wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2LC7
BMRB ID	:	17600
Title	:	Solution structure of the isolated Par-6 PDZ domain
Authors	:	Volkman, B.F.; Whitney, D.S.; Peterson, F.C.
Deposited on	:	2011-04-25

This is a wwPDB NMR Structure Validation Summary 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:

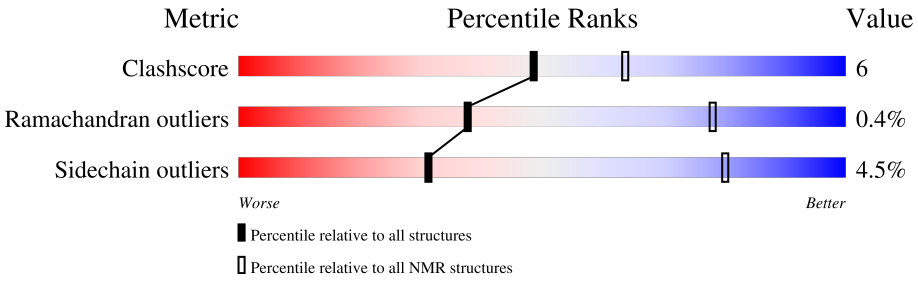
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 is 90%.

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	102	66% 11% 22% .

2 Ensemble composition and analysis

This entry contains 20 models. Model 9 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:158-A:164, A:172-A:181, A:191-A:251 (78)	0.51	9

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 3 clusters and 7 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1386 atoms, of which 630 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Par-6.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	100	1386	470	630	138	146	2	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	154	GLY	-	expression tag	UNP O97111
A	155	SER	-	expression tag	UNP O97111

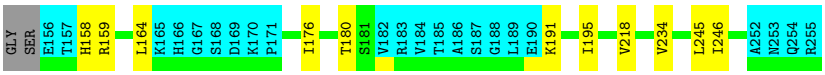
4 Residue-property plots (i)

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: Par-6

Chain A:

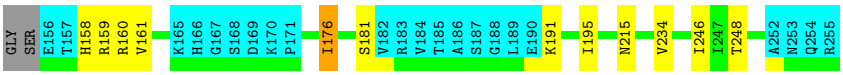


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 9. Colouring as in section 4.1 above.

- Molecule 1: Par-6

Chain A:



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: *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
CYANA	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1218
Number of shifts mapped to atoms	1089
Number of unparsed shifts	0
Number of shifts with mapping errors	129
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	90%

6 Model quality

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.85±0.02	0±0/596 (0.0± 0.0%)	0.67±0.02	0±0/808 (0.0± 0.0%)
All	All	0.85	0/11920 (0.0%)	0.67	1/16160 (0.0%)

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
All	All	0	1

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	250	LYS	CB-CA-C	-5.20	99.99	110.40	1	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	159	ARG	Sidechain	1

6.2 Too-close contacts

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	589	486	618	8±2
All	All	11780	9720	12360	150

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 6.

5 of 62 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:158:HIS:NE2	1:A:219:ILE:HG13	0.62	2.10	7	5
1:A:164:LEU:HG	1:A:242:SER:O	0.62	1.94	20	1
1:A:158:HIS:HB3	1:A:250:LYS:HB3	0.61	1.71	18	2
1:A:160:ARG:HB3	1:A:248:THR:OG1	0.60	1.96	2	2
1:A:216:ASP:OD1	1:A:251:PRO:HA	0.59	1.96	11	2

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	78/102 (76%)	75±1 (96±1%)	3±1 (3±1%)	0±0 (0±1%)	38	78
All	All	1560/2040 (76%)	1501 (96%)	52 (3%)	7 (0%)	38	78

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	164	LEU	4
1	A	244	ASN	3

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	66/85 (78%)	63±1 (96±2%)	3±1 (4±2%)	31 80
All	All	1320/1700 (78%)	1261 (96%)	59 (4%)	31 80

5 of 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	180	THR	15
1	A	176	ILE	11
1	A	158	HIS	7
1	A	164	LEU	5
1	A	160	ARG	4

