wwPDB NMR Structure Validation Summary Report

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PDB ID	:	2KVA
BMRB ID	:	16772
Title	:	SOLUTION STRUCTURE OF CI-MPR ligand-free domain 5
Authors	:	Olson, L.J.; Peterson, F.C.; Volkman, B.F.; Dahms, N.M.
Deposited on	:	2010-03-10

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:

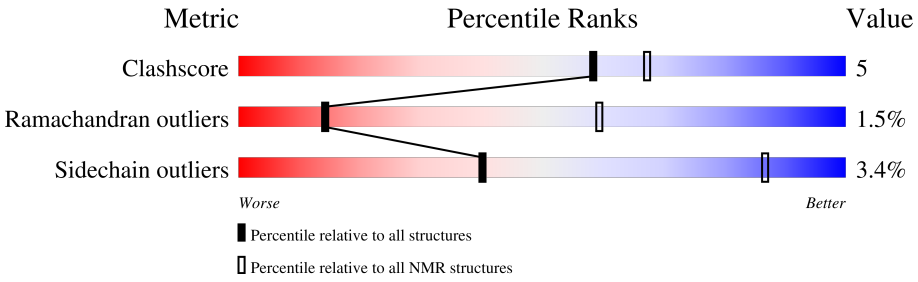
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 87%.

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	148	84% 6% 10%

2 Ensemble composition and analysis

This entry contains 20 models. Model 14 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:586-A:696, A:700-A:707, A:712-A:725 (133)	0.80	14

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2134 atoms, of which 956 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cation-independent mannose-6-phosphate receptor.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	148	2134	734	956	198	239	7	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	578	GLU	-	expression tag	UNP P08169
A	579	ALA	-	expression tag	UNP P08169
A	580	GLU	-	expression tag	UNP P08169
A	581	ALA	-	expression tag	UNP P08169
A	582	GLU	-	expression tag	UNP P08169
A	583	PHE	-	expression tag	UNP P08169

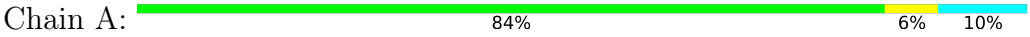
4 Residue-property plots

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: Cation-independent mannose-6-phosphate receptor

Chain A:

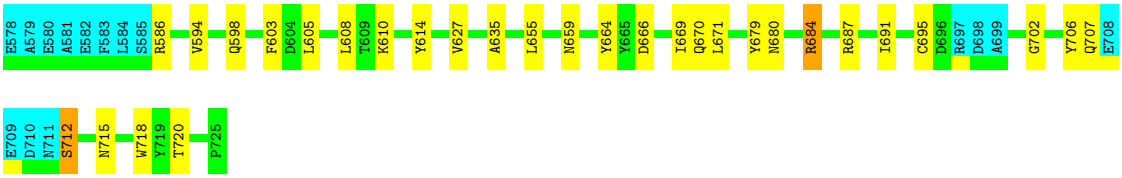


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 14. Colouring as in section 4.1 above.

- Molecule 1: Cation-independent mannose-6-phosphate receptor

Chain A:



5 Refinement protocol and experimental data overview

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

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	1608
Number of shifts mapped to atoms	1498
Number of unparsed shifts	0
Number of shifts with mapping errors	110
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

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±0/1087 (0.0± 0.0%)	0.68±0.01	0±0/1475 (0.0± 0.0%)
All	All	0.85	1/21740 (0.0%)	0.68	2/29500 (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±0.3
All	All	0	2

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	687	ARG	CZ-NH2	-5.79	1.25	1.33	9	1

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
1	A	679	TYR	CB-CG-CD2	-5.53	117.68	121.00	1	1
1	A	679	TYR	CB-CG-CD1	5.03	124.02	121.00	1	1

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	A	647	ARG	Sidechain	1

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Mol	Chain	Res	Type	Group	Models (Total)
1	A	586	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	1058	864	985	10±3
All	All	21160	17280	19700	201

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.

