Full wwPDB NMR Structure Validation Report (i)

Mar 1, 2022 – 01:01 PM EST

PDB ID	:	2FI2
Title	:	Solution structure of the SCAN homodimer from MZF-1/ZNF42
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Deposited on	:	2005-12-27

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:

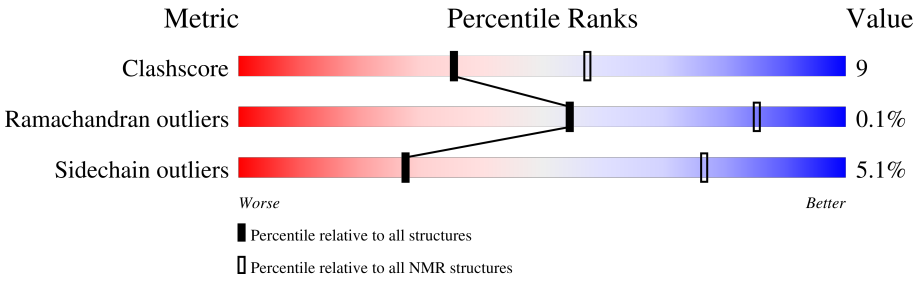
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	94	74% 15% 11%
1	B	94	73% 17% 10%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 5 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:40-A:123, B:39-B:123 (169)	0.46	5

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2941 atoms, of which 1464 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Zinc finger protein 42.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	94	1471	459	733	139	137	3	0
1	B	94	1470	459	731	139	138	3	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	GLY	-	cloning artifact	UNP P28698
A	36	SER	-	cloning artifact	UNP P28698
B	35	GLY	-	cloning artifact	UNP P28698
B	36	SER	-	cloning artifact	UNP P28698

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

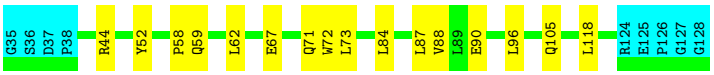
These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for 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: Zinc finger protein 42

Chain A: 74% 15% 11%

• Molecule 1: Zinc finger protein 42

Chain B: 73% 17% 10%



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: Zinc finger protein 42

Chain A: 68% 19% • 11%

• Molecule 1: Zinc finger protein 42

Chain B: 68% 20% • 10%

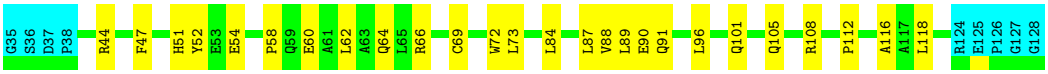
4.2.2 Score per residue for model 2

- Molecule 1: Zinc finger protein 42

Chain A: 65% 22% • 11%

- Molecule 1: Zinc finger protein 42

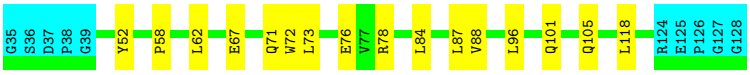
Chain B: 63% 28% 10%



4.2.3 Score per residue for model 3

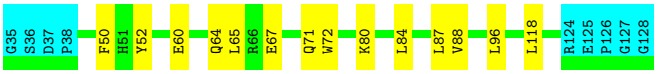
- Molecule 1: Zinc finger protein 42

Chain A: 72% 17% 11%



- Molecule 1: Zinc finger protein 42

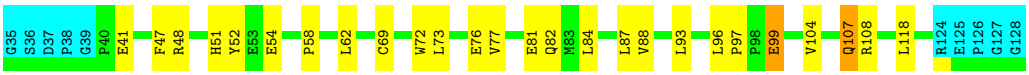
Chain B: 76% 15% 10%



4.2.4 Score per residue for model 4

- Molecule 1: Zinc finger protein 42

Chain A: 62% 26% • 11%



- Molecule 1: Zinc finger protein 42

Chain B: 61% 28% • 10%

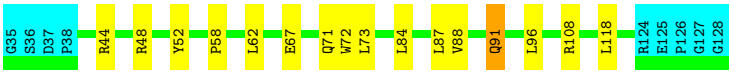
4.2.5 Score per residue for model 5 (medoid)

