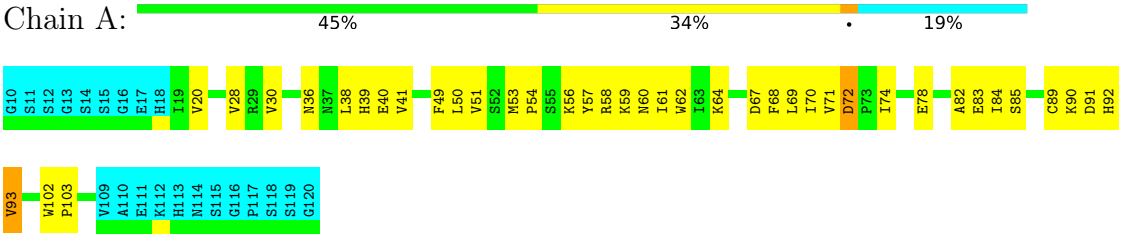
G10 S11 S12 G13 S14 S15 G16 E17 H18 I19 V20 P21 Q24 I27 V28 R29 V30 N36 N37 L38 H39 E40 V41 A44 F49 L50 V51 S52 M53 Y57 R58 K59 I63 F68 L69 I70 V71 D72 P73 I74 E75 E76 K79 A82 E83 I84 S85 F86 V87 L88

C89 K90 D91 H92 V93 R94 S95 L96 W102 P103 E104 A105 V109 A110 E111 K112 H113 N114 S115 G116 P117 S118 S119 G120

4.2.10 Score per residue for model 10

- Molecule 1: MGC11102 protein

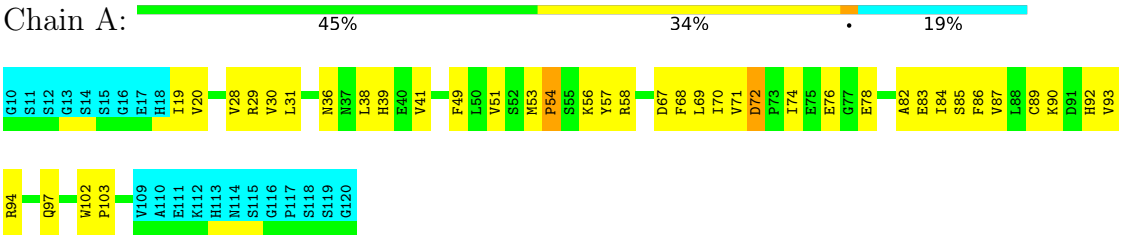
Chain A:



4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: MGC11102 protein

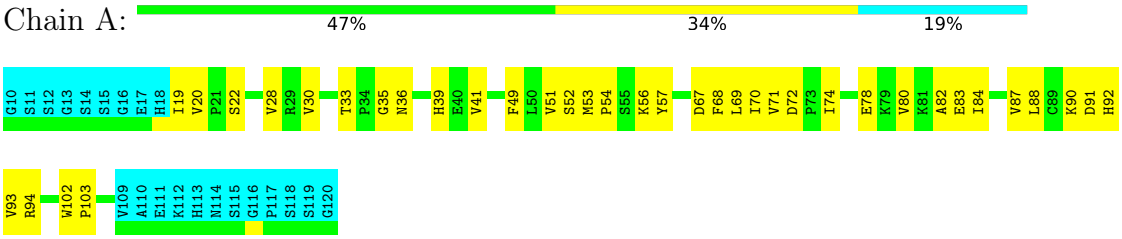
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: MGC11102 protein

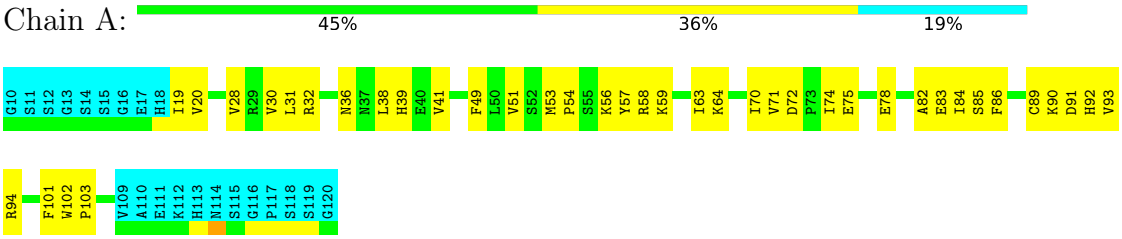
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: MGC11102 protein

