Full wwPDB NMR Structure Validation Report (i)

Feb 22, 2022 – 10:11 AM EST

PDB ID	:	1WJT
Title	:	Solution structure of the N-terminal Domain I of mouse transcription elongation factor S-II protein 3
Authors	:	Yoneyama, M.; Tochio, N.; Koshiba, S.; Inoue, M.; Kigawa, T.; 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:

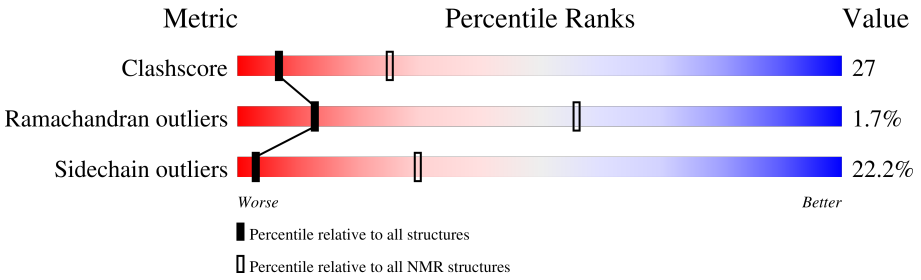
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	103	25% 41% • 30%

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:10-A:65, A:69-A:84 (72)	0.21	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 4 clusters and 1 single-model cluster was found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1622 atoms, of which 841 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcription elongation factor S-II protein 3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	103	1622	481	841	146	149	5	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	cloning artifact	UNP P23881
A	2	SER	-	cloning artifact	UNP P23881
A	3	SER	-	cloning artifact	UNP P23881
A	4	GLY	-	cloning artifact	UNP P23881
A	5	SER	-	cloning artifact	UNP P23881
A	6	SER	-	cloning artifact	UNP P23881
A	7	GLY	-	cloning artifact	UNP P23881
A	98	SER	-	cloning artifact	UNP P23881
A	99	GLY	-	cloning artifact	UNP P23881
A	100	PRO	-	cloning artifact	UNP P23881
A	101	SER	-	cloning artifact	UNP P23881
A	102	SER	-	cloning artifact	UNP P23881
A	103	GLY	-	cloning artifact	UNP P23881

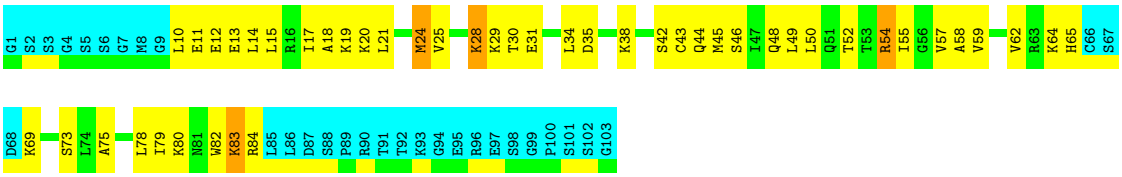
4 Residue-property plots (i)

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: Transcription elongation factor S-II protein 3

Chain A: 25% 41% • 30%



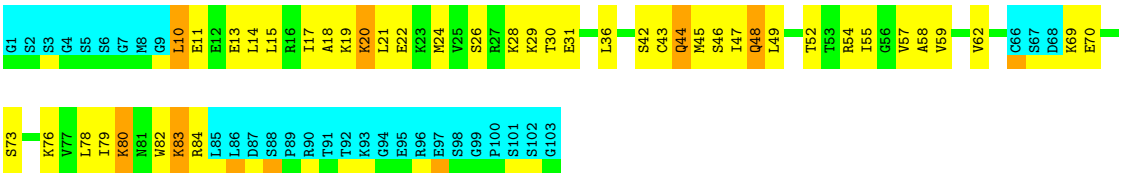
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Transcription elongation factor S-II protein 3

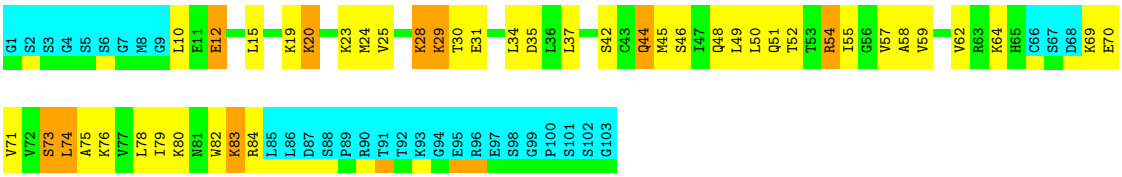
Chain A: 28% 36% 6% 30%



4.2.2 Score per residue for model 2

• Molecule 1: Transcription elongation factor S-II protein 3

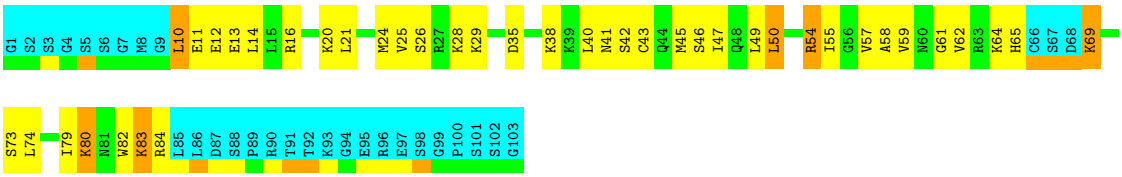
Chain A: 27% 34% 9% 30%



4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Transcription elongation factor S-II protein 3

