Full wwPDB NMR Structure Validation Report (i)

Feb 27, 2022 – 02:40 PM EST

PDB ID	:	2DZM
Title	:	Solution Structure of the Ubiquitin-like Domain in Human FAS-associated factor 1 (hFAF1)
Authors	:	Zhao, C.; Sato, M.; Koshiba, S.; Watanabe, S.; Harada, T.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2006-09-29

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:

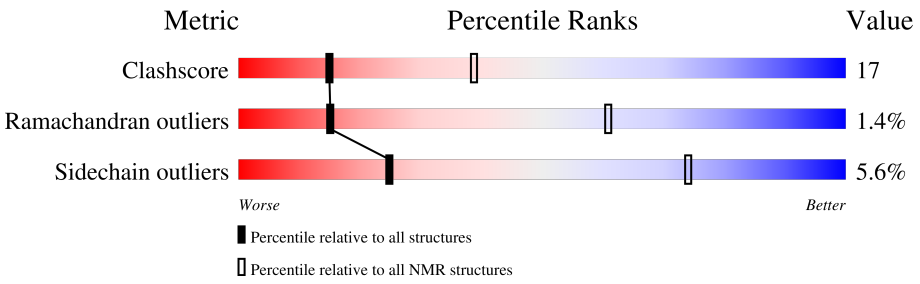
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	100	49% 22% • 28%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:8-A:54, A:59-A:83 (72)	0.17	1

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 and 2 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1538 atoms, of which 771 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called FAS-associated factor 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	100	1538	477	771	131	156	3	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q9UNN5
A	2	SER	-	expression tag	UNP Q9UNN5
A	3	SER	-	expression tag	UNP Q9UNN5
A	4	GLY	-	expression tag	UNP Q9UNN5
A	5	SER	-	expression tag	UNP Q9UNN5
A	6	SER	-	expression tag	UNP Q9UNN5
A	7	GLY	-	expression tag	UNP Q9UNN5

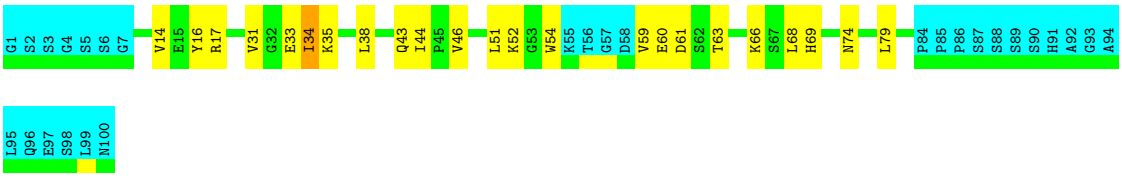
4 Residue-property plots (i)

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: FAS-associated factor 1

Chain A: 49% 22% • 28%



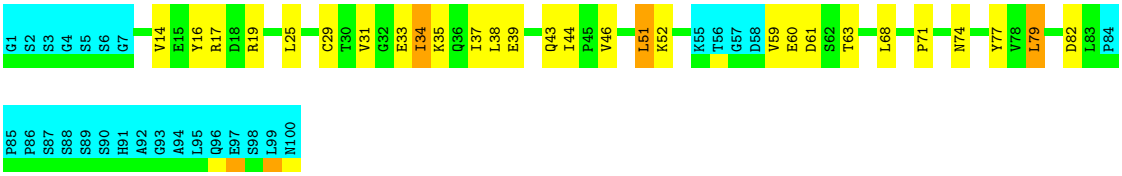
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: FAS-associated factor 1