5 of 76 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:679:TYR:OH	1:A:712:SER:HA	0.70	1.87	16	6
1:A:676:GLY:HA3	1:A:687:ARG:NH2	0.69	2.03	9	1
1:A:586:ARG:HA	1:A:664:TYR:O	0.62	1.94	5	8
1:A:655:LEU:HA	1:A:687:ARG:NH2	0.62	2.10	9	1
1:A:655:LEU:HD23	1:A:714:TYR:CD1	0.60	2.32	17	4

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	132/148 (89%)	120±2 (91±1%)	10±2 (7±2%)	2±1 (1±1%)	14	59
All	All	2640/2960 (89%)	2405 (91%)	196 (7%)	39 (1%)	14	59

5 of 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	684	ARG	11
1	A	712	SER	7
1	A	666	ASP	5
1	A	667	GLY	4
1	A	635	ALA	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	116/128 (91%)	112±1 (97±1%)	4±1 (3±1%)	40 87
All	All	2320/2560 (91%)	2242 (97%)	78 (3%)	40 87

5 of 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	615	LYS	16
1	A	598	GLN	12
1	A	684	ARG	7
1	A	671	LEU	6
1	A	659	ASN	5

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

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 87% for the well-defined parts and 83% 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	1608
Number of shifts mapped to atoms	1498
Number of unparsed shifts	0
Number of shifts with mapping errors	110
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

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 110) occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	584	LEU	HD11	0.924	0.005	2
1	A	584	LEU	HD12	0.924	0.005	2
1	A	584	LEU	HD22	0.893	0.020	2
1	A	584	LEU	HD23	0.893	0.020	2
1	A	587	THR	HG22	1.442	0.020	1
1	A	587	THR	HG23	1.442	0.020	1
1	A	593	THR	HG22	1.269	0.020	1
1	A	593	THR	HG23	1.269	0.020	1
1	A	594	VAL	HG11	0.907	0.020	2
1	A	594	VAL	HG12	0.907	0.020	2
1	A	594	VAL	HG22	1.016	0.020	2
1	A	594	VAL	HG23	1.016	0.020	2
1	A	598	GLN	HE22	6.855	0.020	2
1	A	605	LEU	HD11	-0.058	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	605	LEU	HD12	-0.058	0.020	2
1	A	605	LEU	HD22	-0.107	0.020	2
1	A	605	LEU	HD23	-0.107	0.020	2
1	A	606	THR	HG22	1.417	0.001	1
1	A	606	THR	HG23	1.417	0.001	1
1	A	608	LEU	HD11	0.608	0.020	2
1	A	608	LEU	HD12	0.608	0.020	2
1	A	608	LEU	HD22	0.35	0.020	2
1	A	608	LEU	HD23	0.35	0.020	2
1	A	609	THR	HG22	1.286	0.020	1
1	A	609	THR	HG23	1.286	0.020	1
1	A	616	VAL	HG11	1.292	0.020	2
1	A	616	VAL	HG12	1.292	0.020	2
1	A	616	VAL	HG22	0.979	0.020	2
1	A	616	VAL	HG23	0.979	0.020	2
1	A	618	THR	HG22	1.485	0.020	1
1	A	618	THR	HG23	1.485	0.020	1
1	A	625	ILE	HD12	0.003	0.020	1
1	A	625	ILE	HD13	0.003	0.020	1
1	A	625	ILE	HG13	0.828	0.020	2
1	A	625	ILE	HG21	0.665	0.020	1
1	A	625	ILE	HG22	0.665	0.020	1
1	A	626	ASN	HD22	7.174	0.020	2
1	A	627	VAL	HG11	0.665	0.020	2
1	A	627	VAL	HG12	0.665	0.020	2
1	A	627	VAL	HG22	0.66	0.020	2
1	A	627	VAL	HG23	0.66	0.020	2
1	A	631	VAL	HG11	0.89	0.020	2
1	A	631	VAL	HG12	0.89	0.020	2
1	A	631	VAL	HG22	0.911	0.020	2
1	A	631	VAL	HG23	0.911	0.020	2
1	A	633	VAL	HG11	0.467	0.020	2
1	A	633	VAL	HG12	0.467	0.020	2
1	A	633	VAL	HG22	0.562	0.001	2
1	A	633	VAL	HG23	0.562	0.001	2
1	A	644	GLN	HE22	3.719	0.020	2
1	A	645	VAL	HG11	0.908	0.020	2
1	A	645	VAL	HG12	0.908	0.020	2
1	A	645	VAL	HG22	0.859	0.020	2
1	A	645	VAL	HG23	0.859	0.020	2
1	A	654	ASN	HD22	6.287	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	655	LEU	HD11	0.244	0.020	2
1	A	655	LEU	HD12	0.244	0.020	2
1	A	655	LEU	HD22	0.604	0.020	2
1	A	655	LEU	HD23	0.604	0.020	2
1	A	659	ASN	HD22	7.872	0.020	2
1	A	662	LEU	HD11	0.673	0.020	2
1	A	662	LEU	HD12	0.673	0.020	2
1	A	662	LEU	HD22	0.559	0.020	2
1	A	662	LEU	HD23	0.559	0.020	2
1	A	669	ILE	HD12	0.083	0.020	1
1	A	669	ILE	HD13	0.083	0.020	1
1	A	669	ILE	HG13	0.628	0.020	2
1	A	669	ILE	HG21	0.831	0.001	1
1	A	669	ILE	HG22	0.831	0.001	1
1	A	670	GLN	HE22	6.869	0.020	2
1	A	671	LEU	HD11	1.083	0.020	2
1	A	671	LEU	HD12	1.083	0.020	2
1	A	671	LEU	HD22	1.068	0.020	2
1	A	671	LEU	HD23	1.068	0.020	2
1	A	672	THR	HG22	1.167	0.020	1
1	A	672	THR	HG23	1.167	0.020	1
1	A	677	THR	HG22	1.767	0.020	1
1	A	677	THR	HG23	1.767	0.020	1
1	A	680	ASN	HD22	6.951	0.020	2
1	A	681	ASN	HD22	6.873	0.020	2
1	A	685	THR	HG22	1.459	0.020	1
1	A	685	THR	HG23	1.459	0.020	1
1	A	689	THR	HG22	1.206	0.020	1
1	A	689	THR	HG23	1.206	0.020	1
1	A	690	LEU	HD11	0.825	0.020	2
1	A	690	LEU	HD12	0.825	0.020	2
1	A	690	LEU	HD22	0.813	0.020	2
1	A	690	LEU	HD23	0.813	0.020	2
1	A	691	ILE	HD12	0.634	0.020	1
1	A	691	ILE	HD13	0.634	0.020	1
1	A	691	ILE	HG13	0.555	0.003	2
1	A	691	ILE	HG21	0.018	0.004	1
1	A	691	ILE	HG22	0.018	0.004	1
1	A	692	THR	HG22	1.146	0.020	1
1	A	692	THR	HG23	1.146	0.020	1
1	A	694	LEU	HD11	0.868	0.020	2

