Full wwPDB NMR Structure Validation Report (i)

Feb 22, 2022 – 12:29 PM EST

PDB ID	:	1WJ6
Title	:	Solution structure of RSGI RUH-024, a PB1 domain in human cDNA, KIAA0049
Authors	:	Hamada, T.; Hirota, H.; Hayashi, F.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2004-05-29

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:

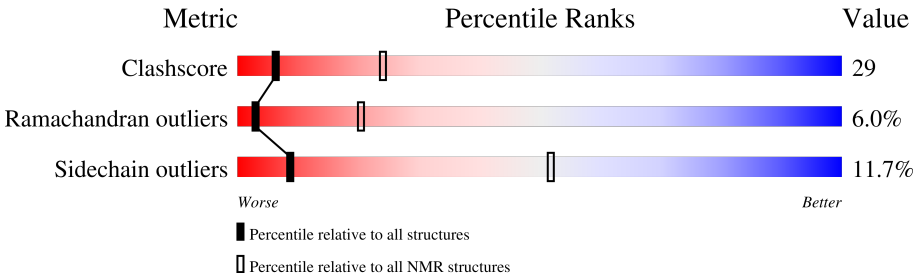
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	101	36% 41% • 20%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 3 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:14-A:94 (81)	0.13	3

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 2 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1502 atoms, of which 729 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called KIAA0049 protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	101	1502	475	729	126	168	4	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP Q14596
A	2	SER	-	cloning artifact	UNP Q14596
A	3	SER	-	cloning artifact	UNP Q14596
A	4	GLY	-	cloning artifact	UNP Q14596
A	5	SER	-	cloning artifact	UNP Q14596
A	6	SER	-	cloning artifact	UNP Q14596
A	7	GLY	-	cloning artifact	UNP Q14596
A	96	SER	-	cloning artifact	UNP Q14596
A	97	GLY	-	cloning artifact	UNP Q14596
A	98	PRO	-	cloning artifact	UNP Q14596
A	99	SER	-	cloning artifact	UNP Q14596
A	100	SER	-	cloning artifact	UNP Q14596
A	101	GLY	-	cloning artifact	UNP Q14596

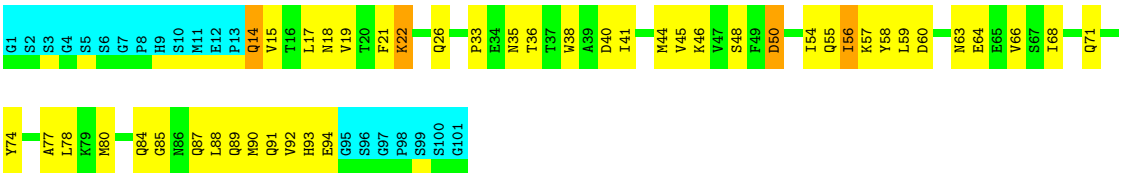
4 Residue-property plots (i)

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: KIAA0049 protein

Chain A: 36% 41% • 20%



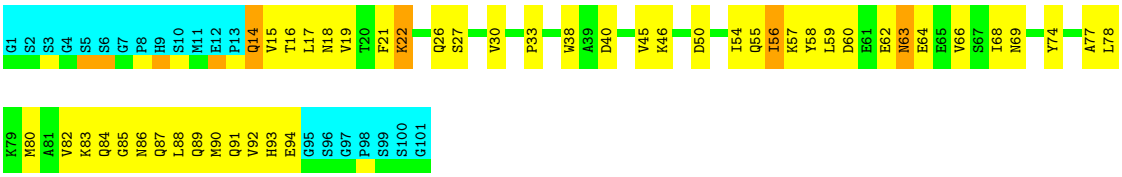
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: KIAA0049 protein

