Full wwPDB NMR Structure Validation Report (i)

Feb 27, 2022 – 10:25 PM EST

PDB ID	:	2DBH
Title	:	Solution structure of the carboxyl-terminal CARD-like domain in human TNFR-related death receptor-6
Authors	:	Saito, K.; Inoue, M.; Koshiba, S.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2005-12-15

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:

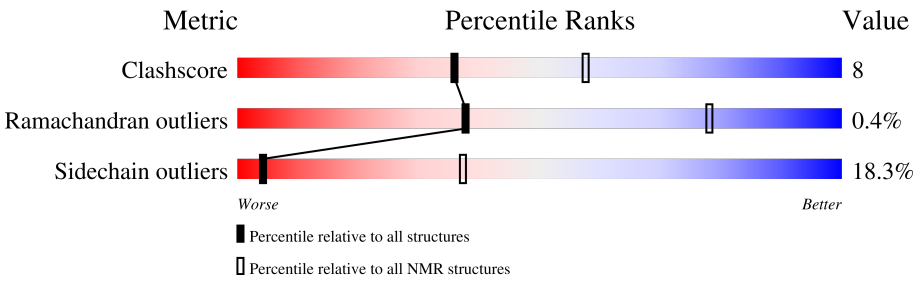
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	102	57% 21% 23%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 14 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:17-A:95 (79)	0.31	14

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 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1567 atoms, of which 780 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Tumor necrosis factor receptor superfamily member 21.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	102	1567	489	780	133	163	2	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP O75509
A	2	SER	-	cloning artifact	UNP O75509
A	3	SER	-	cloning artifact	UNP O75509
A	4	GLY	-	cloning artifact	UNP O75509
A	5	SER	-	cloning artifact	UNP O75509
A	6	SER	-	cloning artifact	UNP O75509
A	7	GLY	-	cloning artifact	UNP O75509
A	97	SER	-	cloning artifact	UNP O75509
A	98	GLY	-	cloning artifact	UNP O75509
A	99	PRO	-	cloning artifact	UNP O75509
A	100	SER	-	cloning artifact	UNP O75509
A	101	SER	-	cloning artifact	UNP O75509
A	102	GLY	-	cloning artifact	UNP O75509

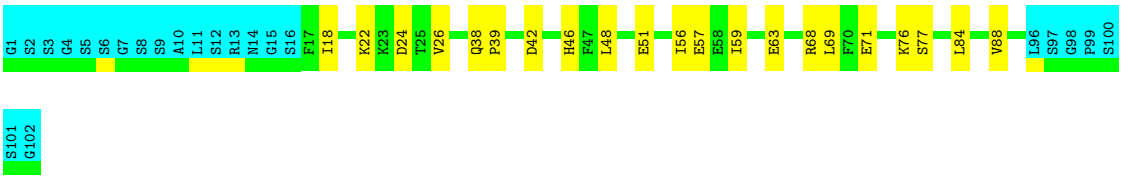
4 Residue-property plots (i)

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: Tumor necrosis factor receptor superfamily member 21

Chain A: 57% 21% 23%



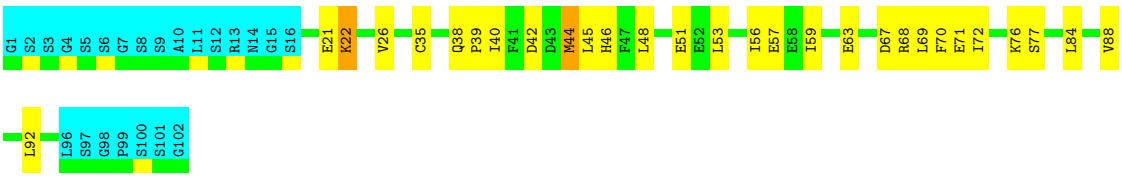
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Tumor necrosis factor receptor superfamily member 21

