



Full wwPDB NMR Structure Validation Report ⓘ

Feb 27, 2022 – 02:34 PM EST

PDB ID : 2ED8
Title : Solution structure of the second fibronectin type III domain of human Netrin receptor DCC
Authors : Tochio, N.; Koshiba, S.; Tomizawa, T.; Kigawa, T.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-02-14

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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

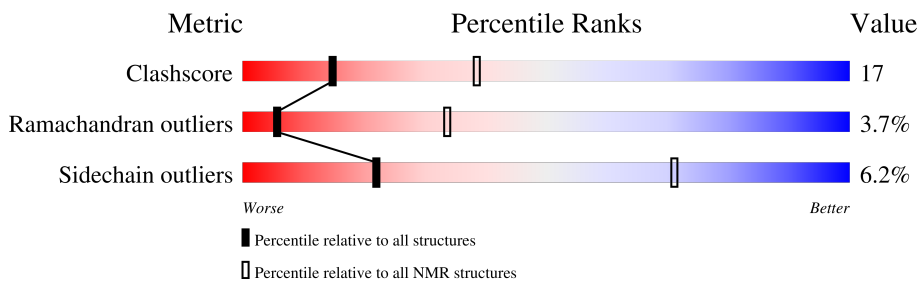
1 Overall quality at a glance

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	106	

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 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:8-A:99 (92)	0.14	7

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 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1550 atoms, of which 761 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Netrin receptor DCC.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	106	1550	496	761	127	165	1	0

There are 13 discrepancies between the modelled and reference sequences:

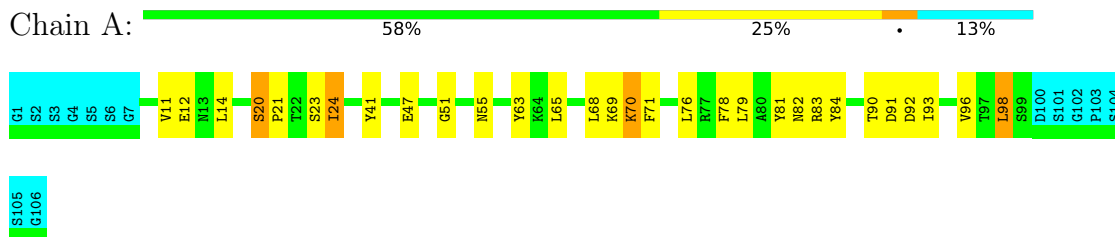
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P43146
A	2	SER	-	expression tag	UNP P43146
A	3	SER	-	expression tag	UNP P43146
A	4	GLY	-	expression tag	UNP P43146
A	5	SER	-	expression tag	UNP P43146
A	6	SER	-	expression tag	UNP P43146
A	7	GLY	-	expression tag	UNP P43146
A	101	SER	-	expression tag	UNP P43146
A	102	GLY	-	expression tag	UNP P43146
A	103	PRO	-	expression tag	UNP P43146
A	104	SER	-	expression tag	UNP P43146
A	105	SER	-	expression tag	UNP P43146
A	106	GLY	-	expression tag	UNP P43146