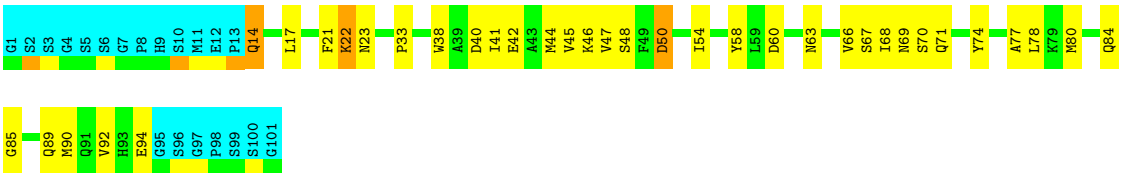
Chain A: 34% 43% • 20%



4.2.2 Score per residue for model 2

• Molecule 1: KIAA0049 protein

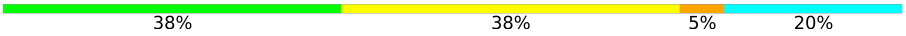
Chain A: 45% 33% • 20%

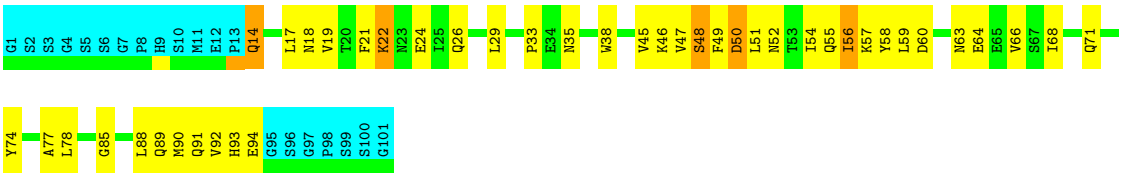


4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: KIAA0049 protein

Chain A:

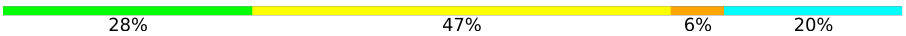


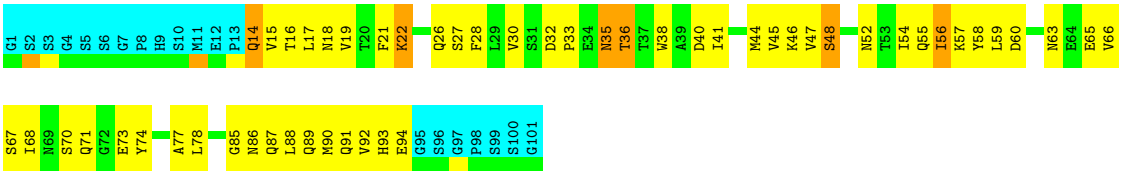


4.2.4 Score per residue for model 4

- Molecule 1: KIAA0049 protein

Chain A:

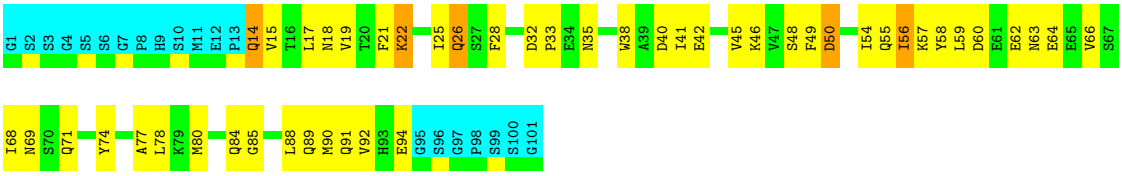




4.2.5 Score per residue for model 5

- Molecule 1: KIAA0049 protein

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: KIAA0049 protein

Chain A: 35% 37% 8% • 20%

G1 S2 S3 G4 S5 S6 G7 P8 H9 S10 M11 E12 P13 Q14 V15 T16 L17 N18 V19 T20 F21 K22 Q26 S27 F28 L29 V30 P33 T36 T37 W38 A39 D40 I41 M44 V45 K46 V47 S48 F49 D50 I54 Q55 I56 K57 Y58 L59 D60 E61 E62 N63 V66 S67 I68

Q71 Y74 E75 E76 A77 L78 K79 G85 L88 Q89 M90 Q91 V92 H93 E94 G95 S96 G97 P98 S99 S100 G101

4.2.7 Score per residue for model 7

- Molecule 1: KIAA0049 protein

Chain A: 32% 44% • • 20%

G1 S2 S3 G4 S5 S6 G7 P8 H9 S10 M11 E12 P13 Q14 V15 T16 L17 N18 V19 T20 F21 K22 S27 D32 P33 E34 N35 T36 T37 W38 A39 D40 A43 M44 V45 K46 V47 S48 F49 D50 L51 N52 T53 I54 Q55 I56 K57 Y58 L59 D60 N63 I68 N69 S70

E73 Y74 E75 E76 A77 L78 K79 M80 A81 V82 K83 Q84 G85 N86 Q87 L88 Q89 M90 Q91 V92 H93 E94 G95 S96 G97 P98 S99 S100 G101

4.2.8 Score per residue for model 8

- Molecule 1: KIAA0049 protein

Chain A: 32% 44% 5% 20%

G1 S2 S3 G4 S5 S6 G7 P8 H9 S10 M11 E12 P13 Q14 V15 T16 L17 N18 V19 T20 F21 K22 N23 E24 I25 Q26 S27 F28 S31 D32 P33 W38 A39 D40 I41 E42 A43 M44 V45 K46 V47 S48 F49 D50 I54 Q55 I56 K57 Y58 L59 E62 N63 I68 Y74