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List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	694	LEU	HD12	0.868	0.020	2
1	A	694	LEU	HD22	0.517	0.020	2
1	A	694	LEU	HD23	0.517	0.020	2
1	A	701	VAL	HG11	1.633	0.020	2
1	A	701	VAL	HG12	1.633	0.020	2
1	A	701	VAL	HG22	1.454	0.020	2
1	A	701	VAL	HG23	1.454	0.020	2
1	A	707	GLN	HE22	6.693	0.020	2
1	A	711	ASN	HD22	6.78	0.020	2
1	A	713	THR	HG22	1.117	0.020	1
1	A	713	THR	HG23	1.117	0.020	1
1	A	715	ASN	HD22	6.87	0.020	2
1	A	720	THR	HG22	1.194	0.020	1
1	A	720	THR	HG23	1.194	0.020	1

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	141	-0.44 ± 0.07	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	130	-0.61 ± 0.09	Should be applied
$^{13}C'$	135	0.07 ± 0.17	None needed (< 0.5 ppm)
^{15}N	135	-0.31 ± 0.46	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 87%, i.e. 1511 atoms were assigned a chemical shift out of a possible 1743. 0 out of 14 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	649/659 (98%)	268/268 (100%)	256/266 (96%)	125/125 (100%)
Sidechain	748/892 (84%)	498/573 (87%)	237/277 (86%)	13/42 (31%)
Aromatic	114/192 (59%)	70/91 (77%)	42/97 (43%)	2/4 (50%)
Overall	1511/1743 (87%)	836/932 (90%)	535/640 (84%)	140/171 (82%)