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: Netrin receptor DCC

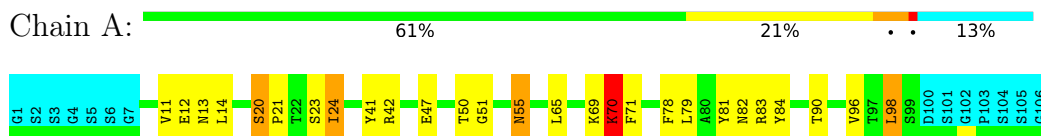


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

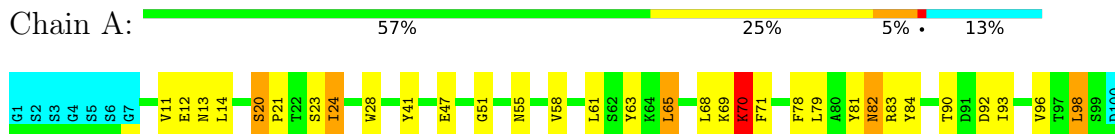
4.2.1 Score per residue for model 1

- Molecule 1: Netrin receptor DCC



4.2.2 Score per residue for model 2

- Molecule 1: Netrin receptor DCC



S101
G102
P103
S104
S105
G106

4.2.3 Score per residue for model 3

- Molecule 1: Netrin receptor DCC

Chain A: 58% 25% 13%

G1 S2 S3 S4 S5 S6 S7 V11 E12 M13 L14 G15 A16 V17 S20 S21 T22 S23 T24 Y33 Y41 E47 D59 Y63 K64 L65 L68 K69 K70 F71 Y74 S75 L76 R77 F78 L79 A80 Y81 N82 R83 T90 I93 Y96 T97 L98 S99 D100 S101

G102
P103
S104
S105
G106

4.2.4 Score per residue for model 4

- Molecule 1: Netrin receptor DCC

Chain A: 53% 30% 13%

G1 S2 S3 S4 S5 S6 S7 V11 E12 M13 L14 S20 P21 T22 I24 P30 V38 Q39 G40 Y41 E47 T50 G51 N55 L61 S62 Y63 K64 L65 L68 K69 K70 F71 T72 E73 Y74 S75 L76 R77 F78 Y81 N82 R83 Y84 D91 D92 I93

V96
I97
L98
S99
D100
S101
G102
P103
S104
S105
G106

4.2.5 Score per residue for model 5

- Molecule 1: Netrin receptor DCC

Chain A: 62% 19% 6% 13%

G1 S2 S3 S4 S5 S6 S7 E12 M13 L14 S20 S23 I24 W28 Y41 E47 G51 N55 L65 L68 K69 K70 F71 L76 R77 F78 Y81 N82 R83 Y84 T90 D91 D92 I93 V96 T97 L98 S99 D100 S101 G102 P103 S104 G106

4.2.6 Score per residue for model 6

- Molecule 1: Netrin receptor DCC

Chain A: 52% 29% 6% 13%

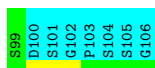
G1 S2 S3 S4 S5 S6 S7 L14 V17 S20 S23 I24 W28 Y33 Y41 R42 E47 T50 G51 V58 D59 S62 Y63 K64 L65 L68 K69 K70 F71 L76 R77 F78 L79 A80 Y81 N82 R83 Y84 G85 V88 T90 D91 D92 I93



