Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2NCM
Title	:	NEURAL CELL ADHESION MOLECULE, NMR, 20 STRUCTURES
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Deposited on	:	1996-12-16

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 (1)) were used in the production of this report:

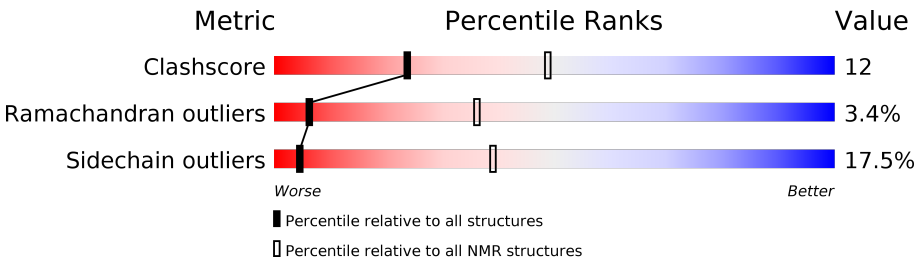
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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	99	54% 31% • 11%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 10 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:3-A:27, A:34-A:40, A:44-A:99 (88)	0.21	10

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. No single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1499 atoms, of which 735 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called NEURAL CELL ADHESION MOLECULE.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	99	1499	476	735	126	160	2	0

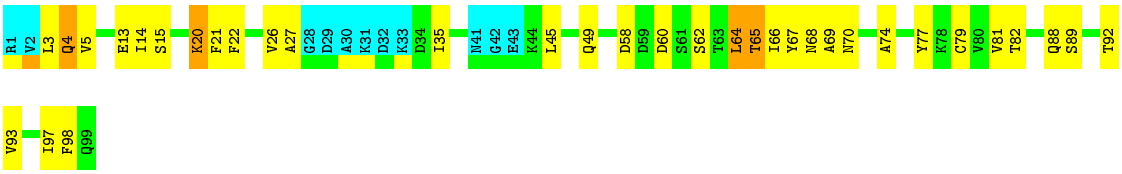
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: NEURAL CELL ADHESION MOLECULE

Chain A: 54% 31% • 11%



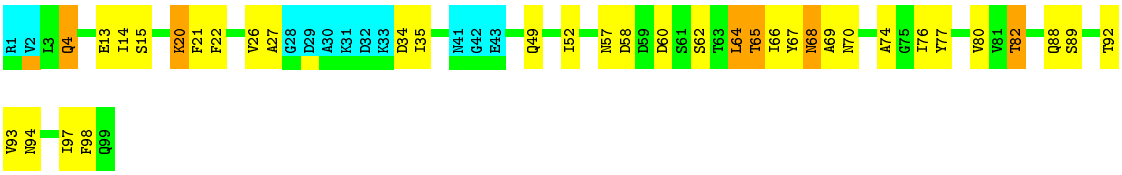
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: NEURAL CELL ADHESION MOLECULE