• Molecule 1: Zinc finger protein 42

Chain A: 69% 19% • 11%

• Molecule 1: Zinc finger protein 42

Chain B: 73% 16% • 10%



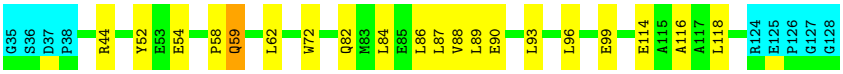
4.2.6 Score per residue for model 6

• Molecule 1: Zinc finger protein 42

Chain A: 60% 27% • 11%

• Molecule 1: Zinc finger protein 42

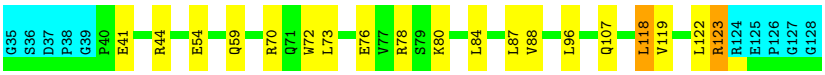
Chain B: 69% 20% • 10%



4.2.7 Score per residue for model 7

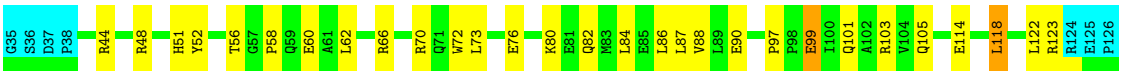
• Molecule 1: Zinc finger protein 42

Chain A: 69% 18% • 11%



• Molecule 1: Zinc finger protein 42

Chain B: 60% 29% • 10%



4.2.8 Score per residue for model 8

- Molecule 1: Zinc finger protein 42

Chain A:

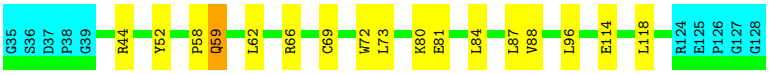
- Molecule 1: Zinc finger protein 42

Chain B:

4.2.9 Score per residue for model 9

- Molecule 1: Zinc finger protein 42

Chain A:



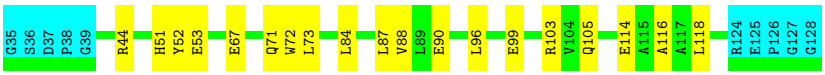
- Molecule 1: Zinc finger protein 42

Chain B:

4.2.10 Score per residue for model 10

- Molecule 1: Zinc finger protein 42

Chain A:



- Molecule 1: Zinc finger protein 42

Chain B: 64% 26% • 10%

G35 S36 D37 P38 R44 H51 Y52 T56 G57 P58 Q59 E60 E67 Q71 W72 L73 Q82 M83 L84 E85 L86 L87 V88 L89 E90 L93 L96 E99 R103 V104 Q105 E114 L118 R124 E125 P126 G127 G128

4.2.11 Score per residue for model 11

- Molecule 1: Zinc finger protein 42

Chain A: 66% 23% 11%

G35 S36 D37 P38 G39 R48 Y52 P58 Q59 E60 A61 L62 A63 Q64 C69 R70 Q71 W72 L73 Q82 M83 L84 E85 L86 L87 V88 L96 E99 R103 E114 A115 A116 A117 L118 R124 E125 P126 G127 G128

- Molecule 1: Zinc finger protein 42

Chain B: 65% 21% • 10%

G35 S36 D37 P38 R44 Y52 P58 Q59 L62 W72 L73 Q82 M83 L84 E85 L86 L87 V88 L89 E90 Q91 L96 E99 R103 V104 Q105 G106 Q107 R108 L118 V119 L122 R123 R124 E125 P126 G127 G128