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

The completeness of assignment taking into account all chemical shift lists is 90% for the well-defined parts and 90% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1218
Number of shifts mapped to atoms	1089
Number of unparsed shifts	0
Number of shifts with mapping errors	129
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. First 5 (of 129) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	157	THR	HG22	1.201	0.000	1
1	A	157	THR	HG23	1.201	0.000	1
1	A	161	VAL	HG11	0.802	0.000	1
1	A	161	VAL	HG12	0.802	0.000	1
1	A	163	LEU	HD11	0.792	0.007	2
1	A	163	LEU	HD12	0.792	0.007	2
1	A	163	LEU	HD22	0.76	0.002	2
1	A	163	LEU	HD23	0.76	0.002	2
1	A	164	LEU	HD11	0.874	0.001	2
1	A	164	LEU	HD12	0.874	0.001	2
1	A	164	LEU	HD22	0.876	0.000	2
1	A	164	LEU	HD23	0.876	0.000	2
1	A	172	LEU	HD11	0.887	0.000	2
1	A	172	LEU	HD12	0.887	0.000	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	172	LEU	HD22	0.892	0.000	2
1	A	172	LEU	HD23	0.892	0.000	2
1	A	176	ILE	HG21	0.882	0.000	1
1	A	176	ILE	HG22	0.882	0.000	1
1	A	176	ILE	HG13	1.11	0.004	2
1	A	176	ILE	HD12	0.826	0.000	1
1	A	176	ILE	HD13	0.826	0.000	1
1	A	180	THR	HG22	1.102	0.004	1
1	A	180	THR	HG23	1.102	0.004	1
1	A	182	VAL	HG11	0.873	0.000	2
1	A	182	VAL	HG12	0.873	0.000	2
1	A	182	VAL	HG22	0.923	0.000	2
1	A	182	VAL	HG23	0.923	0.000	2
1	A	184	VAL	HG11	0.951	0.004	2
1	A	184	VAL	HG12	0.951	0.004	2
1	A	184	VAL	HG22	0.923	0.000	2
1	A	184	VAL	HG23	0.923	0.000	2
1	A	185	THR	HG22	1.141	0.003	1
1	A	185	THR	HG23	1.141	0.003	1
1	A	189	LEU	HD11	0.843	0.000	1
1	A	189	LEU	HD12	0.843	0.000	1
1	A	192	GLN	HE22	6.788	0.000	2
1	A	195	ILE	HG21	0.793	0.001	1
1	A	195	ILE	HG22	0.793	0.001	1
1	A	195	ILE	HG13	1.267	0.005	2
1	A	195	ILE	HD12	0.765	0.006	1
1	A	195	ILE	HD13	0.765	0.006	1
1	A	197	ILE	HG21	0.856	0.003	1
1	A	197	ILE	HG22	0.856	0.003	1
1	A	197	ILE	HG13	1.177	0.006	2
1	A	197	ILE	HD12	0.529	0.003	1
1	A	197	ILE	HD13	0.529	0.003	1
1	A	200	LEU	HD11	0.859	0.000	2
1	A	200	LEU	HD12	0.859	0.000	2
1	A	200	LEU	HD22	0.774	0.006	2
1	A	200	LEU	HD23	0.774	0.006	2
1	A	201	VAL	HG11	1.031	0.000	2
1	A	201	VAL	HG12	1.031	0.000	2
1	A	201	VAL	HG22	0.956	0.005	2
1	A	201	VAL	HG23	0.956	0.005	2
1	A	209	THR	HG22	1.453	0.000	1