4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: Netrin receptor DCC

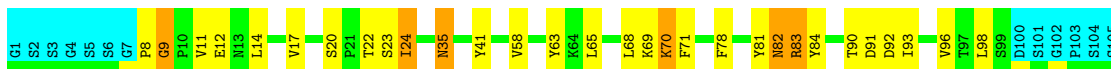
Chain A: 57% 25% • • 13%



4.2.8 Score per residue for model 8

- Molecule 1: Netrin receptor DCC

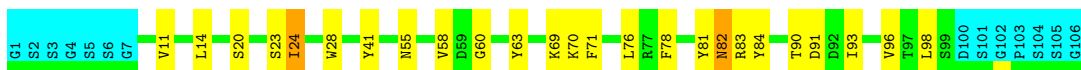
Chain A: 58% 23% 6% 13%



4.2.9 Score per residue for model 9

- Molecule 1: Netrin receptor DCC

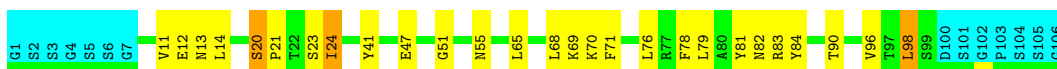
Chain A: 63% 22% • 13%



4.2.10 Score per residue for model 10

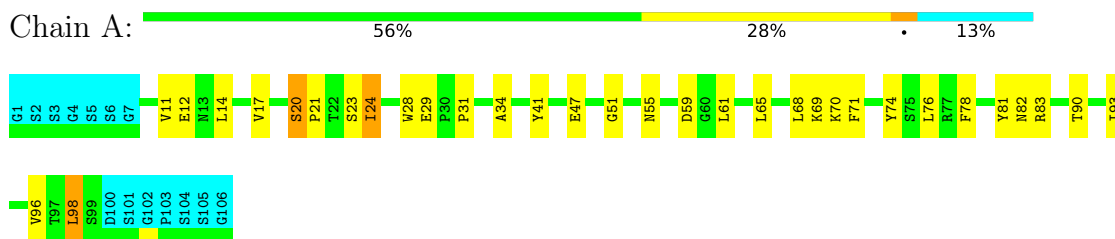
- Molecule 1: Netrin receptor DCC

Chain A: 61% 23% • 13%



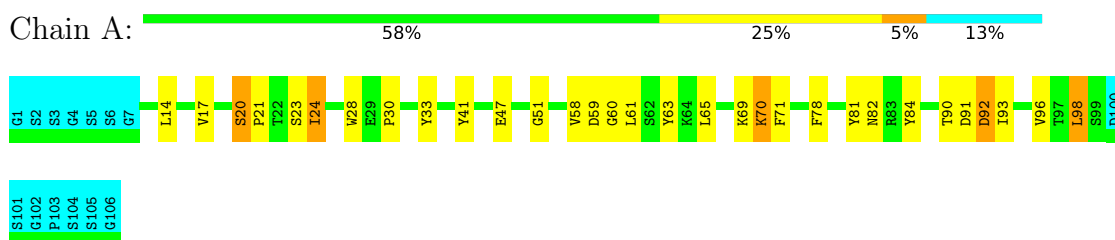
4.2.11 Score per residue for model 11

