Full wwPDB NMR Structure Validation Report (i)

Feb 22, 2022 – 11:40 AM EST

PDB ID	:	1WIS
Title	:	Solution structure of the fifth FNIII domain from human KIAA1514 protein
Authors	:	Suetake, T.; Hayashi, F.; 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 (i) symbol.

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

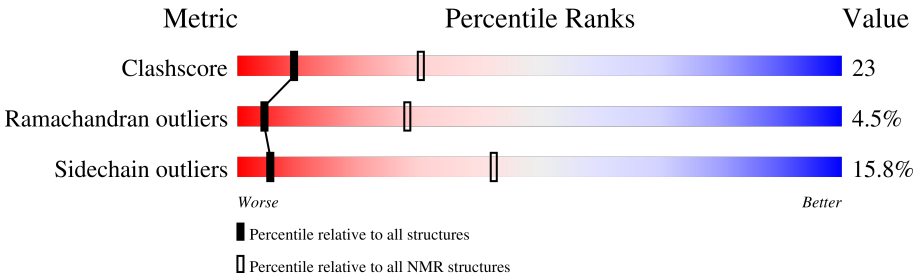
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	124	45% 34% • 18%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 16 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:13-A:60, A:65-A:118 (102)	0.20	16

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 5 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1830 atoms, of which 906 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called KIAA1514 protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	124	1830	574	906	163	184	3	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	GB 7959295
A	2	SER	-	cloning artifact	GB 7959295
A	3	SER	-	cloning artifact	GB 7959295
A	4	GLY	-	cloning artifact	GB 7959295
A	5	SER	-	cloning artifact	GB 7959295
A	6	SER	-	cloning artifact	GB 7959295
A	7	GLY	-	cloning artifact	GB 7959295
A	119	SER	-	cloning artifact	GB 7959295
A	120	GLY	-	cloning artifact	GB 7959295
A	121	PRO	-	cloning artifact	GB 7959295
A	122	SER	-	cloning artifact	GB 7959295
A	123	SER	-	cloning artifact	GB 7959295
A	124	GLY	-	cloning artifact	GB 7959295

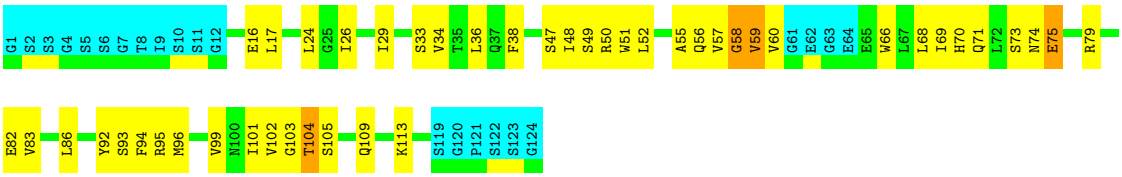
4 Residue-property plots (i)

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: KIAA1514 protein

Chain A: 45% 34% • 18%



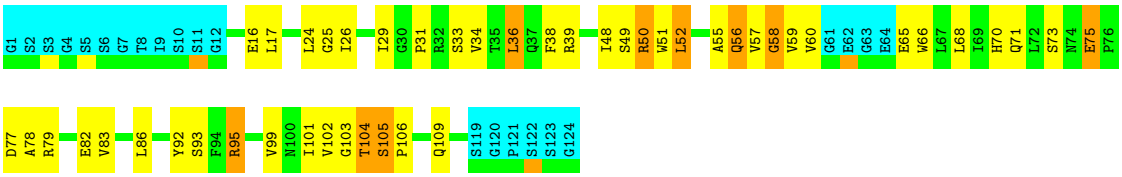
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: KIAA1514 protein

