Full wwPDB NMR Structure Validation Report (i)

Jun 12, 2024 – 07:09 AM EDT

PDB ID	:	2ENJ
Title	:	Solution structure of the C2 domain from human protein kinase C theta
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Deposited on	:	2007-03-28

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

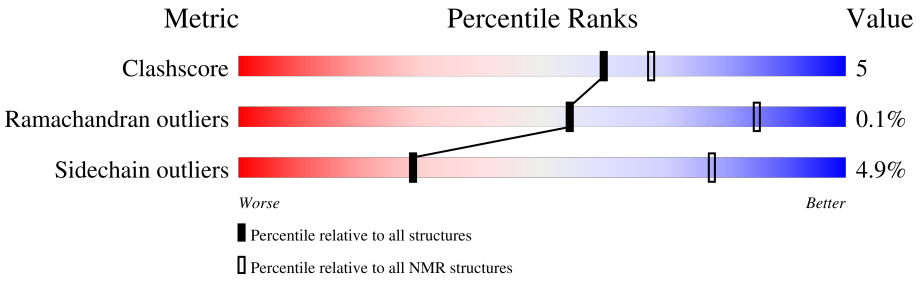
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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	138	60% • 36%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 2 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:2-A:14, A:27-A:34, A:50-A:75, A:82-A:123 (89)	0.42	2

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 5 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2124 atoms, of which 1054 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Protein kinase C theta type.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	138	2124	669	1054	183	206	12	0

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP Q04759
A	-5	SER	-	expression tag	UNP Q04759
A	-4	SER	-	expression tag	UNP Q04759
A	-3	GLY	-	expression tag	UNP Q04759
A	-2	SER	-	expression tag	UNP Q04759
A	-1	SER	-	expression tag	UNP Q04759
A	0	GLY	-	expression tag	UNP Q04759
A	126	SER	-	expression tag	UNP Q04759
A	127	GLY	-	expression tag	UNP Q04759
A	128	PRO	-	expression tag	UNP Q04759
A	129	SER	-	expression tag	UNP Q04759
A	130	SER	-	expression tag	UNP Q04759
A	131	GLY	-	expression tag	UNP Q04759

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: Protein kinase C theta type

Chain A: 60% • 36%

G-6 S-5 S-4 G-3 S-2 S-1 G0 M1 L5 G15 S16 C17 Q18 S19 C20 Q21 G22 E23 A24 V25 N26 A30 E35 Y36 V37 E38 S39 E40 N41 G42 Q43 M44 Y45 I46 Q47 K48 K49 P50 T51 V74 K75 G76 K77 N78 V79 D80 L81 A93 K102 E124 M125 S126

G127 P128 S129 S130 G131

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: Protein kinase C theta type

Chain A: 57% 7% 36%

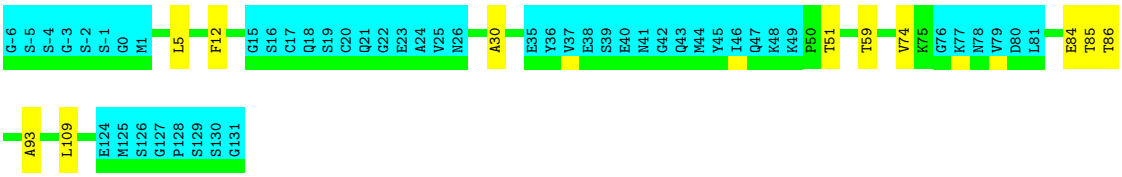
G-6 S-5 S-4 G-3 S-2 S-1 G0 M1 L5 G15 S16 C17 Q18 S19 C20 Q21 G22 E23 A24 V25 N26 E35 Y36 V37 E38 S39 E40 N41 G42 Q43 M44 Y45 I46 Q47 K48 K49 D57 S58 T59 I64 G76 K77 N78 V79 D80 L81 L92 A93 R114 A119

F122 L123 E124 M125 S126 G127 P128 S129 S130 G131

4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: Protein kinase C theta type