7.1.4 Statistically unusual chemical shifts (i)

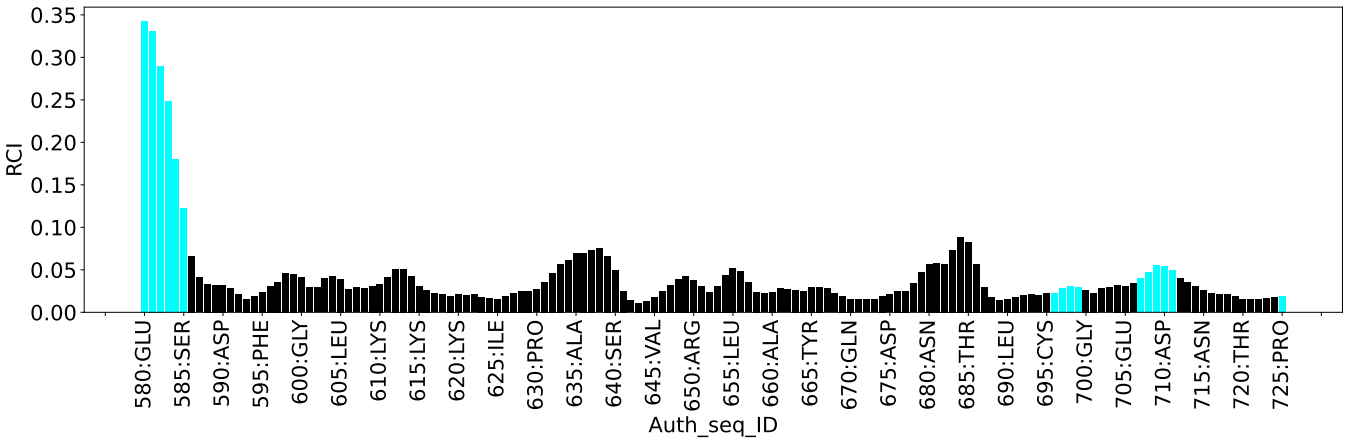
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	618	THR	HG1	5.85	0.08 – 2.19	22.3
1	A	720	THR	HG1	5.34	0.08 – 2.19	19.9
1	A	644	GLN	HE22	3.72	4.88 – 9.19	-7.7
1	A	704	PRO	HD3	0.86	1.76 – 5.48	-7.4

7.1.5 Random Coil Index (RCI) plots (i)

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:



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	1763
Intra-residue (|i-j|=0)	329
Sequential (|i-j|=1)	389
Medium range (|i-j|>1 and |i-j|<5)	170
Long range (|i-j|≥5)	866
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	9
Total dihedral-angle restraints	0
Number of unmapped restraints	551
Number of restraints per residue	11.9
Number of long range restraints per residue[1]	5.9

[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)	26.9	0.2
0.2-0.5 (Medium)	53.2	0.5
>0.5 (Large)	110.5	3.33

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)

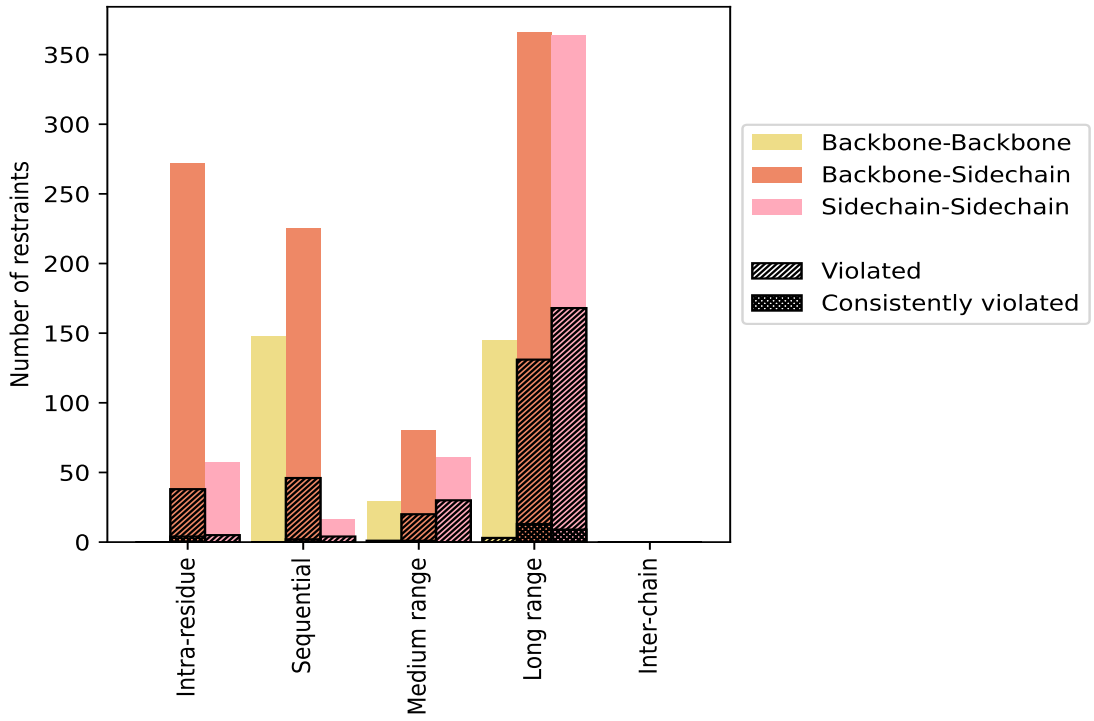
9.1 Summary of distance violations (i)