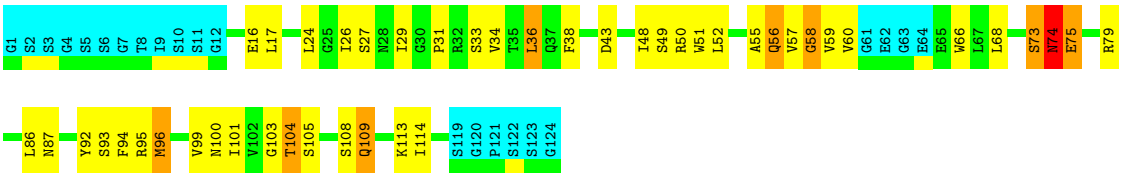
Chain A: 44% 31% 7% 18%



4.2.2 Score per residue for model 2

• Molecule 1: KIAA1514 protein

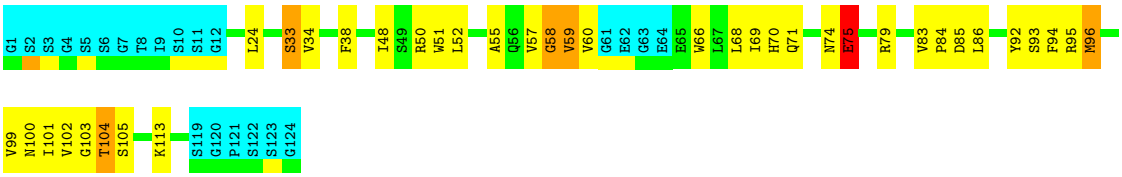
Chain A: 45% 30% 6% • 18%



4.2.3 Score per residue for model 3

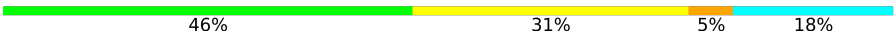
- Molecule 1: KIAA1514 protein

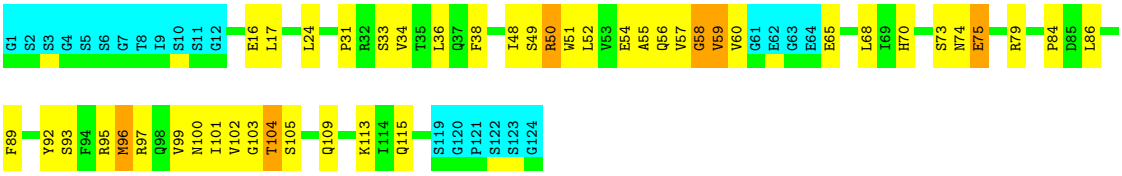
Chain A:



4.2.4 Score per residue for model 4

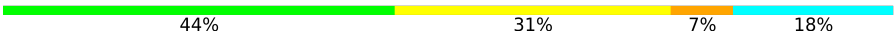
- Molecule 1: KIAA1514 protein

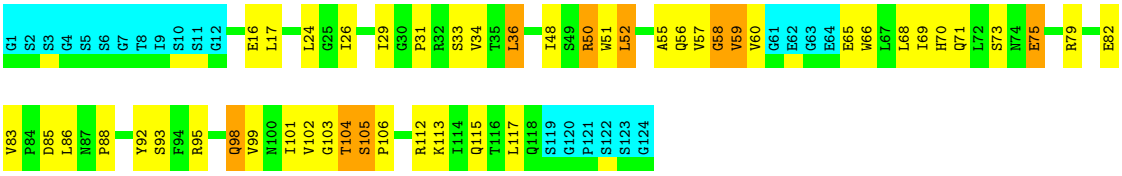
Chain A: 



4.2.5 Score per residue for model 5

- Molecule 1: KIAA1514 protein

Chain A: 



4.2.6 Score per residue for model 6

- Molecule 1: KIAA1514 protein

Chain A: 44% 32% 6% 18%

G1 S2 S3 G4 S5 S6 G7 T8 I9 S10 S11 G12 E16 L17 L24 R32 S33 V34 T35 L36 Q37 F38 G41 Y42 D43 T46 S47 I48 S49 R50 W51 L52 V53 E54 A55 Q56 V57 G58 V59 V60 G61 E62 G63 E64 L68 I69 H70 Q71 L72 S73 N74 E75 P76 D77

A78 R79 E82 V83 L86 Y92 S93 F94 R95 M96 R97 Q98 V99 N100 I101 V102 G103 T104 Q109 K113 I114 Q115 S119 G120 P121 S122 S123 G124

4.2.7 Score per residue for model 7

- Molecule 1: KIAA1514 protein

Chain A: 42% 35% • • 18%

G1 S2 S3 G4 S5 S6 G7 T8 I9 S10 S11 G12 E16 L24 G25 I26 I29 G30 S33 V34 T35 L36 Q37 F38 I48 S49 R50 W51 L52 A55 Q56 V57 G58 V59 V60 G61 E62 G63 E64 E65 W66 L67 L68 I69 H70 Q71 L72 S73 N74 E75 A78 R79 S80

M81 E82 V83 P84 D85 L86 N87 P88 Y92 S93 F94 R95 M96 V99 N100 I101 V102 G103 T104 S105 P106 P107 S108 Q109 L117 Q118 S119 G120 P121 S122 S123 G124

4.2.8 Score per residue for model 8

- Molecule 1: KIAA1514 protein

Chain A: 48% 29% 6% 18%

G1 S2 S3 G4 S5 S6 G7 T8 I9 S10 S11 G12 P15 E16 L24 G25 I26 I29 G30 S33 V34 T35 L36 Q37 F38 I48 S49 R50 W51 L52 A55 Q56 V57 G58 V59 V60 G61 E62 G63 E64 E65 W66 L67 L68 I69 H70 Q71 L72 S73 N74 E75 A78