4.2.12 Score per residue for model 12

- Molecule 1: Zinc finger protein 42

Chain A: 64% 24% • 11%

G35 S36 D37 P38 G39 P40 E41 R44 L45 Y52 Q59 E60 Q64 E67 L68 Q71 W72 K80 L84 L87 V88 L89 E90 Q91 L96 E99 I100 Q101 Q105 R108 L118 L122 R123 R124 E125 P126 G127 G128

- Molecule 1: Zinc finger protein 42

Chain B: 70% 19% • 10%

G35 S36 D37 P38 Y52 P58 Q59 Q64 E67 L68 Q71 W72 K80 L84 L87 V88 L89 E90 Q91 L96 E99 P112 E113 E114 L118 R124 E125 P126 G127 G128

4.2.13 Score per residue for model 13

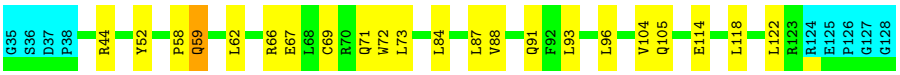
- Molecule 1: Zinc finger protein 42

Chain A: 68% 21% 11%

G35 S36 D37 P38 G39 R44 H51 Y52 R66 E67 L68 C69 R70 Q71 W72 L84 L87 V88 Q91 F92 L93 L96 V104 E114 A115 A116 A117 L118 L122 R123 R124 E125 P126 G127 G128

- Molecule 1: Zinc finger protein 42

Chain B: 67% 22% • 10%



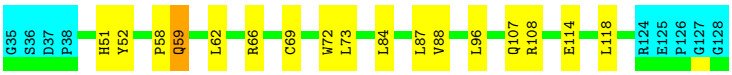
4.2.14 Score per residue for model 14

- Molecule 1: Zinc finger protein 42

Chain A: 63% 26% • 11%

- Molecule 1: Zinc finger protein 42

Chain B: 72% 17% • 10%



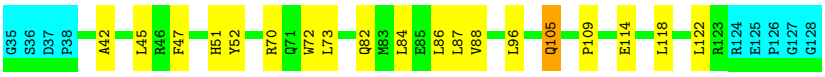
4.2.15 Score per residue for model 15

- Molecule 1: Zinc finger protein 42

Chain A: 68% 21% 11%

- Molecule 1: Zinc finger protein 42

Chain B: 70% 19% • 10%



4.2.16 Score per residue for model 16

- Molecule 1: Zinc finger protein 42

Chain A: 71% 18% 11%

- Molecule 1: Zinc finger protein 42

Chain B: 70% 19% • 10%

G35 S36 D37 P38 R44 H51 Y52 T56 G57 P58 Q59 E60 E67 Q71 W72 L73 L84 L87 V88 L89 E90 L93 L96 V104 L118 R124 E125 P126 G127 G128

4.2.17 Score per residue for model 17

• Molecule 1: Zinc finger protein 42

Chain A: 63% 23% • 11%

G35 S36 D37 P38 G39 Y52 T56 G57 P58 Q59 E60 Q64 L65 R66 E67 L68 C69 W72 S79 K80 E81 Q82 M83 L84 E85 L86 L87 V88 L96 Q101 Q105 R108 L118 V119 L122 R123 R124 E125 P126 G127 G128

• Molecule 1: Zinc finger protein 42

Chain B: 66% 22% • 10%

G35 S36 D37 P38 E41 Y52 P58 L62 R66 E67 L68 C69 R70 Q71 W72 L73 S79 K80 E81 L84 L87 V88 L89 E90 L96 Q101 Q105 E114 A115 A116 A117 L118 L122 R123 R124 E125 P126 G127 G128