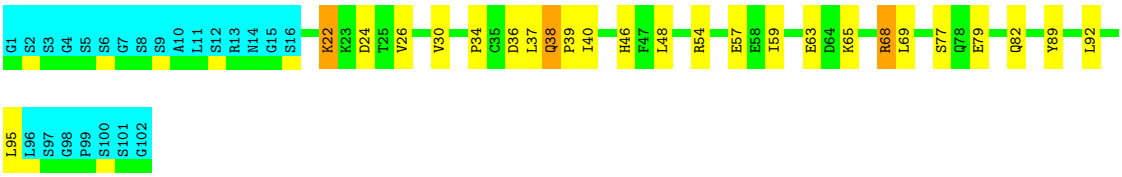
Chain A: 49% 26% • 23%



4.2.2 Score per residue for model 2

• Molecule 1: Tumor necrosis factor receptor superfamily member 21

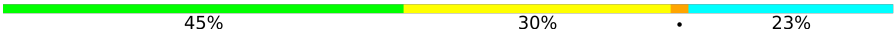
Chain A: 53% 22% • 23%

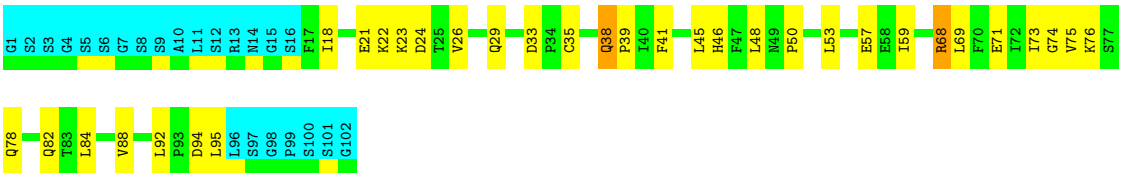


4.2.3 Score per residue for model 3

- Molecule 1: Tumor necrosis factor receptor superfamily member 21

Chain A:

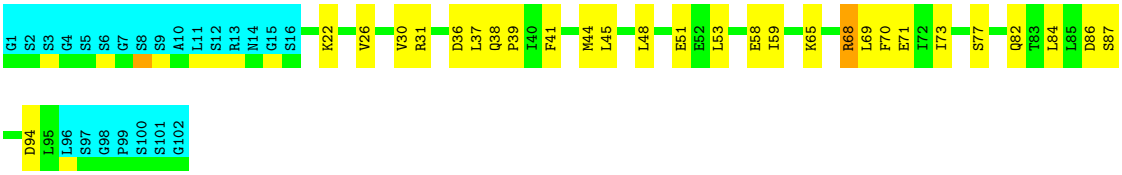




4.2.4 Score per residue for model 4

- Molecule 1: Tumor necrosis factor receptor superfamily member 21

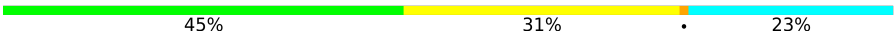
Chain A:

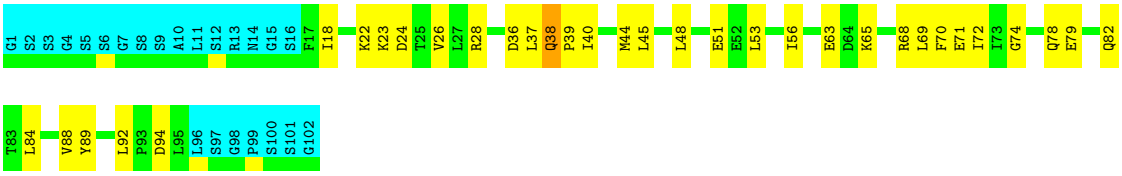


4.2.5 Score per residue for model 5

- Molecule 1: Tumor necrosis factor receptor superfamily member 21

Chain A:

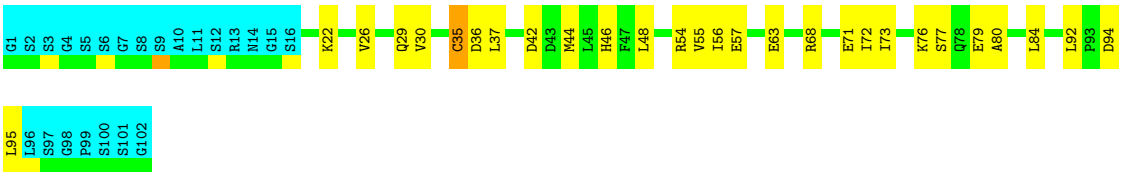




4.2.6 Score per residue for model 6

- Molecule 1: Tumor necrosis factor receptor superfamily member 21

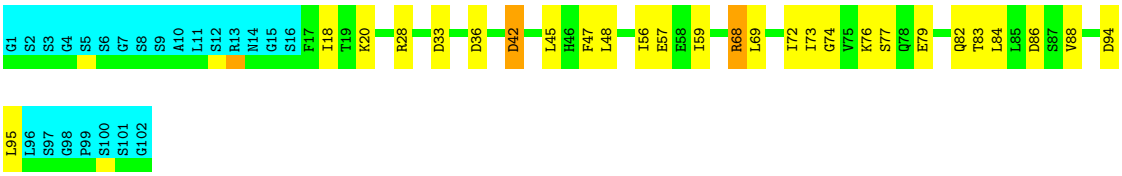
Chain A: 50% 26% • 23%



4.2.7 Score per residue for model 7

- Molecule 1: Tumor necrosis factor receptor superfamily member 21

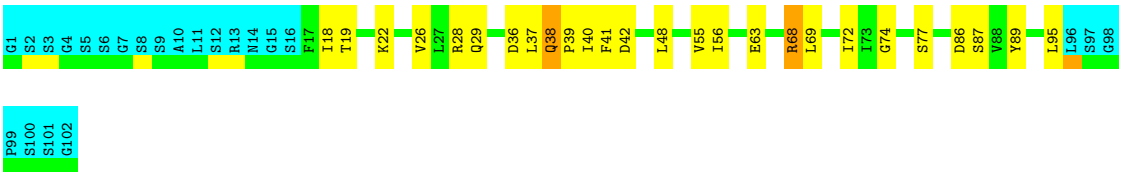
Chain A: 51% 25% • 23%



4.2.8 Score per residue for model 8

- Molecule 1: Tumor necrosis factor receptor superfamily member 21

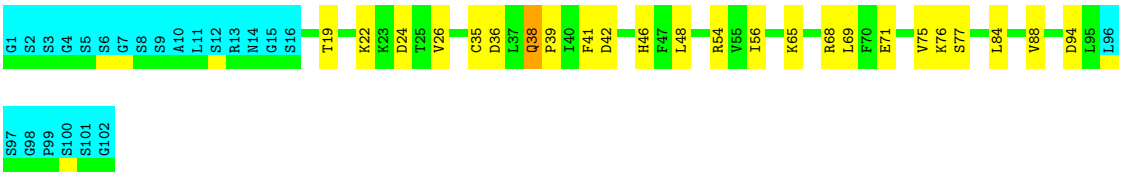
Chain A: 52% 24% • 23%



4.2.9 Score per residue for model 9

- Molecule 1: Tumor necrosis factor receptor superfamily member 21

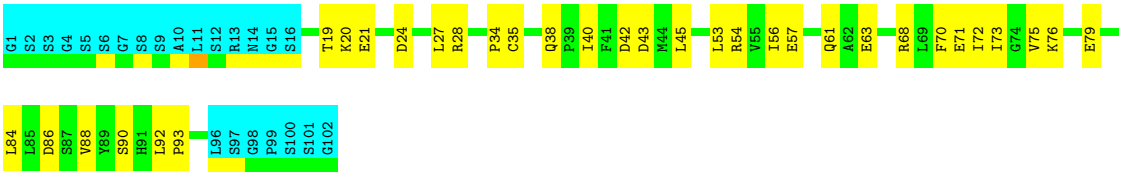
Chain A: 54% 23% • 23%



4.2.10 Score per residue for model 10

• Molecule 1: Tumor necrosis factor receptor superfamily member 21

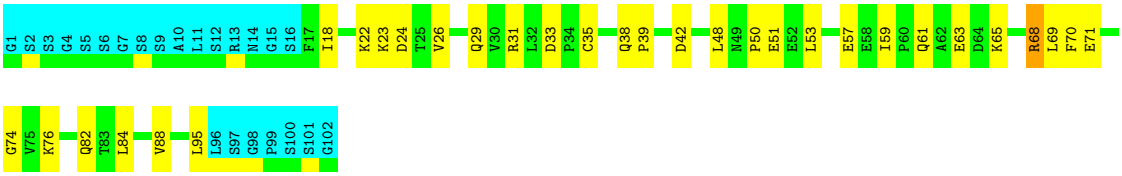
Chain A: 45% 32% 23%



4.2.11 Score per residue for model 11

• Molecule 1: Tumor necrosis factor receptor superfamily member 21

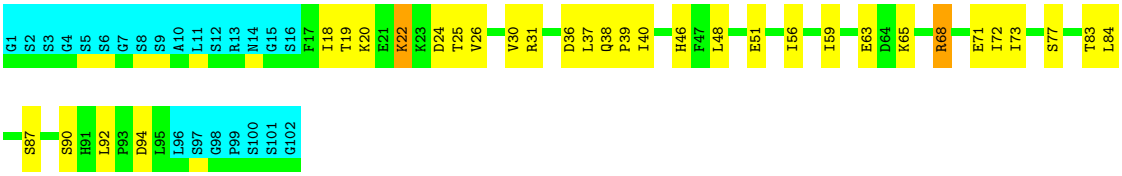
Chain A: 47% 29% • 23%



4.2.12 Score per residue for model 12

• Molecule 1: Tumor necrosis factor receptor superfamily member 21

Chain A: 46% 29% • 23%



4.2.13 Score per residue for model 13

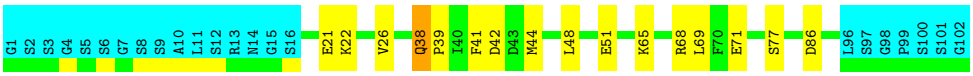
• Molecule 1: Tumor necrosis factor receptor superfamily member 21