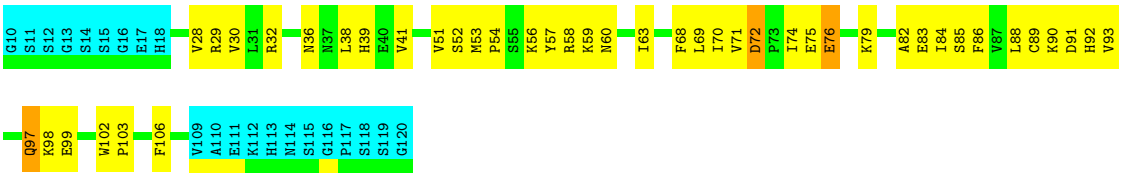
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: MGC11102 protein

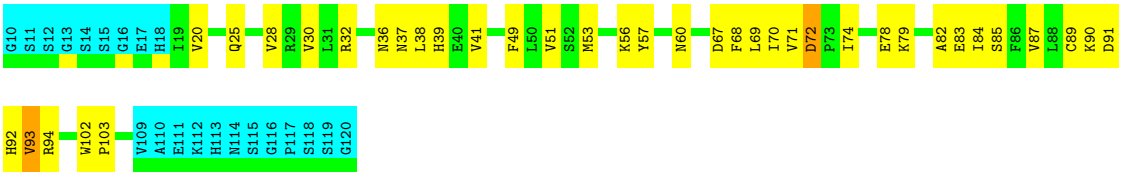
Chain A: 41% 37% • 19%



4.2.15 Score per residue for model 15

- Molecule 1: MGC11102 protein

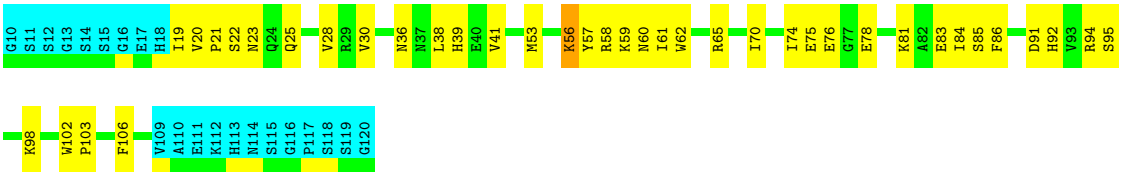
Chain A: 47% 32% • 19%



4.2.16 Score per residue for model 16

- Molecule 1: MGC11102 protein

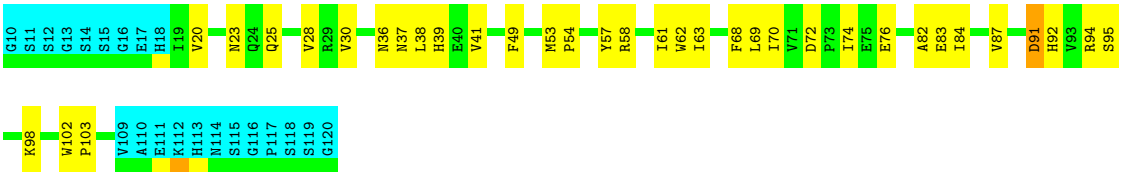
Chain A: 46% 34% • 19%



4.2.17 Score per residue for model 17

- Molecule 1: MGC11102 protein

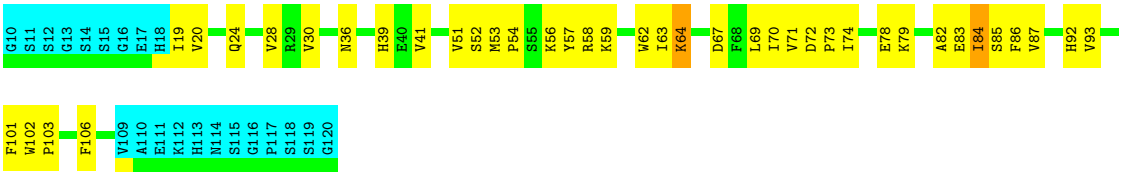
Chain A: 50% 31% • 19%