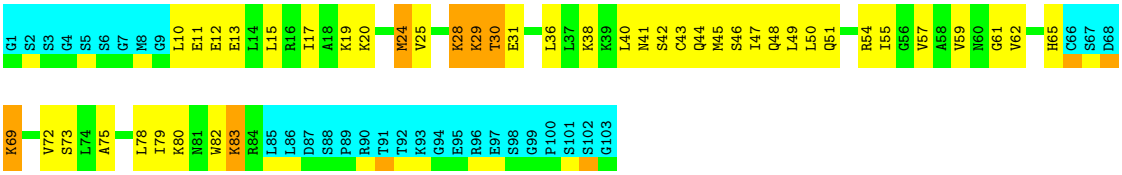
Chain A: 30% 34% 6% 30%



4.2.4 Score per residue for model 4

- Molecule 1: Transcription elongation factor S-II protein 3

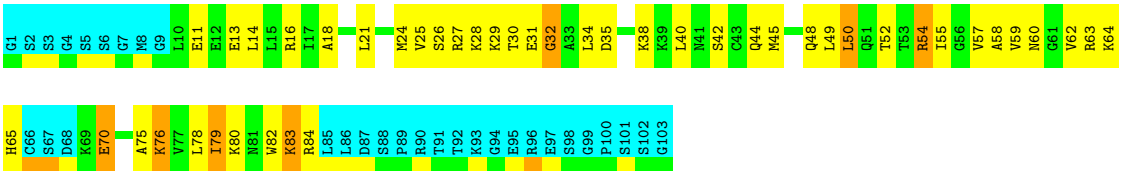
Chain A: 27% 37% 6% 30%



4.2.5 Score per residue for model 5

- Molecule 1: Transcription elongation factor S-II protein 3

Chain A: 26% 37% 7% 30%



4.2.6 Score per residue for model 6

- Molecule 1: Transcription elongation factor S-II protein 3

Chain A: 32% 35% • 30%

G1 S2 S3 G4 S5 S6 G7 M8 G9 L10 E11 E12 E13 L14 L15 R16 I17 A18 L21 E22 K23 M24 K28 K29 T30 E31 L40 N41 S42 C43 Q44 M45 S46 I47 Q48 L49 L50 R54 I55 G56 V57 A58 V59 V62 R63 K64 H65 C66 S67 D68 V71 V72 S73 L74

A75 K76 V77 L78 I79 K80 N81 W82 K83 R84 L85 L86 D87 S88 P89 R90 T91 T92 K93 G94 E95 R96 E97 S98 G99 P100 S101 S102 G103

4.2.7 Score per residue for model 7

- Molecule 1: Transcription elongation factor S-II protein 3

Chain A: 30% 30% 10% 30%

G1 S2 S3 G4 S5 S6 G7 M8 G9 L10 E11 E12 E13 L14 L15 R16 I17 A18 K19 K20 M24 V25 S26 R27 K28 K29 T30 A33 L34 D35 L36 L37 K38 K39 L40 N41 S42 C43 Q44 M45 L49 L50 R54 I55 G56 V57 A58 V59 V62 R63 K64 H65 C66 S67 D68

K69 E70 V71 V72 S73 L74 A75 L78 I79 K80 N81 W82 K83 R84 L85 L86 D87 S88 P89 R90 T91 T92 K93 G94 E95 R96 E97 S98 G99 P100 S101 S102 G103

4.2.8 Score per residue for model 8

- Molecule 1: Transcription elongation factor S-II protein 3

Chain A: 27% 36% 7% 30%

G1 S2 S3 G4 S5 S6 G7 M8 G9 L10 E11 E12 E13 L14 L15 R16 K19 M24 R27 K28 K29 T30 E31 L34 D35 L36 L37 K38 K39 L40 N41 S42 M45 S46 I47 Q48 L49 L50 R54 I55 G56 V57 A58 V59 N60 G61 V62 H65 C66 S67 D68 K69 E70

V71 V72 S73 L74 A75 L78 I79 K80 N81 W82 K83 R84 L85 L86 D87 S88 P89 R90 T91 T92 K93 G94 E95 R96 E97 S98 G99 P100 S101 S102 G103