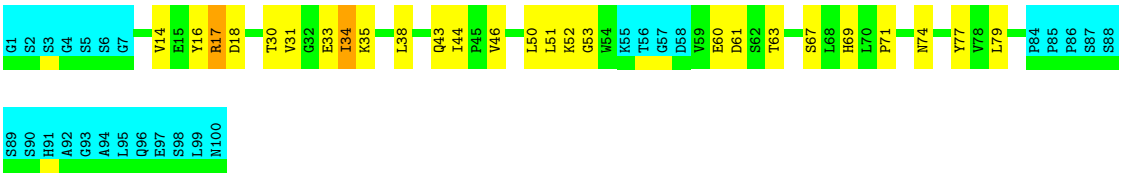
Chain A: 44% 25% • 28%



4.2.2 Score per residue for model 2

• Molecule 1: FAS-associated factor 1

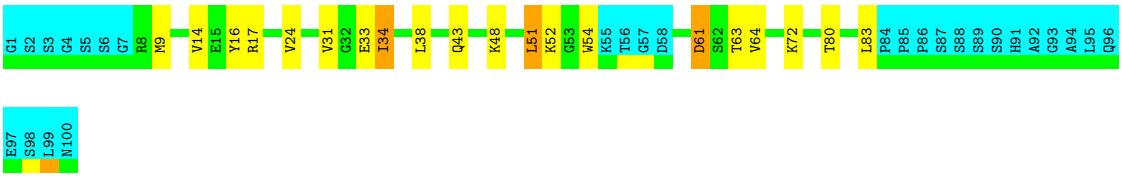
Chain A: 46% 24% • 28%



4.2.3 Score per residue for model 3

- Molecule 1: FAS-associated factor 1

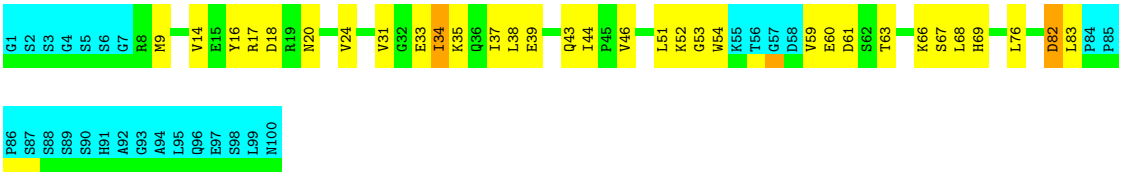
Chain A: 52% 17% • 28%



4.2.4 Score per residue for model 4

- Molecule 1: FAS-associated factor 1

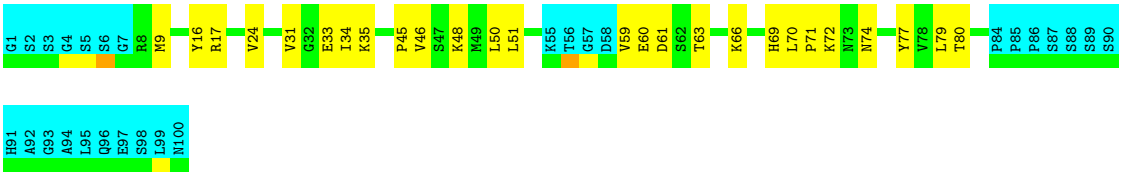
Chain A: 40% 30% • 28%



4.2.5 Score per residue for model 5

- Molecule 1: FAS-associated factor 1

Chain A: 46% 26% 28%



4.2.6 Score per residue for model 6

- Molecule 1: FAS-associated factor 1

Chain A: 43% 26% • 28%

G1 S2 S3 G4 S5 S6 G7 F12 R13 V14 E15 Y16 R17 L25 E26 D27 V31 G32 E33 I34 K35 L38 Q43 I44 P45 K48 L51 K52 G53 W54 K55 T56 G57 D58 V59 E60 D61 S62 T63 L68 H69 N74 L79 D82 L83 P84 P85 P86 S87 S88 S89 S90 H91 A92 G93 A94 L95 Q96 E97 S98 L99 N100