4.2.18 Score per residue for model 18

- Molecule 1: MGC11102 protein

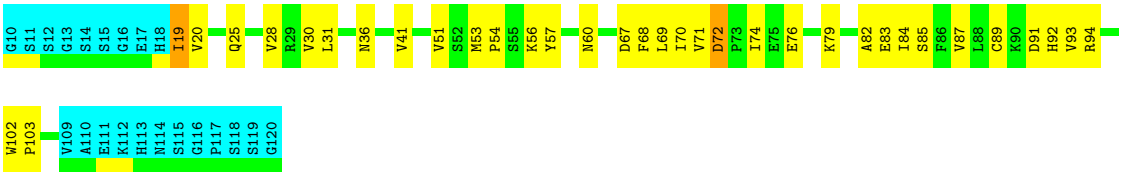
Chain A: 45% 34% • 19%



4.2.19 Score per residue for model 19

- Molecule 1: MGC11102 protein

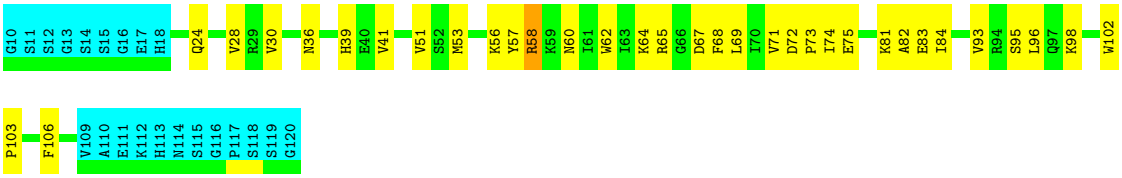
Chain A: 50% 30% • 19%



4.2.20 Score per residue for model 20

- Molecule 1: MGC11102 protein

Chain A: 50% 30% • 19%



5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *target function, structures with the lowest energy, structures with the least restraint violations.*

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	736	744	742	27±5
All	All	14720	14880	14840	547