- Molecule 1: Netrin receptor DCC



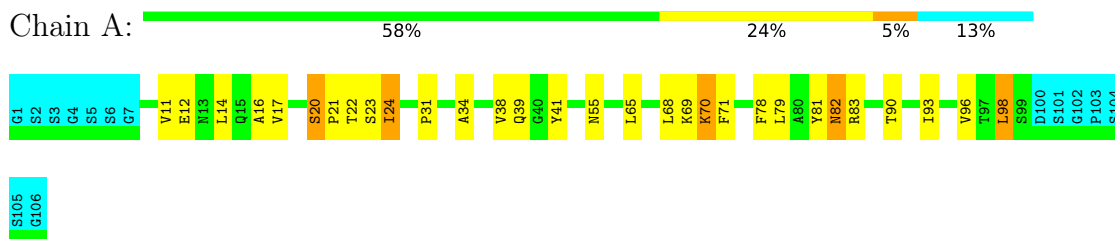
4.2.12 Score per residue for model 12

- Molecule 1: Netrin receptor DCC



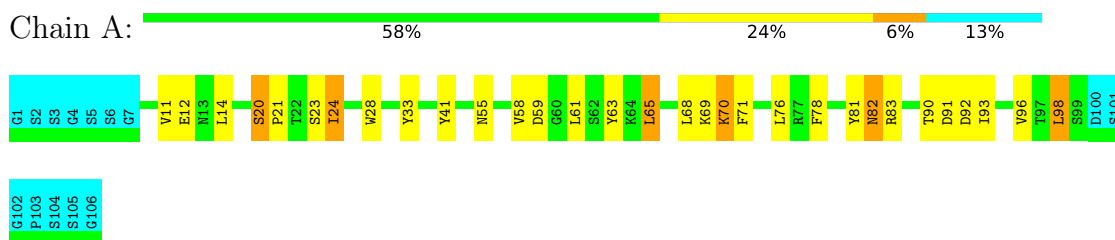
4.2.13 Score per residue for model 13

- Molecule 1: Netrin receptor DCC



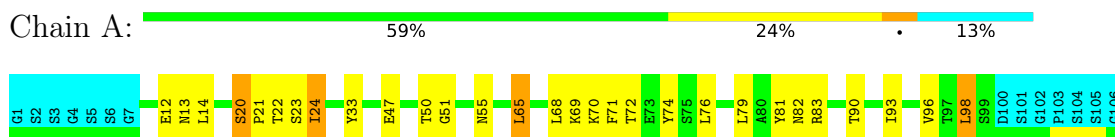
4.2.14 Score per residue for model 14

- Molecule 1: Netrin receptor DCC



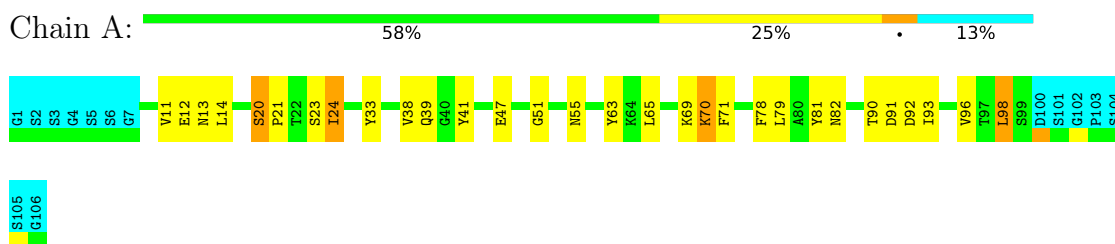
4.2.15 Score per residue for model 15

- Molecule 1: Netrin receptor DCC



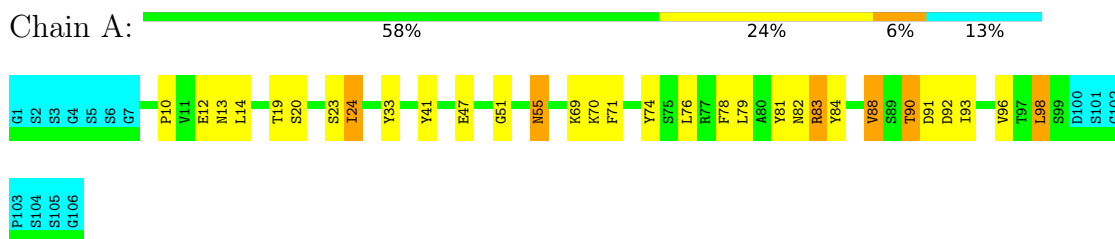
4.2.16 Score per residue for model 16

- Molecule 1: Netrin receptor DCC