E82 V83 P84 D85 L86 N87 P88 F89 Y92 S93 F94 R95 M96 I101 V102 G103 T104 Q109 K113 S119 G120 P121 S122 S123 G124

4.2.9 Score per residue for model 9

- Molecule 1: KIAA1514 protein

Chain A: 46% 31% 6% 18%

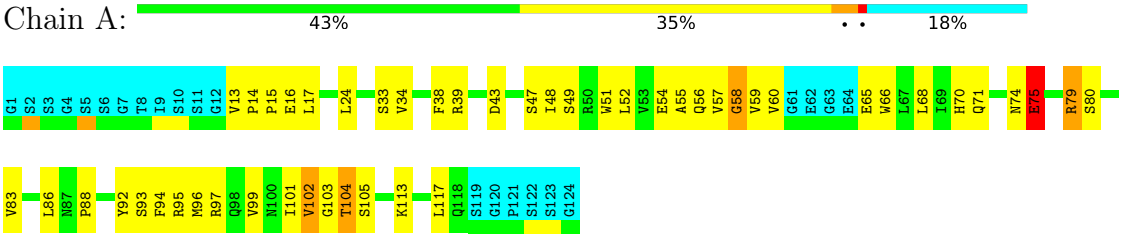
G1 S2 S3 G4 S5 S6 G7 T8 I9 S10 S11 G12 P15 E16 L17 L24 G25 I26 P31 R32 S33 V34 T35 L36 I48 S49 R50 W51 L52 A55 Q56 V57 G58 V59 V60 G61 E62 G63 E64 E65 W66 L67 L68 I69 H70 S73 N74 E75 E82 V83 L86 N87

P88 Y92 S93 F94 R95 V99 N100 I101 V102 G103 T104 Q109 P110 S111 R112 K113 I114 L117 Q118 S119 G120 P121 S122 S123 G124

4.2.10 Score per residue for model 10

- Molecule 1: KIAA1514 protein

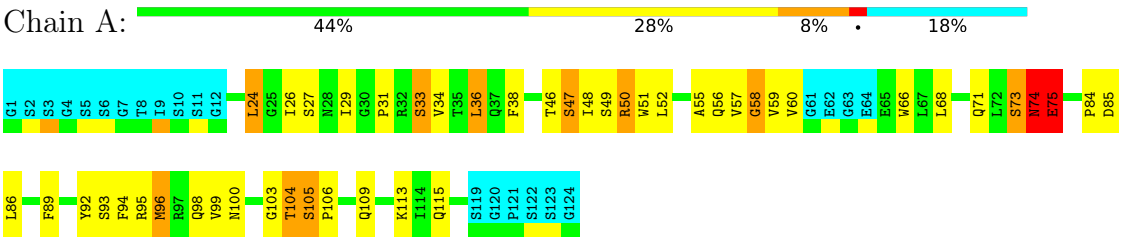
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: KIAA1514 protein

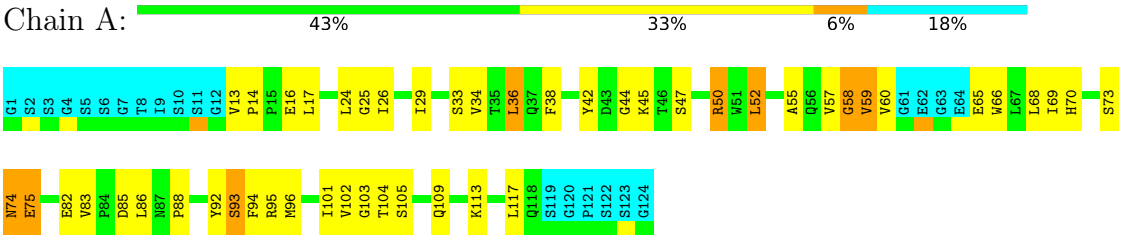
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: KIAA1514 protein

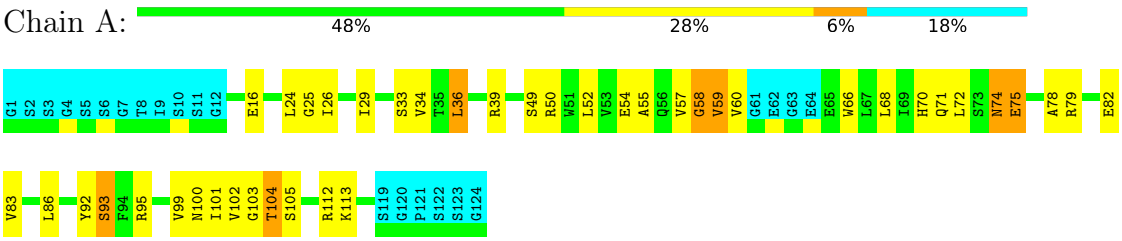
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: KIAA1514 protein