4.2.9 Score per residue for model 9

- Molecule 1: Transcription elongation factor S-II protein 3

Chain A: 24% 38% 8% 30%

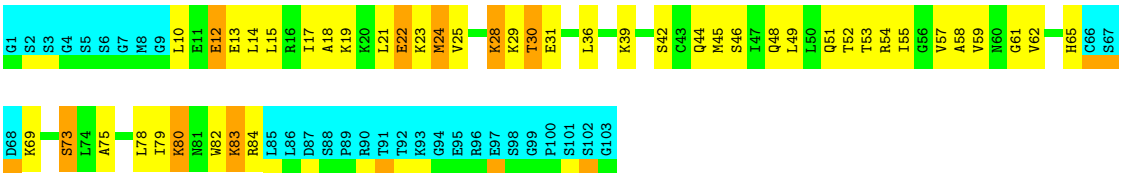
G1 S2 S3 G4 S5 S6 G7 M8 G9 L10 E11 E12 E13 L14 L15 R16 I17 A18 K19 K20 L21 E22 K23 M24 V25 S26 R27 K28 K29 G32 A33 L34 D35 K38 K39 L40 N41 S42 C43 S46 I47 Q48 L49 L50 Q51 T52 T53 R54 I55 G56 V57 A58 V59 V62 R63

C66 S67 D68 K69 E70 V71 V72 S73 L74 A75 L78 I79 K80 N81 W82 K83 R84 L85 L86 D87 S88 P89 R90 T91 T92 K93 G94 E95 R96 E97 S98 G99 P100 S101 S102 G103

