



Full wwPDB NMR Structure Validation Report ⓘ

Dec 13, 2023 – 11:36 PM EST

PDB ID : 2JPE
BMRB ID : 15242
Title : FHA domain of NIPP1
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Deposited on : 2007-05-07

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 ⓘ 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 ⓘ](#)) were used in the production of this report:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
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) : 2.36

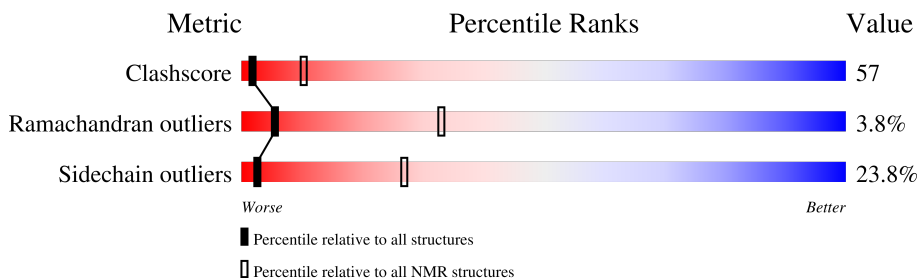
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 93%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	140	

2 Ensemble composition and analysis

This entry contains 20 models. Model 6 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:17-A:117, A:123-A:130 (109)	0.19	6

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 4 clusters. No single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2090 atoms, of which 1047 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Nuclear inhibitor of protein phosphatase 1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	132	2090	669	1047	184	186	4	0

There are 8 discrepancies between the modelled and reference sequences:

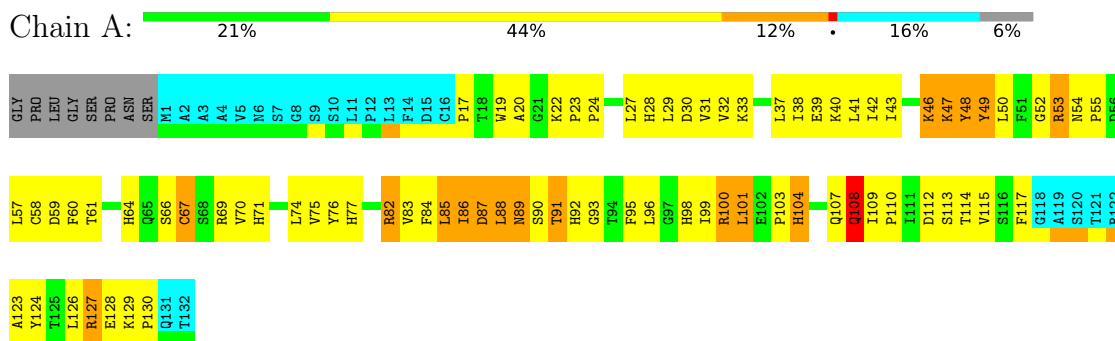
Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	GLY	-	cloning artifact	UNP Q8R3G1
A	-6	PRO	-	cloning artifact	UNP Q8R3G1
A	-5	LEU	-	cloning artifact	UNP Q8R3G1
A	-4	GLY	-	cloning artifact	UNP Q8R3G1
A	-3	SER	-	cloning artifact	UNP Q8R3G1
A	-2	PRO	-	cloning artifact	UNP Q8R3G1
A	-1	ASN	-	cloning artifact	UNP Q8R3G1
A	0	SER	-	cloning artifact	UNP Q8R3G1

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: Nuclear inhibitor of protein phosphatase 1