Chain A: 60% 18% 23%

4.2.14 Score per residue for model 14 (medoid)

- Molecule 1: Tumor necrosis factor receptor superfamily member 21

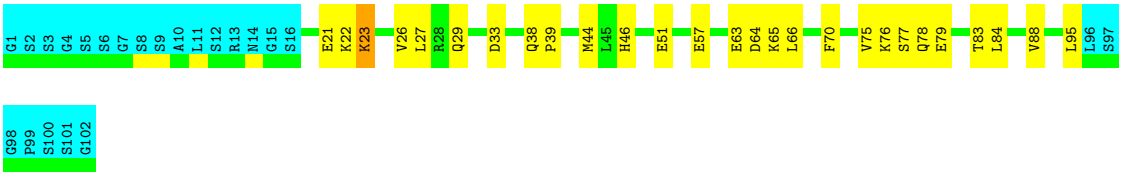
Chain A: 62% 15% • 23%



4.2.15 Score per residue for model 15

- Molecule 1: Tumor necrosis factor receptor superfamily member 21

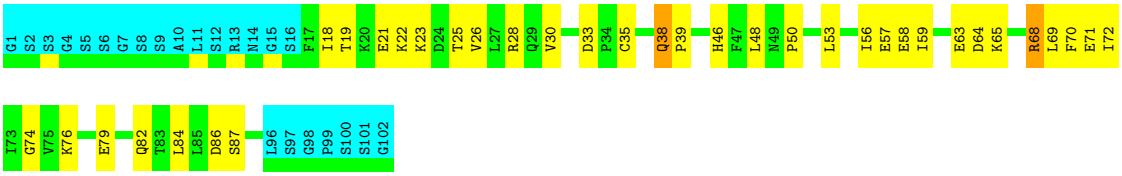
Chain A: 51% 25% • 23%



4.2.16 Score per residue for model 16

- Molecule 1: Tumor necrosis factor receptor superfamily member 21

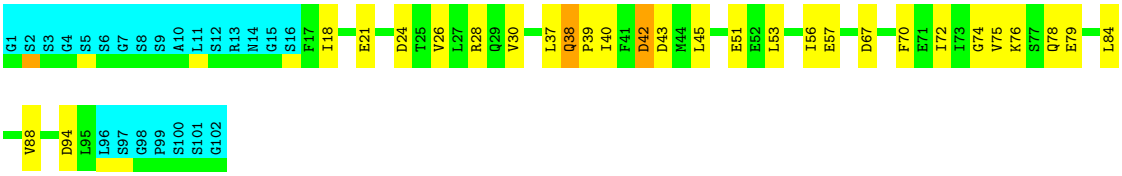
Chain A: 42% 33% • 23%



4.2.17 Score per residue for model 17

- Molecule 1: Tumor necrosis factor receptor superfamily member 21

Chain A: 50% 25% • 23%



4.2.18 Score per residue for model 18

- Molecule 1: Tumor necrosis factor receptor superfamily member 21

Chain A: 48% 27% • 23%

G1 S2 S3 G4 S5 S6 G7 S8 S9 A10 L11 S12 R13 N14 G15 S16 F17 I18 K22 K23 D24 T25 V26 L27 R28 R31 Q38 P39 D42 D43 M44 L45 H46 F47 L48 E51 E52 L53 E57 E58 I59 D64 K65 R68 L69 F70 E71 I72 I73 K76

E79 L84 V88 Y89 D94 L95 L96 S97 G98 P99 S100 S101 G102

4.2.19 Score per residue for model 19

- Molecule 1: Tumor necrosis factor receptor superfamily member 21

Chain A: 52% 24% • 23%

G1 S2 S3 G4 S5 S6 G7 S8 S9 A10 L11 S12 R13 N14 G15 S16 F17 I18 T19 K20 E21 K22 K23 P34 C35 Q38 P39 I40 F41 H46 F47 L48 E51 I56 I59 P60 Q61 L66 D67 R68 L69 F70 E71 I72 I73 G74 L84 L92 L96 S97

G98 P99 S100 S101 G102

4.2.20 Score per residue for model 20

- Molecule 1: Tumor necrosis factor receptor superfamily member 21

Chain A: 47% 29% • 23%

G1 S2 S3 G4 S5 S6 G7 S8 S9 A10 L11 S12 R13 N14 G15 S16 F17 I18 E21 K22 K23 D24 T25 V26 V30 D33 P34 L37 Q38 P39 I40 L45 H46 F47 L48 L53 R54 E57 E58 I59 E63 D64 R68 L69 F70 V75 K76 S77 Q78 E79

Q82 T83 L84 V88 L96 S97 G98 P99 S100 S101 G102

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
CNS	structure solution	1.1
CNS	refinement	1.1

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	649	652	652	11±4
All	All	12980	13040	13040	221

