wwPDB NMR Structure Validation Summary Report

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PDB ID	:	8K2S
BMRB ID	:	36581
Title	:	The structure of HtpG M domain in complex with unstructured D131D binding site a
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Deposited on	:	2023-07-13

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

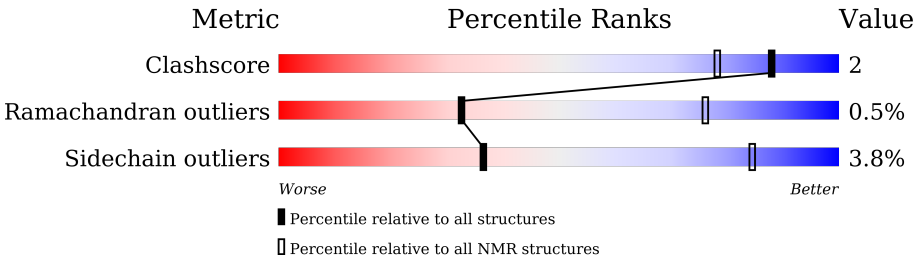
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 25%.

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	292	83% · 5% 9%
2	B	77	5% · 71% 21%

2 Ensemble composition and analysis

This entry contains 20 models. Model 1 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:232-A:482, B:625-B:630 (257)	0.88	1

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 2 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5302 atoms, of which 2643 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Molecular chaperone HtpG (Fragment).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	265	4333	1390	2146	371	419	7	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	203	MET	-	initiating methionine	UNP A0A7A6VTW3
A	204	LYS	-	expression tag	UNP A0A7A6VTW3
A	205	HIS	-	expression tag	UNP A0A7A6VTW3
A	206	HIS	-	expression tag	UNP A0A7A6VTW3
A	207	HIS	-	expression tag	UNP A0A7A6VTW3
A	208	HIS	-	expression tag	UNP A0A7A6VTW3
A	209	HIS	-	expression tag	UNP A0A7A6VTW3
A	210	HIS	-	expression tag	UNP A0A7A6VTW3
A	211	PRO	-	expression tag	UNP A0A7A6VTW3
A	212	MET	-	expression tag	UNP A0A7A6VTW3
A	213	SER	-	expression tag	UNP A0A7A6VTW3
A	214	ASP	-	expression tag	UNP A0A7A6VTW3
A	215	TYR	-	expression tag	UNP A0A7A6VTW3
A	216	ASP	-	expression tag	UNP A0A7A6VTW3
A	217	ILE	-	expression tag	UNP A0A7A6VTW3
A	218	PRO	-	expression tag	UNP A0A7A6VTW3
A	219	THR	-	expression tag	UNP A0A7A6VTW3
A	220	THR	-	expression tag	UNP A0A7A6VTW3
A	221	GLU	-	expression tag	UNP A0A7A6VTW3
A	222	ASN	-	expression tag	UNP A0A7A6VTW3
A	223	LEU	-	expression tag	UNP A0A7A6VTW3
A	224	TYR	-	expression tag	UNP A0A7A6VTW3
A	225	PHE	-	expression tag	UNP A0A7A6VTW3
A	226	GLN	-	expression tag	UNP A0A7A6VTW3
A	227	GLY	-	expression tag	UNP A0A7A6VTW3
A	228	HIS	-	expression tag	UNP A0A7A6VTW3
A	229	MET	-	expression tag	UNP A0A7A6VTW3

- Molecule 2 is a protein called Disordered protein (D131D).

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	61	969	302	497	77	89	4	0

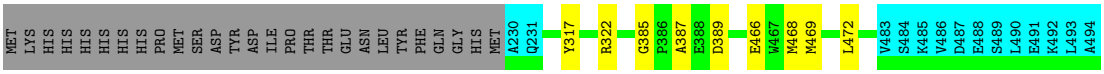
4 Residue-property plots

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.