E75 E76 A77 L78 K79 M80 Q84 G85 L88 Q89 M90 Q91 V92 H93 E94 G95 S96 G97 P98 S99 S100 G101

4.2.9 Score per residue for model 9

- Molecule 1: KIAA0049 protein

Chain A: 33% 45% • • 20%

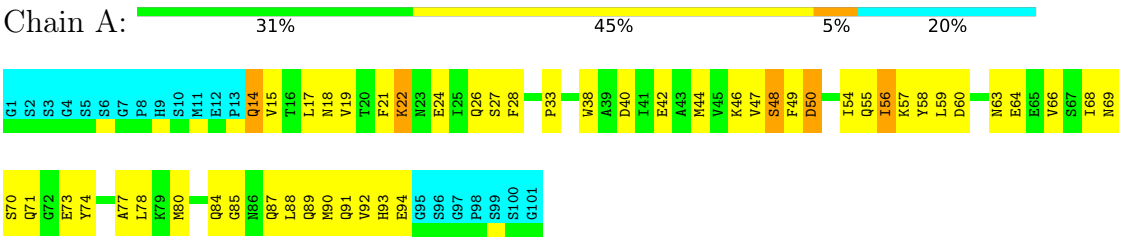
G1 S2 S3 G4 S5 S6 G7 P8 H9 S10 M11 E12 P13 Q14 V15 T16 L17 N18 V19 T20 F21 K22 N23 Q26 P33 W38 A39 D40 I41 E42 A43 M44 V45 K46 F49 D50 L51 N52 T53 I54 Q55 I56 K57 Y58 L59 D60 N63 E64 E65 V66 S67 I68 N69 S70 Q71

Y74 E75 E76 A77 L78 K79 M80 Q84 G85 N86 Q87 L88 Q89 M90 Q91 V92 G95 S96 G97 P98 S99 S100 G101

4.2.10 Score per residue for model 10

- Molecule 1: KIAA0049 protein

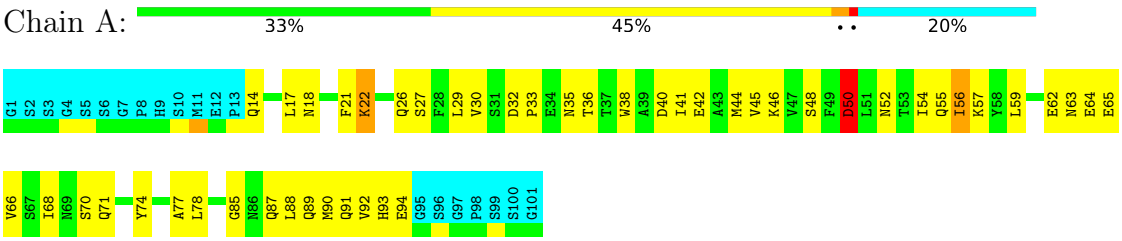
Chain A:



4.2.11 Score per residue for model 11

- Molecule 1: KIAA0049 protein

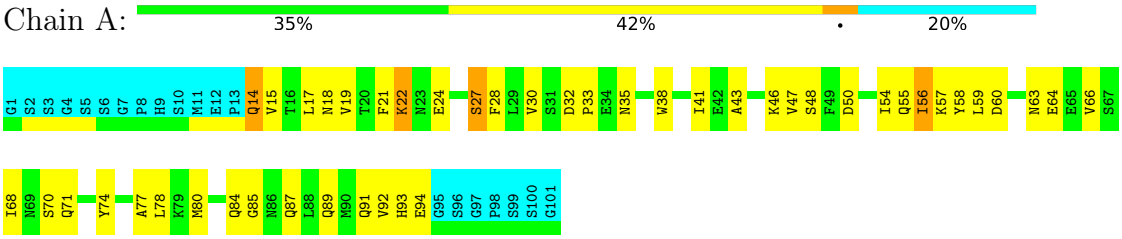
Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: KIAA0049 protein

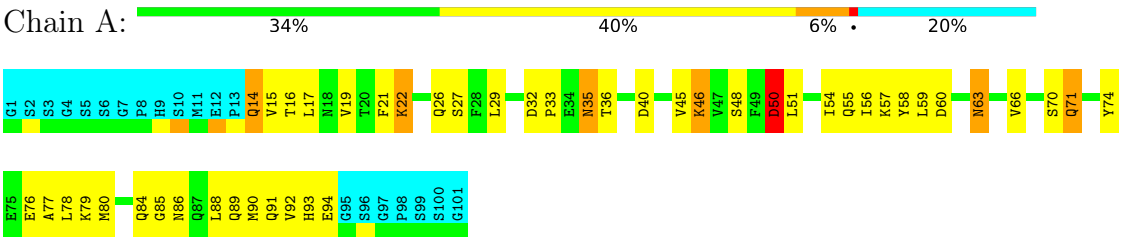
Chain A:



4.2.13 Score per residue for model 13

- Molecule 1: KIAA0049 protein

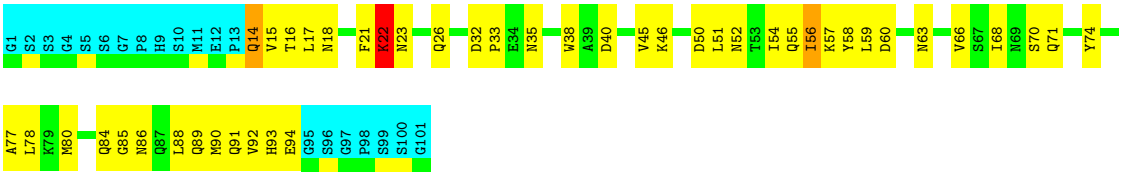
Chain A:



4.2.14 Score per residue for model 14

- Molecule 1: KIAA0049 protein

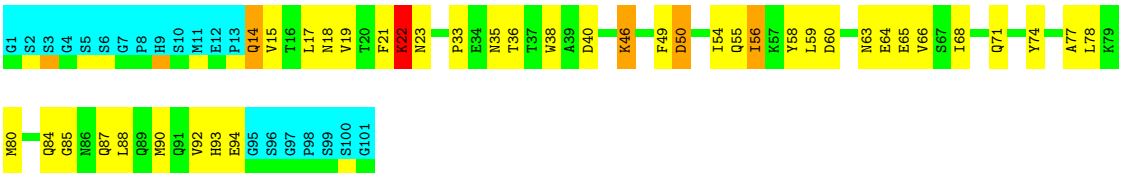
Chain A: 36% 42% • • 20%



4.2.15 Score per residue for model 15

- Molecule 1: KIAA0049 protein

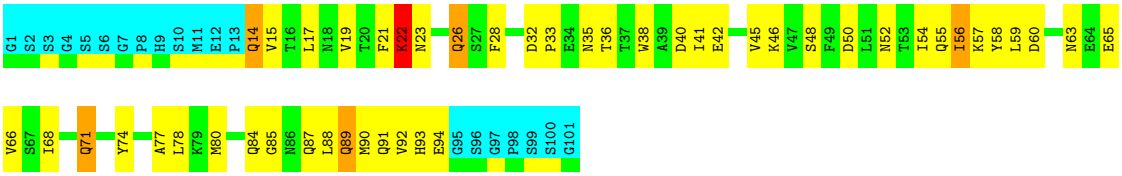
Chain A: 41% 35% • • 20%



4.2.16 Score per residue for model 16

- Molecule 1: KIAA0049 protein

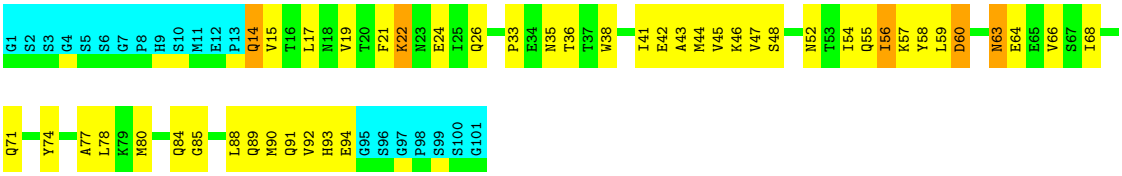
Chain A: 33% 42% 5% • 20%



4.2.17 Score per residue for model 17

- Molecule 1: KIAA0049 protein

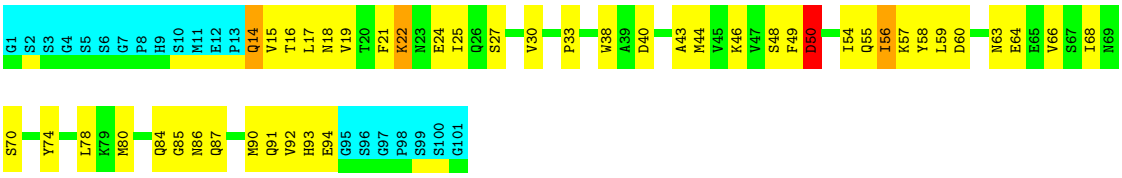
Chain A: 35% 41% 5% 20%



4.2.18 Score per residue for model 18

- Molecule 1: KIAA0049 protein

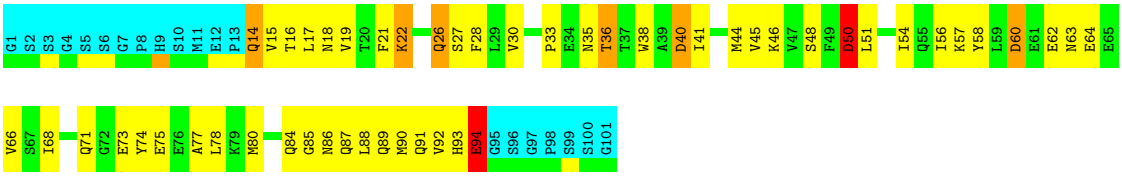
Chain A: 36% 41% • • 20%



4.2.19 Score per residue for model 19

- Molecule 1: KIAA0049 protein

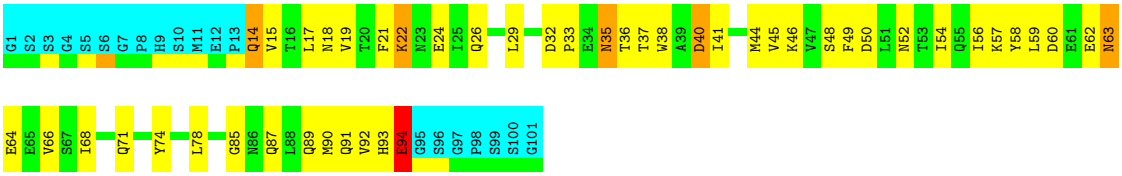
Chain A: 29% 44% 6% • 20%



4.2.20 Score per residue for model 20

- Molecule 1: KIAA0049 protein

Chain A: 34% 41% 5% • 20%