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 19.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:VAL:HG21	1:A:41:VAL:HG21	0.95	1.37	14	17
1:A:74:ILE:HD11	1:A:83:GLU:CG	0.88	1.98	17	18
1:A:74:ILE:HD11	1:A:83:GLU:HG3	0.82	1.50	11	20
1:A:68:PHE:O	1:A:69:LEU:HD23	0.81	1.75	20	13
1:A:51:VAL:HG11	1:A:71:VAL:HG11	0.79	1.53	20	15
1:A:53:MET:SD	1:A:84:ILE:HD12	0.77	2.19	9	19
1:A:93:VAL:HG13	1:A:102:TRP:CZ3	0.73	2.19	1	2
1:A:41:VAL:HG23	1:A:49:PHE:CE1	0.69	2.22	13	7
1:A:41:VAL:HG23	1:A:49:PHE:CZ	0.69	2.23	3	11
1:A:74:ILE:HD11	1:A:83:GLU:HG2	0.69	1.62	17	1
1:A:30:VAL:HA	1:A:41:VAL:HG12	0.67	1.65	7	13
1:A:39:HIS:O	1:A:51:VAL:HG22	0.66	1.89	14	12
1:A:93:VAL:HG13	1:A:102:TRP:CH2	0.65	2.27	1	4
1:A:30:VAL:HG23	1:A:67:ASP:O	0.65	1.92	5	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:VAL:CG2	1:A:41:VAL:HG21	0.62	2.19	14	3
1:A:41:VAL:CG2	1:A:49:PHE:CZ	0.62	2.83	13	6
1:A:39:HIS:CE1	1:A:63:ILE:HD13	0.61	2.31	18	1
1:A:39:HIS:CE1	1:A:63:ILE:HD12	0.61	2.31	4	6
1:A:93:VAL:HG22	1:A:102:TRP:CZ3	0.60	2.32	2	3
1:A:39:HIS:CE1	1:A:63:ILE:CD1	0.58	2.86	18	6
1:A:62:TRP:CZ2	1:A:64:LYS:NZ	0.58	2.72	18	1
1:A:93:VAL:HG22	1:A:102:TRP:CH2	0.57	2.35	2	4
1:A:38:LEU:O	1:A:39:HIS:CD2	0.56	2.58	7	11
1:A:38:LEU:C	1:A:39:HIS:CD2	0.56	2.80	6	16
1:A:72:ASP:O	1:A:82:ALA:HB1	0.55	2.02	1	8
1:A:21:PRO:CG	1:A:27:ILE:HD11	0.55	2.30	2	2
1:A:51:VAL:HG11	1:A:71:VAL:CG1	0.55	2.28	20	1
1:A:38:LEU:HD23	1:A:52:SER:HA	0.55	1.78	14	5
1:A:74:ILE:HD11	1:A:83:GLU:CD	0.55	2.21	6	8
1:A:88:LEU:HD23	1:A:92:HIS:CE1	0.55	2.37	6	2
1:A:85:SER:O	1:A:86:PHE:CD2	0.55	2.60	18	2
1:A:72:ASP:C	1:A:82:ALA:HB1	0.54	2.22	1	18
1:A:85:SER:O	1:A:86:PHE:CG	0.54	2.60	16	7
1:A:44:ALA:O	1:A:105:ALA:HB2	0.54	2.03	1	1
1:A:27:ILE:HD11	1:A:96:LEU:HD13	0.54	1.80	9	2
1:A:103:PRO:HG2	1:A:106:PHE:CD2	0.53	2.38	2	4
1:A:52:SER:OG	1:A:80:VAL:HG21	0.53	2.02	6	2
1:A:56:LYS:HG3	1:A:57:TYR:CD1	0.52	2.39	16	16
1:A:74:ILE:CD1	1:A:83:GLU:CG	0.52	2.83	17	1
1:A:72:ASP:N	1:A:72:ASP:OD1	0.52	2.43	10	2
1:A:37:ASN:O	1:A:38:LEU:HD23	0.52	2.05	15	2
1:A:22:SER:H	1:A:25:GLN:NE2	0.52	2.03	16	1
1:A:21:PRO:HG2	1:A:27:ILE:HD11	0.52	1.82	2	2
1:A:103:PRO:CG	1:A:106:PHE:CD2	0.51	2.94	2	2
1:A:33:THR:HG22	1:A:35:GLY:H	0.51	1.66	2	3
1:A:39:HIS:CE1	1:A:63:ILE:HG21	0.51	2.41	17	1
1:A:72:ASP:O	1:A:82:ALA:CB	0.50	2.59	1	7
1:A:70:ILE:O	1:A:85:SER:N	0.50	2.45	14	14