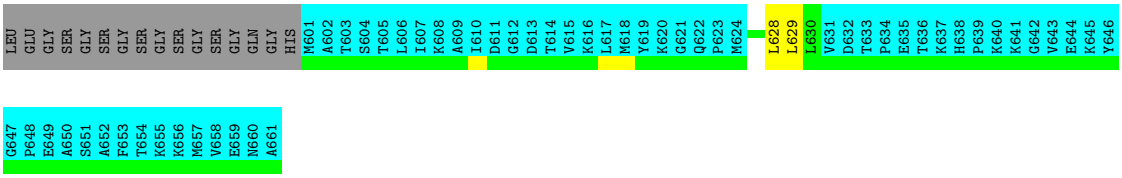
• Molecule 1: Molecular chaperone HtpG (Fragment)

Chain A:



• Molecule 2: Disordered protein (D131D)

Chain B:

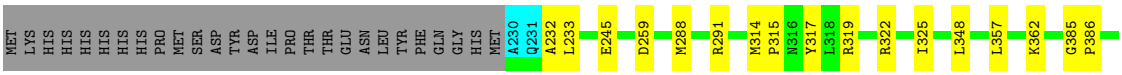


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

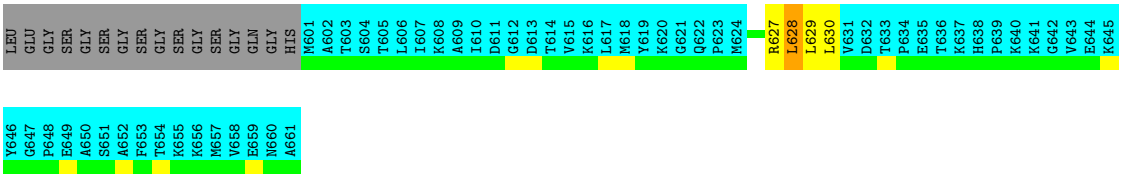
• Molecule 1: Molecular chaperone HtpG (Fragment)

Chain A:



• Molecule 2: Disordered protein (D131D)

Chain B:


LEU GLU GLY SER GLY SER GLY SER GLY SER GLY SER GLY GLN GLY HIS M601 A602 T603 S604 T605 L606 I607 K608 A609 I610 D611 G612 D613 T614 V615 K616 L617 M618 Y619 K620 G621 Q622 P623 M624 R627 L628 L629 L630 V631 D632 T633 P634 E635 T636 K637 H638 P639 K640 K641 G642 V643 E644 K645
Y646 G647 P648 E649 A650 S651 A652 F653 T654 K655 K656 M657 V658 E659 N660 A661

5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular 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
CNS	refinement	
CYANA	structure calculation	

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	955
Number of shifts mapped to atoms	955
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	25%

6 Model quality

6.1 Standard geometry

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

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	2081	2036	2029	8±2
2	B	53	62	62	2±2
All	All	42680	41960	41820	161

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 2.

5 of 89 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:389:ASP:HB3	2:B:629:LEU:HD12	0.64	1.67	10	14
1:A:462:ASP:HB2	1:A:465:ASP:HB2	0.61	1.73	1	1
1:A:387:ALA:HB2	1:A:468:MET:HA	0.59	1.73	5	12
1:A:317:TYR:HB3	1:A:384:GLU:HB2	0.58	1.75	5	3
1:A:462:ASP:HB3	1:A:465:ASP:HB2	0.57	1.75	15	1

6.3 Torsion angles

6.3.1 Protein backbone

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	251/292 (86%)	242±2 (96±1%)	9±2 (3±1%)	0±0 (0±0%)	54 85
2	B	6/77 (8%)	3±1 (47±15%)	2±1 (35±12%)	1±1 (18±14%)	0 3
All	All	5140/7380 (70%)	4895 (95%)	217 (4%)	28 (1%)	32 76

5 of 7 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	627	ARG	9
2	B	628	LEU	7
1	A	232	ALA	4
2	B	629	LEU	3
1	A	472	LEU	2

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	226/264 (86%)	217±2 (96±1%)	9±2 (4±1%)	36 84
2	B	6/61 (10%)	6±0 (98±6%)	0±0 (2±6%)	50 91
All	All	4640/6500 (71%)	4464 (96%)	176 (4%)	36 84

5 of 56 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	317	TYR	16
1	A	322	ARG	12
1	A	472	LEU	10
1	A	314	MET	9
1	A	295	HIS	7

6.3.3 RNA

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates

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 25% for the well-defined parts and 21% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_0*