4.2.18 Score per residue for model 18

• Molecule 1: Zinc finger protein 42

Chain A: 72% 17% 11%

G35 S36 D37 P38 G39 R44 Y52 P58 L62 E67 Q71 W72 L84 L87 V88 L89 E90 L93 L96 V104 Q107 R108 R124 E125 P126 G127 G128

• Molecule 1: Zinc finger protein 42

Chain B: 77% 13% • 10%

G35 S36 D37 P38 Y52 E67 L68 C69 R70 Q71 W72 L73 L84 L87 V88 L96 Q107 L118 L122 R123 R124 E125 P126 G127 G128

4.2.19 Score per residue for model 19

• Molecule 1: Zinc finger protein 42

Chain A: 71% 17% • 11%

G35 S36 D37 P38 G39 R44 Y52 P58 Q59 L62 E67 R70 Q71 W72 L84 L87 V88 L89 E90 Q91 L96 R108 A116 R124 E125 P126 G127 G128

• Molecule 1: Zinc finger protein 42

Chain B: 67% 20% • 10%

G35 S36 D37 P38 R44 H51 Y52 P58 Q59 L62 S79 K80 E81 L84 L87 V88 L89 E90 Q91 L96 Q101 Q105 R108 E114 A115 A116 A117 L118 L122 R123 R124 E125 P126 G127 G128

4.2.20 Score per residue for model 20

- Molecule 1: Zinc finger protein 42

Chain A: 67% 21% • 11%

G35 S36 D37 P38 G39 P40 E41 R44 Y52 T56 E60 E67 Q71 W72 L73 L84 L87 V88 L89 E90 Q91 L96 E99 R103 V104 Q107 L118 L122 R123 R124 E125 P126 G127 G128

- Molecule 1: Zinc finger protein 42

Chain B: 71% 19% 10%

G35 S36 D37 P38 R44 R48 Y52 P58 L62 R66 E67 L68 C69 R70 Q71 W72 Q82 M83 L84 E85 L86 L87 V88 L89 E90 L96 R124 E125 P126 G127 G128

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *AUTOMATED METHODS WERE USED FOR BACKBONE CHEMICAL SHIFT ASSIGNMENT AND ITERATIVE NOE REFINEMENT. FINAL STRUCTURES WERE OBTAINED BY MOLECULAR DYNAMICS IN EXPLICIT SOLVENT.*

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

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

Software name	Classification	Version
XPLOR-NIH	refinement	2.9.3.
CYANA	structure solution	2.1

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.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.1±0.2
1	B	0.0±0.0	0.1±0.3
All	All	0	3

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	B	48	ARG	Sidechain	1
1	A	44	ARG	Sidechain	1
1	B	123	ARG	Sidechain	1

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	674	677	676	16±3
1	B	678	680	679	16±3
All	All	27040	27140	27100	468