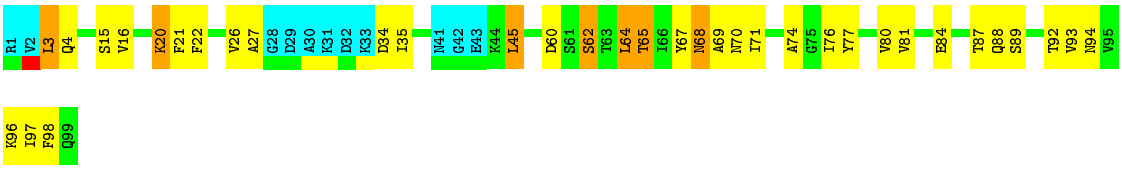
Chain A: 53% 30% 6% 11%



4.2.2 Score per residue for model 2

• Molecule 1: NEURAL CELL ADHESION MOLECULE

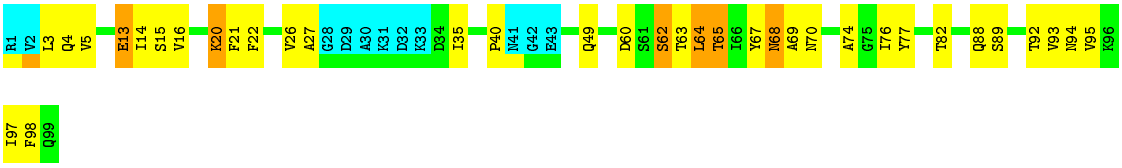
Chain A: 53% 29% 7% 11%



4.2.3 Score per residue for model 3

- Molecule 1: NEURAL CELL ADHESION MOLECULE

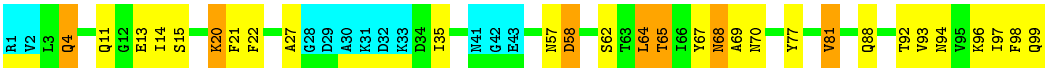
Chain A: 53% 30% 6% 11%



4.2.4 Score per residue for model 4

- Molecule 1: NEURAL CELL ADHESION MOLECULE

Chain A: 60% 22% 7% 11%



4.2.5 Score per residue for model 5

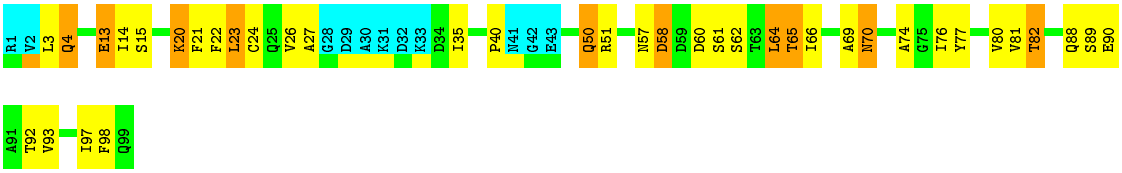
- Molecule 1: NEURAL CELL ADHESION MOLECULE

Chain A: 61% 22% 6% 11%

4.2.6 Score per residue for model 6

- Molecule 1: NEURAL CELL ADHESION MOLECULE

Chain A: 49% 29% 10% 11%



4.2.7 Score per residue for model 7

- Molecule 1: NEURAL CELL ADHESION MOLECULE

Chain A: 60% 24% 5% 11%

R1 V2 L3 Q4 E13 I14 S15 K20 F21 A27 G28 D29 A30 K31 D32 K33 D34 I35 N41 G42 E43 K44 L45 S46 Q49 Q50 R51 I52 N57 D58 S62 T63 L64 T65 I66 Y67 N68 A69 N70 Y77 K78 Q88 T92 I97 F98 Q99

4.2.8 Score per residue for model 8

- Molecule 1: NEURAL CELL ADHESION MOLECULE

Chain A: 58% 28% • 11%

R1 V2 L3 Q4 G12 E13 I14 S15 V16 K20 F21 F22 A27 G28 D29 A30 K31 D32 K33 D34 I35 N41 G42 E43 D58 D59 D60 L64 T65 I66 Y67 N68 A69 N70 A74 Y77 V80 V81 T82 Q88 S89 T92 V93 K96 I97 F98 Q99

4.2.9 Score per residue for model 9

- Molecule 1: NEURAL CELL ADHESION MOLECULE

Chain A: 47% 35% 6% 11%

R1 V2 L3 Q4 V5 D6 I7 E13 I14 S15 V16 G17 E18 S19 K20 F21 F22 V26 A27 G28 D29 A30 K31 D32 K33 D34 I35 N41 G42 E43 S46 Q49 I52 N57 D58 D59 D60 S61 S62 T63 L64 T65 I66 Y67 N68 A69 N70 I71 D72 D73 A74 Y77

K78 C79 V80 V81 T82 Q88 S89 T92 V93 N94 I97 F98 Q99

4.2.10 Score per residue for model 10 (medoid)

- Molecule 1: NEURAL CELL ADHESION MOLECULE

Chain A: 51% 32% 6% 11%

R1 V2 L3 Q4 V5 S15 V16 K20 F21 F22 L23 V26 A27 G28 D29 A30 K31 D32 K33 D34 I35 S36 W37 P40 N41 G42 E43 K44 Q49 I52 D58 D59 D60 S61 S62 T63 L64 T65 I66 Y67 N68 A69 N70 A74 Y77 K78 C79 T82 Q88