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	209	THR	HG23	1.453	0.000	1
1	A	211	LEU	HD11	0.876	0.000	1
1	A	211	LEU	HD12	0.876	0.000	1
1	A	211	LEU	HD22	0.876	0.000	1
1	A	211	LEU	HD23	0.876	0.000	1
1	A	212	LEU	HD11	0.654	0.007	2
1	A	212	LEU	HD12	0.654	0.007	2
1	A	212	LEU	HD22	0.434	0.003	2
1	A	212	LEU	HD23	0.434	0.003	2
1	A	214	VAL	HG11	0.969	0.004	1
1	A	214	VAL	HG12	0.969	0.004	1
1	A	215	ASN	HD22	6.99	0.000	2
1	A	218	VAL	HG11	0.671	0.000	1
1	A	218	VAL	HG12	0.671	0.000	1
1	A	219	ILE	HG21	0.841	0.008	1
1	A	219	ILE	HG22	0.841	0.008	1
1	A	219	ILE	HG13	0.745	0.000	2
1	A	219	ILE	HD12	0.405	0.006	1
1	A	219	ILE	HD13	0.405	0.006	1
1	A	221	VAL	HG11	0.843	0.002	2
1	A	221	VAL	HG12	0.843	0.002	2
1	A	221	VAL	HG22	0.799	0.000	2
1	A	221	VAL	HG23	0.799	0.000	2
1	A	222	ASN	HD22	7.323	0.001	2
1	A	224	ILE	HG21	0.941	0.002	1
1	A	224	ILE	HG22	0.941	0.002	1
1	A	224	ILE	HG13	1.205	0.006	2
1	A	224	ILE	HD12	0.848	0.005	1
1	A	224	ILE	HD13	0.848	0.005	1
1	A	226	VAL	HG11	0.753	0.002	2
1	A	226	VAL	HG12	0.753	0.002	2
1	A	226	VAL	HG22	0.689	0.004	2
1	A	226	VAL	HG23	0.689	0.004	2
1	A	230	THR	HG22	1.342	0.004	1
1	A	230	THR	HG23	1.342	0.004	1
1	A	231	LEU	HD11	0.926	0.005	1
1	A	231	LEU	HD12	0.926	0.005	1
1	A	231	LEU	HD22	0.926	0.005	1
1	A	231	LEU	HD23	0.926	0.005	1
1	A	233	GLN	HE22	6.833	0.000	2
1	A	234	VAL	HG11	1.001	0.006	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	234	VAL	HG12	1.001	0.006	2
1	A	234	VAL	HG22	0.88	0.000	2
1	A	234	VAL	HG23	0.88	0.000	2
1	A	235	THR	HG22	1.245	0.006	1
1	A	235	THR	HG23	1.245	0.006	1
1	A	239	VAL	HG11	1.073	0.004	2
1	A	239	VAL	HG12	1.073	0.004	2
1	A	239	VAL	HG22	0.95	0.001	2
1	A	239	VAL	HG23	0.95	0.001	2
1	A	241	ASN	HD22	7.085	0.000	2
1	A	244	ASN	HD22	6.661	0.000	2
1	A	245	LEU	HD11	1.049	0.000	1
1	A	245	LEU	HD12	1.049	0.000	1
1	A	245	LEU	HD22	1.05	0.000	1
1	A	245	LEU	HD23	1.05	0.000	1
1	A	246	ILE	HG21	0.675	0.003	1
1	A	246	ILE	HG22	0.675	0.003	1
1	A	246	ILE	HG13	0.784	0.008	2
1	A	246	ILE	HD12	0.802	0.000	1
1	A	246	ILE	HD13	0.802	0.000	1
1	A	247	ILE	HG21	0.907	0.000	1
1	A	247	ILE	HG22	0.907	0.000	1
1	A	247	ILE	HG13	1.035	0.004	2
1	A	247	ILE	HD12	0.63	0.000	1
1	A	247	ILE	HD13	0.63	0.000	1
1	A	248	THR	HG22	0.962	0.000	1
1	A	248	THR	HG23	0.962	0.000	1
1	A	249	VAL	HG11	0.705	0.004	2
1	A	249	VAL	HG12	0.705	0.004	2
1	A	249	VAL	HG22	0.797	0.000	2
1	A	249	VAL	HG23	0.797	0.000	2
1	A	253	ASN	HD22	6.915	0.000	2
1	A	254	GLN	HE22	6.924	0.000	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	100	-0.63 ± 0.13	Should be checked
$^{13}C_{\beta}$	90	-0.18 ± 0.09	None needed (< 0.5 ppm)

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Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C'$	97	-0.29 ± 0.14	None needed (< 0.5 ppm)
^{15}N	95	-0.07 ± 0.59	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 90%, i.e. 966 atoms were assigned a chemical shift out of a possible 1068. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	389/392 (99%)	161/161 (100%)	153/156 (98%)	75/75 (100%)
Sidechain	553/639 (87%)	371/420 (88%)	176/195 (90%)	6/24 (25%)
Aromatic	24/37 (65%)	15/18 (83%)	9/17 (53%)	0/2 (0%)
Overall	966/1068 (90%)	547/599 (91%)	338/368 (92%)	81/101 (80%)

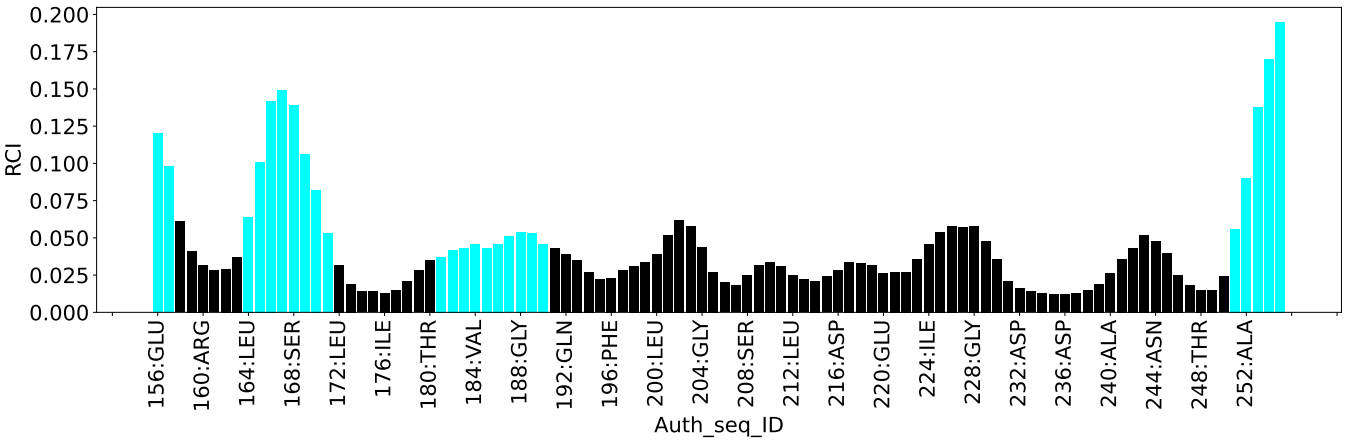
7.1.4 Statistically unusual chemical shifts