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	955
Number of shifts mapped to atoms	955
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	255	-0.01 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	246	0.94 ± 0.12	Should be checked
$^{13}C'$	0	—	None (insufficient data)
^{15}N	227	-0.02 ± 0.23	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 25%, i.e. 899 atoms were assigned a chemical shift out of a possible 3668. 0 out of 42 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	667/1277 (52%)	213/514 (41%)	241/514 (47%)	213/249 (86%)
Sidechain	232/2035 (11%)	0/1314 (0%)	232/635 (37%)	0/86 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	0/356 (0%)	0/172 (0%)	0/164 (0%)	0/20 (0%)
Overall	899/3668 (25%)	213/2000 (11%)	473/1313 (36%)	213/355 (60%)

7.1.4 Statistically unusual chemical shifts (i)

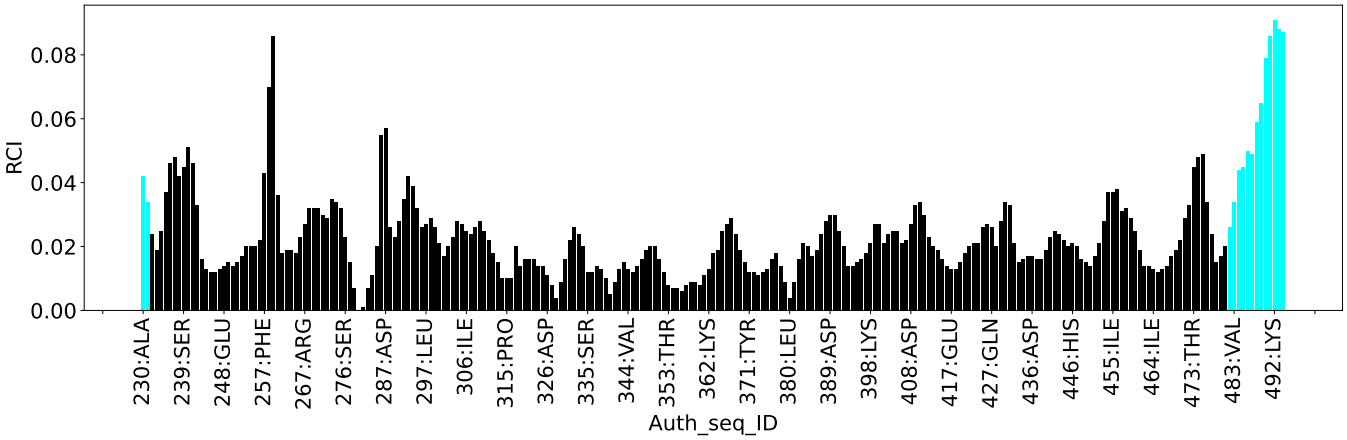
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	279	TYR	H	117.59	4.70 – 11.88	152.2
1	A	328	SER	H	31.14	5.45 – 11.10	40.5
1	A	340	GLN	H	29.41	5.39 – 11.05	37.5
1	A	279	TYR	N	9.63	100.12 – 140.79	-27.2
1	A	380	LEU	CB	57.53	33.11 – 51.34	8.4
1	A	335	SER	CB	51.64	56.28 – 71.32	-8.1
1	A	462	ASP	CB	53.22	32.98 – 48.76	7.8
1	A	380	LEU	CA	40.90	45.17 – 66.21	-7.0
1	A	360	LEU	CB	30.11	33.11 – 51.34	-6.7
1	A	353	THR	CB	58.99	61.12 – 78.27	-6.2

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:


RCI
0.00
0.02
0.04
0.06
0.08
230:ALA
239:SER
248:GLU
257:PHE
267:ARG
276:SER
287:ASP
297:LEU
306:ILE
315:PRO
326:ASP
335:SER
344:VAL
353:THR
362:LYS
371:TYR
380:LEU
389:ASP
398:LYS
408:ASP
417:GLU
427:GLN
436:ASP
446:HIS
455:ILE
464:ILE
473:THR
483:VAL
492:LYS
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	3707
Intra-residue (|i-j|=0)	0
Sequential (|i-j|=1)	809
Medium range (|i-j|>1 and |i-j|<5)	1161
Long range (|i-j|≥5)	1698
Inter-chain	37
Hydrogen bond restraints	2
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	10.0
Number of long range restraints per residue[1]	4.6

[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)	50.1	0.2
0.2-0.5 (Medium)	98.3	0.5
>0.5 (Large)	5.0	3.63