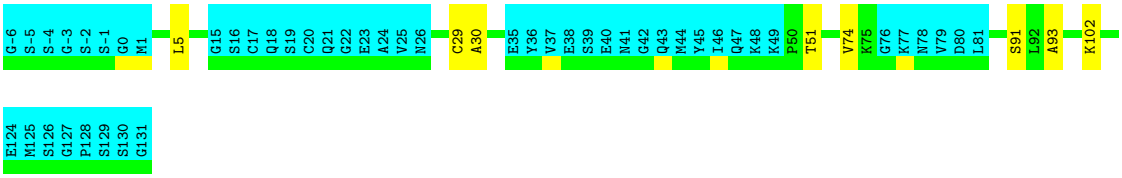
Chain A: 57% 8% 36%



4.2.3 Score per residue for model 3

- Molecule 1: Protein kinase C theta type

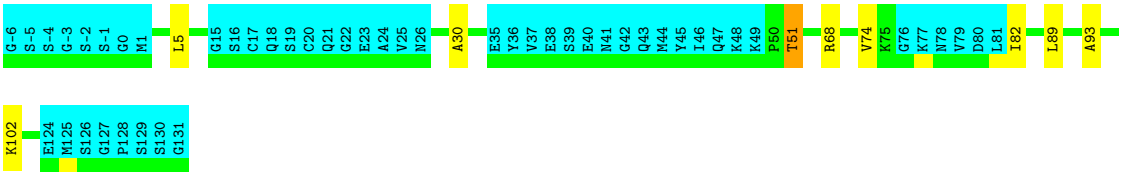
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: Protein kinase C theta type

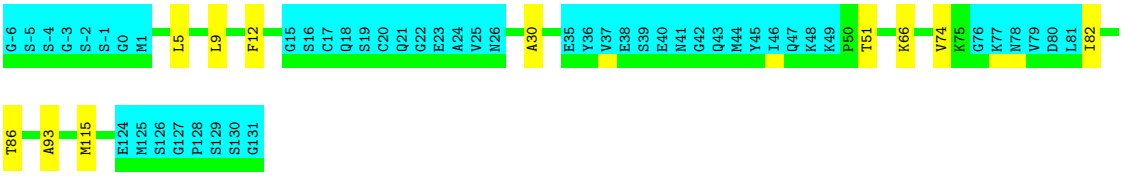
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: Protein kinase C theta type

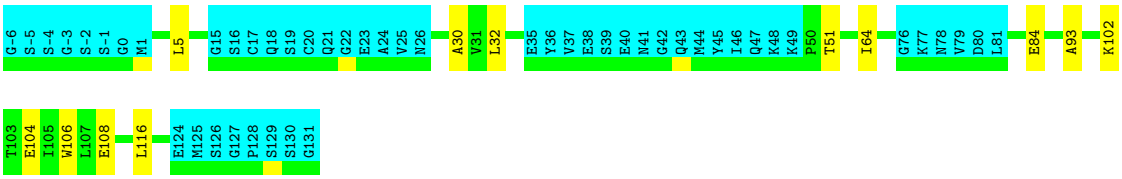
Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Protein kinase C theta type

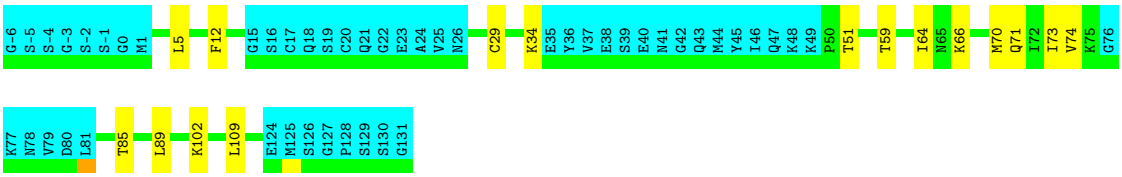
Chain A:



4.2.7 Score per residue for model 7

- Molecule 1: Protein kinase C theta type

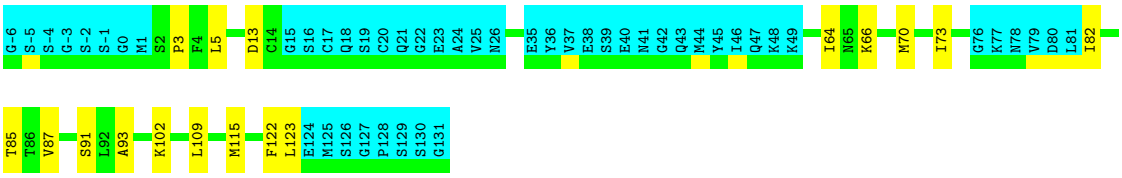
Chain A:



4.2.8 Score per residue for model 8

- Molecule 1: Protein kinase C theta type

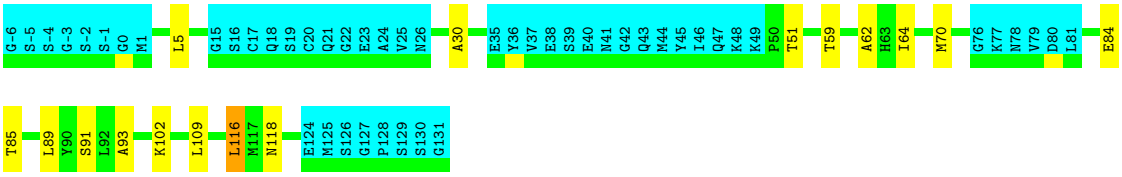
Chain A:



4.2.9 Score per residue for model 9

- Molecule 1: Protein kinase C theta type

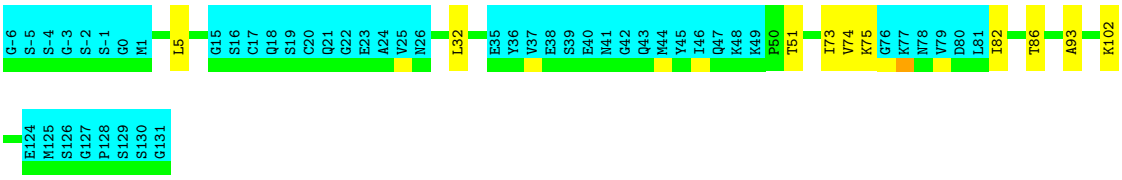
Chain A:



4.2.10 Score per residue for model 10

- Molecule 1: Protein kinase C theta type

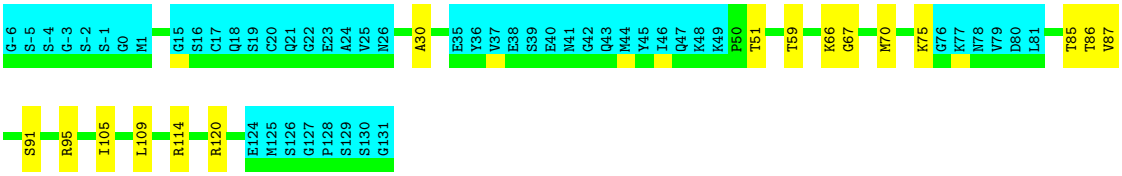
Chain A: 57% 7% 36%



4.2.11 Score per residue for model 11

- Molecule 1: Protein kinase C theta type

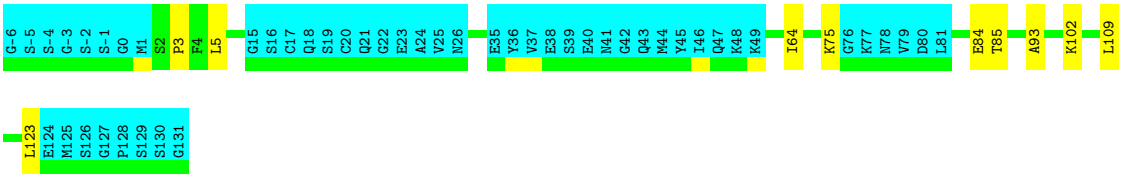
Chain A: 53% 12% 36%



4.2.12 Score per residue for model 12

- Molecule 1: Protein kinase C theta type

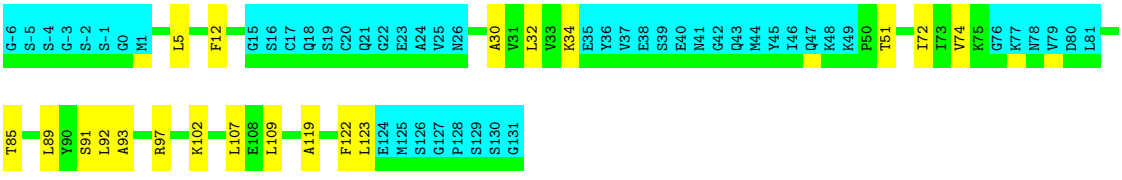
Chain A: 57% 7% 36%



4.2.13 Score per residue for model 13

- Molecule 1: Protein kinase C theta type

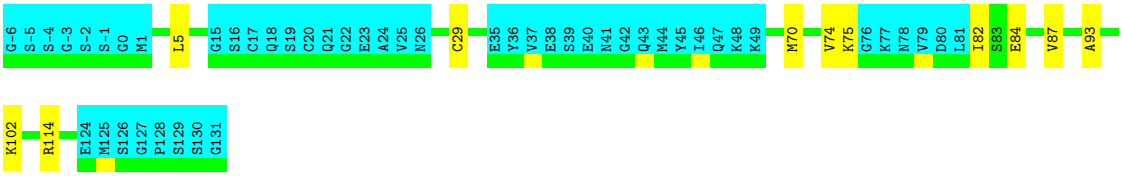
Chain A: 50% 14% 36%



4.2.14 Score per residue for model 14

- Molecule 1: Protein kinase C theta type

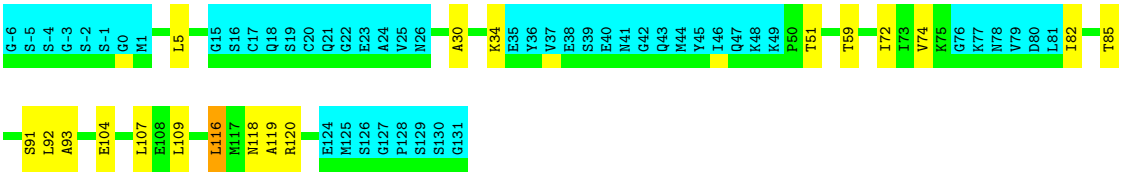
Chain A: 57% 8% 36%



4.2.15 Score per residue for model 15

- Molecule 1: Protein kinase C theta type

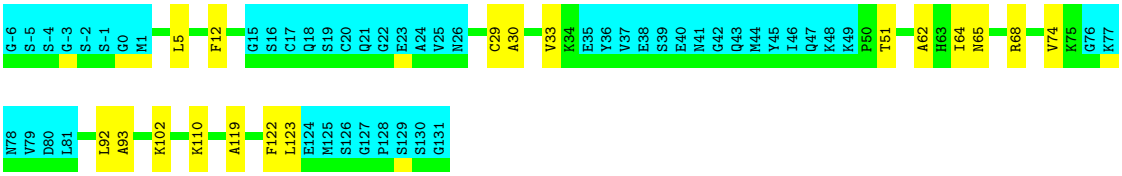
Chain A: 51% 13% • 36%



4.2.16 Score per residue for model 16

- Molecule 1: Protein kinase C theta type

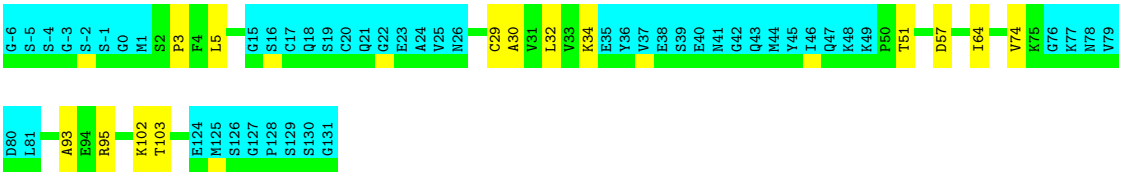
Chain A: 51% 13% 36%



4.2.17 Score per residue for model 17

- Molecule 1: Protein kinase C theta type

Chain A: 54% 10% 36%



4.2.18 Score per residue for model 18

- Molecule 1: Protein kinase C theta type

Chain A: 53% 11% • 36%