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:


RCI
0.200
0.175
0.150
0.125
0.100
0.075
0.050
0.025
0.000
156:GLU
160:ARG
164:LEU
168:SER
172:LEU
176:ILE
180:THR
184:VAL
188:GLY
192:GLN
196:PHE
200:LEU
204:GLY
208:SER
212:LEU
216:ASP
220:GLU
224:ILE
228:GLY
232:ASP
236:ASP
240:ALA
244:ASN
248:THR
252:ALA
Auth_seq_ID

8 NMR restraints analysis

8.1 Conformationally restricting restraints

The following table provides the summary of experimentally observed NMR restraints in different categories. Restraints are classified into different categories based on the sequence separation of the atoms involved.

Description	Value
Total distance restraints	1233
Intra-residue (|i-j|=0)	303
Sequential (|i-j|=1)	325
Medium range (|i-j|>1 and |i-j|<5)	169
Long range (|i-j|≥5)	436
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	501
Number of restraints per residue	12.1
Number of long range restraints per residue[1]	4.3

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations

This section provides the overview of the restraint violations analysis. The violations are binned as small, medium and large violations based on its absolute value. Average number of violations per model is calculated by dividing the total number of violations in each bin by the size of the ensemble.

8.2.1 Average number of distance violations per model

Distance violations less than 0.1 Å are not included in the calculation.

Bins (Å)	Average number of violations per model	Max (Å)
0.1-0.2 (Small)	28.4	0.2
0.2-0.5 (Medium)	65.5	0.5
>0.5 (Large)	135.6	3.5

8.2.2 Average number of dihedral-angle violations per model (i)

Dihedral-angle violations less than 1° are not included in the calculation.There are no dihedral-angle violations

9 Distance violation analysis (i)

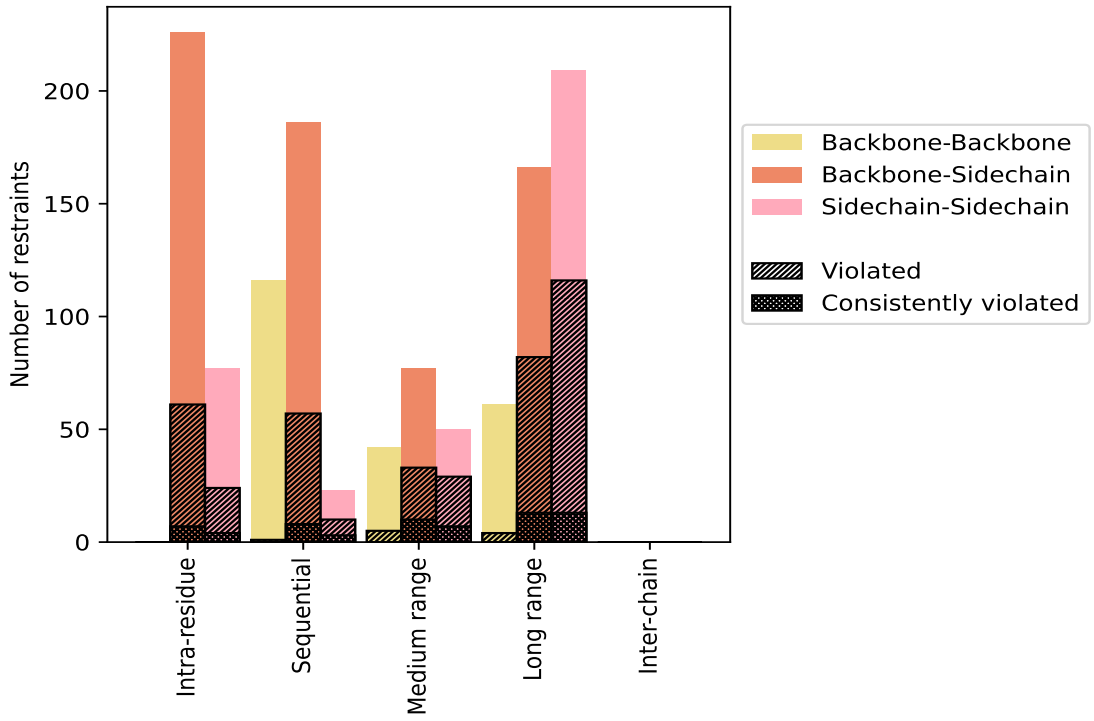
9.1 Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
Intra-residue (|i-j|=0)	303	24.6	85	28.1	6.9	11	3.6	0.9
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	226	18.3	61	27.0	4.9	7	3.1	0.6
Sidechain-Sidechain	77	6.2	24	31.2	1.9	4	5.2	0.3
Sequential (|i-j|=1)	325	26.4	68	20.9	5.5	11	3.4	0.9
Backbone-Backbone	116	9.4	1	0.9	0.1	0	0.0	0.0
Backbone-Sidechain	186	15.1	57	30.6	4.6	8	4.3	0.6
Sidechain-Sidechain	23	1.9	10	43.5	0.8	3	13.0	0.2
Medium range (|i-j|>1 & |i-j|<5)	169	13.7	67	39.6	5.4	17	10.1	1.4
Backbone-Backbone	42	3.4	5	11.9	0.4	0	0.0	0.0
Backbone-Sidechain	77	6.2	33	42.9	2.7	10	13.0	0.8
Sidechain-Sidechain	50	4.1	29	58.0	2.4	7	14.0	0.6
Long range (|i-j|≥5)	436	35.4	202	46.3	16.4	26	6.0	2.1
Backbone-Backbone	61	4.9	4	6.6	0.3	0	0.0	0.0
Backbone-Sidechain	166	13.5	82	49.4	6.7	13	7.8	1.1
Sidechain-Sidechain	209	17.0	116	55.5	9.4	13	6.2	1.1
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1233	100.0	422	34.2	34.2	65	5.3	5.3
Backbone-Backbone	219	17.8	10	4.6	0.8	0	0.0	0.0
Backbone-Sidechain	655	53.1	233	35.6	18.9	38	5.8	3.1
Sidechain-Sidechain	359	29.1	179	49.9	14.5	27	7.5	2.2