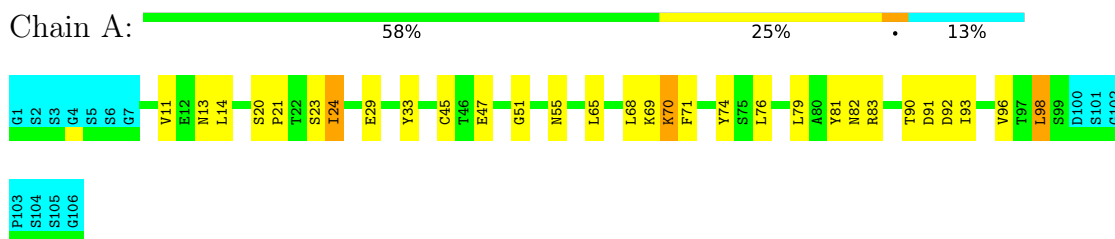
4.2.17 Score per residue for model 17

- Molecule 1: Netrin receptor DCC



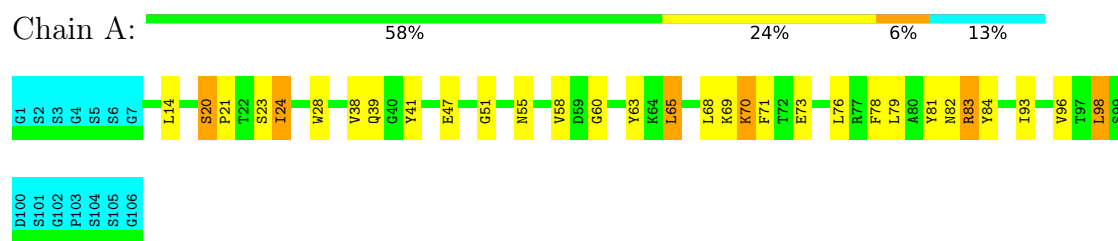
4.2.18 Score per residue for model 18

- Molecule 1: Netrin receptor DCC



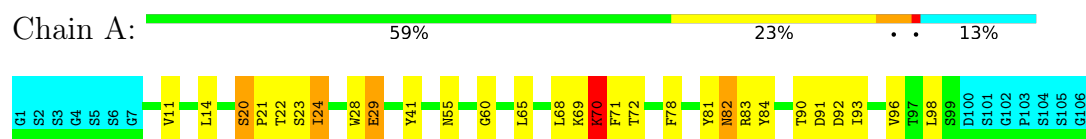
4.2.19 Score per residue for model 19

- Molecule 1: Netrin receptor DCC



4.2.20 Score per residue for model 20

- Molecule 1: Netrin receptor DCC



5 Refinement protocol and experimental data overview

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	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	712	700	700	24±3
All	All	14240	14000	14000	478