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, structures with the lowest energy, target function*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
KUJIRA	structure solution	0.8995
CYANA	structure solution	1.0.8
CYANA	refinement	1.0.8

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	653	628	628	37±6
All	All	13060	12560	12560	733

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 29.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:TYR:CE2	1:A:78:LEU:HD11	0.96	1.96	7	18
1:A:43:ALA:O	1:A:47:VAL:HG22	0.92	1.64	12	1
1:A:74:TYR:CZ	1:A:78:LEU:HD11	0.90	1.99	1	17
1:A:77:ALA:HB1	1:A:88:LEU:HD21	0.74	1.60	15	16
1:A:33:PRO:HB2	1:A:78:LEU:HD13	0.72	1.61	2	20
1:A:59:LEU:HD22	1:A:63:ASN:C	0.71	2.06	5	17
1:A:77:ALA:HB1	1:A:88:LEU:CD2	0.68	2.18	15	10
1:A:50:ASP:O	1:A:51:LEU:HD23	0.67	1.89	19	4
1:A:54:ILE:HD11	1:A:56:ILE:HD11	0.66	1.68	18	2
1:A:17:LEU:HD22	1:A:90:MET:SD	0.66	2.31	15	19
1:A:58:TYR:CE2	1:A:77:ALA:HB2	0.63	2.28	2	11
1:A:21:PHE:CZ	1:A:22:LYS:CE	0.63	2.81	17	4
1:A:19:VAL:CG1	1:A:92:VAL:HG23	0.63	2.24	5	16
1:A:33:PRO:CB	1:A:78:LEU:HD22	0.63	2.23	15	10