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 8.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:48:LEU:HD11	1:A:69:LEU:CD1	0.82	2.05	20	12
1:A:48:LEU:HD11	1:A:69:LEU:HD12	0.82	1.52	19	2
1:A:48:LEU:HD11	1:A:69:LEU:HD11	0.79	1.54	1	5
1:A:45:LEU:HD23	1:A:53:LEU:HD22	0.78	1.55	17	3
1:A:84:LEU:O	1:A:88:VAL:HG23	0.75	1.80	17	12
1:A:22:LYS:O	1:A:26:VAL:HG23	0.72	1.84	12	15
1:A:70:PHE:CD1	1:A:84:LEU:HD21	0.69	2.21	16	8
1:A:18:ILE:HD12	1:A:74:GLY:HA2	0.68	1.63	16	8
1:A:45:LEU:HD23	1:A:53:LEU:CD2	0.67	2.20	18	3
1:A:26:VAL:O	1:A:30:VAL:HG23	0.67	1.90	2	5
1:A:56:ILE:HD11	1:A:72:ILE:HD12	0.66	1.65	1	10
1:A:56:ILE:HD11	1:A:72:ILE:CD1	0.64	2.23	16	4
1:A:41:PHE:CE1	1:A:66:LEU:HD12	0.63	2.28	19	1
1:A:37:LEU:HD23	1:A:40:ILE:HD12	0.62	1.68	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:VAL:HG11	1:A:37:LEU:HD11	0.62	1.70	6	3
1:A:40:ILE:HD11	1:A:92:LEU:HD12	0.62	1.72	19	2
1:A:40:ILE:HD11	1:A:92:LEU:CD1	0.62	2.25	1	6
1:A:42:ASP:HA	1:A:45:LEU:HD12	0.61	1.72	18	3
1:A:18:ILE:CD1	1:A:84:LEU:HD23	0.61	2.26	18	3
1:A:55:VAL:HG12	1:A:68:ARG:HD3	0.60	1.73	6	2
1:A:73:ILE:HD12	1:A:84:LEU:HD13	0.59	1.74	4	2
1:A:40:ILE:HD11	1:A:92:LEU:HD11	0.57	1.76	1	2
1:A:36:ASP:O	1:A:37:LEU:HD23	0.57	1.98	4	1
1:A:45:LEU:CD2	1:A:53:LEU:HD22	0.57	2.30	10	2
1:A:37:LEU:CD2	1:A:40:ILE:HD12	0.56	2.30	2	1
1:A:59:ILE:HD11	1:A:68:ARG:HD2	0.56	1.76	19	11
1:A:44:MET:HG3	1:A:69:LEU:HD21	0.55	1.78	1	1
1:A:26:VAL:HG13	1:A:88:VAL:HG11	0.55	1.77	15	3
1:A:40:ILE:HD11	1:A:92:LEU:HG	0.55	1.79	2	1
1:A:40:ILE:HD12	1:A:88:VAL:HA	0.55	1.78	17	1
1:A:69:LEU:HD23	1:A:84:LEU:HD11	0.55	1.78	7	2
1:A:48:LEU:HD21	1:A:69:LEU:HD12	0.54	1.78	16	1
1:A:73:ILE:HG23	1:A:80:ALA:HB1	0.54	1.80	6	1
1:A:45:LEU:HA	1:A:48:LEU:HD12	0.53	1.78	20	2
1:A:48:LEU:HD21	1:A:69:LEU:CD1	0.53	2.33	3	1
1:A:59:ILE:HD11	1:A:68:ARG:CD	0.53	2.34	1	4
1:A:27:LEU:HD23	1:A:66:LEU:HD23	0.53	1.80	15	1
1:A:29:GLN:HB3	1:A:95:LEU:HD22	0.52	1.82	11	3
1:A:75:VAL:O	1:A:75:VAL:HG12	0.52	2.05	9	5