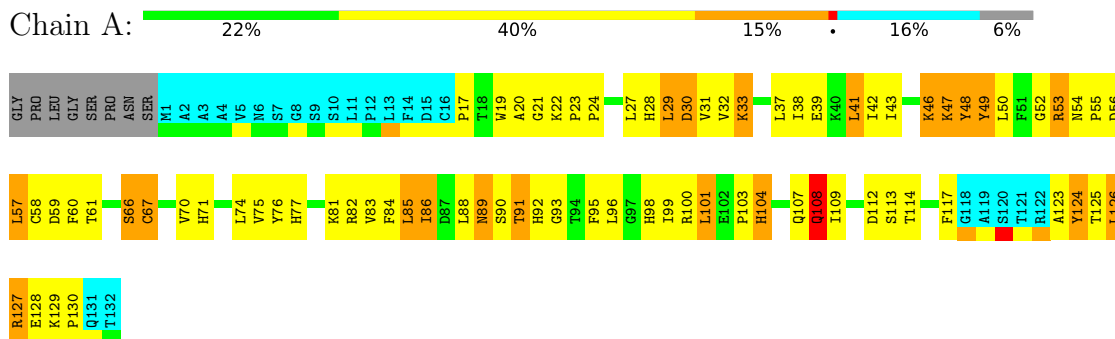


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

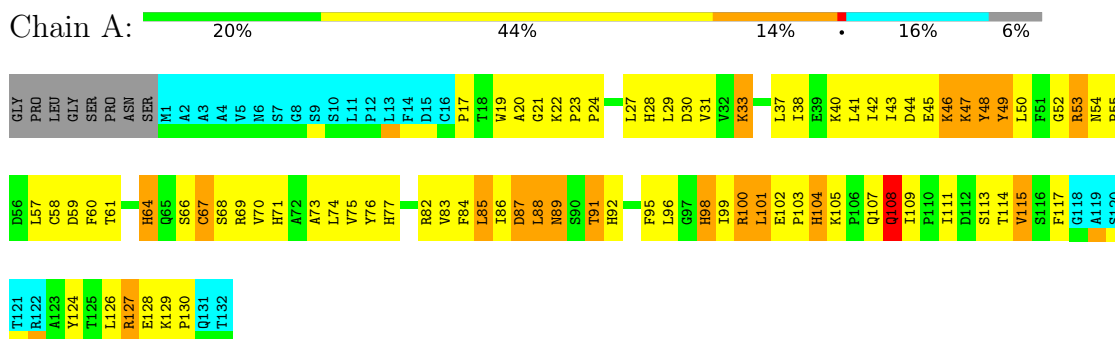
4.2.1 Score per residue for model 1

- Molecule 1: Nuclear inhibitor of protein phosphatase 1



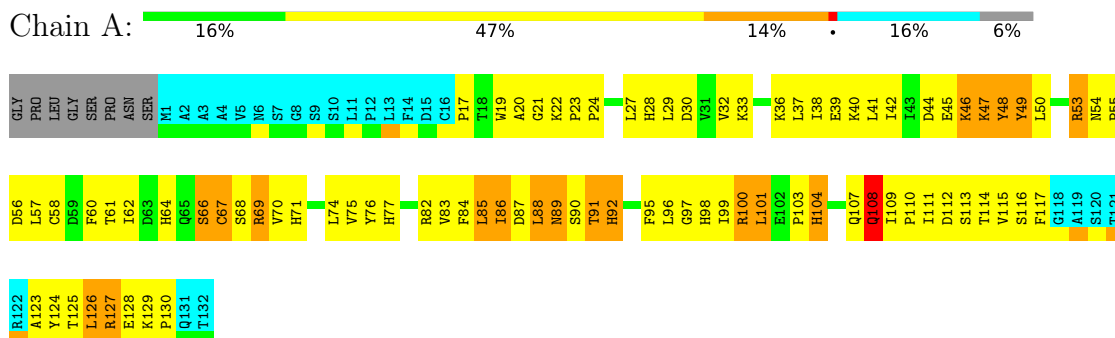
4.2.2 Score per residue for model 2

- Molecule 1: Nuclear inhibitor of protein phosphatase 1



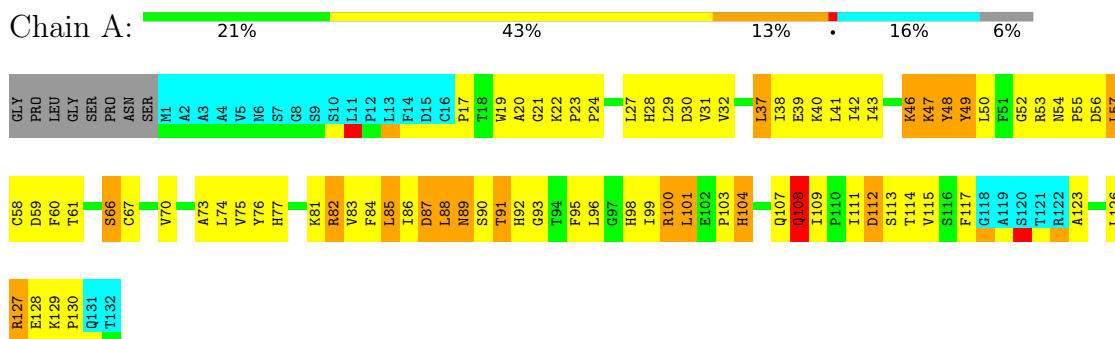
4.2.3 Score per residue for model 3

- Molecule 1: Nuclear inhibitor of protein phosphatase 1



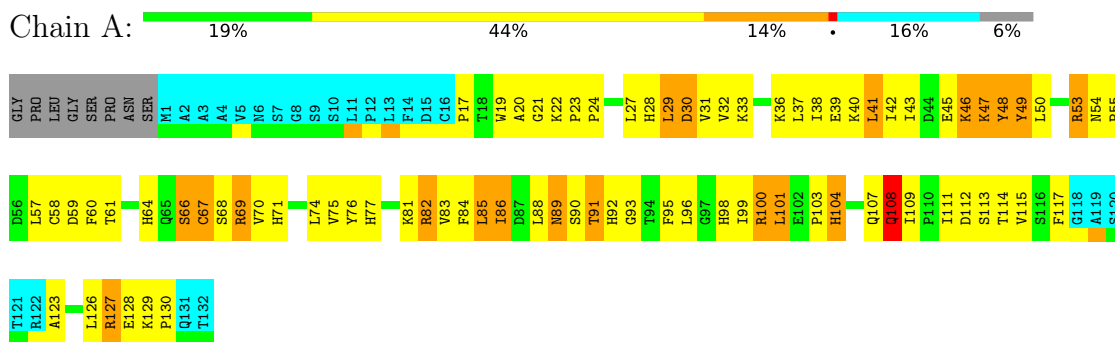