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 9.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:LEU:HD21	1:B:72:TRP:CZ3	0.75	2.16	13	7
1:A:66:ARG:HA	1:A:69:CYS:SG	0.74	2.21	14	6
1:A:44:ARG:HG2	1:A:72:TRP:CE2	0.70	2.22	12	1
1:B:44:ARG:HD3	1:B:72:TRP:CZ2	0.69	2.22	9	3
1:A:72:TRP:CZ3	1:B:87:LEU:HD21	0.69	2.22	11	9
1:A:72:TRP:CH2	1:B:87:LEU:HD21	0.66	2.24	7	14
1:A:73:LEU:HD11	1:B:87:LEU:HD23	0.65	1.67	1	13
1:B:66:ARG:HA	1:B:69:CYS:SG	0.65	2.32	14	7
1:A:84:LEU:O	1:A:88:VAL:HG23	0.63	1.93	17	20
1:A:87:LEU:HD23	1:B:73:LEU:HD11	0.63	1.70	16	13
1:B:84:LEU:O	1:B:88:VAL:HG23	0.63	1.93	17	20
1:B:67:GLU:O	1:B:71:GLN:HG3	0.63	1.94	12	8
1:A:87:LEU:HD21	1:B:72:TRP:CH2	0.63	2.28	10	14
1:A:67:GLU:O	1:A:71:GLN:HG3	0.62	1.95	20	5
1:B:59:GLN:HE21	1:B:59:GLN:N	0.61	1.93	13	9
1:A:59:GLN:N	1:A:59:GLN:HE21	0.59	1.95	6	6
1:A:52:TYR:CD2	1:B:96:LEU:HD23	0.58	2.33	9	19
1:A:96:LEU:HD23	1:B:52:TYR:CD2	0.58	2.32	11	20
1:A:88:VAL:HG22	1:B:69:CYS:SG	0.58	2.38	2	6
1:A:67:GLU:O	1:A:71:GLN:HG2	0.57	1.99	6	5
1:B:99:GLU:O	1:B:103:ARG:HG2	0.57	2.00	10	4
1:A:87:LEU:HD13	1:B:87:LEU:HD13	0.56	1.78	12	16
1:A:104:VAL:HA	1:A:107:GLN:OE1	0.55	2.01	20	2
1:B:60:GLU:O	1:B:64:GLN:HG3	0.55	2.01	3	2
1:B:41:GLU:O	1:B:45:LEU:HG	0.55	2.00	1	1
1:B:44:ARG:HD2	1:B:90:GLU:OE1	0.54	2.01	2	7
1:B:101:GLN:O	1:B:105:GLN:HG2	0.54	2.01	17	3
1:B:105:GLN:HE21	1:B:105:GLN:N	0.54	2.01	15	2
1:A:58:PRO:O	1:A:62:LEU:HG	0.54	2.02	2	13
1:A:58:PRO:HG2	1:A:59:GLN:NE2	0.54	2.18	6	6
1:A:73:LEU:HD12	1:B:84:LEU:HD13	0.53	1.81	8	3
1:B:93:LEU:HD11	1:B:104:VAL:HG11	0.53	1.79	10	1
1:A:44:ARG:HD3	1:A:72:TRP:CZ2	0.53	2.39	7	4
1:A:114:GLU:O	1:A:118:LEU:HG	0.53	2.03	11	5
1:A:69:CYS:SG	1:B:88:VAL:HG22	0.53	2.44	9	5
1:B:82:GLN:O	1:B:86:LEU:HG	0.53	2.03	4	8
1:A:123:ARG:HB2	1:B:54:GLU:OE1	0.53	2.04	6	1
1:A:99:GLU:O	1:A:103:ARG:HG2	0.52	2.05	20	5
1:B:44:ARG:O	1:B:48:ARG:HG3	0.52	2.04	5	1
1:A:118:LEU:O	1:A:122:LEU:HG	0.52	2.05	12	7
1:A:91:GLN:OE1	1:B:48:ARG:HD3	0.52	2.05	20	1
1:B:104:VAL:HA	1:B:107:GLN:OE1	0.52	2.05	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:89:LEU:HD23	1:B:112:PRO:HA	0.52	1.82	2	2
1:B:58:PRO:O	1:B:62:LEU:HG	0.51	2.05	7	14
1:B:58:PRO:HG2	1:B:59:GLN:NE2	0.51	2.21	11	8
1:B:118:LEU:O	1:B:122:LEU:HG	0.51	2.06	7	10
1:A:56:THR:O	1:A:60:GLU:HB3	0.51	2.06	1	4
1:A:79:SER:HB2	1:A:81:GLU:OE2	0.51	2.06	17	2
1:B:44:ARG:HD2	1:B:90:GLU:OE2	0.50	2.06	19	1
1:B:114:GLU:O	1:B:118:LEU:HG	0.50	2.07	10	7
1:A:59:GLN:NE2	1:B:116:ALA:HB1	0.50	2.22	2	5
1:A:101:GLN:O	1:A:105:GLN:HB2	0.50	2.06	12	2
1:A:116:ALA:HB1	1:B:59:GLN:NE2	0.50	2.22	19	7
1:A:84:LEU:HD13	1:B:73:LEU:HD12	0.49	1.83	15	6
1:A:54:GLU:OE1	1:B:123:ARG:HB2	0.49	2.08	4	1
1:B:66:ARG:HA	1:B:69:CYS:HG	0.49	1.68	2	2
1:A:73:LEU:O	1:A:78:ARG:HD2	0.49	2.06	5	3
1:B:67:GLU:O	1:B:71:GLN:HG2	0.49	2.07	10	3
1:B:79:SER:HB2	1:B:81:GLU:OE2	0.49	2.08	17	2
1:A:44:ARG:HD2	1:A:90:GLU:OE1	0.48	2.07	10	4