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:PRO:O	1:A:78:LEU:HD13	0.62	1.94	15	11
1:A:36:THR:CG2	1:A:41:ILE:HD11	0.62	2.24	6	3
1:A:54:ILE:HD12	1:A:92:VAL:HG22	0.61	1.72	20	6
1:A:45:VAL:HG11	1:A:92:VAL:CG2	0.61	2.26	7	10
1:A:26:GLN:OE1	1:A:28:PHE:CZ	0.60	2.55	16	2
1:A:38:TRP:CD1	1:A:68:ILE:HG22	0.60	2.31	16	9
1:A:21:PHE:CD1	1:A:92:VAL:HG12	0.57	2.33	5	19
1:A:45:VAL:CG1	1:A:92:VAL:CG2	0.57	2.83	9	13
1:A:36:THR:HG21	1:A:41:ILE:HD11	0.57	1.76	6	2
1:A:14:GLN:HB2	1:A:29:LEU:HD11	0.57	1.76	20	2
1:A:26:GLN:OE1	1:A:49:PHE:CE1	0.57	2.58	10	1
1:A:33:PRO:HB3	1:A:78:LEU:HD22	0.57	1.77	6	3
1:A:21:PHE:CE1	1:A:22:LYS:CE	0.56	2.87	17	5
1:A:58:TYR:CE2	1:A:66:VAL:CG1	0.56	2.89	4	11
1:A:74:TYR:CE2	1:A:78:LEU:CD1	0.56	2.82	7	1
1:A:59:LEU:HD13	1:A:63:ASN:OD1	0.56	2.00	17	2
1:A:19:VAL:HG13	1:A:92:VAL:HG23	0.55	1.78	17	9
1:A:80:MET:CE	1:A:84:GLN:NE2	0.55	2.70	10	14
1:A:19:VAL:HG11	1:A:45:VAL:CG1	0.55	2.31	13	5
1:A:17:LEU:HD11	1:A:74:TYR:OH	0.55	2.02	13	5
1:A:46:LYS:HG3	1:A:54:ILE:HD13	0.54	1.79	13	3
1:A:37:THR:O	1:A:41:ILE:HD12	0.54	2.03	20	1
1:A:49:PHE:O	1:A:50:ASP:CB	0.53	2.57	15	6
1:A:59:LEU:HD22	1:A:63:ASN:O	0.53	2.02	18	4
1:A:58:TYR:CD2	1:A:68:ILE:HD11	0.53	2.39	6	2
1:A:26:GLN:OE1	1:A:49:PHE:CZ	0.53	2.62	10	1
1:A:46:LYS:O	1:A:50:ASP:N	0.53	2.42	10	18
1:A:21:PHE:CZ	1:A:22:LYS:HE3	0.53	2.39	17	4
1:A:21:PHE:CE1	1:A:22:LYS:HE2	0.52	2.40	17	7
1:A:68:ILE:HD13	1:A:74:TYR:HA	0.52	1.81	7	7
1:A:21:PHE:CE1	1:A:22:LYS:HE3	0.52	2.39	6	5
1:A:21:PHE:CE1	1:A:22:LYS:HG2	0.51	2.40	14	4
1:A:33:PRO:O	1:A:78:LEU:CD1	0.51	2.58	12	15
1:A:35:ASN:HD22	1:A:36:THR:N	0.51	2.03	13	4
1:A:55:GLN:OE1	1:A:57:LYS:CE	0.51	2.59	6	1
1:A:58:TYR:C	1:A:58:TYR:CD1	0.51	2.84	16	7
1:A:28:PHE:N	1:A:28:PHE:CD1	0.51	2.79	10	1
1:A:17:LEU:CD1	1:A:30:VAL:HG21	0.50	2.34	18	7
1:A:40:ASP:O	1:A:44:MET:CB	0.50	2.59	6	4
1:A:19:VAL:HG11	1:A:45:VAL:HG11	0.50	1.82	13	1
1:A:62:GLU:O	1:A:63:ASN:CB	0.50	2.58	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:74:TYR:CZ	1:A:78:LEU:HD21	0.50	2.42	20	1
1:A:58:TYR:CE2	1:A:66:VAL:HB	0.50	2.41	20	7
1:A:55:GLN:OE1	1:A:57:LYS:CG	0.50	2.60	6	1
1:A:74:TYR:CE1	1:A:78:LEU:HG	0.50	2.42	16	2
1:A:33:PRO:C	1:A:78:LEU:HD13	0.50	2.27	11	1
1:A:14:GLN:HB3	1:A:29:LEU:HD11	0.49	1.84	3	2
1:A:21:PHE:CZ	1:A:22:LYS:HE2	0.49	2.43	11	9
1:A:21:PHE:HB3	1:A:49:PHE:CE1	0.49	2.42	9	1
1:A:38:TRP:CE2	1:A:68:ILE:HG22	0.49	2.43	16	4
1:A:46:LYS:HG2	1:A:54:ILE:HG23	0.48	1.85	19	3
1:A:19:VAL:HG11	1:A:45:VAL:HG13	0.48	1.85	7	2
1:A:58:TYR:CD1	1:A:58:TYR:C	0.48	2.87	7	11