4.2.10 Score per residue for model 10

- Molecule 1: Transcription elongation factor S-II protein 3

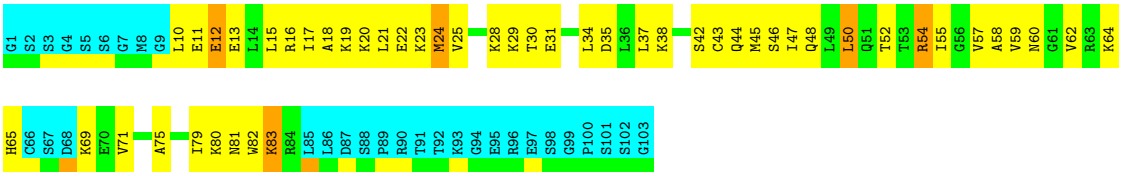
Chain A: 26% 36% 8% 30%



4.2.11 Score per residue for model 11

- Molecule 1: Transcription elongation factor S-II protein 3

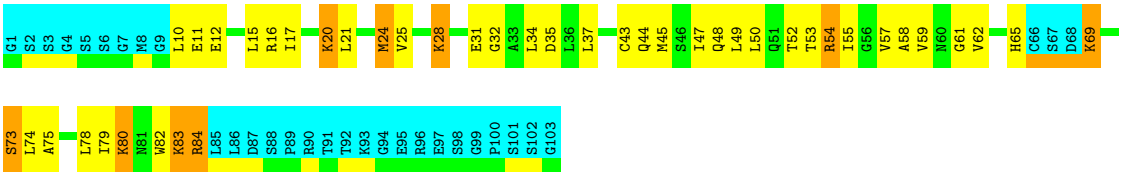
Chain A: 22% 43% 5% 30%



4.2.12 Score per residue for model 12

- Molecule 1: Transcription elongation factor S-II protein 3

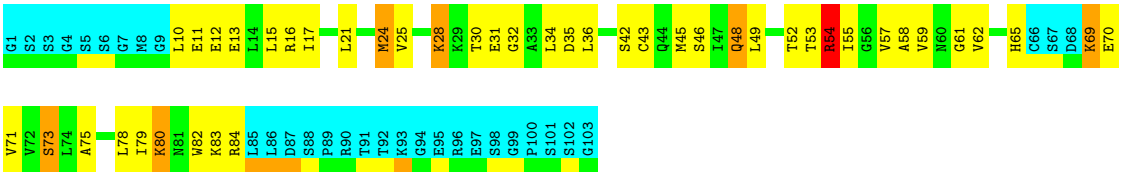
Chain A: 28% 33% 9% 30%



4.2.13 Score per residue for model 13

- Molecule 1: Transcription elongation factor S-II protein 3

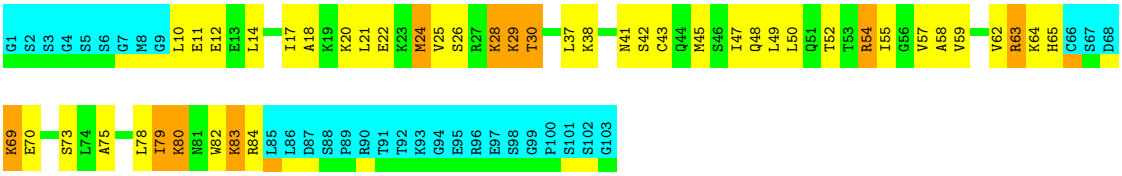
Chain A: 27% 36% 6% • 30%



4.2.14 Score per residue for model 14

• Molecule 1: Transcription elongation factor S-II protein 3

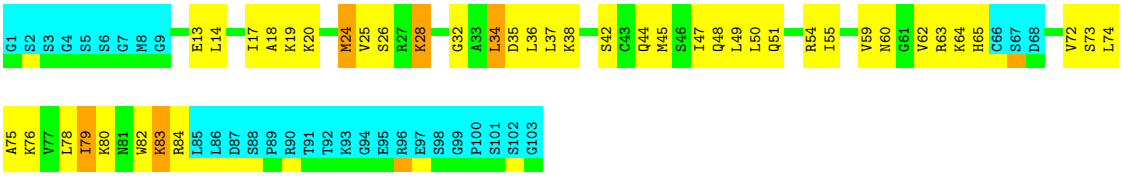
Chain A: 26% 34% 10% 30%



4.2.15 Score per residue for model 15

• Molecule 1: Transcription elongation factor S-II protein 3

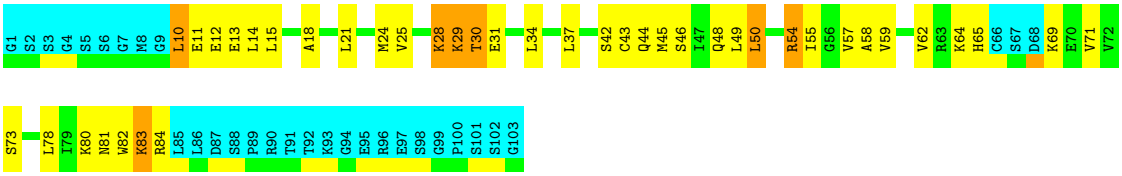
Chain A: 28% 37% 5% 30%



4.2.16 Score per residue for model 16

• Molecule 1: Transcription elongation factor S-II protein 3

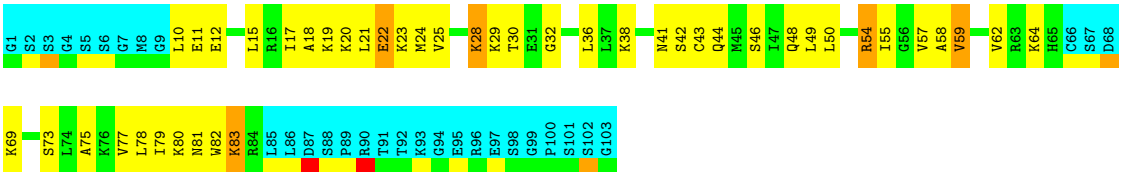
Chain A: 30% 33% 7% 30%



4.2.17 Score per residue for model 17

• Molecule 1: Transcription elongation factor S-II protein 3

Chain A: 27% 38% 5% 30%



4.2.18 Score per residue for model 18

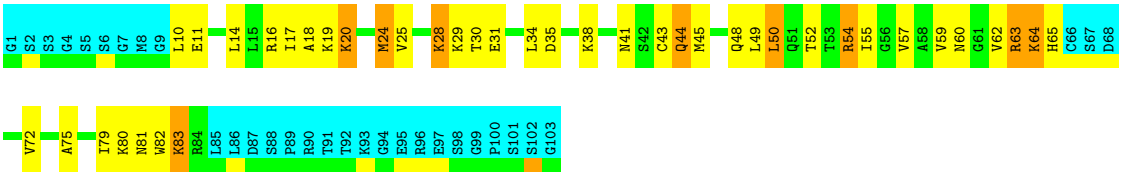
- Molecule 1: Transcription elongation factor S-II protein 3

Chain A: 21% 43% 6% 30%

4.2.19 Score per residue for model 19

- Molecule 1: Transcription elongation factor S-II protein 3

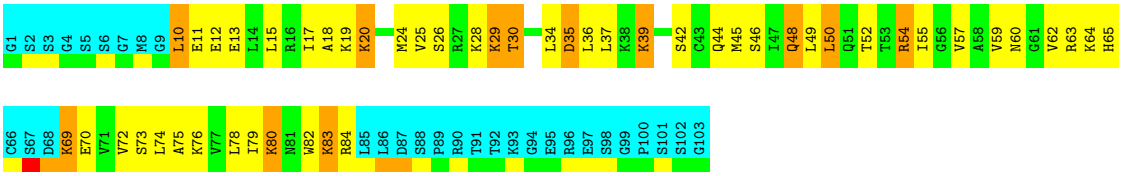
Chain A: 30% 31% 9% 30%



4.2.20 Score per residue for model 20

- Molecule 1: Transcription elongation factor S-II protein 3

Chain A: 21% 37% 12% 30%



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	576	652	652	34±5
All	All	11520	13040	13040	672