4.2.7 Score per residue for model 7

- Molecule 1: FAS-associated factor 1

Chain A: 43% 26% • 28%

G1 S2 S3 G4 S5 S6 G7 V14 E15 Y16 R17 D18 V31 G32 E33 I34 K35 L38 L42 Q43 V46 L51 K52 G53 W54 K55 T56 G57 D58 V59 E60 D61 S62 T63 S67 L68 H69 L70 P71 N74 S75 L76 Y77 V78 L79 T80 P84 P85 P86 S87 S88 S89 S90 H91 A92 G93 A94 L95 Q96 E97 S98 L99 N100

4.2.8 Score per residue for model 8

- Molecule 1: FAS-associated factor 1

Chain A: 38% 33% • 28%

G1 S2 S3 G4 S5 S6 G7 R8 M9 F12 R13 V14 E15 Y16 R17 D18 R19 N20 V21 D22 V23 V24 L25 E26 C29 T30 V31 G32 E33 I34 K35 Q36 I37 L38 Q43 V46 L51 K52 G53 W54 K55 T56 G57 D58 V59 E60 D61 S62 T63 V64 L65 K66 S67 L68 H69 Y77 V78 P84 P85 P86 S87 S88 S89 S90 H91 A92 G93 A94 L95 Q96 E97 S98 L99 N100

4.2.9 Score per residue for model 9

- Molecule 1: FAS-associated factor 1

Chain A: 45% 24% • 28%

G1 S2 S3 G4 S5 S6 G7 F12 R13 V14 E15 Y16 R17 D18 L25 T30 V31 G32 E33 I34 K35 Q36 I37 L38 Q43 I44 P45 V46 L51 K52 G53 W54 K55 T56 G57 D58 V59 E60 D61 S62 T63 L68 H69 L76 Y77 V78 D82 L83 P84 P85 P86 S87 S88 S89 S90 H91 A92 G93 A94 L95 Q96 E97 S98 L99 N100

4.2.10 Score per residue for model 10

- Molecule 1: FAS-associated factor 1

Chain A: 52% 17% • 28%

G1 S2 S3 G4 S5 S6 G7 F12 R13 V14 E15 Y16 R17 N20 V31 G32 E33 I34 K35 Q43 V46 L51 W54 K55 T56 G57 D58 V59 E60 D61 S62 T63 P71 N74 V78 P84 P85 P86 S87 S88 S89 S90 H91 A92 G93 A94 L95 Q96 E97 S98 L99 N100

4.2.11 Score per residue for model 11

- Molecule 1: FAS-associated factor 1

Chain A: 46% 23% • 28%

G1 S2 S3 G4 S5 S6 G7 R8 M9 F12 Y16 R17 D18 R19 V31 G32 E33 I34 Q43 I44 M49 L50 L51 K52 G53 W54 K55 T56 G57 D58 V59 E60 D61 S62 T63 L68 H69 L70 N74 Y77 V78 L79 P84 P85 P86 S87 S88 S89 S90 H91 A92 G93 A94 L95 Q96 E97 S98 L99 N100

4.2.12 Score per residue for model 12

- Molecule 1: FAS-associated factor 1

Chain A: 49% 22% • 28%

G1 S2 S3 G4 S5 S6 G7 V14 E15 Y16 R17 D18 R19 D27 T30 V31 G32 E33 I34 L38 Q43 I44 M49 L50 L51 K52 K55 T56 G57 D58 V59 E60 D61 S62 T63 L68 H69 L76 P84 P85 P86 S87 S88 S89 S90 H91 A92 G93 A94 L95 Q96 E97 S98 L99 N100