G-6 S-5 S-4 G-3 S-2 S-1 G0 M1 S2 P3 F4 L5 G15 S16 C17 Q18 S19 C20 Q21 C22 E23 A24 V25 N26 E35 Y36 V37 E38 S39 E40 M41 G42 Q43 M44 Y45 I46 Q47 K48 K49 T59 I64 I72 I73 G76 K77 N78 V79 D80 L81 I82 A93 K102

L107 M115 L116 M117 N118 F122 L123 E124 M125 S126 G127 P128 S129 S130 G131

4.2.19 Score per residue for model 19

- Molecule 1: Protein kinase C theta type

Chain A: 48% 16% • 36%

G-6 S-5 S-4 G-3 S-2 S-1 G0 M1 S2 P3 F4 L5 S10 G15 S16 C17 Q18 S19 C20 Q21 C22 E23 A24 V25 N26 A30 K34 E35 Y36 V37 E38 S39 E40 M41 G42 Q43 M44 Y45 I46 Q47 K48 K49 P50 T51 T59 I64 N65 K66 I73 V74 K75 G76 K77

N78 V79 D80 L81 I82 T85 S91 L92 A93 K102 L109 L116 M117 N118 A119 F122 L123 E124 M125 S126 G127 P128 S129 S130 G131

4.2.20 Score per residue for model 20

- Molecule 1: Protein kinase C theta type

Chain A: 54% 10% 36%

G-6 S-5 S-4 G-3 S-2 S-1 G0 M1 L5 F12 G15 S16 C17 Q18 S19 C20 Q21 C22 E23 A24 V25 N26 L32 V33 K34 E35 Y36 V37 E38 S39 E40 N41 G42 Q43 M44 Y45 I46 Q47 K48 K49 T59 H63 V74 K75 G76 K77 N78 V79 D80 L81 I82 T85

T86 A93 K102 L109 E124 M125 S126 G127 P128 S129 S130 G131

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	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	725	738	738	7±2
All	All	14500	14760	14760	137