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:LEU:HD21	1:A:93:ILE:HD11	0.92	1.37	20	18
1:A:71:PHE:CZ	1:A:96:VAL:HG11	0.84	2.07	18	20
1:A:14:LEU:HD22	1:A:90:THR:HG21	0.83	1.51	9	18
1:A:69:LYS:NZ	1:A:72:THR:HG21	0.81	1.89	20	1
1:A:65:LEU:HD23	1:A:68:LEU:HD11	0.73	1.58	13	13
1:A:47:GLU:OE2	1:A:50:THR:HG23	0.71	1.85	15	4
1:A:29:GLU:OE2	1:A:61:LEU:HD13	0.68	1.88	7	1
1:A:71:PHE:CE1	1:A:96:VAL:HG11	0.64	2.27	13	19
1:A:42:ARG:NH1	1:A:81:TYR:CD2	0.63	2.66	7	3
1:A:79:LEU:C	1:A:79:LEU:HD12	0.63	2.14	6	12
1:A:65:LEU:CD2	1:A:68:LEU:HD21	0.63	2.24	5	3
1:A:81:TYR:O	1:A:81:TYR:CD1	0.60	2.54	9	2
1:A:81:TYR:CD1	1:A:81:TYR:O	0.60	2.54	6	18
1:A:10:PRO:HB3	1:A:88:VAL:HG11	0.59	1.73	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:TYR:HE1	1:A:65:LEU:HD12	0.59	1.57	16	2
1:A:71:PHE:CZ	1:A:96:VAL:CG1	0.59	2.84	18	19
1:A:24:ILE:HG21	1:A:76:LEU:HD11	0.57	1.77	3	12
1:A:47:GLU:CD	1:A:74:TYR:CE1	0.57	2.78	18	2
1:A:28:TRP:CE3	1:A:61:LEU:O	0.56	2.59	11	2
1:A:47:GLU:OE2	1:A:74:TYR:CE1	0.56	2.58	18	1
1:A:23:SER:O	1:A:24:ILE:CG1	0.55	2.55	8	20
1:A:47:GLU:OE2	1:A:74:TYR:CZ	0.55	2.59	18	2
1:A:71:PHE:CE1	1:A:96:VAL:CG1	0.54	2.90	13	19
1:A:55:ASN:ND2	1:A:55:ASN:H	0.54	2.00	5	3
1:A:28:TRP:CZ2	1:A:60:GLY:O	0.54	2.61	12	4
1:A:41:TYR:HB3	1:A:78:PHE:CZ	0.53	2.39	13	18
1:A:29:GLU:HG2	1:A:61:LEU:HD23	0.53	1.80	11	1
1:A:65:LEU:HD23	1:A:68:LEU:HD21	0.53	1.80	5	3
1:A:20:SER:CB	1:A:21:PRO:CD	0.53	2.87	2	12
1:A:20:SER:CA	1:A:98:LEU:HD12	0.52	2.34	15	12
1:A:22:THR:HG21	1:A:68:LEU:O	0.52	2.04	3	4
1:A:41:TYR:CB	1:A:78:PHE:CZ	0.52	2.92	13	9
1:A:10:PRO:CB	1:A:88:VAL:HG11	0.52	2.35	17	1
1:A:69:LYS:O	1:A:70:LYS:C	0.52	2.47	1	20
1:A:58:VAL:CG1	1:A:63:TYR:CD2	0.51	2.93	8	7
1:A:47:GLU:O	1:A:51:GLY:N	0.50	2.45	17	14
1:A:82:ASN:O	1:A:83:ARG:C	0.50	2.50	14	13
1:A:79:LEU:HD12	1:A:79:LEU:O	0.50	2.07	6	1
1:A:69:LYS:HZ1	1:A:72:THR:HG21	0.50	1.63	20	1
1:A:22:THR:CG2	1:A:68:LEU:O	0.50	2.59	3	5
1:A:63:TYR:CE1	1:A:65:LEU:HD12	0.49	2.41	16	1
1:A:82:ASN:OD1	1:A:84:TYR:N	0.49	2.45	12	2
1:A:16:ALA:O	1:A:17:VAL:HG13	0.49	2.08	3	2
1:A:20:SER:CB	1:A:21:PRO:HD2	0.49	2.38	2	5
1:A:81:TYR:CD1	1:A:81:TYR:C	0.49	2.86	18	16
1:A:24:ILE:HD13	1:A:76:LEU:HD11	0.49	1.85	17	4
1:A:14:LEU:CD2	1:A:90:THR:HG21	0.49	2.36	17	2
1:A:83:ARG:HD2	1:A:84:TYR:CD1	0.49	2.43	19	2
1:A:41:TYR:HB3	1:A:78:PHE:CE2	0.48	2.44	3	4
1:A:14:LEU:CD2	1:A:93:ILE:HD11	0.48	2.33	8	1
1:A:58:VAL:HG11	1:A:63:TYR:CD2	0.48	2.44	8	3
1:A:58:VAL:HG12	1:A:63:TYR:CD2	0.48	2.44	2	1
1:A:83:ARG:HG3	1:A:84:TYR:CD1	0.48	2.44	10	2
1:A:82:ASN:OD1	1:A:84:TYR:CD2	0.48	2.67	20	3