1:A:69:LEU:HD22	1:A:87:VAL:HA	0.50	1.84	12	10
1:A:57:TYR:O	1:A:59:LYS:N	0.49	2.45	4	10
1:A:68:PHE:C	1:A:69:LEU:HD23	0.49	2.27	9	1
1:A:84:ILE:HG22	1:A:85:SER:N	0.49	2.23	5	4
1:A:85:SER:O	1:A:86:PHE:CD1	0.49	2.66	13	1
1:A:39:HIS:ND1	1:A:63:ILE:HG21	0.49	2.22	17	1
1:A:28:VAL:HG11	1:A:49:PHE:CZ	0.49	2.43	17	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:LEU:CD2	1:A:92:HIS:CE1	0.49	2.94	6	1
1:A:33:THR:HG23	1:A:38:LEU:O	0.48	2.08	3	4
1:A:56:LYS:HD2	1:A:57:TYR:CE1	0.48	2.43	16	1
1:A:89:CYS:O	1:A:93:VAL:HG23	0.47	2.10	19	1
1:A:20:VAL:HG13	1:A:21:PRO:HD2	0.47	1.84	1	3
1:A:24:GLN:O	1:A:73:PRO:CD	0.47	2.62	9	4
1:A:31:LEU:HD12	1:A:40:GLU:HG2	0.47	1.86	2	1
1:A:31:LEU:HD11	1:A:42:GLU:HB3	0.47	1.85	7	1
1:A:91:ASP:O	1:A:94:ARG:N	0.47	2.47	7	7
1:A:54:PRO:HG2	1:A:57:TYR:CD2	0.47	2.45	13	15
1:A:95:SER:O	1:A:98:LYS:N	0.47	2.48	4	3
1:A:44:ALA:HA	1:A:105:ALA:HB3	0.46	1.87	5	3
1:A:28:VAL:HG21	1:A:41:VAL:CG2	0.46	2.35	1	3
1:A:106:PHE:N	1:A:106:PHE:CD1	0.46	2.81	2	1
1:A:56:LYS:HG3	1:A:57:TYR:CE1	0.45	2.46	6	2
1:A:62:TRP:C	1:A:62:TRP:CD1	0.45	2.88	18	1
1:A:62:TRP:CZ2	1:A:64:LYS:HE2	0.45	2.46	10	2
1:A:30:VAL:HG12	1:A:31:LEU:N	0.45	2.27	11	4
1:A:85:SER:C	1:A:86:PHE:CD1	0.45	2.90	13	1
1:A:91:ASP:O	1:A:92:HIS:C	0.45	2.55	13	12
1:A:68:PHE:CE1	1:A:106:PHE:HB3	0.45	2.46	4	1
1:A:89:CYS:O	1:A:90:LYS:C	0.45	2.55	13	11
1:A:92:HIS:O	1:A:93:VAL:C	0.45	2.55	10	7
1:A:84:ILE:CG2	1:A:85:SER:N	0.45	2.80	18	4
1:A:40:GLU:OE2	1:A:49:PHE:C	0.45	2.55	4	2
1:A:102:TRP:CG	1:A:103:PRO:HD2	0.44	2.47	19	14
1:A:56:LYS:HE2	1:A:57:TYR:CE1	0.44	2.47	6	1
1:A:104:GLU:O	1:A:106:PHE:N	0.44	2.51	2	1
1:A:22:SER:CB	1:A:25:GLN:OE1	0.44	2.65	3	1
1:A:23:ASN:OD1	1:A:23:ASN:C	0.44	2.56	16	1
1:A:104:GLU:O	1:A:107:SER:N	0.44	2.50	2	1
1:A:29:ARG:HB2	1:A:68:PHE:CD1	0.44	2.48	5	1
1:A:93:VAL:HG12	1:A:97:GLN:HG3	0.44	1.90	14	1
1:A:93:VAL:O	1:A:94:ARG:C	0.43	2.57	15	1
1:A:29:ARG:NH2	1:A:65:ARG:NH2	0.43	2.67	4	1
1:A:29:ARG:HB2	1:A:68:PHE:CE1	0.43	2.48	5	2
1:A:61:ILE:CG2	1:A:62:TRP:N	0.43	2.81	10	3
1:A:25:GLN:HE21	1:A:70:ILE:HG21	0.43	1.74	17	3
1:A:58:ARG:CZ	1:A:58:ARG:HB3	0.42	2.44	3	1
1:A:30:VAL:CG1	1:A:31:LEU:N	0.42	2.82	8	1
1:A:28:VAL:HG11	1:A:49:PHE:HZ	0.42	1.71	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:21:PRO:HG2	1:A:27:ILE:CD1	0.42	2.45	8	1
1:A:72:ASP:C	1:A:82:ALA:CB	0.42	2.88	1	1
1:A:101:PHE:O	1:A:102:TRP:C	0.42	2.58	18	2
1:A:75:GLU:O	1:A:76:GLU:C	0.42	2.57	16	3