1:A:45:LEU:HD22	1:A:53:LEU:CD2	0.52	2.33	20	1
1:A:45:LEU:HD23	1:A:53:LEU:HD21	0.52	1.82	4	2
1:A:50:PRO:HA	1:A:53:LEU:HD12	0.51	1.81	16	3
1:A:36:ASP:O	1:A:92:LEU:HD21	0.51	2.06	5	1
1:A:37:LEU:HA	1:A:40:ILE:HD12	0.51	1.83	20	3
1:A:70:PHE:CG	1:A:84:LEU:HD21	0.50	2.42	11	5
1:A:41:PHE:CE1	1:A:69:LEU:HD13	0.49	2.41	4	1
1:A:41:PHE:CE1	1:A:69:LEU:HD22	0.49	2.42	3	3
1:A:48:LEU:HD13	1:A:56:ILE:HD12	0.48	1.86	8	2
1:A:92:LEU:HD12	1:A:95:LEU:HD11	0.48	1.84	2	1
1:A:30:VAL:CG1	1:A:37:LEU:HD11	0.47	2.39	6	2
1:A:45:LEU:HD22	1:A:53:LEU:HD22	0.47	1.86	10	1
1:A:92:LEU:HD13	1:A:95:LEU:HD11	0.47	1.87	3	1
1:A:37:LEU:HD23	1:A:92:LEU:HD11	0.47	1.87	5	1
1:A:47:PHE:CZ	1:A:83:THR:HG21	0.46	2.45	7	1
1:A:73:ILE:HD13	1:A:76:LYS:HE3	0.46	1.87	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:88:VAL:HG12	1:A:95:LEU:CD1	0.46	2.40	7	1
1:A:48:LEU:HD13	1:A:56:ILE:CD1	0.45	2.42	9	1
1:A:35:CYS:SG	1:A:92:LEU:HD22	0.45	2.51	6	1
1:A:38:GLN:N	1:A:39:PRO:HD2	0.45	2.27	18	1
1:A:92:LEU:HB2	1:A:95:LEU:HD12	0.45	1.87	3	1
1:A:27:LEU:HD22	1:A:63:GLU:HG2	0.44	1.87	10	1
1:A:18:ILE:HD12	1:A:74:GLY:CA	0.44	2.40	16	2
1:A:40:ILE:HD11	1:A:92:LEU:CG	0.44	2.41	2	1
1:A:48:LEU:HD11	1:A:69:LEU:HD13	0.44	1.87	16	1
1:A:73:ILE:HB	1:A:84:LEU:HD22	0.44	1.90	6	3
1:A:44:MET:O	1:A:48:LEU:HD12	0.43	2.14	6	1
1:A:48:LEU:CD1	1:A:56:ILE:HD12	0.42	2.44	9	1
1:A:38:GLN:N	1:A:39:PRO:CD	0.42	2.82	4	11
1:A:70:PHE:CE1	1:A:84:LEU:HD11	0.42	2.49	1	1
1:A:69:LEU:HG	1:A:73:ILE:HD12	0.42	1.90	18	1
1:A:38:GLN:CB	1:A:39:PRO:CD	0.42	2.98	2	3
1:A:44:MET:HG3	1:A:84:LEU:HD12	0.42	1.91	4	1
1:A:29:GLN:CD	1:A:95:LEU:HD22	0.42	2.34	8	2
1:A:92:LEU:CB	1:A:95:LEU:HD12	0.42	2.45	3	1
1:A:44:MET:SD	1:A:84:LEU:HD13	0.41	2.56	1	1
1:A:23:LYS:CG	1:A:70:PHE:CD2	0.41	3.04	15	1
1:A:44:MET:HE2	1:A:84:LEU:HD13	0.41	1.93	15	1
1:A:26:VAL:CG1	1:A:88:VAL:HG11	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	79/102 (77%)	73±2 (92±2%)	6±2 (8±2%)	0±1 (0±1%)	38	78
All	All	1580/2040 (77%)	1454 (92%)	119 (8%)	7 (0%)	38	78