1:B:56:THR:O	1:B:60:GLU:HB3	0.47	2.09	7	3
1:A:120:ASP:O	1:A:123:ARG:HG2	0.47	2.10	14	1
1:A:44:ARG:O	1:A:48:ARG:HG3	0.47	2.10	15	1
1:A:44:ARG:HG2	1:A:72:TRP:NE1	0.47	2.24	12	1
1:A:62:LEU:O	1:A:66:ARG:HG2	0.47	2.10	16	2
1:A:81:GLU:HG3	1:A:82:GLN:NE2	0.46	2.26	4	1
1:B:119:VAL:O	1:B:123:ARG:HG3	0.46	2.11	11	1
1:B:93:LEU:HD22	1:B:104:VAL:HG11	0.46	1.88	4	3
1:A:93:LEU:HD22	1:A:104:VAL:HG11	0.46	1.88	2	5
1:A:119:VAL:O	1:A:123:ARG:HG3	0.46	2.11	7	2
1:B:119:VAL:O	1:B:123:ARG:HG2	0.46	2.11	4	1
1:A:82:GLN:O	1:A:86:LEU:HG	0.46	2.11	11	4
1:A:64:GLN:O	1:A:68:LEU:HG	0.46	2.11	17	3
1:A:54:GLU:HB3	1:B:123:ARG:CZ	0.45	2.41	7	1
1:B:62:LEU:O	1:B:66:ARG:HG2	0.45	2.11	7	1
1:B:64:GLN:O	1:B:68:LEU:HG	0.45	2.12	12	1
1:A:47:PHE:CE1	1:A:69:CYS:HB3	0.45	2.47	4	1
1:A:42:ALA:O	1:A:46:ARG:HG3	0.45	2.12	16	1
1:A:115:ALA:O	1:A:119:VAL:HG12	0.44	2.11	15	1
1:B:118:LEU:H	1:B:118:LEU:HD23	0.44	1.73	8	2
1:B:107:GLN:NE2	1:B:118:LEU:HD13	0.44	2.27	11	1
1:A:76:GLU:HG3	1:A:77:VAL:HG23	0.44	1.90	8	2
1:A:97:PRO:HB2	1:A:99:GLU:OE1	0.44	2.12	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:ARG:HA	1:A:69:CYS:HG	0.44	1.73	9	1
1:A:48:ARG:NH1	1:B:91:GLN:HA	0.44	2.27	5	2
1:B:42:ALA:O	1:B:45:LEU:HB3	0.44	2.13	15	2
1:B:47:PHE:CE1	1:B:69:CYS:HB3	0.43	2.48	2	1
1:A:41:GLU:OE1	1:A:110:GLY:HA2	0.43	2.13	6	1
1:A:91:GLN:HB2	1:B:47:PHE:CZ	0.43	2.48	8	1
1:A:87:LEU:O	1:A:90:GLU:HB3	0.43	2.13	20	1
1:A:103:ARG:HB2	1:A:122:LEU:HD13	0.43	1.91	20	1
1:B:105:GLN:HG3	1:B:108:ARG:CZ	0.42	2.43	11	1
1:B:69:CYS:O	1:B:73:LEU:HD12	0.42	2.14	18	1
1:B:50:PHE:CD2	1:B:65:LEU:HD21	0.42	2.49	3	1
1:B:114:GLU:O	1:B:118:LEU:HD23	0.42	2.14	7	3
1:A:41:GLU:O	1:A:45:LEU:HG	0.42	2.14	12	1
1:A:101:GLN:O	1:A:105:GLN:HG2	0.42	2.13	16	2
1:A:91:GLN:HB3	1:B:47:PHE:CZ	0.42	2.50	15	1
1:B:89:LEU:O	1:B:93:LEU:HG	0.42	2.15	6	1
1:A:82:GLN:O	1:A:85:GLU:HB3	0.42	2.15	17	1
1:B:97:PRO:HB2	1:B:99:GLU:OE1	0.41	2.16	7	1
1:A:87:LEU:HD22	1:B:87:LEU:HD22	0.41	1.92	1	1
1:A:48:ARG:HD3	1:B:91:GLN:OE1	0.41	2.16	4	1
1:A:60:GLU:O	1:A:64:GLN:HG2	0.41	2.16	11	3
1:A:105:GLN:HG3	1:A:108:ARG:CZ	0.41	2.46	1	1
1:A:107:GLN:NE2	1:A:118:LEU:HD13	0.41	2.31	7	1
1:A:69:CYS:SG	1:B:87:LEU:HD23	0.41	2.56	11	1
1:B:70:ARG:C	1:B:70:ARG:HD3	0.41	2.37	7	1
1:B:40:PRO:HG3	1:B:78:ARG:NH2	0.41	2.31	1	1
1:A:47:PHE:CZ	1:B:91:GLN:HB2	0.41	2.51	5	1
1:A:51:HIS:CE1	1:A:53:GLU:HB3	0.41	2.51	10	1
1:B:101:GLN:O	1:B:105:GLN:HB2	0.40	2.17	2	1
1:B:44:ARG:HD3	1:B:72:TRP:CE2	0.40	2.51	6	1
1:B:44:ARG:NH1	1:B:108:ARG:HH11	0.40	2.14	2	1
1:A:70:ARG:C	1:A:70:ARG:HD2	0.40	2.36	11	1
1:A:44:ARG:HD3	1:A:90:GLU:OE2	0.40	2.16	12	1
1:A:89:LEU:O	1:A:93:LEU:HG	0.40	2.16	6	1
1:A:105:GLN:OE1	1:A:108:ARG:HD2	0.40	2.16	12	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	84/94 (89%)	80±1 (96±1%)	3±1 (4±1%)	0±0 (0±0%)	54	85
1	B	85/94 (90%)	82±1 (96±1%)	3±1 (4±1%)	0±0 (0±0%)	54	85
All	All	3380/3760 (90%)	3241 (96%)	136 (4%)	3 (0%)	54	85