1:A:69:LEU:CD2	1:A:87:VAL:HG13	0.42	2.44	4	1
1:A:20:VAL:HG11	1:A:101:PHE:CE2	0.42	2.49	8	1
1:A:53:MET:SD	1:A:84:ILE:CD1	0.42	3.06	17	2
1:A:27:ILE:CD1	1:A:96:LEU:HD13	0.42	2.43	1	1
1:A:102:TRP:CD2	1:A:103:PRO:HD2	0.42	2.50	19	12
1:A:81:LYS:N	1:A:81:LYS:HE2	0.41	2.29	2	1
1:A:89:CYS:O	1:A:92:HIS:N	0.41	2.53	6	1
1:A:54:PRO:HB2	1:A:57:TYR:CG	0.41	2.50	12	1
1:A:63:ILE:O	1:A:64:LYS:CE	0.41	2.69	4	2
1:A:31:LEU:HD13	1:A:48:ARG:HD3	0.41	1.92	7	1
1:A:62:TRP:NE1	1:A:64:LYS:CG	0.41	2.84	18	1
1:A:95:SER:O	1:A:96:LEU:C	0.41	2.58	20	1
1:A:90:LYS:O	1:A:94:ARG:CD	0.41	2.69	1	1
1:A:62:TRP:CZ2	1:A:64:LYS:HE3	0.41	2.51	20	1
1:A:98:LYS:HG3	1:A:99:GLU:N	0.41	2.31	14	1
1:A:29:ARG:NH1	1:A:42:GLU:OE2	0.41	2.53	6	1
1:A:28:VAL:CG2	1:A:41:VAL:CG2	0.41	2.97	14	1
1:A:64:LYS:N	1:A:64:LYS:HD3	0.41	2.30	18	1
1:A:74:ILE:HG22	1:A:75:GLU:N	0.41	2.31	20	1
1:A:20:VAL:CG1	1:A:21:PRO:HD2	0.41	2.46	16	2
1:A:19:ILE:HB	1:A:92:HIS:CE1	0.41	2.51	5	1
1:A:21:PRO:HD3	1:A:96:LEU:HD21	0.41	1.91	9	1
1:A:40:GLU:OE1	1:A:50:LEU:HD21	0.41	2.16	10	1
1:A:88:LEU:HD23	1:A:92:HIS:ND1	0.40	2.30	6	1
1:A:70:ILE:O	1:A:85:SER:CB	0.40	2.69	9	1
1:A:29:ARG:HB2	1:A:68:PHE:CE2	0.40	2.51	11	1
1:A:70:ILE:HD11	1:A:88:LEU:HD21	0.40	1.92	12	1
1:A:93:VAL:HG13	1:A:102:TRP:CZ2	0.40	2.51	20	3
1:A:72:ASP:OD1	1:A:73:PRO:O	0.40	2.40	8	1
1:A:32:ARG:CZ	1:A:32:ARG:HB3	0.40	2.47	15	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	90/111 (81%)	71±2 (79±3%)	15±2 (17±2%)	3±1 (4±1%)	5 33
All	All	1800/2220 (81%)	1424 (79%)	308 (17%)	68 (4%)	5 33

All 12 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	36	ASN	20
1	A	58	ARG	13
1	A	78	GLU	10
1	A	60	ASN	6
1	A	76	GLU	5
1	A	54	PRO	4
1	A	19	ILE	3
1	A	93	VAL	3
1	A	105	ALA	1
1	A	22	SER	1
1	A	75	GLU	1
1	A	84	ILE	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	82/97 (85%)	79±1 (97±1%)	3±1 (3±1%)	41 87
All	All	1640/1940 (85%)	1586 (97%)	54 (3%)	41 87

All 20 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	72	ASP	9
1	A	79	LYS	6
1	A	94	ARG	5
1	A	65	ARG	4

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Mol	Chain	Res	Type	Models (Total)
1	A	58	ARG	3
1	A	60	ASN	3
1	A	64	LYS	3
1	A	81	LYS	3
1	A	90	LYS	2
1	A	67	ASP	2
1	A	23	ASN	2
1	A	56	LYS	2
1	A	91	ASP	2
1	A	32	ARG	2
1	A	76	GLU	1
1	A	24	GLN	1
1	A	78	GLU	1
1	A	97	GLN	1
1	A	52	SER	1
1	A	98	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