T92 V93 I97 F98 Q99

4.2.11 Score per residue for model 11

- Molecule 1: NEURAL CELL ADHESION MOLECULE

Chain A: 58% 25% 6% 11%

R1 V2 L3 Q4 V5 D6 I7 S15 K20 F21 A27 G28 D29 A30 K31 D32 K33 D34 I35 S39 P40 N41 G42 E43 K44 L45 Q49 N57 D58 D59 S62 T63 L64 T65 A69 N70 A74 G75 I76 Y77 K78 C79 T82 Q88 S89 T92 V93 N94

I97 F98 Q99

4.2.12 Score per residue for model 12

- Molecule 1: NEURAL CELL ADHESION MOLECULE

Chain A: 55% 29% 5% 11%

R1 V2 L3 Q4 G12 E13 I14 S15 V16 K20 F21 F22 L23 V26 A27 G28 D29 A30 K31 D32 K33 D34 I35 P40 N41 G42 E43 K44 L45 Q49 I52 D59 D60 S61 S62 T63 L64 T65 I66 Y67 N68 A69 N70 I71 D72 D73 A74 V81 E84 T92

V93 I97 F98 Q99

4.2.13 Score per residue for model 13

- Molecule 1: NEURAL CELL ADHESION MOLECULE

Chain A: 53% 31% 5% 11%

R1 V2 L3 Q4 I7 G12 E13 I14 S15 K20 F21 F22 V26 A27 G28 D29 A30 K31 D32 K33 D34 I35 P40 N41 G42 E43 K44 L45 Q49 Q50 R51 I52 S53 V54 N57 D58 D59 D60 S61 S62 T63 L64 T65 I66 Y67 N68 A69 N70 A74 Y77 K78

C79 V80 V81 T82 T92 V93 I97 F98 Q99

4.2.14 Score per residue for model 14

- Molecule 1: NEURAL CELL ADHESION MOLECULE

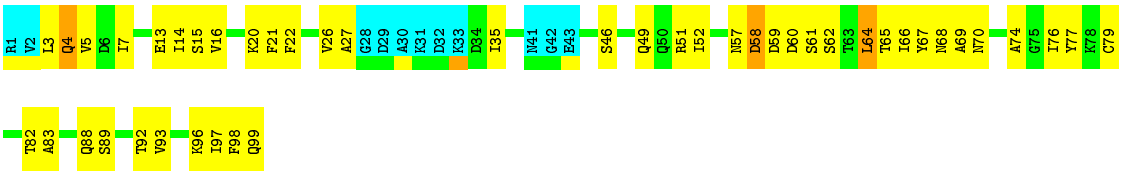
Chain A: 57% 28% • 11%

R1 V2 L3 Q4 V5 S15 E18 S19 K20 F21 F22 L23 A27 G28 D29 A30 K31 D32 K33 D34 N41 G42 E43 Q49 I52 D58 L64 T65 I66 Y67 N68 A69 N70 A74 Y77 K78 C79 V80 V81 T87 Q88 T92 V93 K96 I97 F98 Q99

4.2.15 Score per residue for model 15

- Molecule 1: NEURAL CELL ADHESION MOLECULE

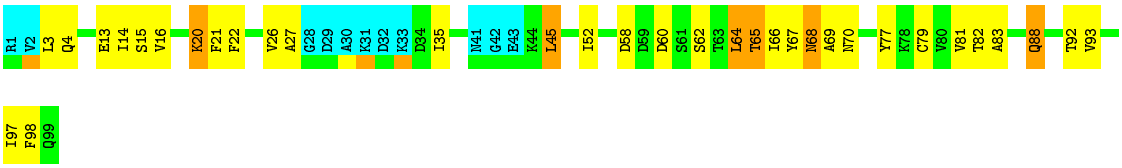
Chain A: 43% 42% • 11%



4.2.16 Score per residue for model 16

- Molecule 1: NEURAL CELL ADHESION MOLECULE

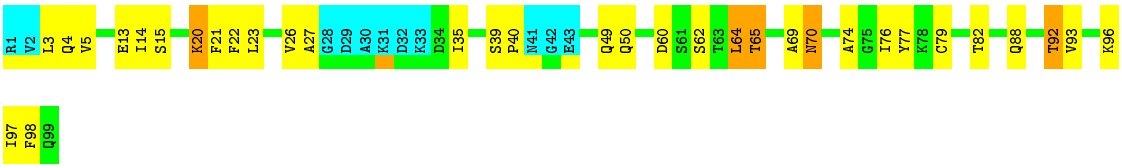
Chain A:



4.2.17 Score per residue for model 17

- Molecule 1: NEURAL CELL ADHESION MOLECULE

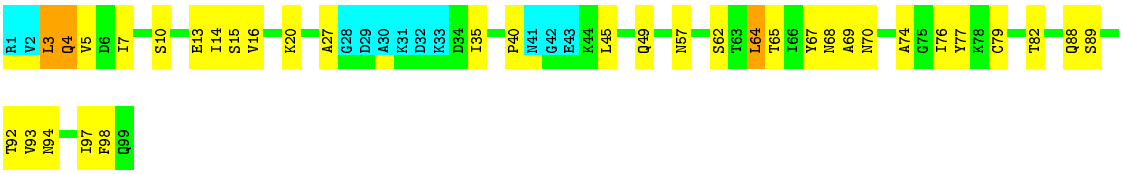
Chain A:



4.2.18 Score per residue for model 18

- Molecule 1: NEURAL CELL ADHESION MOLECULE

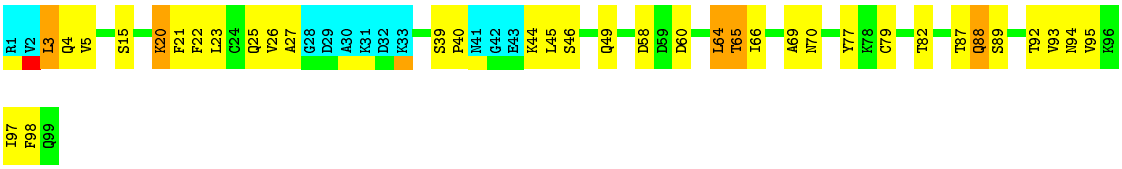
Chain A:



4.2.19 Score per residue for model 19

- Molecule 1: NEURAL CELL ADHESION MOLECULE

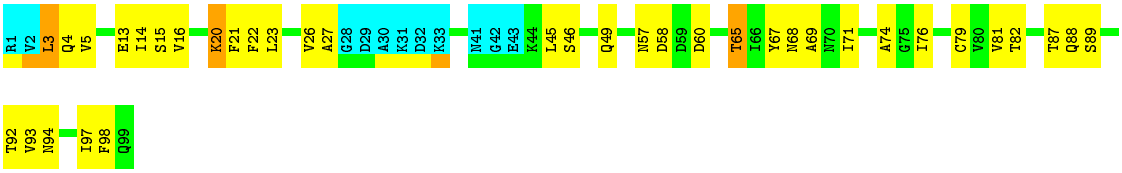
Chain A:



4.2.20 Score per residue for model 20

- Molecule 1: NEURAL CELL ADHESION MOLECULE

Chain A:



5 Refinement protocol and experimental data overview (i)

Of the ? calculated structures, 20 were deposited, based on the following criterion: *?*.

The authors did not provide any information on software used for structure solution, optimization or refinement.

No chemical shift data was provided. No validations of the models with respect to experimental NMR restraints is performed at this time.