1:A:60:ASP:OD1	1:A:64:GLU:N	0.48	2.47	19	1
1:A:44:MET:O	1:A:48:SER:N	0.48	2.47	17	1
1:A:21:PHE:O	1:A:23:ASN:N	0.47	2.47	9	4
1:A:64:GLU:O	1:A:66:VAL:HG23	0.47	2.09	11	11
1:A:38:TRP:CZ2	1:A:68:ILE:HB	0.47	2.45	5	17
1:A:43:ALA:O	1:A:47:VAL:N	0.47	2.44	17	1
1:A:38:TRP:CD2	1:A:68:ILE:CG2	0.47	2.98	18	1
1:A:57:LYS:O	1:A:91:GLN:N	0.47	2.48	7	18
1:A:58:TYR:CZ	1:A:66:VAL:HG11	0.47	2.45	4	1
1:A:38:TRP:NE1	1:A:68:ILE:HG22	0.47	2.25	16	2
1:A:27:SER:C	1:A:28:PHE:CD1	0.47	2.88	12	1
1:A:58:TYR:O	1:A:66:VAL:N	0.47	2.48	4	6
1:A:55:GLN:N	1:A:93:HIS:O	0.46	2.48	12	14
1:A:45:VAL:CG1	1:A:92:VAL:HG21	0.46	2.40	4	5
1:A:35:ASN:C	1:A:35:ASN:ND2	0.46	2.69	4	4
1:A:41:ILE:HG13	1:A:74:TYR:CE2	0.46	2.46	12	3
1:A:21:PHE:CD1	1:A:92:VAL:CG1	0.46	2.98	10	10
1:A:17:LEU:HD11	1:A:30:VAL:HG21	0.46	1.86	12	2
1:A:71:GLN:O	1:A:74:TYR:N	0.46	2.49	5	15
1:A:28:PHE:HZ	1:A:48:SER:HG	0.46	1.49	6	4
1:A:21:PHE:CE2	1:A:22:LYS:HE2	0.45	2.46	8	3
1:A:19:VAL:HG11	1:A:92:VAL:HG23	0.45	1.88	9	2
1:A:55:GLN:NE2	1:A:56:ILE:O	0.45	2.49	6	1
1:A:74:TYR:CZ	1:A:78:LEU:CD1	0.45	2.89	1	4
1:A:68:ILE:HG23	1:A:73:GLU:HB2	0.45	1.89	7	1
1:A:46:LYS:CG	1:A:54:ILE:HG23	0.45	2.42	19	1
1:A:18:ASN:ND2	1:A:87:GLN:OE1	0.45	2.50	10	10
1:A:21:PHE:N	1:A:24:GLU:O	0.45	2.50	10	5
1:A:38:TRP:NE1	1:A:68:ILE:O	0.45	2.49	4	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:28:PHE:CD1	1:A:28:PHE:N	0.45	2.85	12	1
1:A:18:ASN:O	1:A:90:MET:N	0.45	2.49	5	5
1:A:46:LYS:CG	1:A:54:ILE:HD13	0.45	2.42	17	6
1:A:47:VAL:CG2	1:A:48:SER:N	0.45	2.80	7	1
1:A:60:ASP:OD2	1:A:66:VAL:CG2	0.45	2.65	17	1
1:A:46:LYS:CG	1:A:54:ILE:CD1	0.44	2.96	17	5
1:A:44:MET:O	1:A:47:VAL:HG22	0.44	2.12	4	2
1:A:28:PHE:HE1	1:A:48:SER:HG	0.44	1.54	4	2
1:A:37:THR:O	1:A:40:ASP:N	0.44	2.51	6	1
1:A:43:ALA:O	1:A:46:LYS:N	0.44	2.50	9	2
1:A:26:GLN:CD	1:A:49:PHE:CZ	0.44	2.91	10	1
1:A:19:VAL:O	1:A:26:GLN:N	0.44	2.49	5	3
1:A:55:GLN:O	1:A:56:ILE:C	0.44	2.55	15	13
1:A:80:MET:O	1:A:83:LYS:N	0.43	2.51	7	2
1:A:87:GLN:NE2	1:A:89:GLN:OE1	0.43	2.52	16	1
1:A:46:LYS:HG3	1:A:54:ILE:CD1	0.43	2.43	14	7
1:A:46:LYS:HG2	1:A:54:ILE:HD13	0.43	1.91	18	1
1:A:62:GLU:O	1:A:62:GLU:CD	0.43	2.57	19	1
1:A:76:GLU:O	1:A:79:LYS:N	0.43	2.51	6	4
1:A:44:MET:O	1:A:48:SER:CB	0.43	2.66	11	1
1:A:32:ASP:N	1:A:32:ASP:OD1	0.43	2.51	12	1
1:A:21:PHE:CD1	1:A:22:LYS:HG2	0.43	2.49	14	2
1:A:38:TRP:CE2	1:A:68:ILE:CG2	0.43	3.02	16	2
1:A:33:PRO:CB	1:A:78:LEU:HD13	0.43	2.41	7	2
1:A:46:LYS:O	1:A:49:PHE:N	0.43	2.51	9	2
1:A:49:PHE:O	1:A:50:ASP:C	0.43	2.57	18	1
1:A:32:ASP:CG	1:A:32:ASP:O	0.43	2.57	4	1
1:A:38:TRP:CH2	1:A:56:ILE:HD13	0.43	2.48	15	1