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1 Bar chart : Distribution of distance restraints and violations



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories. The hydrogen bonds and disulfied bonds are counted in their appropriate category on the x-axis

9.2 Distance violation statistics for each model

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	42	34	36	125	0	237	0.74	2.51	0.52	0.64
2	47	39	39	112	0	237	0.75	3.5	0.55	0.64
3	34	34	31	107	0	206	0.8	2.73	0.53	0.68
4	46	38	41	117	0	242	0.75	2.66	0.56	0.58
5	45	38	32	121	0	236	0.75	3.02	0.55	0.62
6	34	38	35	121	0	228	0.8	2.54	0.54	0.67
7	45	37	35	121	0	238	0.73	2.9	0.55	0.54
8	41	36	37	119	0	233	0.81	2.72	0.55	0.73
9	41	36	37	117	0	231	0.77	3.37	0.58	0.63
10	43	35	36	114	0	228	0.79	2.75	0.54	0.68
11	38	42	38	121	0	239	0.83	3.2	0.58	0.68

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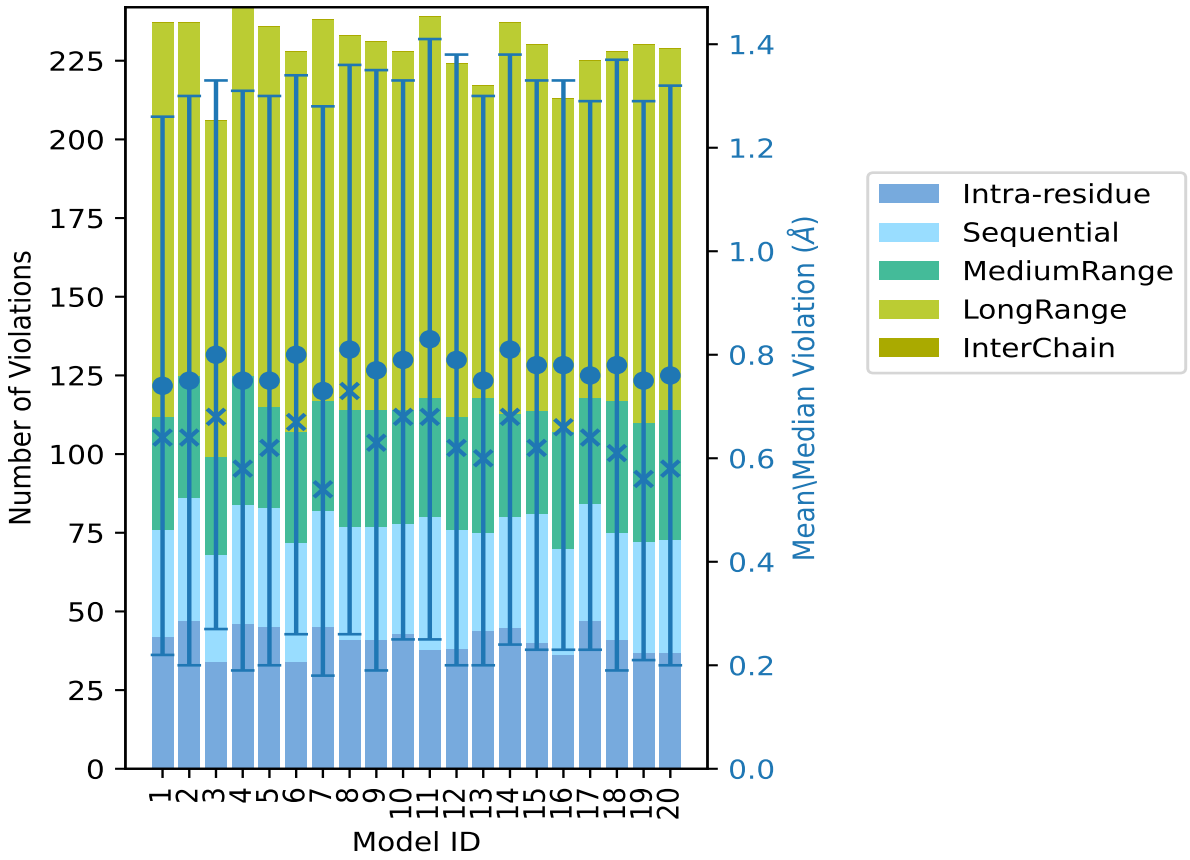
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	38	38	36	112	0	224	0.79	2.89	0.59	0.62
13	44	31	43	99	0	217	0.75	2.33	0.55	0.6
14	45	35	33	124	0	237	0.81	3.41	0.57	0.68
15	40	41	33	116	0	230	0.78	2.84	0.55	0.62
16	36	34	37	106	0	213	0.78	2.65	0.55	0.66
17	47	37	34	107	0	225	0.76	2.86	0.53	0.64
18	41	34	42	111	0	228	0.78	3.46	0.59	0.61
19	37	35	38	120	0	230	0.75	2.28	0.54	0.56
20	37	36	41	115	0	229	0.76	2.89	0.56	0.58