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	682	654	654	16±4
All	All	13640	13080	13080	322

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 12.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:35:ILE:HD13	1:A:81:VAL:HG23	0.80	1.50	13	3
1:A:70:ASN:O	1:A:97:ILE:HD12	0.72	1.84	17	19
1:A:26:VAL:HG21	1:A:60:ASP:CB	0.71	2.16	16	11
1:A:69:ALA:HB1	1:A:97:ILE:HD13	0.69	1.64	15	13
1:A:13:GLU:O	1:A:14:ILE:HD13	0.69	1.86	1	1
1:A:3:LEU:HD21	1:A:83:ALA:HB2	0.68	1.64	15	1
1:A:16:VAL:HG13	1:A:69:ALA:O	0.68	1.88	9	10
1:A:22:PHE:CD2	1:A:93:VAL:HG21	0.68	2.24	15	15
1:A:20:LYS:NZ	1:A:97:ILE:HD11	0.68	2.04	18	20
1:A:35:ILE:HG21	1:A:62:SER:OG	0.68	1.89	11	13
1:A:21:PHE:HB3	1:A:65:THR:HG23	0.67	1.64	3	17
1:A:76:ILE:HD13	1:A:94:ASN:HA	0.66	1.65	3	6
1:A:4:GLN:CB	1:A:27:ALA:HB3	0.66	2.20	12	7
1:A:39:SER:OG	1:A:45:LEU:HD11	0.66	1.91	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:LEU:HD11	1:A:77:TYR:CD2	0.65	2.27	18	18
1:A:20:LYS:HE3	1:A:66:ILE:HD12	0.64	1.69	19	1
1:A:82:THR:HG23	1:A:88:GLN:CG	0.61	2.26	11	7
1:A:35:ILE:CD1	1:A:81:VAL:HG23	0.59	2.27	12	3
1:A:82:THR:HG23	1:A:88:GLN:HG2	0.58	1.76	9	8
1:A:26:VAL:HG21	1:A:60:ASP:HB2	0.58	1.74	16	10
1:A:4:GLN:HB3	1:A:27:ALA:HB3	0.57	1.75	16	19
1:A:26:VAL:HG21	1:A:60:ASP:HB3	0.57	1.76	2	7
1:A:35:ILE:HD11	1:A:60:ASP:HA	0.57	1.75	8	2
1:A:35:ILE:HD13	1:A:81:VAL:HG22	0.56	1.76	9	1
1:A:12:GLY:O	1:A:14:ILE:HD12	0.55	2.02	12	3
1:A:10:SER:O	1:A:93:VAL:HG23	0.55	2.02	18	1
1:A:22:PHE:CD1	1:A:93:VAL:HG21	0.54	2.37	14	2
1:A:20:LYS:HZ1	1:A:97:ILE:HD11	0.53	1.61	18	3
1:A:52:ILE:HG12	1:A:66:ILE:HG23	0.53	1.80	9	10
1:A:34:ASP:C	1:A:35:ILE:HD12	0.53	2.23	1	1
1:A:35:ILE:CD1	1:A:81:VAL:HG22	0.52	2.34	9	1
1:A:52:ILE:HG23	1:A:66:ILE:HG12	0.52	1.80	9	3
1:A:45:LEU:O	1:A:45:LEU:HD12	0.51	2.06	16	3
1:A:5:VAL:HG21	1:A:89:SER:O	0.51	2.05	9	7
1:A:14:ILE:HD13	1:A:20:LYS:CB	0.51	2.35	4	2
1:A:74:ALA:N	1:A:97:ILE:HD12	0.51	2.21	20	1
1:A:82:THR:HG23	1:A:88:GLN:HB3	0.50	1.84	8	6
1:A:14:ILE:HG23	1:A:18:GLU:HG3	0.50	1.82	9	1
1:A:23:LEU:HD23	1:A:25:GLN:NE2	0.50	2.21	19	1
1:A:52:ILE:CG2	1:A:64:LEU:HD11	0.50	2.37	12	1
1:A:13:GLU:C	1:A:14:ILE:HD12	0.49	2.27	17	8
1:A:80:VAL:HG13	1:A:89:SER:O	0.49	2.07	2	3
1:A:7:ILE:HD11	1:A:79:CYS:HB2	0.49	1.83	18	5
1:A:3:LEU:HD11	1:A:87:THR:O	0.48	2.08	14	4
1:A:13:GLU:C	1:A:14:ILE:HD13	0.48	2.29	1	1
1:A:20:LYS:CE	1:A:66:ILE:HD12	0.48	2.36	19	1
1:A:35:ILE:HD12	1:A:35:ILE:N	0.46	2.25	7	2
1:A:35:ILE:N	1:A:35:ILE:HD12	0.46	2.25	1	2
1:A:34:ASP:O	1:A:81:VAL:HG22	0.46	2.11	2	2
1:A:20:LYS:HD2	1:A:66:ILE:HD12	0.45	1.88	6	2
1:A:20:LYS:HZ3	1:A:97:ILE:HD11	0.45	1.70	19	1
1:A:74:ALA:HB2	1:A:97:ILE:HG13	0.45	1.88	3	13
1:A:4:GLN:CD	1:A:27:ALA:HB3	0.45	2.32	14	1
1:A:45:LEU:HD11	1:A:54:VAL:CG2	0.44	2.42	13	1
1:A:22:PHE:CZ	1:A:95:VAL:HG22	0.44	2.47	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:82:THR:HG23	1:A:88:GLN:HG3	0.44	1.90	11	1
1:A:7:ILE:HD11	1:A:79:CYS:CB	0.43	2.43	15	2
1:A:3:LEU:HD11	1:A:83:ALA:HB2	0.43	1.89	16	1
1:A:23:LEU:HD13	1:A:24:CYS:N	0.43	2.29	6	1
1:A:20:LYS:NZ	1:A:95:VAL:HG11	0.42	2.29	19	1
1:A:76:ILE:O	1:A:76:ILE:HG22	0.42	2.14	6	2
1:A:14:ILE:HG23	1:A:18:GLU:CG	0.42	2.44	9	1
1:A:39:SER:HB3	1:A:45:LEU:HD23	0.41	1.91	19	1
1:A:37:TRP:CE3	1:A:78:LYS:O	0.41	2.74	10	1
1:A:76:ILE:HG23	1:A:92:THR:HB	0.41	1.92	17	1
1:A:3:LEU:HD23	1:A:81:VAL:HG12	0.41	1.93	12	1
1:A:80:VAL:HG13	1:A:90:GLU:HB3	0.41	1.93	6	1
1:A:39:SER:OG	1:A:45:LEU:HD23	0.41	2.15	11	1
1:A:93:VAL:O	1:A:93:VAL:HG13	0.40	2.16	19	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	87/99 (88%)	72±3 (82±4%)	13±3 (14±3%)	3±1 (3±1%)	6 36
All	All	1740/1980 (88%)	1431 (82%)	250 (14%)	59 (3%)	6 36