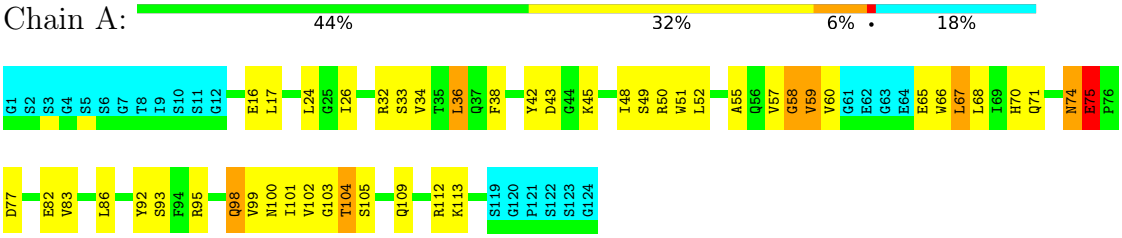
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: KIAA1514 protein

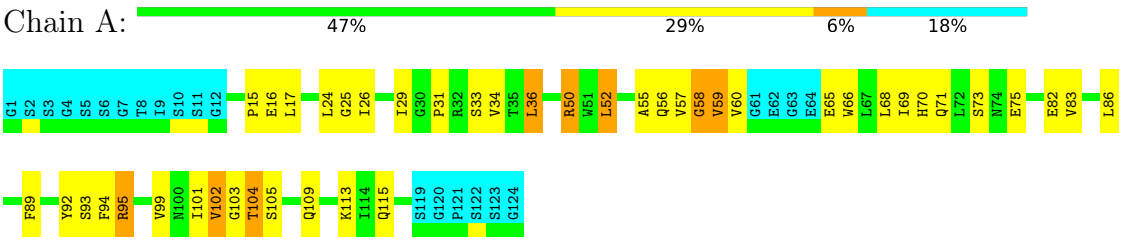
Chain A:



4.2.15 Score per residue for model 15

- Molecule 1: KIAA1514 protein

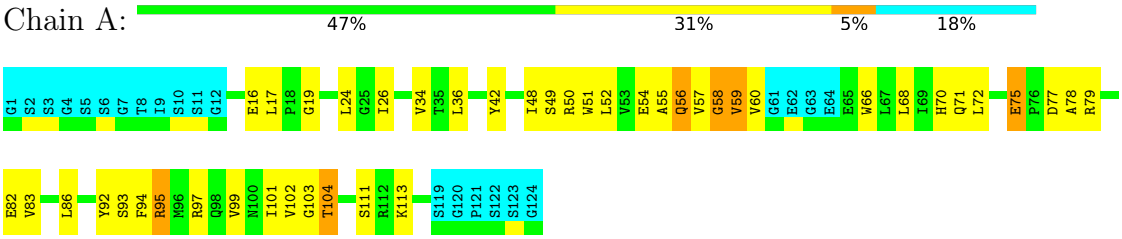
Chain A:



4.2.16 Score per residue for model 16 (medoid)

- Molecule 1: KIAA1514 protein

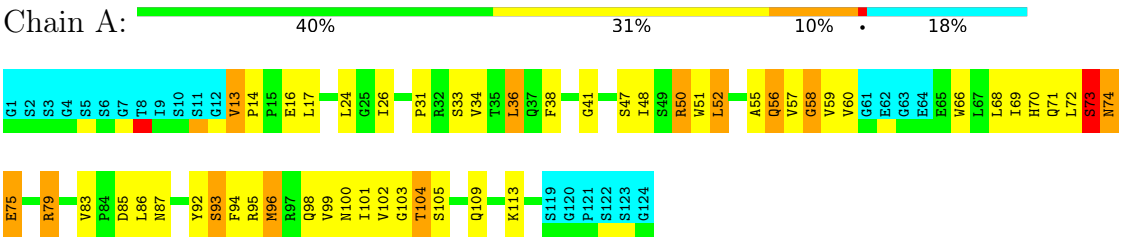
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: KIAA1514 protein

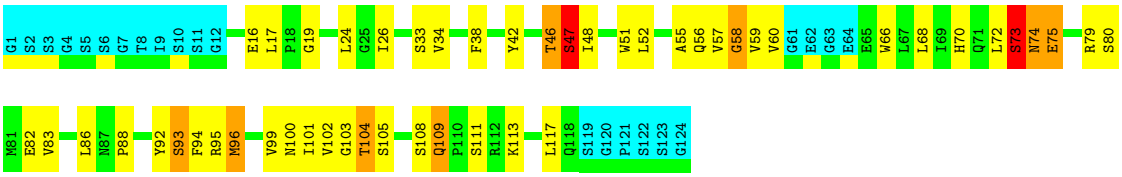
Chain A:



4.2.18 Score per residue for model 18

- Molecule 1: KIAA1514 protein

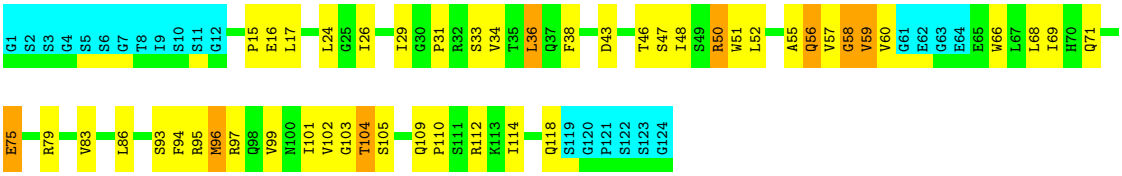
Chain A: 42% 32% 6% • 18%



4.2.19 Score per residue for model 19

- Molecule 1: KIAA1514 protein

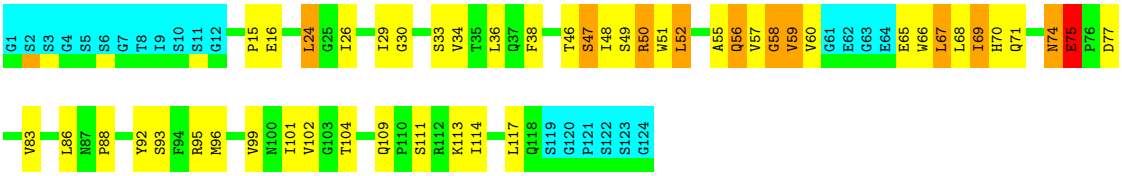
Chain A: 44% 32% 6% 18%



4.2.20 Score per residue for model 20

- Molecule 1: KIAA1514 protein

Chain A: 43% 31% 8% • 18%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle 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	798	800	800	36±5
All	All	15960	16000	16000	723

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:26:ILE:CG2	1:A:29:ILE:HD11	0.95	1.91	2	1
1:A:99:VAL:HG22	1:A:104:THR:OG1	0.93	1.63	14	18
1:A:58:GLY:O	1:A:60:VAL:HG23	0.88	1.69	12	15
1:A:60:VAL:HG21	1:A:93:SER:HB2	0.83	1.49	19	5
1:A:57:VAL:HG22	1:A:92:TYR:OH	0.83	1.74	16	17
1:A:16:GLU:O	1:A:102:VAL:HG21	0.81	1.74	20	15
1:A:52:LEU:HG	1:A:68:LEU:HD13	0.80	1.53	10	20
1:A:34:VAL:HG13	1:A:86:LEU:HD12	0.78	1.56	12	20
1:A:70:HIS:HB2	1:A:83:VAL:HG13	0.77	1.56	18	12
1:A:57:VAL:HG13	1:A:92:TYR:OH	0.76	1.81	20	12
1:A:26:ILE:HG22	1:A:29:ILE:HD11	0.75	1.58	2	4
1:A:68:LEU:HD21	1:A:71:GLN:CD	0.72	2.05	7	2
1:A:60:VAL:HG21	1:A:93:SER:CB	0.70	2.16	19	5
1:A:34:VAL:HG13	1:A:86:LEU:CD1	0.68	2.18	15	16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:LEU:HD21	1:A:71:GLN:NE2	0.67	2.02	19	2
1:A:70:HIS:CB	1:A:83:VAL:HG13	0.67	2.19	18	15
1:A:29:ILE:HD12	1:A:114:ILE:HD13	0.66	1.67	2	1
1:A:29:ILE:HD13	1:A:34:VAL:HB	0.65	1.68	2	1
1:A:58:GLY:O	1:A:60:VAL:HG12	0.64	1.92	19	5
1:A:24:LEU:HD11	1:A:96:MET:HB2	0.64	1.70	20	1
1:A:66:TRP:CD2	1:A:95:ARG:CZ	0.62	2.82	9	4
1:A:68:LEU:HD11	1:A:71:GLN:HG2	0.62	1.70	7	1
1:A:66:TRP:CG	1:A:95:ARG:CZ	0.61	2.84	20	2
1:A:93:SER:O	1:A:94:PHE:CD1	0.60	2.54	9	8
1:A:46:THR:O	1:A:46:THR:HG23	0.60	1.96	18	2
1:A:66:TRP:CE3	1:A:95:ARG:NE	0.60	2.69	9	4
1:A:66:TRP:CG	1:A:95:ARG:NH2	0.60	2.70	12	14
1:A:66:TRP:CD2	1:A:95:ARG:NH2	0.60	2.70	11	12
1:A:56:GLN:O	1:A:92:TYR:CD2	0.60	2.55	4	4
1:A:70:HIS:CD2	1:A:82:GLU:O	0.60	2.55	6	4
1:A:38:PHE:CD2	1:A:96:MET:SD	0.59	2.95	19	8
1:A:29:ILE:HD13	1:A:114:ILE:HD13	0.59	1.75	20	2
1:A:72:LEU:HD21	1:A:78:ALA:CB	0.59	2.28	8	3
1:A:57:VAL:HG22	1:A:92:TYR:CZ	0.58	2.33	14	13
1:A:56:GLN:O	1:A:92:TYR:CD1	0.58	2.57	9	1
1:A:59:VAL:HG13	1:A:59:VAL:O	0.58	1.98	13	2
1:A:26:ILE:HG22	1:A:29:ILE:CG1	0.57	2.29	15	8
1:A:68:LEU:HD21	1:A:71:GLN:HE21	0.57	1.58	19	2
1:A:38:PHE:CE1	1:A:79:ARG:O	0.56	2.58	10	6
1:A:68:LEU:HD21	1:A:71:GLN:OE1	0.56	2.00	15	6
1:A:13:VAL:HG13	1:A:14:PRO:HD2	0.56	1.75	17	3
1:A:38:PHE:CG	1:A:96:MET:SD	0.56	2.99	2	8
1:A:38:PHE:CD2	1:A:96:MET:HE2	0.55	2.36	20	4
1:A:56:GLN:OE1	1:A:60:VAL:HG23	0.55	2.01	8	1
1:A:99:VAL:HG22	1:A:104:THR:HG1	0.55	1.59	6	2
1:A:16:GLU:C	1:A:102:VAL:HG11	0.55	2.22	12	2
1:A:38:PHE:CD1	1:A:79:ARG:O	0.54	2.61	6	3
1:A:48:ILE:CG1	1:A:51:TRP:CH2	0.54	2.91	2	6
1:A:85:ASP:O	1:A:86:LEU:HD23	0.54	2.02	5	4
1:A:66:TRP:CD1	1:A:95:ARG:NH2	0.53	2.76	7	5
1:A:34:VAL:HG22	1:A:86:LEU:HD11	0.53	1.80	15	1
1:A:70:HIS:CE1	1:A:82:GLU:O	0.53	2.61	15	2
1:A:55:ALA:HB1	1:A:93:SER:O	0.53	2.03	3	18
1:A:48:ILE:HG13	1:A:51:TRP:CH2	0.53	2.39	3	17
1:A:50:ARG:NE	1:A:52:LEU:CD1	0.53	2.72	4	3