4.2.13 Score per residue for model 13

- Molecule 1: FAS-associated factor 1

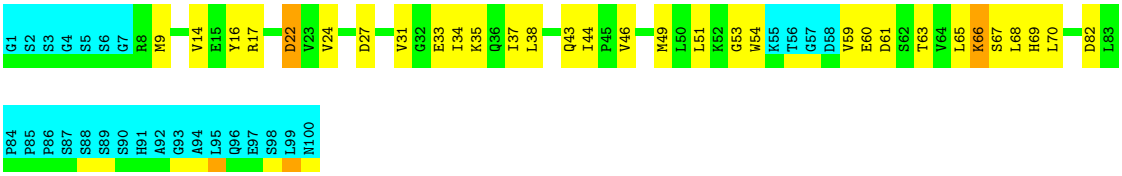
Chain A: 34% 35% • 28%

G1 S2 S3 G4 S5 S6 G7 R8 M9 F12 R13 V14 E15 Y16 R17 D18 R19 N20 V21 D22 V23 T30 V31 G32 E33 I34 K35 L38 E39 Q43 I44 P45 V46 L51 K52 K55 T56 G57 D58 V59 E60 D61 S62 T63 V64 L65 K66 S67 L68 H69 L70 P71 N74 S75 L76 Y77 V78 L79 D82 L83 P84 P85 P86 S87 S88 S89 S90 H91 A92 G93 A94 L95 Q96 E97 S98 L99 N100