1:A:62:GLU:O	1:A:62:GLU:CG	0.43	2.66	19	1
1:A:46:LYS:CD	1:A:54:ILE:HG12	0.42	2.44	3	5
1:A:59:LEU:HD13	1:A:63:ASN:O	0.42	2.14	8	1
1:A:21:PHE:CD1	1:A:22:LYS:HE2	0.42	2.48	15	3
1:A:21:PHE:HB3	1:A:49:PHE:CE2	0.42	2.49	15	1
1:A:41:ILE:O	1:A:42:GLU:C	0.42	2.58	5	7
1:A:35:ASN:ND2	1:A:36:THR:N	0.42	2.66	4	2
1:A:44:MET:O	1:A:47:VAL:CG2	0.42	2.68	4	1
1:A:55:GLN:NE2	1:A:69:ASN:HD21	0.42	2.13	1	1
1:A:59:LEU:HD22	1:A:64:GLU:N	0.42	2.29	5	2
1:A:33:PRO:HB2	1:A:78:LEU:HD22	0.42	1.92	9	1
1:A:24:GLU:HG3	1:A:25:ILE:N	0.42	2.29	18	1
1:A:93:HIS:O	1:A:94:GLU:C	0.42	2.57	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:81:ALA:HB2	1:A:88:LEU:HB2	0.42	1.90	7	1
1:A:74:TYR:CE1	1:A:78:LEU:CG	0.42	3.02	16	1
1:A:16:THR:N	1:A:86:ASN:O	0.41	2.48	18	8
1:A:32:ASP:O	1:A:32:ASP:CG	0.41	2.59	20	1
1:A:35:ASN:ND2	1:A:35:ASN:C	0.41	2.74	7	1
1:A:24:GLU:CG	1:A:25:ILE:N	0.41	2.83	8	1
1:A:23:ASN:O	1:A:23:ASN:CG	0.41	2.59	8	2
1:A:59:LEU:HD23	1:A:65:GLU:N	0.41	2.31	15	4
1:A:68:ILE:HG23	1:A:73:GLU:CB	0.41	2.45	4	2
1:A:47:VAL:HG23	1:A:48:SER:N	0.41	2.30	10	2
1:A:47:VAL:O	1:A:48:SER:C	0.41	2.59	3	1
1:A:43:ALA:O	1:A:44:MET:C	0.41	2.59	7	3
1:A:74:TYR:O	1:A:75:GLU:C	0.41	2.60	19	1
1:A:46:LYS:CG	1:A:54:ILE:HG12	0.40	2.46	9	1
1:A:59:LEU:HD23	1:A:64:GLU:C	0.40	2.36	9	1
1:A:25:ILE:O	1:A:26:GLN:OE1	0.40	2.39	5	1
1:A:55:GLN:CD	1:A:55:GLN:O	0.40	2.59	6	1
1:A:55:GLN:CD	1:A:55:GLN:C	0.40	2.80	6	1
1:A:46:LYS:NZ	1:A:52:ASN:O	0.40	2.48	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	81/101 (80%)	68±2 (84±2%)	8±2 (10±2%)	5±1 (6±1%)	3 20
All	All	1620/2020 (80%)	1358 (84%)	165 (10%)	97 (6%)	3 20

All 7 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	22	LYS	20
1	A	85	GLY	20
1	A	14	GLN	19

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Mol	Chain	Res	Type	Models (Total)
1	A	56	ILE	19
1	A	50	ASP	12
1	A	36	THR	5
1	A	94	GLU	2

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	75/89 (84%)	66±2 (88±3%)	9±2 (12±3%)	9 52
All	All	1500/1780 (84%)	1324 (88%)	176 (12%)	9 52

All 27 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	94	GLU	19
1	A	60	ASP	18
1	A	89	GLN	18
1	A	40	ASP	16
1	A	26	GLN	13
1	A	70	SER	10
1	A	35	ASN	10
1	A	27	SER	9
1	A	63	ASN	8
1	A	48	SER	8
1	A	52	ASN	7
1	A	32	ASP	6
1	A	50	ASP	6
1	A	62	GLU	5
1	A	22	LYS	4
1	A	71	GLN	4
1	A	69	ASN	3
1	A	67	SER	2
1	A	46	LYS	2
1	A	51	LEU	1
1	A	55	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	53	THR	1
1	A	76	GLU	1
1	A	31	SER	1
1	A	42	GLU	1
1	A	73	GLU	1
1	A	36	THR	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