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:TRP:CE2	1:A:95:ARG:NH2	0.53	2.77	9	2
1:A:26:ILE:CD1	1:A:111:SER:CB	0.52	2.88	16	4
1:A:25:GLY:O	1:A:36:LEU:HD23	0.52	2.04	12	4
1:A:44:GLY:O	1:A:45:LYS:CB	0.52	2.57	12	1
1:A:68:LEU:HD11	1:A:71:GLN:HB3	0.52	1.81	8	7
1:A:55:ALA:CB	1:A:93:SER:O	0.51	2.59	9	19
1:A:26:ILE:HD13	1:A:36:LEU:HG	0.51	1.81	2	7
1:A:83:VAL:O	1:A:86:LEU:HD11	0.51	2.05	5	4
1:A:57:VAL:HG13	1:A:92:TYR:CZ	0.51	2.41	20	5
1:A:57:VAL:HA	1:A:92:TYR:CE1	0.51	2.41	9	1
1:A:17:LEU:HD21	1:A:103:GLY:CA	0.51	2.36	18	14
1:A:70:HIS:CE1	1:A:84:PRO:HD2	0.51	2.41	4	3
1:A:36:LEU:HD11	1:A:94:PHE:CB	0.50	2.37	17	1
1:A:88:PRO:CB	1:A:117:LEU:O	0.50	2.60	18	7
1:A:66:TRP:CE3	1:A:95:ARG:HG2	0.50	2.42	20	2
1:A:54:GLU:OE2	1:A:97:ARG:CZ	0.50	2.60	6	2
1:A:55:ALA:CB	1:A:69:ILE:HD13	0.50	2.36	5	1
1:A:51:TRP:CZ3	1:A:98:GLN:HG3	0.50	2.42	5	2
1:A:57:VAL:CG1	1:A:92:TYR:OH	0.49	2.60	13	3
1:A:29:ILE:HD13	1:A:34:VAL:CB	0.49	2.36	2	1
1:A:52:LEU:CG	1:A:68:LEU:HD13	0.49	2.36	2	8
1:A:38:PHE:CE2	1:A:96:MET:HE1	0.49	2.42	7	3
1:A:50:ARG:NH1	1:A:52:LEU:HD13	0.49	2.23	19	1
1:A:73:SER:O	1:A:74:ASN:C	0.48	2.52	17	5
1:A:38:PHE:CD2	1:A:96:MET:CE	0.48	2.97	20	2
1:A:87:ASN:HB2	1:A:92:TYR:CE1	0.48	2.44	2	2
1:A:16:GLU:O	1:A:100:ASN:ND2	0.47	2.48	2	7
1:A:87:ASN:OD1	1:A:92:TYR:CZ	0.47	2.68	17	1
1:A:44:GLY:C	1:A:45:LYS:CG	0.47	2.81	12	1
1:A:69:ILE:HD11	1:A:83:VAL:HG11	0.47	1.87	19	3
1:A:83:VAL:O	1:A:86:LEU:CD1	0.47	2.63	13	2
1:A:70:HIS:NE2	1:A:82:GLU:O	0.46	2.49	12	10
1:A:24:LEU:HD11	1:A:96:MET:HG3	0.46	1.88	11	1
1:A:42:TYR:CE2	1:A:44:GLY:HA2	0.46	2.45	12	1
1:A:57:VAL:CG2	1:A:92:TYR:OH	0.46	2.59	17	5
1:A:16:GLU:C	1:A:102:VAL:HG21	0.46	2.31	4	6
1:A:30:GLY:N	1:A:33:SER:O	0.46	2.49	20	3
1:A:30:GLY:CA	1:A:33:SER:O	0.46	2.64	20	1
1:A:69:ILE:CG1	1:A:70:HIS:N	0.46	2.79	17	8
1:A:56:GLN:HG3	1:A:66:TRP:CD1	0.46	2.46	19	2
1:A:57:VAL:O	1:A:59:VAL:N	0.46	2.49	14	18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:36:LEU:HD11	1:A:94:PHE:HB3	0.46	1.86	6	2
1:A:54:GLU:OE2	1:A:68:LEU:N	0.46	2.49	13	1
1:A:56:GLN:OE1	1:A:66:TRP:NE1	0.45	2.50	9	1
1:A:66:TRP:CH2	1:A:93:SER:HB3	0.45	2.47	5	4
1:A:51:TRP:NE1	1:A:74:ASN:O	0.45	2.49	17	1
1:A:108:SER:OG	1:A:109:GLN:N	0.45	2.49	2	1
1:A:58:GLY:O	1:A:60:VAL:N	0.45	2.50	20	5
1:A:57:VAL:HG22	1:A:92:TYR:CE2	0.45	2.47	6	1
1:A:56:GLN:CD	1:A:66:TRP:NE1	0.45	2.70	18	3
1:A:72:LEU:CD2	1:A:78:ALA:CB	0.45	2.95	8	1
1:A:59:VAL:O	1:A:59:VAL:CG1	0.45	2.65	13	1
1:A:50:ARG:CD	1:A:52:LEU:CD1	0.45	2.95	15	4
1:A:66:TRP:CZ3	1:A:95:ARG:HG2	0.45	2.46	20	2
1:A:19:GLY:N	1:A:42:TYR:O	0.45	2.50	18	2
1:A:46:THR:O	1:A:46:THR:CG2	0.45	2.63	18	1
1:A:57:VAL:HA	1:A:92:TYR:CZ	0.44	2.47	13	14