4.2.14 Score per residue for model 14

- Molecule 1: FAS-associated factor 1

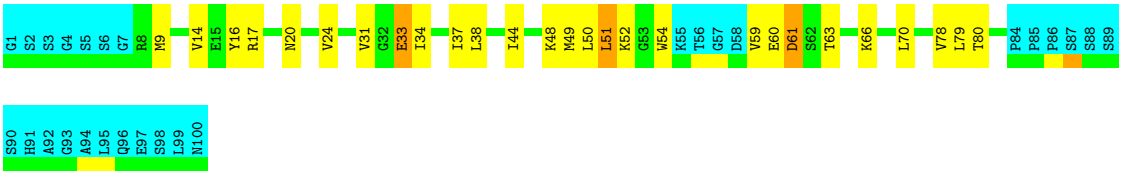
Chain A: 41% 29% • 28%



4.2.15 Score per residue for model 15

- Molecule 1: FAS-associated factor 1

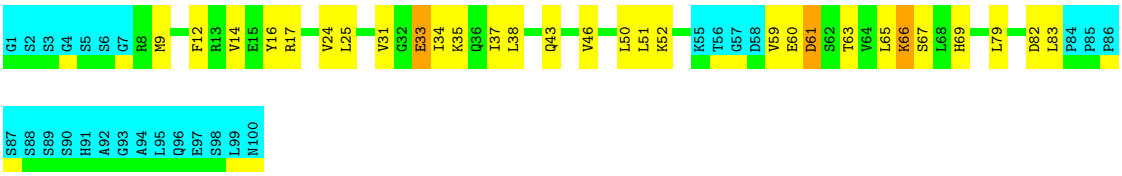
Chain A: 45% 24% • 28%



4.2.16 Score per residue for model 16

- Molecule 1: FAS-associated factor 1

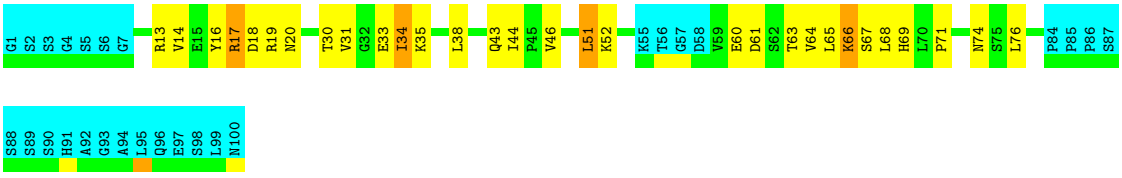
Chain A: 43% 26% • 28%



4.2.17 Score per residue for model 17

- Molecule 1: FAS-associated factor 1

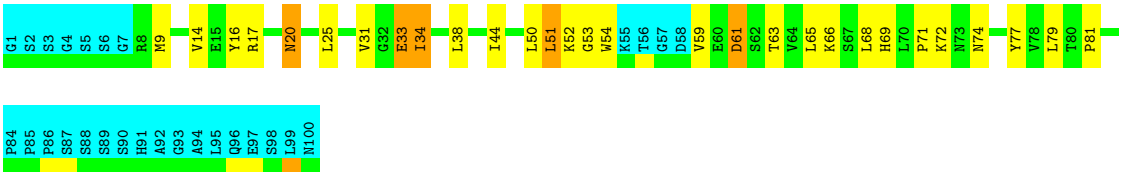
Chain A: 42% 26% • 28%



4.2.18 Score per residue for model 18

- Molecule 1: FAS-associated factor 1

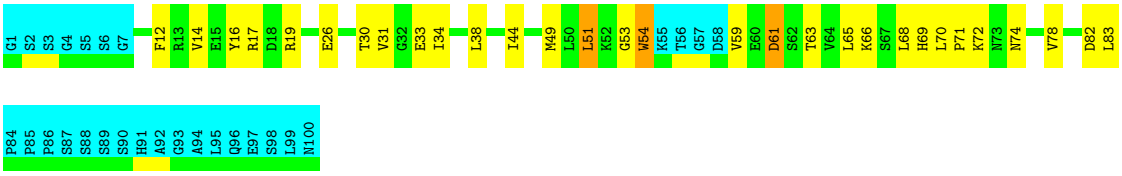
Chain A: 43% 24% 5% 28%



4.2.19 Score per residue for model 19

- Molecule 1: FAS-associated factor 1

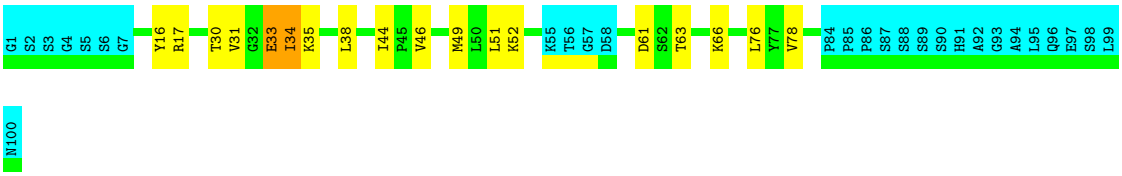
Chain A: 42% 27% • 28%



4.2.20 Score per residue for model 20

- Molecule 1: FAS-associated factor 1

Chain A: 54% 16% • 28%



5 Refinement protocol and experimental data overview (i)

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

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

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

Software name	Classification	Version
CYANA	structure solution	2.0.17
CYANA	refinement	2.0.17

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	586	606	605	20±4
All	All	11720	12120	12100	401