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)

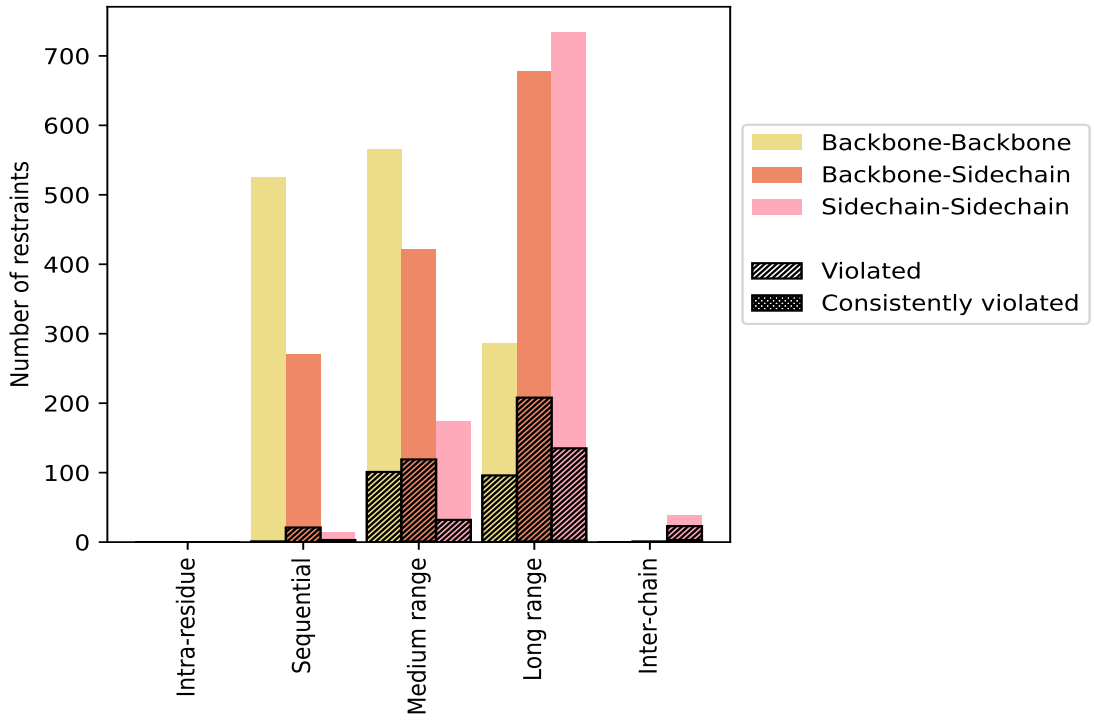
9.1 Summary of distance violations (i)

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)	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
Sequential (|i-j|=1)	809	21.8	25	3.1	0.7	0	0.0	0.0
Backbone-Backbone	525	14.2	1	0.2	0.0	0	0.0	0.0
Backbone-Sidechain	270	7.3	21	7.8	0.6	0	0.0	0.0
Sidechain-Sidechain	14	0.4	3	21.4	0.1	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	1161	31.3	252	21.7	6.8	1	0.1	0.0
Backbone-Backbone	565	15.2	101	17.9	2.7	0	0.0	0.0
Backbone-Sidechain	422	11.4	119	28.2	3.2	1	0.2	0.0
Sidechain-Sidechain	174	4.7	32	18.4	0.9	0	0.0	0.0
Long range (|i-j|≥5)	1698	45.8	439	25.9	11.8	3	0.2	0.1
Backbone-Backbone	286	7.7	96	33.6	2.6	0	0.0	0.0
Backbone-Sidechain	678	18.3	208	30.7	5.6	1	0.1	0.0
Sidechain-Sidechain	734	19.8	135	18.4	3.6	2	0.3	0.1
Inter-chain	37	1.0	22	59.5	0.6	3	8.1	0.1
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	1	0.0	1	100.0	0.0	0	0.0	0.0
Sidechain-Sidechain	36	1.0	21	58.3	0.6	3	8.3	0.1
Hydrogen bond	2	0.1	2	100.0	0.1	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	3707	100.0	740	20.0	20.0	7	0.2	0.2
Backbone-Backbone	1376	37.1	198	14.4	5.3	0	0.0	0.0
Backbone-Sidechain	1371	37.0	349	25.5	9.4	2	0.1	0.1
Sidechain-Sidechain	960	25.9	193	20.1	5.2	5	0.5	0.1