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)	329	18.7	43	13.1	2.4	4	1.2	0.2
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	272	15.4	38	14.0	2.2	4	1.5	0.2
Sidechain-Sidechain	57	3.2	5	8.8	0.3	0	0.0	0.0
Sequential (|i-j|=1)	389	22.1	50	12.9	2.8	2	0.5	0.1
Backbone-Backbone	148	8.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	225	12.8	46	20.4	2.6	2	0.9	0.1
Sidechain-Sidechain	16	0.9	4	25.0	0.2	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	170	9.6	51	30.0	2.9	1	0.6	0.1
Backbone-Backbone	29	1.6	1	3.4	0.1	0	0.0	0.0
Backbone-Sidechain	80	4.5	20	25.0	1.1	1	1.2	0.1
Sidechain-Sidechain	61	3.5	30	49.2	1.7	0	0.0	0.0
Long range (|i-j|≥5)	866	49.1	302	34.9	17.1	22	2.5	1.2
Backbone-Backbone	145	8.2	3	2.1	0.2	0	0.0	0.0
Backbone-Sidechain	366	20.8	131	35.8	7.4	13	3.6	0.7
Sidechain-Sidechain	355	20.1	168	47.3	9.5	9	2.5	0.5
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	9	0.5	0	0.0	0.0	0	0.0	0.0
Total	1763	100.0	446	25.3	25.3	29	1.6	1.6
Backbone-Backbone	322	18.3	4	1.2	0.2	0	0.0	0.0
Backbone-Sidechain	943	53.5	235	24.9	13.3	20	2.1	1.1
Sidechain-Sidechain	498	28.2	207	41.6	11.7	9	1.8	0.5

[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	15	19	19	142	0	195	0.72	2.78	0.52	0.62
2	23	18	18	136	0	195	0.74	2.4	0.55	0.59
3	21	18	18	146	0	203	0.7	3.08	0.47	0.6
4	18	22	26	134	0	200	0.73	3.04	0.5	0.62
5	20	19	18	139	0	196	0.77	2.26	0.53	0.6
6	18	19	15	125	0	177	0.73	2.65	0.53	0.62
7	21	18	23	124	0	186	0.67	2.91	0.5	0.54
8	18	18	13	153	0	202	0.73	2.38	0.5	0.59
9	12	17	22	114	0	165	0.7	2.35	0.49	0.59
10	17	16	22	129	0	184	0.67	2.19	0.46	0.56
11	20	21	19	127	0	187	0.75	2.16	0.47	0.68