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 17.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:14:VAL:HG21	1:A:38:LEU:HD21	0.86	1.47	12	16
1:A:34:ILE:HA	1:A:37:ILE:HD12	0.77	1.54	8	5
1:A:59:VAL:HG21	1:A:68:LEU:HD11	0.73	1.61	18	9
1:A:52:LYS:CD	1:A:79:LEU:HD12	0.73	2.13	18	4
1:A:31:VAL:HG11	1:A:59:VAL:HG11	0.67	1.65	12	8
1:A:16:TYR:CE2	1:A:44:ILE:HD11	0.66	2.24	6	2
1:A:31:VAL:HG23	1:A:61:ASP:HA	0.65	1.68	14	20
1:A:48:LYS:O	1:A:80:THR:HG22	0.64	1.92	5	3
1:A:31:VAL:HG21	1:A:60:GLU:O	0.64	1.93	11	15
1:A:31:VAL:HG22	1:A:63:THR:O	0.63	1.92	17	20
1:A:35:LYS:HB3	1:A:46:VAL:HG13	0.61	1.72	8	13
1:A:77:TYR:CD2	1:A:79:LEU:HD11	0.60	2.31	11	3
1:A:12:PHE:CE2	1:A:74:ASN:OD1	0.59	2.55	19	1
1:A:52:LYS:HD2	1:A:79:LEU:HD12	0.58	1.73	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:12:PHE:CE2	1:A:25:LEU:HD21	0.58	2.33	16	3
1:A:66:LYS:O	1:A:69:HIS:CE1	0.57	2.57	14	8
1:A:66:LYS:O	1:A:69:HIS:CD2	0.57	2.57	16	2
1:A:52:LYS:HD3	1:A:79:LEU:HD12	0.57	1.76	18	1
1:A:79:LEU:HD12	1:A:79:LEU:N	0.56	2.14	11	3
1:A:52:LYS:HD2	1:A:79:LEU:HD13	0.56	1.78	11	1
1:A:51:LEU:HD12	1:A:54:TRP:NE1	0.56	2.16	18	6
1:A:16:TYR:CD2	1:A:18:ASP:OD1	0.54	2.60	17	5
1:A:42:LEU:C	1:A:43:GLN:NE2	0.54	2.60	7	1
1:A:70:LEU:HD12	1:A:74:ASN:OD1	0.54	2.02	5	1
1:A:34:ILE:CA	1:A:37:ILE:HD12	0.54	2.30	8	3
1:A:38:LEU:HD13	1:A:78:VAL:HG21	0.54	1.79	15	3
1:A:14:VAL:HG11	1:A:78:VAL:HG23	0.53	1.81	19	1
1:A:14:VAL:CG1	1:A:78:VAL:HG23	0.53	2.34	19	6
1:A:59:VAL:HG21	1:A:68:LEU:CD1	0.52	2.34	12	4
1:A:68:LEU:O	1:A:69:HIS:CG	0.52	2.62	6	3
1:A:59:VAL:HG12	1:A:60:GLU:N	0.52	2.19	7	1
1:A:53:GLY:HA3	1:A:77:TYR:CE2	0.51	2.40	2	1
1:A:31:VAL:HG12	1:A:54:TRP:CH2	0.51	2.40	3	2
1:A:12:PHE:CD2	1:A:25:LEU:HD21	0.51	2.39	6	1
1:A:16:TYR:CE1	1:A:17:ARG:HG2	0.51	2.41	18	3
1:A:68:LEU:C	1:A:69:HIS:CG	0.51	2.84	9	4
1:A:12:PHE:CD1	1:A:74:ASN:HB2	0.51	2.41	11	2
1:A:52:LYS:O	1:A:76:LEU:HD22	0.50	2.05	7	6
1:A:33:GLU:HG3	1:A:37:ILE:HD11	0.50	1.83	4	2
1:A:16:TYR:CE1	1:A:17:ARG:HD3	0.50	2.42	13	2
1:A:16:TYR:CE2	1:A:44:ILE:CD1	0.50	2.94	18	5
1:A:33:GLU:OE2	1:A:37:ILE:CG1	0.50	2.60	15	1
1:A:12:PHE:CD1	1:A:74:ASN:HB3	0.50	2.42	10	2
1:A:53:GLY:HA3	1:A:77:TYR:CE1	0.50	2.41	18	2