[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	0	4	41	105	12	162	0.25	0.75	0.12	0.23
2	0	9	46	107	9	171	0.26	0.75	0.11	0.26
3	0	3	43	101	13	160	0.28	2.66	0.22	0.26
4	0	5	64	75	13	157	0.28	2.05	0.17	0.26
5	0	8	54	88	15	165	0.25	0.79	0.12	0.24
6	0	8	41	90	12	151	0.28	2.4	0.2	0.26
7	0	5	47	97	13	162	0.27	1.58	0.15	0.25
8	0	5	58	76	11	150	0.26	0.58	0.1	0.26
9	0	7	54	76	14	151	0.29	2.71	0.26	0.26
10	0	5	54	87	11	157	0.25	0.75	0.11	0.24

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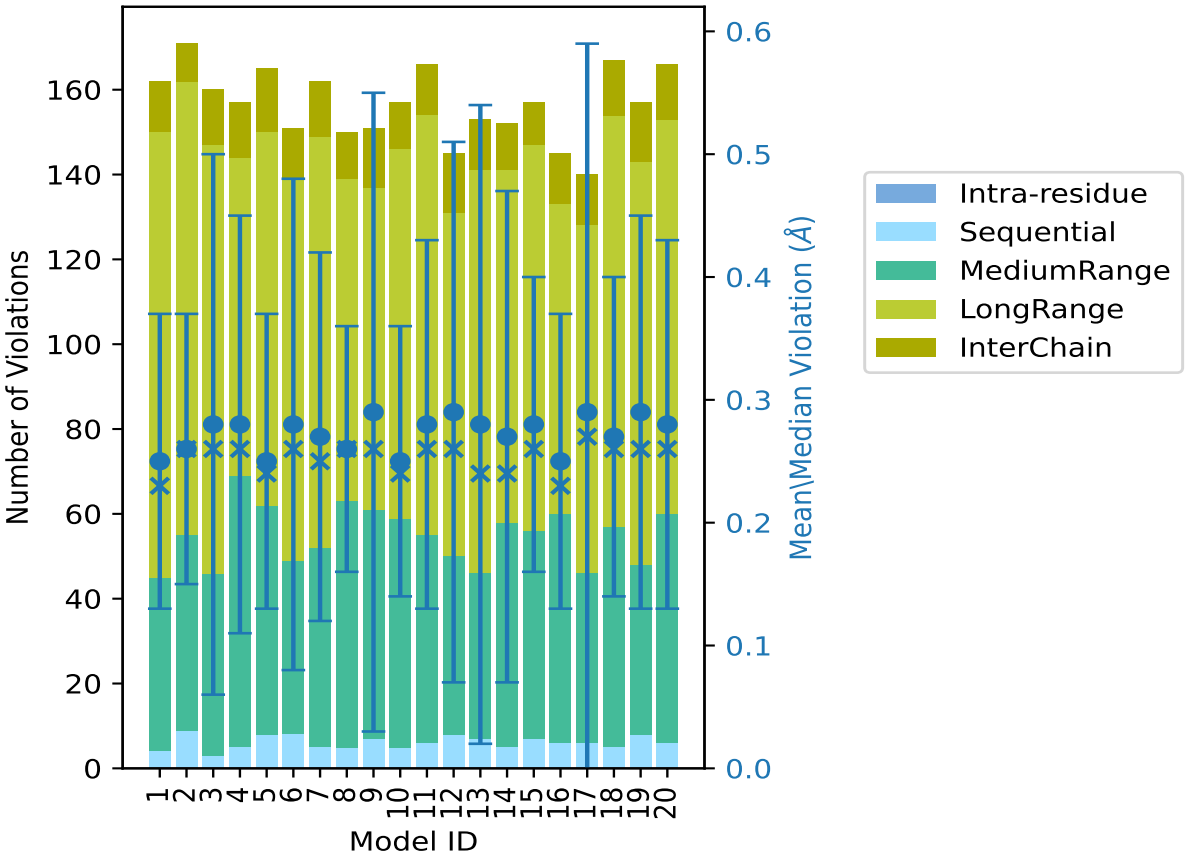
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	0	6	49	99	12	166	0.28	1.52	0.15	0.26
12	0	8	42	81	14	145	0.29	2.55	0.22	0.26
13	0	7	39	95	12	153	0.28	3.02	0.26	0.24
14	0	5	53	83	11	152	0.27	2.29	0.2	0.24
15	0	7	49	91	10	157	0.28	0.88	0.12	0.26
16	0	6	54	73	12	145	0.25	0.69	0.12	0.23
17	0	6	40	82	12	140	0.29	3.63	0.3	0.27
18	0	5	52	97	13	167	0.27	1.18	0.13	0.26
19	0	8	40	95	14	157	0.29	1.14	0.16	0.26
20	0	6	54	93	13	166	0.28	1.69	0.15	0.26