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 27.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:18:ALA:HB2	1:A:55:ILE:HD12	0.97	1.32	18	10
1:A:10:LEU:HD21	1:A:43:CYS:O	0.88	1.68	4	1
1:A:10:LEU:HD12	1:A:13:GLU:OE2	0.86	1.71	11	3
1:A:24:MET:HG3	1:A:30:THR:HG22	0.81	1.51	17	3
1:A:54:ARG:O	1:A:57:VAL:HG12	0.80	1.77	19	19
1:A:48:GLN:O	1:A:52:THR:HG23	0.78	1.78	12	11
1:A:58:ALA:O	1:A:62:VAL:HG23	0.78	1.77	11	16
1:A:21:LEU:O	1:A:25:VAL:HG23	0.76	1.80	18	6
1:A:11:GLU:O	1:A:15:LEU:HD12	0.74	1.83	11	6
1:A:18:ALA:CB	1:A:55:ILE:HD12	0.74	2.13	18	7
1:A:46:SER:HB2	1:A:49:LEU:HD12	0.73	1.60	3	5
1:A:11:GLU:OE2	1:A:49:LEU:HD23	0.73	1.84	9	6
1:A:10:LEU:HD11	1:A:43:CYS:HB3	0.73	1.61	16	7
1:A:75:ALA:O	1:A:79:ILE:HD12	0.72	1.85	14	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:55:ILE:HG23	1:A:82:TRP:CH2	0.71	2.20	19	14
1:A:45:MET:CE	1:A:55:ILE:HG21	0.70	2.17	2	12
1:A:24:MET:CG	1:A:30:THR:HG22	0.69	2.18	17	2
1:A:14:LEU:HD22	1:A:45:MET:CE	0.68	2.18	18	10
1:A:59:VAL:HG21	1:A:82:TRP:CH2	0.67	2.24	17	19
1:A:12:GLU:HA	1:A:15:LEU:HD12	0.66	1.68	12	6
1:A:75:ALA:O	1:A:79:ILE:HD13	0.65	1.91	9	14
1:A:30:THR:HG21	1:A:62:VAL:HG13	0.65	1.69	18	3
1:A:17:ILE:HG22	1:A:55:ILE:HD11	0.64	1.69	7	6
1:A:10:LEU:HD12	1:A:13:GLU:CD	0.63	2.12	4	1
1:A:25:VAL:HG13	1:A:65:HIS:CG	0.62	2.29	5	3
1:A:10:LEU:CD2	1:A:49:LEU:HD13	0.62	2.24	8	1
1:A:59:VAL:HG21	1:A:82:TRP:CZ3	0.62	2.29	18	9
1:A:24:MET:CB	1:A:30:THR:HG22	0.61	2.25	6	1
1:A:50:LEU:HD21	1:A:82:TRP:CD2	0.61	2.31	16	8
1:A:25:VAL:HG13	1:A:65:HIS:CD2	0.60	2.30	11	5
1:A:24:MET:HB3	1:A:30:THR:HG22	0.60	1.72	6	3
1:A:34:LEU:HD12	1:A:74:LEU:HD12	0.60	1.73	9	1
1:A:61:GLY:O	1:A:65:HIS:CD2	0.59	2.55	12	7
1:A:34:LEU:HD22	1:A:38:LYS:HE3	0.58	1.74	15	3
1:A:34:LEU:HD22	1:A:38:LYS:HE2	0.58	1.75	7	2
1:A:34:LEU:CD1	1:A:74:LEU:HD12	0.58	2.28	9	1
1:A:38:LYS:HG2	1:A:74:LEU:HD11	0.58	1.74	9	1
1:A:45:MET:HE1	1:A:55:ILE:HG21	0.58	1.76	2	8
1:A:45:MET:SD	1:A:82:TRP:CE2	0.58	2.97	19	4
1:A:34:LEU:HD22	1:A:38:LYS:CE	0.58	2.29	15	3
1:A:11:GLU:HB2	1:A:49:LEU:HD22	0.57	1.76	6	2
1:A:34:LEU:HD13	1:A:38:LYS:CE	0.57	2.30	15	4
1:A:63:ARG:NE	1:A:79:ILE:HD13	0.57	2.14	14	1
1:A:25:VAL:HG13	1:A:65:HIS:ND1	0.57	2.15	13	1
1:A:34:LEU:HD13	1:A:38:LYS:HE3	0.57	1.77	15	3
1:A:14:LEU:HD21	1:A:43:CYS:HB3	0.57	1.76	1	1
1:A:34:LEU:HD13	1:A:38:LYS:HE2	0.57	1.76	18	2
1:A:34:LEU:CD2	1:A:74:LEU:HD22	0.57	2.29	15	1
1:A:21:LEU:HD12	1:A:55:ILE:HD11	0.56	1.77	13	4
1:A:78:LEU:O	1:A:82:TRP:CG	0.56	2.59	9	16
1:A:13:GLU:O	1:A:17:ILE:HD12	0.56	2.00	1	5
1:A:18:ALA:HB2	1:A:55:ILE:CD1	0.56	2.22	18	5
1:A:45:MET:SD	1:A:82:TRP:CZ2	0.55	3.00	14	3
1:A:10:LEU:HD21	1:A:44:GLN:O	0.55	2.02	2	3
1:A:59:VAL:CG1	1:A:79:ILE:CD1	0.55	2.84	12	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:78:LEU:O	1:A:82:TRP:CD2	0.54	2.60	5	5
1:A:10:LEU:HD23	1:A:49:LEU:HD13	0.54	1.79	17	1
1:A:11:GLU:OE1	1:A:49:LEU:HD23	0.54	2.03	8	1
1:A:59:VAL:CG2	1:A:82:TRP:CH2	0.53	2.91	17	10
1:A:40:LEU:HD11	1:A:55:ILE:HD11	0.53	1.81	3	4
1:A:25:VAL:CG1	1:A:65:HIS:CE1	0.53	2.91	13	1
1:A:46:SER:O	1:A:50:LEU:HD12	0.52	2.04	4	4
1:A:25:VAL:CG2	1:A:62:VAL:HG22	0.52	2.35	10	1