1:A:39:GLU:CG	1:A:44:ILE:O	0.50	2.60	4	3
1:A:9:MET:SD	1:A:24:VAL:CG1	0.50	3.00	5	4
1:A:30:THR:CG2	1:A:61:ASP:O	0.49	2.60	17	6
1:A:31:VAL:CG2	1:A:60:GLU:O	0.49	2.60	2	10
1:A:65:LEU:O	1:A:67:SER:N	0.49	2.44	17	3
1:A:20:ASN:N	1:A:20:ASN:OD1	0.49	2.46	8	2
1:A:12:PHE:CD2	1:A:25:LEU:CD2	0.49	2.96	6	2
1:A:67:SER:O	1:A:69:HIS:CD2	0.49	2.65	2	1
1:A:12:PHE:CZ	1:A:74:ASN:CG	0.49	2.86	19	1
1:A:71:PRO:O	1:A:74:ASN:ND2	0.48	2.46	2	7
1:A:14:VAL:HG21	1:A:38:LEU:HD11	0.48	1.85	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:THR:HG22	1:A:32:GLY:H	0.48	1.68	13	1
1:A:12:PHE:CD2	1:A:74:ASN:HB3	0.48	2.43	19	1
1:A:26:GLU:O	1:A:65:LEU:CD1	0.48	2.61	19	2
1:A:9:MET:HB3	1:A:24:VAL:HG13	0.48	1.86	4	5
1:A:59:VAL:CG1	1:A:60:GLU:N	0.48	2.76	7	1
1:A:48:LYS:HG3	1:A:83:LEU:HD13	0.47	1.84	3	1
1:A:18:ASP:CG	1:A:19:ARG:N	0.47	2.66	13	1
1:A:50:LEU:HD12	1:A:79:LEU:O	0.47	2.08	5	4
1:A:25:LEU:CD1	1:A:65:LEU:HD11	0.47	2.39	18	1
1:A:43:GLN:NE2	1:A:43:GLN:N	0.47	2.63	7	1
1:A:12:PHE:CE1	1:A:25:LEU:HD21	0.47	2.45	9	1
1:A:16:TYR:CE2	1:A:18:ASP:OD1	0.47	2.68	11	1
1:A:51:LEU:HD13	1:A:52:LYS:N	0.47	2.24	18	5
1:A:43:GLN:N	1:A:43:GLN:NE2	0.47	2.63	2	2
1:A:44:ILE:HG22	1:A:49:MET:CG	0.47	2.40	19	5
1:A:16:TYR:O	1:A:17:ARG:C	0.47	2.53	18	20
1:A:39:GLU:O	1:A:43:GLN:N	0.46	2.46	4	2
1:A:22:ASP:OD1	1:A:23:VAL:N	0.46	2.48	13	2
1:A:52:LYS:HB2	1:A:77:TYR:CE1	0.46	2.46	2	1
1:A:18:ASP:N	1:A:18:ASP:OD1	0.46	2.46	12	2
1:A:59:VAL:HG11	1:A:68:LEU:HD11	0.46	1.87	8	1
1:A:59:VAL:CG2	1:A:68:LEU:HD11	0.46	2.40	12	3
1:A:14:VAL:CG2	1:A:38:LEU:HD21	0.46	2.37	8	2
1:A:38:LEU:HD13	1:A:78:VAL:CG2	0.45	2.41	15	2
1:A:26:GLU:CD	1:A:29:CYS:SG	0.45	2.95	8	1
1:A:82:ASP:O	1:A:83:LEU:C	0.45	2.56	4	4
1:A:77:TYR:CE2	1:A:79:LEU:HD11	0.45	2.46	5	2
1:A:71:PRO:O	1:A:72:LYS:C	0.44	2.56	5	3
1:A:65:LEU:C	1:A:67:SER:N	0.44	2.70	17	4
1:A:17:ARG:O	1:A:18:ASP:C	0.44	2.55	2	2
1:A:53:GLY:O	1:A:54:TRP:C	0.44	2.55	14	5
1:A:61:ASP:C	1:A:61:ASP:OD1	0.44	2.55	19	1
1:A:33:GLU:O	1:A:34:ILE:C	0.44	2.56	19	20
1:A:64:VAL:O	1:A:67:SER:CB	0.44	2.65	17	1
1:A:50:LEU:HD12	1:A:81:PRO:HD3	0.44	1.87	18	1
1:A:12:PHE:CE2	1:A:74:ASN:CG	0.44	2.91	19	1
1:A:21:VAL:CG1	1:A:38:LEU:CD2	0.43	2.96	13	1