[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

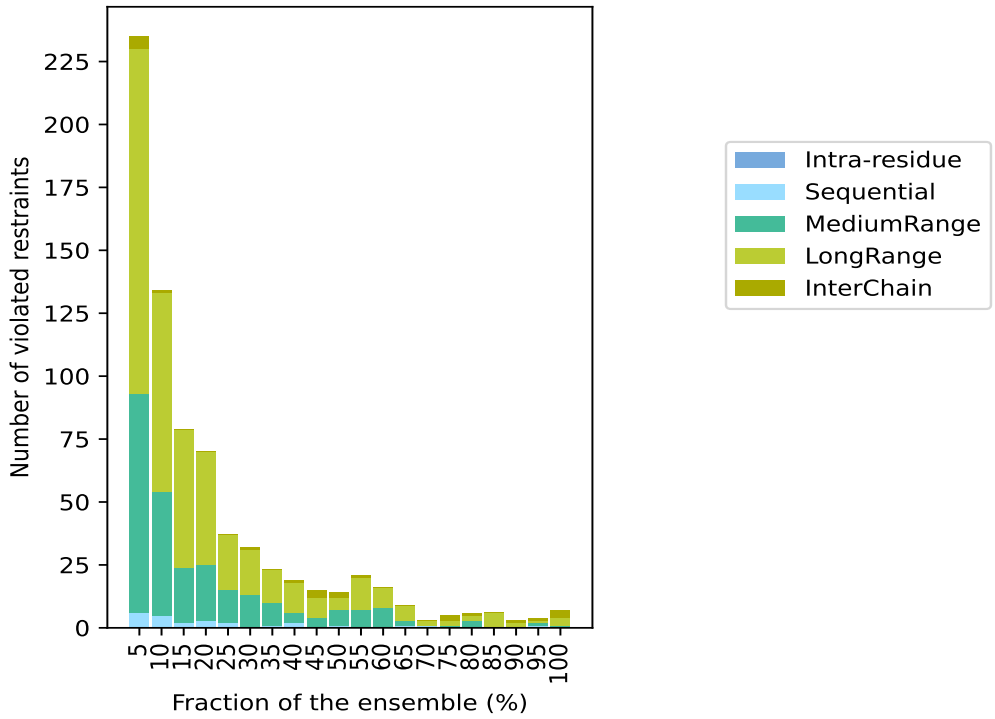
9.3 Distance violation statistics for the ensemble (i)

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, 2967(IR:0, SQ:784, MR:909, LR:1259, IC:15) 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]	%
0	6	87	137	5	235	1	5.0
0	5	49	79	1	134	2	10.0
0	2	22	55	0	79	3	15.0
0	3	22	45	0	70	4	20.0
0	2	13	22	0	37	5	25.0
0	0	13	18	1	32	6	30.0
0	1	9	13	0	23	7	35.0
0	2	4	12	1	19	8	40.0
0	0	4	8	3	15	9	45.0
0	1	6	5	2	14	10	50.0
0	0	7	13	1	21	11	55.0
0	0	8	8	0	16	12	60.0
0	1	2	6	0	9	13	65.0
0	1	0	2	0	3	14	70.0
0	0	1	2	2	5	15	75.0
0	0	3	2	1	6	16	80.0
0	0	0	6	0	6	17	85.0
0	0	0	2	1	3	18	90.0
0	1	1	1	1	4	19	95.0
0	0	1	3	3	7	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