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 5.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:LEU:HD11	1:A:93:ALA:HB2	0.68	1.64	19	3
1:A:30:ALA:HB1	1:A:51:THR:HG21	0.66	1.67	17	6
1:A:5:LEU:HD11	1:A:93:ALA:CA	0.62	2.25	2	18
1:A:32:LEU:HD13	1:A:73:ILE:HD12	0.62	1.71	10	1
1:A:106:TRP:CE2	1:A:116:LEU:HD13	0.60	2.32	6	1
1:A:5:LEU:HD11	1:A:93:ALA:N	0.58	2.13	4	10
1:A:30:ALA:HB3	1:A:73:ILE:HB	0.57	1.75	19	1
1:A:95:ARG:HB3	1:A:103:THR:HG21	0.57	1.75	17	1
1:A:92:LEU:HD11	1:A:119:ALA:CB	0.56	2.31	19	4
1:A:85:THR:HB	1:A:109:LEU:HD23	0.55	1.78	7	8
1:A:116:LEU:HD22	1:A:118:ASN:ND2	0.55	2.17	15	4
1:A:122:PHE:O	1:A:123:LEU:HD22	0.53	2.03	13	6
1:A:12:PHE:CZ	1:A:74:VAL:HG11	0.53	2.38	2	5
1:A:5:LEU:HD11	1:A:93:ALA:CB	0.52	2.33	19	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:29:CYS:SG	1:A:74:VAL:HG22	0.52	2.45	3	5
1:A:30:ALA:HB1	1:A:51:THR:CG2	0.52	2.34	5	10
1:A:71:GLN:NE2	1:A:73:ILE:HD11	0.52	2.19	7	1
1:A:32:LEU:CD1	1:A:73:ILE:HD12	0.52	2.33	10	1
1:A:5:LEU:HD21	1:A:93:ALA:HA	0.51	1.81	6	2
1:A:3:PRO:O	1:A:64:ILE:HD12	0.51	2.05	8	5
1:A:95:ARG:HD3	1:A:105:ILE:HD11	0.51	1.82	11	1
1:A:9:LEU:HD22	1:A:115:MET:SD	0.49	2.48	5	1
1:A:5:LEU:HD11	1:A:93:ALA:HA	0.48	1.84	12	6
1:A:74:VAL:HG12	1:A:82:ILE:HD12	0.48	1.85	15	2
1:A:5:LEU:HG	1:A:64:ILE:HD11	0.47	1.86	7	5
1:A:107:LEU:HD21	1:A:117:MET:SD	0.47	2.50	18	1
1:A:74:VAL:HG12	1:A:82:ILE:HD13	0.47	1.87	4	1
1:A:89:LEU:HD23	1:A:92:LEU:HD23	0.46	1.87	13	1
1:A:72:ILE:HG21	1:A:115:MET:SD	0.45	2.52	18	1
1:A:85:THR:CG2	1:A:109:LEU:HD23	0.44	2.42	9	2
1:A:72:ILE:HD12	1:A:107:LEU:HD13	0.44	1.88	18	2
1:A:33:VAL:HG11	1:A:68:ARG:CZ	0.44	2.43	16	1
1:A:5:LEU:CD1	1:A:93:ALA:HB2	0.44	2.41	19	1
1:A:70:MET:HB3	1:A:87:VAL:HG13	0.43	1.89	11	3
1:A:5:LEU:O	1:A:62:ALA:HB3	0.43	2.13	9	2
1:A:92:LEU:HD21	1:A:119:ALA:HB2	0.43	1.90	16	1
1:A:32:LEU:CD1	1:A:51:THR:HG23	0.43	2.44	6	1
1:A:109:LEU:HD11	1:A:115:MET:HG2	0.42	1.91	8	1
1:A:122:PHE:C	1:A:123:LEU:HD22	0.42	2.35	16	1
1:A:74:VAL:O	1:A:82:ILE:HD12	0.41	2.16	5	2
1:A:12:PHE:CE2	1:A:74:VAL:HG11	0.41	2.50	7	1
1:A:70:MET:CE	1:A:89:LEU:HD21	0.41	2.46	7	1
1:A:70:MET:HB2	1:A:89:LEU:HD11	0.41	1.92	9	1
1:A:72:ILE:HD12	1:A:107:LEU:CD1	0.41	2.46	15	1
1:A:32:LEU:HG	1:A:51:THR:HG23	0.41	1.91	17	1
1:A:68:ARG:HG2	1:A:89:LEU:HD12	0.41	1.93	4	1
1:A:5:LEU:HD23	1:A:120:ARG:O	0.41	2.16	15	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	89/138 (64%)	85±1 (96±1%)	4±1 (4±1%)	0±0 (0±0%)	54 85
All	All	1780/2760 (64%)	1702 (96%)	76 (4%)	2 (0%)	54 85

All 2 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	51	THR	1
1	A	67	GLY	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	81/120 (68%)	77±2 (95±2%)	4±2 (5±2%)	29 78
All	All	1620/2400 (68%)	1540 (95%)	80 (5%)	29 78

All 21 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	102	LYS	15
1	A	59	THR	9
1	A	91	SER	7
1	A	34	LYS	6
1	A	75	LYS	6
1	A	84	GLU	5
1	A	86	THR	5
1	A	66	LYS	5
1	A	116	LEU	4
1	A	114	ARG	3
1	A	51	THR	3
1	A	57	ASP	2
1	A	104	GLU	2
1	A	108	GLU	1
1	A	13	ASP	1

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Mol	Chain	Res	Type	Models (Total)
1	A	120	ARG	1
1	A	97	ARG	1
1	A	65	ASN	1
1	A	110	LYS	1
1	A	10	SER	1
1	A	63	HIS	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