1:A:21:VAL:HG11	1:A:38:LEU:CD2	0.43	2.43	13	1
1:A:22:ASP:C	1:A:22:ASP:OD1	0.43	2.56	14	1
1:A:33:GLU:N	1:A:33:GLU:OE1	0.43	2.51	16	1
1:A:65:LEU:O	1:A:68:LEU:N	0.43	2.51	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:33:GLU:OE1	1:A:33:GLU:CA	0.43	2.66	15	1
1:A:18:ASP:OD1	1:A:18:ASP:N	0.43	2.52	4	3
1:A:25:LEU:HD11	1:A:65:LEU:HD11	0.43	1.89	18	1
1:A:12:PHE:CZ	1:A:74:ASN:OD1	0.43	2.71	19	1
1:A:68:LEU:O	1:A:69:HIS:CD2	0.43	2.72	6	1
1:A:27:ASP:N	1:A:27:ASP:OD1	0.42	2.52	12	1
1:A:12:PHE:CD1	1:A:74:ASN:CB	0.42	3.03	10	1
1:A:43:GLN:N	1:A:43:GLN:CD	0.42	2.72	7	1
1:A:63:THR:HG22	1:A:64:VAL:N	0.42	2.30	3	1
1:A:33:GLU:O	1:A:35:LYS:N	0.42	2.53	6	2
1:A:19:ARG:NH2	1:A:20:ASN:O	0.42	2.52	8	1
1:A:54:TRP:HB3	1:A:59:VAL:HG23	0.42	1.91	11	2
1:A:44:ILE:CG2	1:A:49:MET:CG	0.42	2.98	15	2
1:A:25:LEU:HD12	1:A:29:CYS:CB	0.41	2.45	1	1
1:A:16:TYR:CD1	1:A:17:ARG:N	0.41	2.89	7	1
1:A:44:ILE:O	1:A:49:MET:SD	0.41	2.78	20	3
1:A:70:LEU:HD22	1:A:70:LEU:N	0.41	2.30	19	1
1:A:68:LEU:HB2	1:A:70:LEU:CD2	0.41	2.45	11	2
1:A:17:ARG:NH2	1:A:80:THR:OG1	0.41	2.54	7	1
1:A:45:PRO:HG2	1:A:48:LYS:CG	0.41	2.46	5	2
1:A:30:THR:HG21	1:A:61:ASP:O	0.41	2.15	13	1
1:A:13:ARG:O	1:A:76:LEU:N	0.41	2.54	17	1
1:A:9:MET:SD	1:A:9:MET:N	0.40	2.94	11	2
1:A:44:ILE:CG2	1:A:49:MET:HG3	0.40	2.46	14	1
1:A:9:MET:N	1:A:9:MET:SD	0.40	2.94	18	1
1:A:26:GLU:HG3	1:A:27:ASP:N	0.40	2.32	6	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	72/100 (72%)	63±2 (88±3%)	8±2 (11±3%)	1±1 (1±1%)	15	61
All	All	1440/2000 (72%)	1268 (88%)	152 (11%)	20 (1%)	15	61

All 4 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	ILE	12
1	A	17	ARG	3
1	A	66	LYS	3
1	A	54	TRP	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	70/91 (77%)	66±2 (94±2%)	4±2 (6±2%)	25 74
All	All	1400/1820 (77%)	1322 (94%)	78 (6%)	25 74

All 18 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	51	LEU	20
1	A	43	GLN	10
1	A	61	ASP	7
1	A	20	ASN	7
1	A	33	GLU	6
1	A	82	ASP	5
1	A	19	ARG	4
1	A	79	LEU	4
1	A	66	LYS	3
1	A	30	THR	2
1	A	67	SER	2
1	A	18	ASP	2
1	A	72	LYS	1
1	A	69	HIS	1
1	A	74	ASN	1
1	A	22	ASP	1
1	A	27	ASP	1
1	A	70	LEU	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