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	123	ARG	1
1	B	109	PRO	1
1	A	108	ARG	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	69/75 (92%)	66±2 (95±2%)	3±2 (5±2%)	28	77
1	B	69/75 (92%)	65±1 (95±2%)	4±1 (5±2%)	27	76
All	All	2760/3000 (92%)	2619 (95%)	141 (5%)	27	77

All 31 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	B	118	LEU	12
1	A	118	LEU	9
1	B	59	GLN	9
1	A	59	GLN	9

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Mol	Chain	Res	Type	Models (Total)
1	B	51	HIS	8
1	A	91	GLN	7
1	A	105	GLN	7
1	B	105	GLN	7
1	B	91	GLN	6
1	A	51	HIS	6
1	A	108	ARG	6
1	A	81	GLU	5
1	B	81	GLU	5
1	B	80	LYS	5
1	A	41	GLU	4
1	A	76	GLU	3
1	A	99	GLU	3
1	A	107	GLN	3
1	B	107	GLN	3
1	B	108	ARG	3
1	B	90	GLU	3
1	B	99	GLU	3
1	A	70	ARG	3
1	A	80	LYS	3
1	B	41	GLU	2
1	B	70	ARG	2
1	B	98	PRO	1
1	A	67	GLU	1
1	B	76	GLU	1
1	B	56	THR	1
1	B	123	ARG	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