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6]Standard deviation

9.2.1 Bar graph : Distance Violation statistics for each model



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

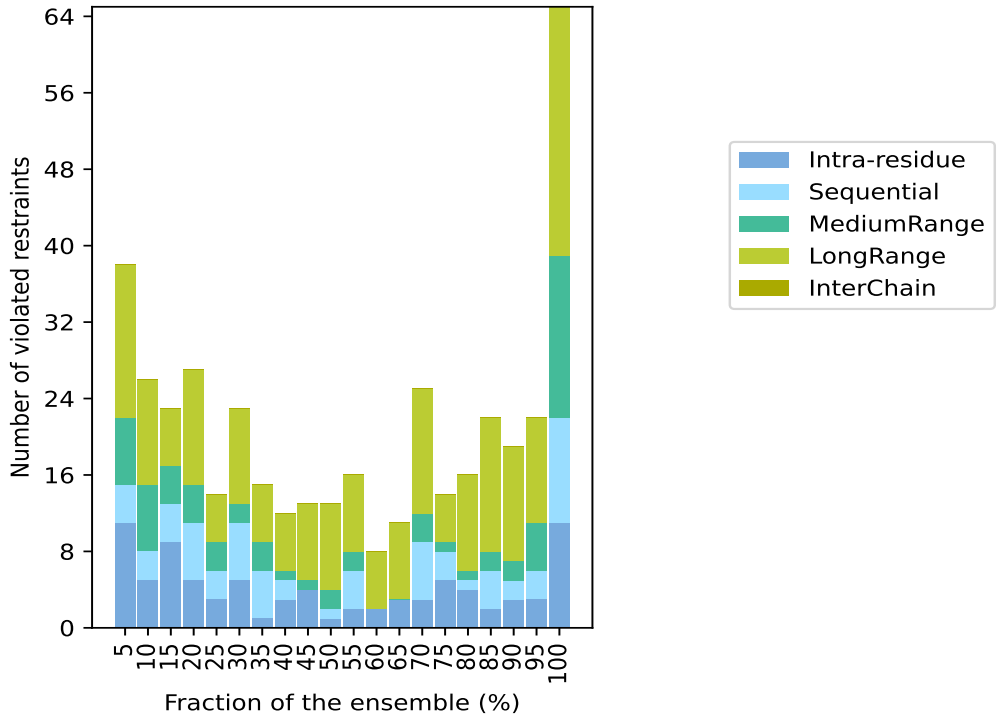
9.3 Distance violation statistics for the ensemble (i)

Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 811(IR:218, SQ:257, MR:102, LR:234, IC:0) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
11	4	7	16	0	38	1	5.0
5	3	7	11	0	26	2	10.0
9	4	4	6	0	23	3	15.0
5	6	4	12	0	27	4	20.0
3	3	3	5	0	14	5	25.0
5	6	2	10	0	23	6	30.0
1	5	3	6	0	15	7	35.0
3	2	1	6	0	12	8	40.0
4	0	1	8	0	13	9	45.0
1	1	2	9	0	13	10	50.0
2	4	2	8	0	16	11	55.0
2	0	0	6	0	8	12	60.0
3	0	0	8	0	11	13	65.0
3	6	3	13	0	25	14	70.0
5	3	1	5	0	14	15	75.0
4	1	1	10	0	16	16	80.0
2	4	2	14	0	22	17	85.0
3	2	2	12	0	19	18	90.0
3	3	5	11	0	22	19	95.0
11	11	17	26	0	65	20	100.0