1:A:33:SER:C	1:A:34:VAL:CG1	0.44	2.85	6	6
1:A:66:TRP:CH2	1:A:110:PRO:HB3	0.44	2.47	19	1
1:A:68:LEU:HD11	1:A:70:HIS:O	0.44	2.12	15	3
1:A:56:GLN:OE1	1:A:59:VAL:HG13	0.44	2.13	2	1
1:A:87:ASN:OD1	1:A:87:ASN:N	0.44	2.49	9	1
1:A:74:ASN:O	1:A:75:GLU:CB	0.44	2.65	20	6
1:A:93:SER:C	1:A:94:PHE:CG	0.43	2.92	10	8
1:A:99:VAL:CG2	1:A:104:THR:OG1	0.43	2.59	17	1
1:A:57:VAL:O	1:A:58:GLY:C	0.43	2.56	10	15
1:A:89:PHE:O	1:A:89:PHE:CD2	0.43	2.72	8	2
1:A:100:ASN:OD1	1:A:103:GLY:N	0.43	2.49	14	3
1:A:57:VAL:HA	1:A:92:TYR:CE2	0.43	2.48	6	1
1:A:26:ILE:HG22	1:A:29:ILE:HG12	0.43	1.90	15	1
1:A:50:ARG:HD3	1:A:52:LEU:CD1	0.43	2.43	9	8
1:A:48:ILE:HG13	1:A:51:TRP:CZ3	0.43	2.48	11	2
1:A:48:ILE:HD12	1:A:98:GLN:HB3	0.43	1.89	11	1
1:A:44:GLY:O	1:A:45:LYS:CG	0.43	2.67	12	1
1:A:50:ARG:NH2	1:A:71:GLN:OE1	0.43	2.52	3	1
1:A:65:GLU:HG3	1:A:67:LEU:HD23	0.43	1.91	20	1
1:A:55:ALA:HA	1:A:66:TRP:CZ3	0.43	2.48	19	4
1:A:56:GLN:NE2	1:A:66:TRP:CD1	0.43	2.87	8	1
1:A:48:ILE:N	1:A:48:ILE:HD13	0.42	2.29	16	2
1:A:38:PHE:CD1	1:A:38:PHE:N	0.42	2.86	20	3
1:A:105:SER:CB	1:A:106:PRO:CD	0.42	2.97	7	4
1:A:65:GLU:HG3	1:A:67:LEU:CD2	0.42	2.45	14	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:72:LEU:O	1:A:73:SER:O	0.42	2.37	17	2
1:A:51:TRP:HB2	1:A:81:MET:HE1	0.42	1.92	7	1
1:A:46:THR:O	1:A:47:SER:O	0.42	2.38	18	3
1:A:54:GLU:OE1	1:A:97:ARG:NH2	0.42	2.53	10	2
1:A:74:ASN:O	1:A:75:GLU:C	0.42	2.57	18	2
1:A:75:GLU:OE1	1:A:75:GLU:CA	0.41	2.69	7	1
1:A:55:ALA:HB3	1:A:69:ILE:HG21	0.41	1.91	20	3
1:A:56:GLN:OE1	1:A:59:VAL:O	0.41	2.39	20	3
1:A:108:SER:O	1:A:109:GLN:C	0.41	2.58	7	2
1:A:26:ILE:CD1	1:A:36:LEU:HG	0.41	2.46	15	2
1:A:47:SER:O	1:A:48:ILE:HD13	0.41	2.14	18	1
1:A:66:TRP:CD2	1:A:95:ARG:NE	0.41	2.88	20	1
1:A:56:GLN:CG	1:A:65:GLU:O	0.41	2.69	4	1
1:A:96:MET:O	1:A:97:ARG:CG	0.41	2.68	19	2
1:A:68:LEU:CD2	1:A:71:GLN:OE1	0.41	2.69	6	2
1:A:100:ASN:OD1	1:A:103:GLY:O	0.41	2.39	11	3
1:A:15:PRO:HB2	1:A:102:VAL:CG2	0.41	2.46	9	6
1:A:87:ASN:CG	1:A:92:TYR:CE1	0.41	2.94	17	1
1:A:38:PHE:CZ	1:A:78:ALA:O	0.41	2.74	1	1
1:A:26:ILE:HG22	1:A:29:ILE:CD1	0.41	2.43	11	1
1:A:87:ASN:CG	1:A:92:TYR:CZ	0.40	2.94	17	1
1:A:75:GLU:CD	1:A:78:ALA:HB2	0.40	2.37	7	1
1:A:70:HIS:HB3	1:A:83:VAL:HG13	0.40	1.94	15	1
1:A:84:PRO:O	1:A:85:ASP:C	0.40	2.59	11	1
1:A:56:GLN:CD	1:A:59:VAL:O	0.40	2.60	2	1
1:A:48:ILE:HD13	1:A:48:ILE:N	0.40	2.31	10	1
1:A:17:LEU:N	1:A:102:VAL:HG11	0.40	2.31	12	1
1:A:42:TYR:O	1:A:43:ASP:C	0.40	2.60	14	1
1:A:58:GLY:O	1:A:59:VAL:C	0.40	2.59	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	102/124 (82%)	82±2 (80±2%)	16±2 (15±2%)	5±1 (4±1%)	4 28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2040/2480 (82%)	1636 (80%)	313 (15%)	91 (4%)	4 28