All 3 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	34	PRO	4
1	A	35	CYS	2
1	A	18	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	76/92 (83%)	62±3 (82±4%)	14±3 (18±4%)	4	37
All	All	1520/1840 (83%)	1242 (82%)	278 (18%)	4	37

All 40 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	68	ARG	16
1	A	71	GLU	14
1	A	57	GLU	13
1	A	77	SER	12
1	A	46	HIS	11
1	A	51	GLU	11
1	A	24	ASP	11
1	A	38	GLN	11
1	A	42	ASP	10
1	A	63	GLU	10
1	A	76	LYS	10
1	A	65	LYS	10
1	A	79	GLU	10
1	A	21	GLU	9
1	A	82	GLN	9
1	A	94	ASP	9
1	A	28	ARG	7
1	A	19	THR	7
1	A	36	ASP	6
1	A	23	LYS	6
1	A	33	ASP	6
1	A	35	CYS	6
1	A	78	GLN	6

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Mol	Chain	Res	Type	Models (Total)
1	A	86	ASP	6
1	A	22	LYS	5
1	A	54	ARG	5
1	A	31	ARG	5
1	A	44	MET	4
1	A	87	SER	4
1	A	64	ASP	4
1	A	58	GLU	3
1	A	20	LYS	3
1	A	48	LEU	3
1	A	43	ASP	3
1	A	61	GLN	3
1	A	25	THR	3
1	A	67	ASP	2
1	A	90	SER	2
1	A	83	THR	2
1	A	41	PHE	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