1:A:34:LEU:HG	1:A:71:VAL:HG22	0.52	1.82	8	3
1:A:24:MET:CG	1:A:25:VAL:N	0.52	2.73	10	3
1:A:63:ARG:HG3	1:A:75:ALA:HB3	0.51	1.81	14	1
1:A:38:LYS:O	1:A:41:ASN:CB	0.51	2.58	4	1
1:A:80:LYS:O	1:A:83:LYS:CB	0.51	2.59	13	11
1:A:69:LYS:O	1:A:73:SER:CB	0.51	2.59	1	4
1:A:46:SER:OG	1:A:49:LEU:HD12	0.51	2.05	6	1
1:A:59:VAL:HG12	1:A:79:ILE:CD1	0.50	2.36	11	8
1:A:10:LEU:CD2	1:A:14:LEU:HD11	0.50	2.36	10	1
1:A:44:GLN:CG	1:A:44:GLN:O	0.50	2.60	4	2
1:A:34:LEU:HA	1:A:37:LEU:HD12	0.50	1.82	16	2
1:A:24:MET:SD	1:A:30:THR:HG22	0.50	2.47	17	2
1:A:11:GLU:OE2	1:A:49:LEU:CD2	0.50	2.60	5	3
1:A:72:VAL:O	1:A:75:ALA:HB3	0.50	2.06	4	1
1:A:11:GLU:OE1	1:A:49:LEU:CD2	0.49	2.61	12	2
1:A:55:ILE:CG2	1:A:82:TRP:CH2	0.49	2.94	19	3
1:A:10:LEU:CD2	1:A:14:LEU:HD12	0.49	2.38	3	1
1:A:17:ILE:HG23	1:A:36:LEU:HB3	0.48	1.83	4	1
1:A:75:ALA:O	1:A:79:ILE:CD1	0.48	2.62	19	12
1:A:34:LEU:O	1:A:35:ASP:C	0.48	2.51	18	7
1:A:69:LYS:O	1:A:73:SER:N	0.48	2.47	3	10
1:A:80:LYS:O	1:A:83:LYS:N	0.47	2.48	5	18
1:A:10:LEU:HD11	1:A:43:CYS:CB	0.47	2.37	16	3
1:A:21:LEU:O	1:A:23:LYS:N	0.47	2.48	10	2
1:A:11:GLU:OE1	1:A:49:LEU:HD21	0.47	2.09	7	1
1:A:10:LEU:HD21	1:A:14:LEU:CD1	0.47	2.40	3	1
1:A:45:MET:HE3	1:A:82:TRP:CZ2	0.47	2.45	20	4
1:A:13:GLU:OE1	1:A:13:GLU:CA	0.47	2.63	16	2
1:A:63:ARG:CZ	1:A:79:ILE:HD13	0.47	2.39	14	1
1:A:79:ILE:O	1:A:83:LYS:N	0.47	2.48	6	5
1:A:34:LEU:HB2	1:A:71:VAL:HG22	0.46	1.87	13	2
1:A:10:LEU:CD2	1:A:44:GLN:O	0.46	2.64	2	1
1:A:17:ILE:O	1:A:20:LYS:N	0.46	2.49	19	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:50:LEU:O	1:A:54:ARG:N	0.46	2.49	6	4
1:A:24:MET:HE2	1:A:36:LEU:CD1	0.46	2.40	13	1
1:A:59:VAL:CG2	1:A:82:TRP:CZ3	0.46	2.99	17	2
1:A:10:LEU:O	1:A:13:GLU:N	0.46	2.49	3	3
1:A:25:VAL:O	1:A:28:LYS:N	0.46	2.48	2	9
1:A:54:ARG:O	1:A:57:VAL:CG1	0.46	2.64	9	6
1:A:24:MET:O	1:A:28:LYS:N	0.46	2.48	17	11
1:A:34:LEU:O	1:A:37:LEU:N	0.46	2.48	18	6
1:A:63:ARG:NE	1:A:76:LYS:CG	0.46	2.79	15	1
1:A:12:GLU:CA	1:A:15:LEU:HD12	0.46	2.38	6	2
1:A:21:LEU:O	1:A:24:MET:N	0.46	2.49	6	3
1:A:14:LEU:HD22	1:A:45:MET:HE1	0.46	1.86	3	2
1:A:20:LYS:O	1:A:23:LYS:CG	0.45	2.64	2	1
1:A:14:LEU:HD22	1:A:45:MET:HE2	0.45	1.88	16	1
1:A:50:LEU:HD21	1:A:82:TRP:CE3	0.45	2.45	16	1
1:A:32:GLY:O	1:A:36:LEU:HD12	0.45	2.11	17	1
1:A:39:LYS:O	1:A:42:SER:N	0.45	2.49	18	2
1:A:14:LEU:CD2	1:A:40:LEU:HD23	0.45	2.42	18	2
1:A:82:TRP:O	1:A:83:LYS:C	0.45	2.55	18	6
1:A:64:LYS:HG2	1:A:65:HIS:CD2	0.45	2.47	15	1
1:A:38:LYS:O	1:A:41:ASN:N	0.45	2.50	14	5
1:A:55:ILE:O	1:A:58:ALA:N	0.45	2.50	14	1
1:A:14:LEU:CD2	1:A:45:MET:CE	0.45	2.95	14	1
1:A:76:LYS:O	1:A:79:ILE:N	0.45	2.50	20	3
1:A:59:VAL:O	1:A:62:VAL:N	0.45	2.50	4	7
1:A:34:LEU:O	1:A:38:LYS:N	0.45	2.49	5	2
1:A:55:ILE:HD12	1:A:58:ALA:HB3	0.44	1.89	9	1
1:A:53:THR:O	1:A:55:ILE:N	0.44	2.50	13	1
1:A:55:ILE:HG23	1:A:82:TRP:CZ3	0.44	2.47	19	1
1:A:21:LEU:CD2	1:A:36:LEU:HD13	0.44	2.42	17	2
1:A:18:ALA:O	1:A:21:LEU:N	0.44	2.50	16	3
1:A:14:LEU:HD21	1:A:43:CYS:CB	0.44	2.40	1	1
1:A:18:ALA:O	1:A:22:GLU:N	0.44	2.49	1	5
1:A:73:SER:O	1:A:76:LYS:N	0.44	2.50	1	1
1:A:37:LEU:CD1	1:A:71:VAL:O	0.44	2.66	7	1
1:A:80:LYS:C	1:A:82:TRP:N	0.44	2.71	16	2
1:A:45:MET:HE3	1:A:55:ILE:HG21	0.44	1.90	5	2