All 11 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	58	GLY	20
1	A	75	GLU	16
1	A	59	VAL	14
1	A	74	ASN	12
1	A	31	PRO	9
1	A	47	SER	7
1	A	102	VAL	5
1	A	112	ARG	3
1	A	41	GLY	2
1	A	73	SER	2
1	A	13	VAL	1

6.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	93/107 (87%)	78±2 (84±3%)	15±2 (16±3%)	5 42
All	All	1860/2140 (87%)	1567 (84%)	293 (16%)	5 42

All 41 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	24	LEU	20
1	A	75	GLU	20
1	A	101	ILE	19
1	A	104	THR	19
1	A	36	LEU	17
1	A	113	LYS	17
1	A	50	ARG	16
1	A	105	SER	15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	33	SER	14
1	A	109	GLN	14
1	A	49	SER	11
1	A	73	SER	11
1	A	79	ARG	10
1	A	56	GLN	9
1	A	52	LEU	8
1	A	96	MET	8
1	A	95	ARG	7
1	A	65	GLU	6
1	A	77	ASP	5
1	A	115	GLN	5
1	A	93	SER	5
1	A	43	ASP	4
1	A	74	ASN	4
1	A	39	ARG	3
1	A	98	GLN	3
1	A	27	SER	2
1	A	85	ASP	2
1	A	89	PHE	2
1	A	32	ARG	2
1	A	46	THR	2
1	A	80	SER	2
1	A	67	LEU	2
1	A	34	VAL	1
1	A	87	ASN	1
1	A	114	ILE	1
1	A	71	GLN	1
1	A	112	ARG	1
1	A	45	LYS	1
1	A	47	SER	1
1	A	118	GLN	1
1	A	69	ILE	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