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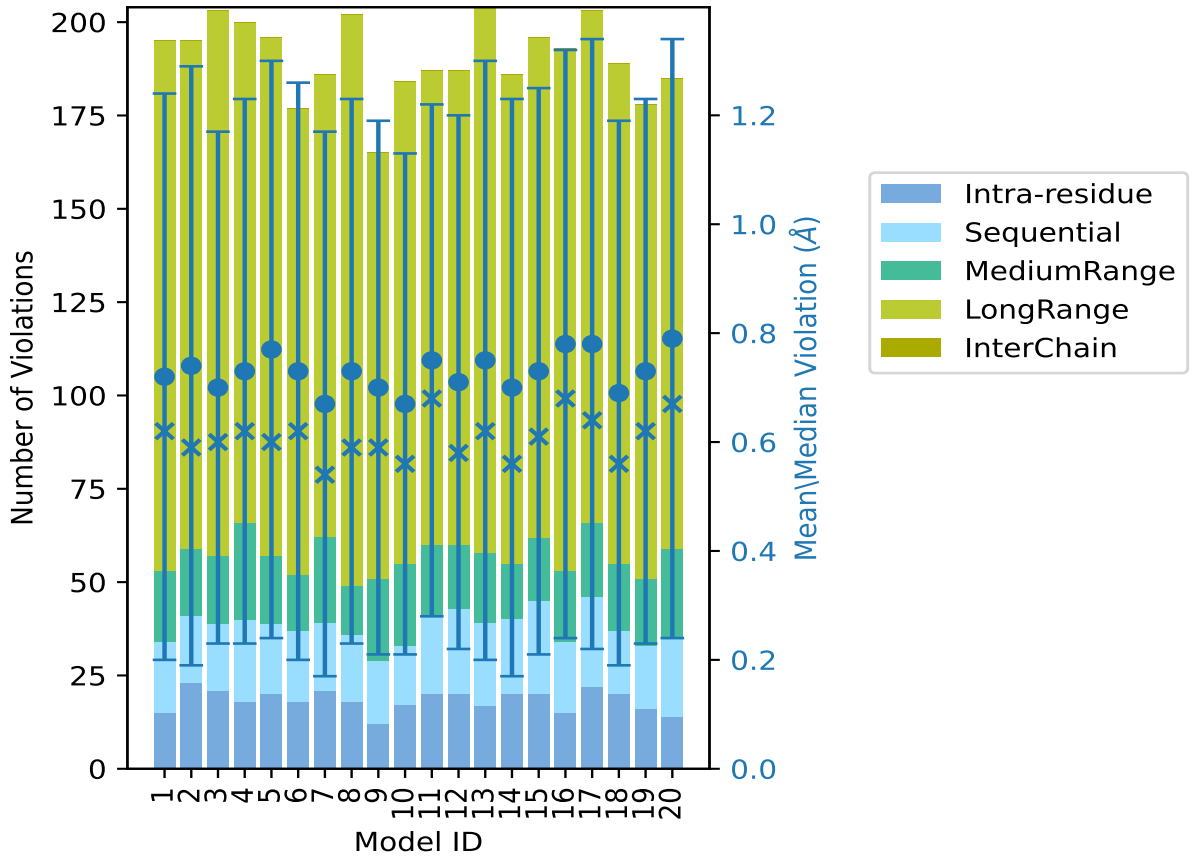
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	20	23	17	127	0	187	0.71	2.93	0.49	0.58
13	17	22	19	146	0	204	0.75	3.33	0.55	0.62
14	20	20	15	131	0	186	0.7	2.94	0.53	0.56
15	20	25	17	134	0	196	0.73	2.48	0.52	0.61
16	15	19	19	140	0	193	0.78	3.25	0.54	0.68
17	22	24	20	137	0	203	0.78	3.09	0.56	0.64
18	20	17	18	134	0	189	0.69	2.92	0.5	0.56
19	16	17	18	127	0	178	0.73	2.29	0.5	0.62
20	14	21	24	126	0	185	0.79	2.63	0.55	0.67

[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

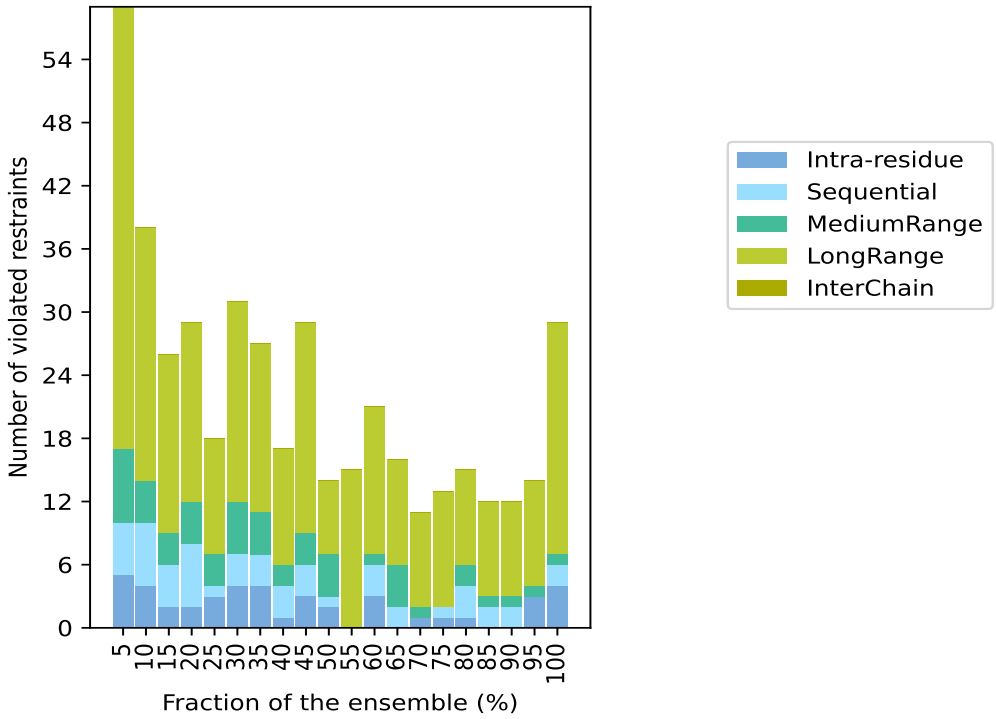
9.3 Distance violation statistics for the ensemble (i)