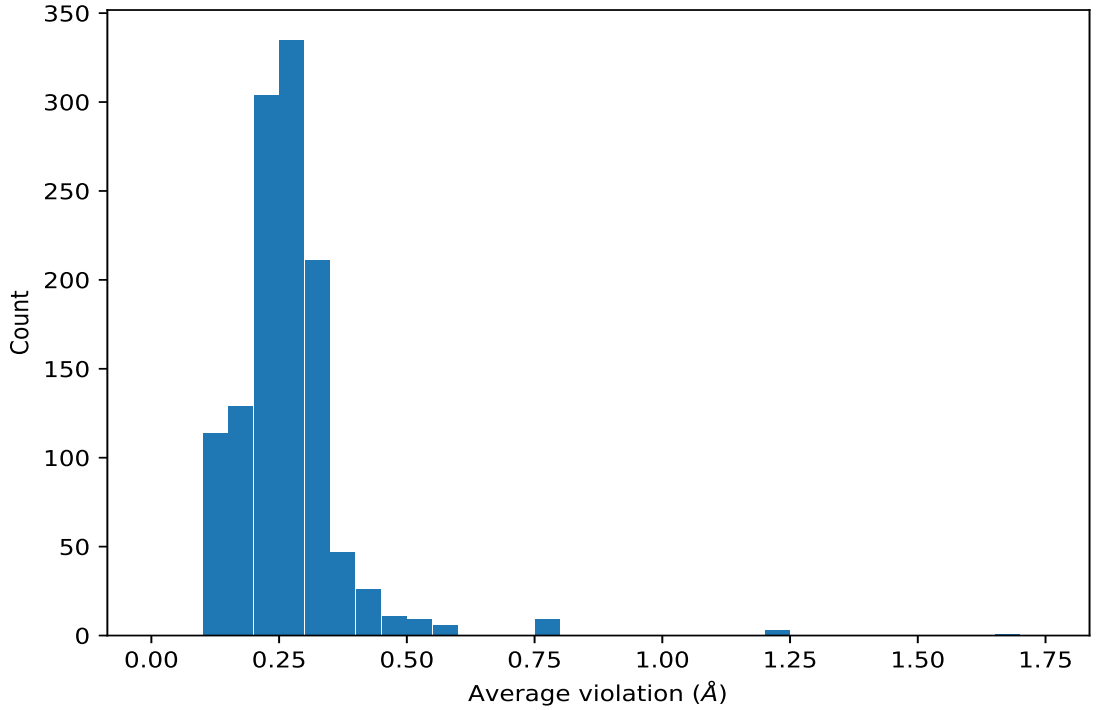
9.3.1 Bar graph : Distance violation statistics for the ensemble



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)
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE1	20	0.6	0.19	0.61
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE2	20	0.6	0.19	0.61
(1,3668)	1:402:A:PHE:HD1	2:618:B:MET:HE3	20	0.6	0.19	0.61
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE1	20	0.6	0.19	0.61
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE2	20	0.6	0.19	0.61
(1,3668)	1:402:A:PHE:HD2	2:618:B:MET:HE3	20	0.6	0.19	0.61
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG21	20	0.46	0.14	0.49
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG22	20	0.46	0.14	0.49
(2,7)	1:338:A:ILE:HD11	1:345:A:THR:HG23	20	0.46	0.14	0.49
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG21	20	0.46	0.14	0.49
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG22	20	0.46	0.14	0.49
(2,7)	1:338:A:ILE:HD12	1:345:A:THR:HG23	20	0.46	0.14	0.49
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG21	20	0.46	0.14	0.49
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG22	20	0.46	0.14	0.49
(2,7)	1:338:A:ILE:HD13	1:345:A:THR:HG23	20	0.46	0.14	0.49
(1,980)	1:286:A:TRP:HZ3	1:289:A:TRP:H	20	0.41	0.06	0.4