[1]Intra-residue restraints, [2]Sequential restraints, [3]Medium range restraints, [4]Long range restraints, [5]Inter-chain restraints, [6] Number of models with violations

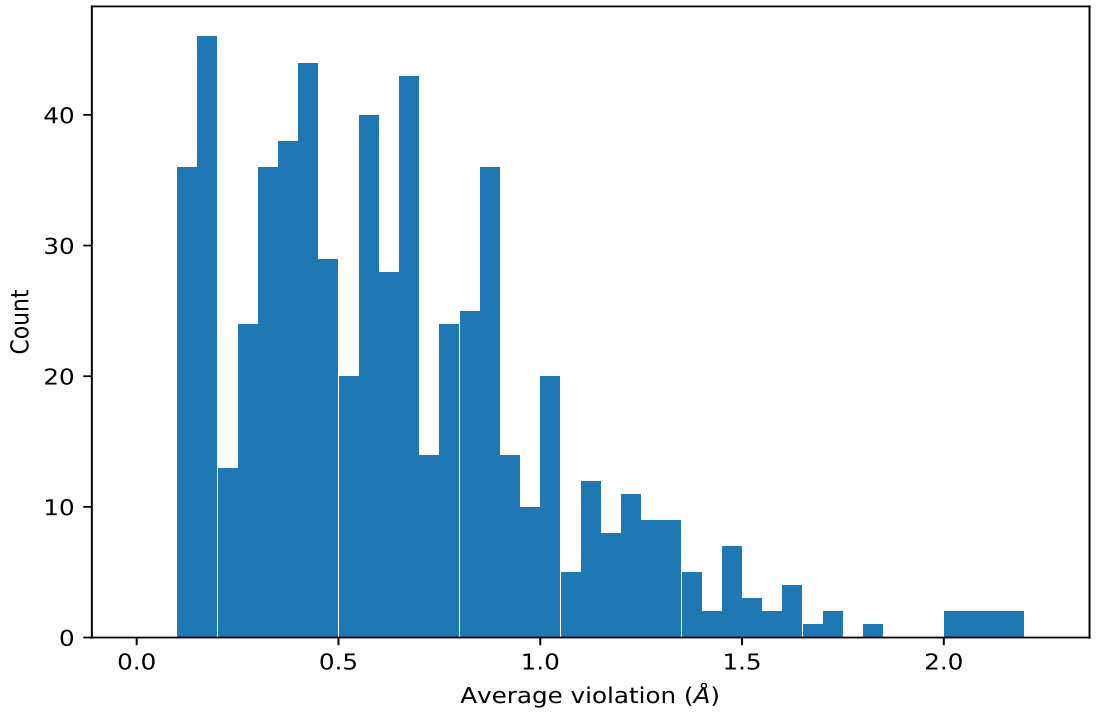
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints (i)

The following table provides the mean and the standard deviation of the violations for the 10 worst performing restraints, sorted by number of violated models and the mean violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