1:A:43:CYS:O	1:A:45:MET:N	0.44	2.50	14	2
1:A:14:LEU:HD22	1:A:45:MET:HE3	0.44	1.89	18	1
1:A:12:GLU:O	1:A:15:LEU:N	0.44	2.51	20	1
1:A:11:GLU:HG2	1:A:15:LEU:HD11	0.44	1.90	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:24:MET:CE	1:A:36:LEU:HD12	0.44	2.43	15	2
1:A:60:ASN:O	1:A:63:ARG:N	0.44	2.51	19	1
1:A:10:LEU:HD21	1:A:14:LEU:HD12	0.44	1.89	3	1
1:A:21:LEU:C	1:A:23:LYS:N	0.44	2.70	17	2
1:A:21:LEU:O	1:A:22:GLU:C	0.43	2.56	10	4
1:A:74:LEU:O	1:A:75:ALA:C	0.43	2.57	20	2
1:A:77:VAL:O	1:A:81:ASN:N	0.43	2.49	17	1
1:A:23:LYS:CG	1:A:24:MET:N	0.43	2.81	9	2
1:A:37:LEU:CB	1:A:74:LEU:HD23	0.43	2.43	20	1
1:A:29:LYS:O	1:A:30:THR:C	0.43	2.57	2	5
1:A:78:LEU:O	1:A:82:TRP:CE3	0.43	2.71	5	1
1:A:10:LEU:O	1:A:12:GLU:N	0.43	2.52	11	1
1:A:52:THR:OG1	1:A:53:THR:N	0.43	2.52	12	1
1:A:80:LYS:O	1:A:82:TRP:N	0.43	2.52	16	2
1:A:83:LYS:O	1:A:84:ARG:C	0.42	2.57	20	4
1:A:10:LEU:HD21	1:A:14:LEU:HD11	0.42	1.91	10	1
1:A:53:THR:C	1:A:55:ILE:N	0.42	2.72	13	1
1:A:24:MET:SD	1:A:30:THR:CB	0.42	3.07	17	1
1:A:14:LEU:CD2	1:A:40:LEU:CD2	0.42	2.97	8	2
1:A:37:LEU:O	1:A:78:LEU:HD11	0.42	2.15	14	1
1:A:49:LEU:C	1:A:51:GLN:N	0.42	2.71	2	4
1:A:62:VAL:C	1:A:64:LYS:N	0.42	2.72	19	4
1:A:30:THR:C	1:A:32:GLY:N	0.42	2.72	5	1
1:A:80:LYS:O	1:A:81:ASN:C	0.42	2.58	16	4
1:A:10:LEU:HD23	1:A:11:GLU:N	0.42	2.30	3	1
1:A:25:VAL:CG1	1:A:65:HIS:ND1	0.42	2.83	4	2
1:A:24:MET:HG3	1:A:25:VAL:N	0.42	2.30	10	2
1:A:20:LYS:HE2	1:A:36:LEU:HD11	0.42	1.91	20	1
1:A:76:LYS:O	1:A:77:VAL:C	0.42	2.58	6	1
1:A:11:GLU:CD	1:A:49:LEU:CD2	0.42	2.88	13	1
1:A:72:VAL:O	1:A:73:SER:C	0.42	2.58	4	1
1:A:48:GLN:O	1:A:52:THR:OG1	0.41	2.38	9	1
1:A:15:LEU:O	1:A:16:ARG:C	0.41	2.59	8	1
1:A:11:GLU:C	1:A:15:LEU:HD12	0.41	2.36	9	1
1:A:25:VAL:HG22	1:A:62:VAL:HG22	0.41	1.91	10	1
1:A:25:VAL:CG1	1:A:65:HIS:CD2	0.41	3.03	20	1
1:A:20:LYS:O	1:A:24:MET:SD	0.41	2.78	7	2
1:A:18:ALA:CA	1:A:55:ILE:HD12	0.41	2.46	17	2
1:A:10:LEU:O	1:A:11:GLU:C	0.41	2.59	4	5
1:A:37:LEU:HB2	1:A:74:LEU:HD23	0.41	1.91	20	1
1:A:11:GLU:O	1:A:12:GLU:C	0.41	2.58	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:34:LEU:HD23	1:A:34:LEU:HA	0.41	1.79	11	1
1:A:20:LYS:HD3	1:A:36:LEU:HD21	0.41	1.92	1	1
1:A:49:LEU:O	1:A:53:THR:N	0.41	2.54	10	1
1:A:32:GLY:O	1:A:36:LEU:CD1	0.41	2.68	17	1
1:A:34:LEU:CD1	1:A:74:LEU:HD22	0.41	2.46	2	1
1:A:17:ILE:O	1:A:18:ALA:C	0.41	2.58	18	3
1:A:59:VAL:O	1:A:60:ASN:C	0.41	2.59	20	2
1:A:53:THR:O	1:A:54:ARG:C	0.41	2.58	13	1
1:A:49:LEU:O	1:A:50:LEU:C	0.41	2.59	17	1
1:A:69:LYS:O	1:A:72:VAL:N	0.41	2.46	20	1
1:A:27:ARG:O	1:A:28:LYS:C	0.41	2.60	5	1
1:A:30:THR:O	1:A:32:GLY:N	0.40	2.54	5	1
1:A:13:GLU:OE1	1:A:13:GLU:O	0.40	2.39	7	2
1:A:13:GLU:CD	1:A:43:CYS:SG	0.40	2.99	13	1
1:A:33:ALA:HB3	1:A:71:VAL:HG13	0.40	1.92	7	1
1:A:55:ILE:HD12	1:A:58:ALA:CB	0.40	2.47	9	1
1:A:14:LEU:HD23	1:A:40:LEU:HD23	0.40	1.92	18	1
1:A:29:LYS:C	1:A:30:THR:OG1	0.40	2.60	4	1
1:A:33:ALA:O	1:A:34:LEU:C	0.40	2.60	7	1
1:A:63:ARG:HG3	1:A:75:ALA:CB	0.40	2.46	14	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	72/103 (70%)	53±2 (73±3%)	18±3 (25±4%)	1±1 (2±1%)	13	56
All	All	1440/2060 (70%)	1054 (73%)	361 (25%)	25 (2%)	13	56