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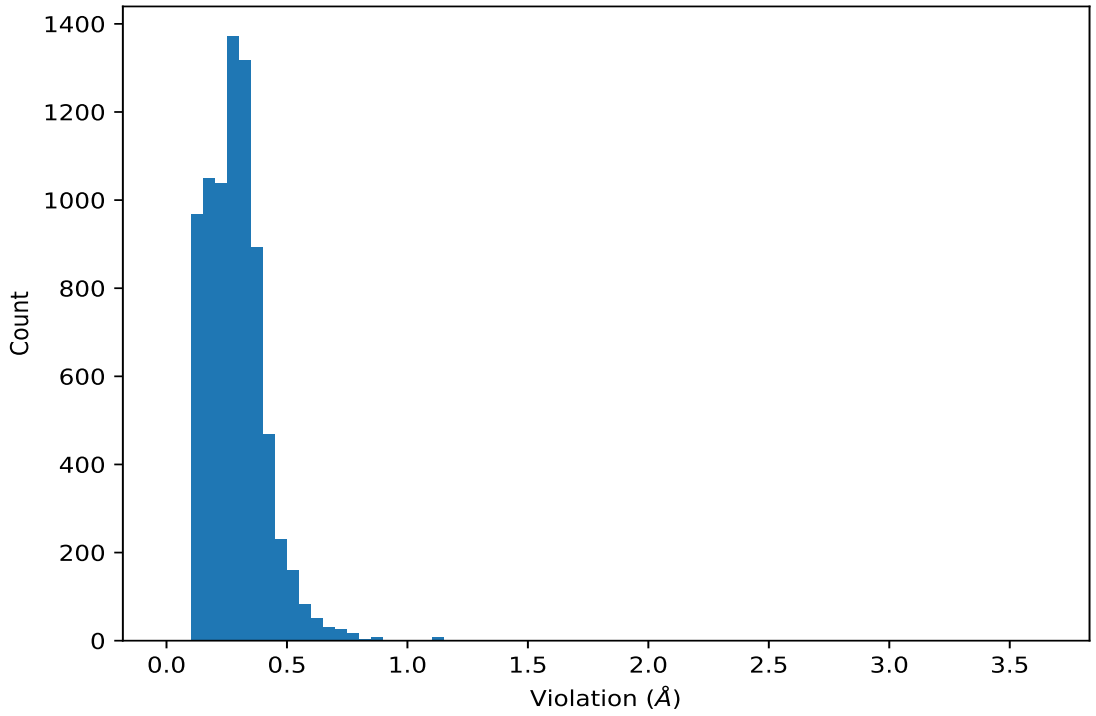
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG21	20	0.41	0.08	0.4
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG22	20	0.41	0.08	0.4
(1,3681)	1:467:A:TRP:HE3	2:625:B:THR:HG23	20	0.41	0.08	0.4
(1,345)	1:250:A:TYR:HB2	1:263:A:TRP:HB2	20	0.4	0.06	0.4
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD11	20	0.35	0.07	0.35
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD12	20	0.35	0.07	0.35
(1,3664)	1:353:A:THR:HG21	2:630:B:LEU:HD13	20	0.35	0.07	0.35
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD11	20	0.35	0.07	0.35
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD12	20	0.35	0.07	0.35
(1,3664)	1:353:A:THR:HG22	2:630:B:LEU:HD13	20	0.35	0.07	0.35
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD11	20	0.35	0.07	0.35
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD12	20	0.35	0.07	0.35
(1,3664)	1:353:A:THR:HG23	2:630:B:LEU:HD13	20	0.35	0.07	0.35
(1,642)	1:268:A:VAL:HG11	1:276:A:SER:H	20	0.34	0.07	0.36
(1,642)	1:268:A:VAL:HG12	1:276:A:SER:H	20	0.34	0.07	0.36
(1,642)	1:268:A:VAL:HG13	1:276:A:SER:H	20	0.34	0.07	0.36
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE1	19	0.37	0.08	0.38
(1,3679)	1:317:A:TYR:HD1	2:626:B:PHE:HE2	19	0.37	0.08	0.38
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE1	19	0.37	0.08	0.38
(1,3679)	1:317:A:TYR:HD2	2:626:B:PHE:HE2	19	0.37	0.08	0.38
(1,2530)	1:388:A:GLU:HA	1:390:A:PHE:H	19	0.32	0.08	0.35
(1,1471)	1:314:A:MET:HA	1:353:A:THR:HA	19	0.29	0.08	0.32

[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)
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	17	3.63
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	13	3.02
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	9	2.71
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	3	2.66
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	12	2.55
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	6	2.4
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	14	2.29
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	4	2.05
(1,1)	1:230:A:ALA:H	1:236:A:ARG:HH11	20	1.69
(1,3442)	1:458:A:LEU:HD11	1:480:A:PHE:HE1	9	1.63

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found