1:A:91:ASP:O	1:A:92:ASP:C	0.47	2.52	6	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:31:PRO:HB2	1:A:34:ALA:HB2	0.47	1.85	11	1
1:A:47:GLU:HG3	1:A:74:TYR:CE1	0.46	2.45	3	2
1:A:12:GLU:O	1:A:13:ASN:C	0.46	2.54	17	7
1:A:84:TYR:CD1	1:A:84:TYR:N	0.46	2.82	1	1
1:A:13:ASN:ND2	1:A:29:GLU:OE1	0.46	2.48	18	1
1:A:55:ASN:OD1	1:A:55:ASN:N	0.46	2.48	1	1
1:A:30:PRO:HD3	1:A:61:LEU:HD21	0.46	1.86	4	2
1:A:28:TRP:CZ3	1:A:62:SER:HA	0.45	2.47	6	1
1:A:77:ARG:NH1	1:A:92:ASP:OD1	0.45	2.50	6	1
1:A:70:LYS:O	1:A:98:LEU:O	0.45	2.35	13	20
1:A:65:LEU:HD23	1:A:68:LEU:CD1	0.45	2.39	19	1
1:A:72:THR:O	1:A:74:TYR:CD2	0.45	2.70	4	2
1:A:63:TYR:HE2	1:A:65:LEU:HD12	0.44	1.72	4	1
1:A:79:LEU:C	1:A:79:LEU:CD1	0.44	2.85	6	1
1:A:28:TRP:C	1:A:29:GLU:OE1	0.44	2.56	20	1
1:A:33:TYR:CD2	1:A:33:TYR:O	0.44	2.70	3	1
1:A:69:LYS:NZ	1:A:72:THR:CG2	0.44	2.73	20	1
1:A:83:ARG:HG3	1:A:84:TYR:N	0.43	2.28	9	1
1:A:20:SER:N	1:A:98:LEU:CD1	0.43	2.82	7	4
1:A:82:ASN:O	1:A:84:TYR:N	0.43	2.51	8	2
1:A:19:THR:C	1:A:98:LEU:HD11	0.43	2.33	17	1
1:A:31:PRO:HG2	1:A:34:ALA:HB2	0.42	1.90	13	1
1:A:24:ILE:HG21	1:A:76:LEU:CD1	0.42	2.44	14	4
1:A:21:PRO:O	1:A:70:LYS:O	0.42	2.37	12	8
1:A:38:VAL:O	1:A:39:GLN:C	0.41	2.58	16	4
1:A:76:LEU:O	1:A:92:ASP:OD1	0.41	2.39	4	1
1:A:12:GLU:OE2	1:A:33:TYR:CE2	0.41	2.73	14	1
1:A:28:TRP:CE2	1:A:61:LEU:HA	0.41	2.49	2	1
1:A:20:SER:HB3	1:A:21:PRO:HD2	0.41	1.93	2	1
1:A:28:TRP:CG	1:A:78:PHE:CE2	0.41	3.09	5	1
1:A:45:CYS:SG	1:A:76:LEU:CD2	0.41	3.09	18	1
1:A:58:VAL:HG12	1:A:63:TYR:CE2	0.40	2.51	12	1
1:A:8:PRO:O	1:A:9:GLY:O	0.40	2.40	8	1
1:A:82:ASN:O	1:A:85:GLY:N	0.40	2.55	6	1
1:A:83:ARG:HB2	1:A:83:ARG:CZ	0.40	2.46	15	1
1:A:12:GLU:OE2	1:A:30:PRO:O	0.40	2.39	7	1
1:A:23:SER:OG	1:A:24:ILE:N	0.40	2.55	20	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	92/106 (87%)	78±2 (85±2%)	10±2 (11±2%)	3±1 (4±1%)	6	34
All	All	1840/2120 (87%)	1564 (85%)	208 (11%)	68 (4%)	6	34

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	24	ILE	20
1	A	98	LEU	17
1	A	11	VAL	14
1	A	70	LYS	10
1	A	90	THR	2
1	A	92	ASP	2
1	A	9	GLY	1
1	A	83	ARG	1
1	A	73	GLU	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	80/89 (90%)	75±1 (94±2%)	5±1 (6±2%)	22	71
All	All	1600/1780 (90%)	1501 (94%)	99 (6%)	22	71

All 15 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	20	SER	20

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Mol	Chain	Res	Type	Models (Total)
1	A	55	ASN	16
1	A	82	ASN	13
1	A	65	LEU	8
1	A	70	LYS	8
1	A	12	GLU	6
1	A	59	ASP	6
1	A	33	TYR	6
1	A	17	VAL	4
1	A	91	ASP	3
1	A	83	ARG	3
1	A	92	ASP	2
1	A	88	VAL	2
1	A	35	ASN	1
1	A	29	GLU	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

No chemical shift data were provided