All 9 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	30	THR	11
1	A	32	GLY	6

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Mol	Chain	Res	Type	Models (Total)
1	A	22	GLU	2
1	A	44	GLN	1
1	A	45	MET	1
1	A	54	ARG	1
1	A	59	VAL	1
1	A	29	LYS	1
1	A	69	LYS	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	65/89 (73%)	51±2 (78±3%)	14±2 (22±3%)	3 30
All	All	1300/1780 (73%)	1012 (78%)	288 (22%)	3 30

All 37 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	28	LYS	18
1	A	24	MET	17
1	A	42	SER	17
1	A	83	LYS	17
1	A	54	ARG	15
1	A	29	LYS	14
1	A	19	LYS	12
1	A	31	GLU	12
1	A	44	GLN	11
1	A	20	LYS	10
1	A	48	GLN	10
1	A	84	ARG	10
1	A	12	GLU	10
1	A	73	SER	10
1	A	69	LYS	10
1	A	80	LYS	9
1	A	64	LYS	9
1	A	16	ARG	9

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Mol	Chain	Res	Type	Models (Total)
1	A	50	LEU	8
1	A	26	SER	7
1	A	70	GLU	7
1	A	35	ASP	7
1	A	10	LEU	5
1	A	46	SER	5
1	A	74	LEU	4
1	A	13	GLU	4
1	A	63	ARG	3
1	A	79	ILE	3
1	A	27	ARG	3
1	A	39	LYS	3
1	A	43	CYS	2
1	A	60	ASN	2
1	A	76	LYS	1
1	A	23	LYS	1
1	A	52	THR	1
1	A	34	LEU	1
1	A	55	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