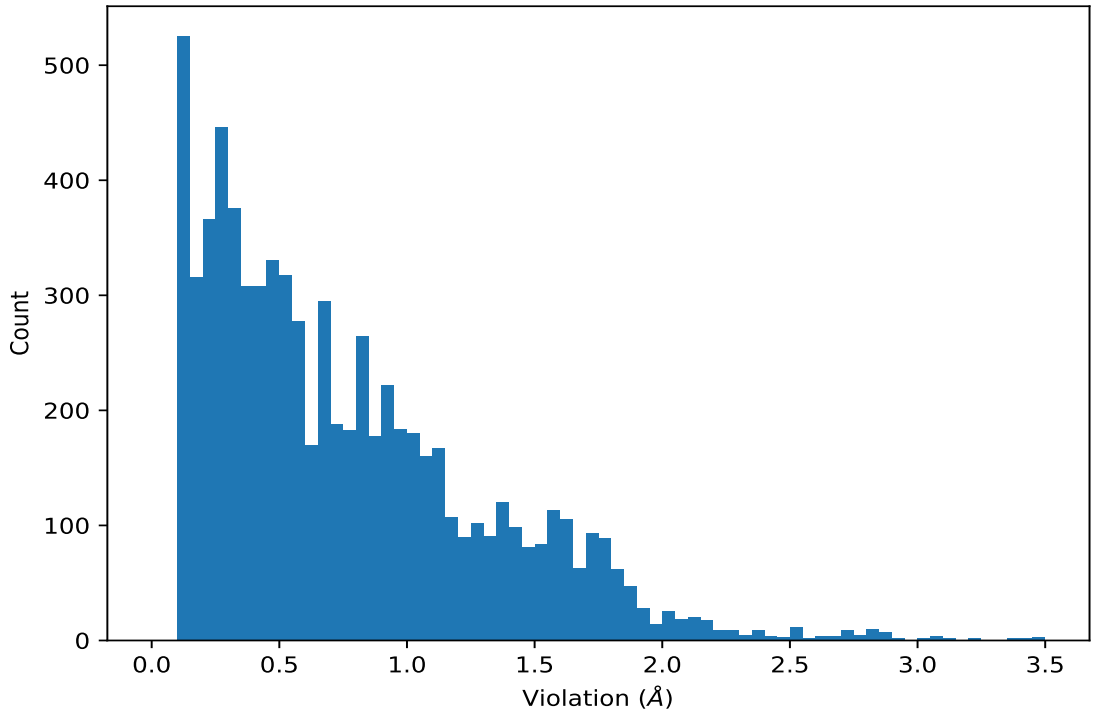
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,550)	1:A:197:ILE:HG23	1:A:214:VAL:HG13	20	2.18	0.63	2.48
(1,550)	1:A:197:ILE:HG23	1:A:214:VAL:HG21	20	2.18	0.63	2.48
(1,837)	1:A:221:VAL:HG13	1:A:222:ASN:HD21	20	2.06	0.71	2.3
(1,837)	1:A:221:VAL:HG21	1:A:222:ASN:HD21	20	2.06	0.71	2.3
(1,782)	1:A:219:ILE:HG23	1:A:248:THR:HG21	20	1.82	0.61	2.0
(1,792)	1:A:220:GLU:HA	1:A:224:ILE:HG23	20	1.73	0.09	1.71
(1,951)	1:A:226:VAL:HG21	1:A:234:VAL:HG13	20	1.69	0.62	2.08
(1,15)	1:A:158:HIS:HE1	1:A:219:ILE:HG12	20	1.6	0.17	1.58
(1,766)	1:A:219:ILE:HD11	1:A:248:THR:HG21	20	1.57	0.55	1.27
(1,813)	1:A:221:VAL:H	1:A:224:ILE:HG23	20	1.55	0.08	1.56
(1,182)	1:A:172:LEU:HD13	1:A:206:ALA:H	20	1.5	0.47	1.73
(1,182)	1:A:172:LEU:HD21	1:A:206:ALA:H	20	1.5	0.47	1.73
(1,547)	1:A:197:ILE:HG23	1:A:214:VAL:H	20	1.49	0.66	1.87

[1]Number of violated models, [2]Standard deviation

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

The following histogram shows the distribution of the absolute value of the violation for all violated restraints in the ensemble.



9.5.2 Table : All distance violations (i)

The following table provides the 10 worst performing restraints, sorted by the violation value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,782)	1:A:219:ILE:HG23	1:A:248:THR:HG21	2	3.5
(1,873)	1:A:222:ASN:HD21	1:A:245:LEU:HD13	18	3.46
(1,873)	1:A:222:ASN:HD21	1:A:245:LEU:HD21	18	3.46
(1,873)	1:A:222:ASN:HD21	1:A:245:LEU:HD13	14	3.41
(1,873)	1:A:222:ASN:HD21	1:A:245:LEU:HD21	14	3.41
(1,694)	1:A:214:VAL:HG13	1:A:215:ASN:HD21	9	3.37
(1,694)	1:A:214:VAL:HG21	1:A:215:ASN:HD21	9	3.37
(1,550)	1:A:197:ILE:HG23	1:A:214:VAL:HG13	11	3.2
(1,550)	1:A:197:ILE:HG23	1:A:214:VAL:HG21	11	3.2
(1,873)	1:A:222:ASN:HD21	1:A:245:LEU:HD13	2	3.15
(1,873)	1:A:222:ASN:HD21	1:A:245:LEU:HD21	2	3.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,694)	1:A:214:VAL:HG13	1:A:215:ASN:HD21	18	3.09
(1,694)	1:A:214:VAL:HG21	1:A:215:ASN:HD21	18	3.09
(1,873)	1:A:222:ASN:HD21	1:A:245:LEU:HD13	11	3.06
(1,873)	1:A:222:ASN:HD21	1:A:245:LEU:HD21	11	3.06
(1,678)	1:A:212:LEU:HD13	1:A:249:VAL:HG21	5	3.02
(1,678)	1:A:212:LEU:HD21	1:A:249:VAL:HG21	5	3.02
(1,873)	1:A:222:ASN:HD21	1:A:245:LEU:HD13	9	2.94

10 Dihedral-angle violation analysis (i)

Dihedral angle analysis failed due to data error in the dihedral angle restraints, possibly missing target value