All 10 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	67	TYR	14
1	A	68	ASN	12
1	A	58	ASP	11
1	A	40	PRO	9
1	A	69	ALA	6
1	A	44	LYS	2
1	A	74	ALA	2
1	A	50	GLN	1

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Mol	Chain	Res	Type	Models (Total)
1	A	49	GLN	1
1	A	59	ASP	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	79/87 (91%)	65±2 (82±3%)	14±2 (18±3%)	4 39
All	All	1580/1740 (91%)	1303 (82%)	277 (18%)	4 39

All 41 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	15	SER	20
1	A	98	PHE	20
1	A	92	THR	20
1	A	65	THR	20
1	A	64	LEU	18
1	A	20	LYS	16
1	A	68	ASN	14
1	A	49	GLN	13
1	A	4	GLN	11
1	A	57	ASN	10
1	A	3	LEU	9
1	A	81	VAL	8
1	A	58	ASP	7
1	A	79	CYS	7
1	A	96	LYS	6
1	A	88	GLN	6
1	A	45	LEU	6
1	A	23	LEU	6
1	A	46	SER	5
1	A	82	THR	5
1	A	99	GLN	4
1	A	5	VAL	4
1	A	62	SER	4

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Mol	Chain	Res	Type	Models (Total)
1	A	70	ASN	4
1	A	94	ASN	4
1	A	13	GLU	4
1	A	51	ARG	4
1	A	59	ASP	3
1	A	61	SER	2
1	A	84	GLU	2
1	A	50	GLN	2
1	A	39	SER	2
1	A	72	ASP	2
1	A	71	ILE	2
1	A	11	GLN	1
1	A	18	GLU	1
1	A	76	ILE	1
1	A	63	THR	1
1	A	21	PHE	1
1	A	89	SER	1
1	A	78	LYS	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 carbohydrates 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