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, 1308(IR:286, SQ:339, MR:119, LR:564, 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]	%
5	5	7	42	0	59	1	5.0
4	6	4	24	0	38	2	10.0
2	4	3	17	0	26	3	15.0
2	6	4	17	0	29	4	20.0
3	1	3	11	0	18	5	25.0
4	3	5	19	0	31	6	30.0
4	3	4	16	0	27	7	35.0
1	3	2	11	0	17	8	40.0
3	3	3	20	0	29	9	45.0
2	1	4	7	0	14	10	50.0
0	0	0	15	0	15	11	55.0
3	3	1	14	0	21	12	60.0
0	2	4	10	0	16	13	65.0
1	0	1	9	0	11	14	70.0
1	1	0	11	0	13	15	75.0
1	3	2	9	0	15	16	80.0
0	2	1	9	0	12	17	85.0
0	2	1	9	0	12	18	90.0
3	0	1	10	0	14	19	95.0
4	2	1	22	0	29	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

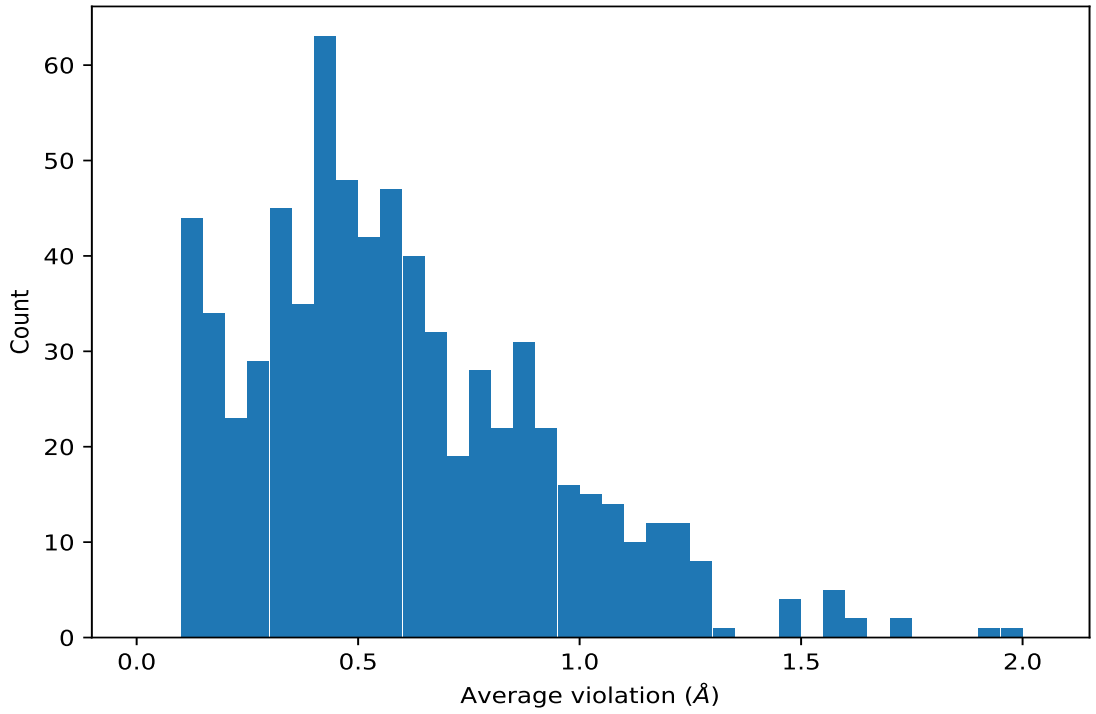
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

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

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.

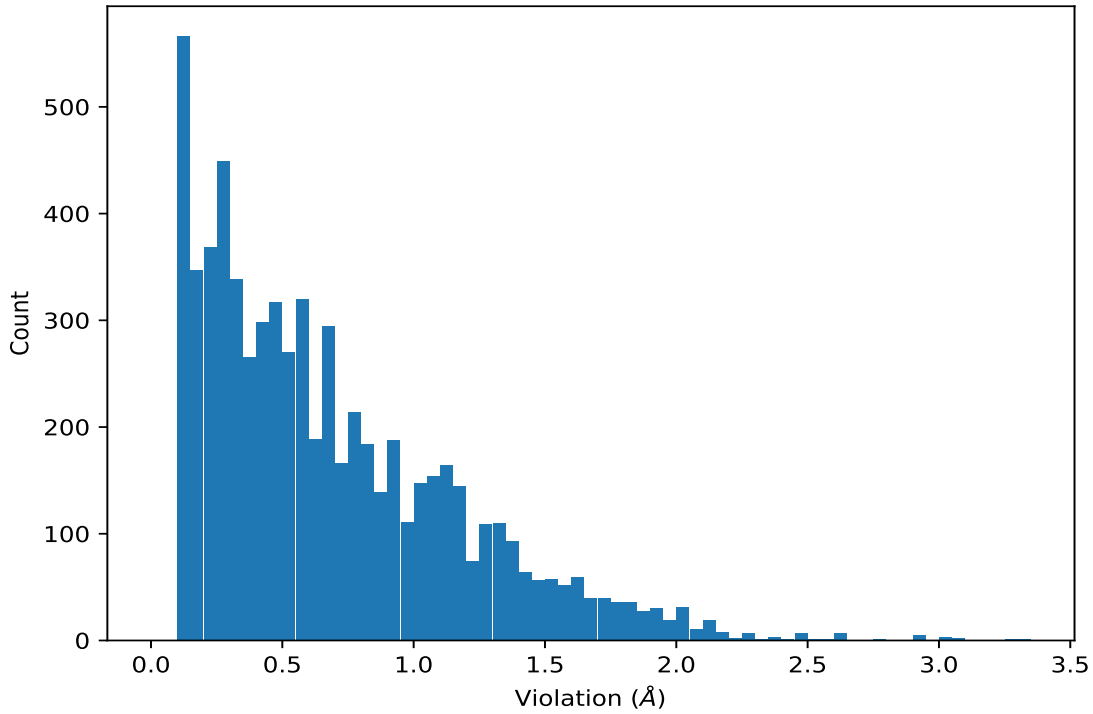
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,668)	1:A:625:ILE:HD11	1:A:691:ILE:HD11	20	1.97	0.72	2.14
(1,35)	1:A:587:THR:HG21	1:A:594:VAL:HG21	20	1.93	0.85	1.94
(1,135)	1:A:594:VAL:HG21	1:A:662:LEU:HD13	20	1.62	0.48	1.62
(1,135)	1:A:594:VAL:HG21	1:A:662:LEU:HD21	20	1.62	0.48	1.62
(1,884)	1:A:644:GLN:HE21	1:A:653:TRP:HA	20	1.46	0.33	1.58
(1,968)	1:A:653:TRP:HA	1:A:654:ASN:HD21	20	1.45	0.57	1.86
(1,62)	1:A:590:ASP:H	1:A:594:VAL:HG21	20	1.3	0.6	1.62
(1,664)	1:A:625:ILE:HD11	1:A:643:CYS:H	20	1.28	0.34	1.42
(1,1188)	1:A:669:ILE:HG23	1:A:692:THR:HA	20	1.27	0.69	1.64
(1,718)	1:A:627:VAL:HG21	1:A:673:TYR:HH	20	1.25	0.51	1.23
(1,215)	1:A:604:ASP:H	1:A:669:ILE:HD11	20	1.24	0.75	0.93

[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)
(1,35)	1:A:587:THR:HG21	1:A:594:VAL:HG21	13	3.33
(1,301)	1:A:608:LEU:HD21	1:A:720:THR:HG21	16	3.25
(1,35)	1:A:587:THR:HG21	1:A:594:VAL:HG21	17	3.09
(1,35)	1:A:587:THR:HG21	1:A:594:VAL:HG21	3	3.08
(1,125)	1:A:594:VAL:HG13	1:A:662:LEU:HD13	4	3.04
(1,125)	1:A:594:VAL:HG13	1:A:662:LEU:HD21	4	3.04
(1,293)	1:A:608:LEU:HD13	1:A:720:THR:HG21	13	3.0
(1,35)	1:A:587:THR:HG21	1:A:594:VAL:HG21	14	2.94
(1,1013)	1:A:655:LEU:HD13	1:A:689:THR:HG21	12	2.93
(1,1013)	1:A:655:LEU:HD21	1:A:689:THR:HG21	12	2.93
(1,35)	1:A:587:THR:HG21	1:A:594:VAL:HG21	18	2.92

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,668)	1:A:625:ILE:HD11	1:A:691:ILE:HD11	7	2.91

10 Dihedral-angle violation analysis (i)

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