4.2.4 Score per residue for model 4

- Molecule 1: Nuclear inhibitor of protein phosphatase 1



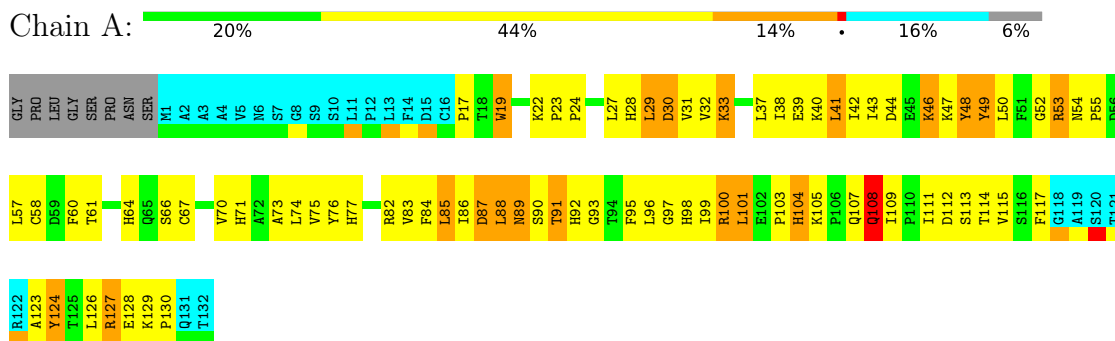
4.2.5 Score per residue for model 5

- Molecule 1: Nuclear inhibitor of protein phosphatase 1



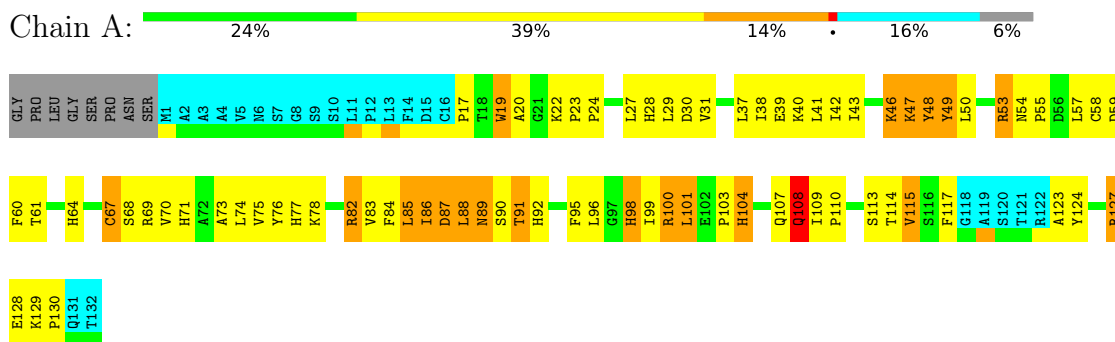
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Nuclear inhibitor of protein phosphatase 1



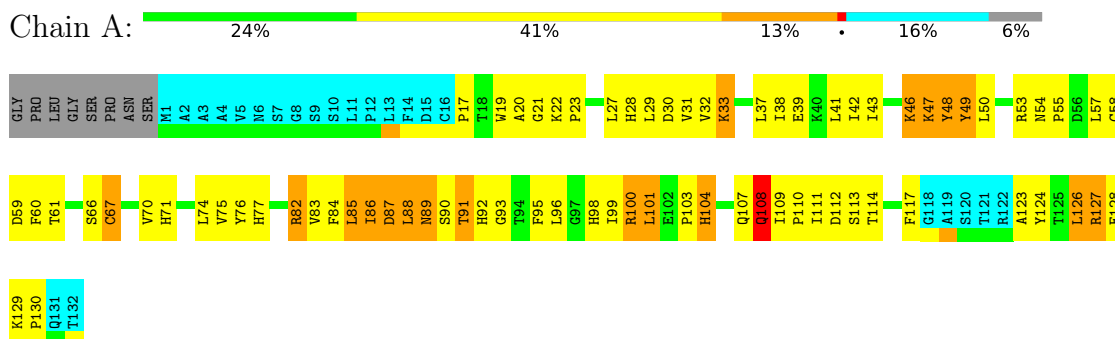
4.2.7 Score per residue for model 7

- Molecule 1: Nuclear inhibitor of protein phosphatase 1



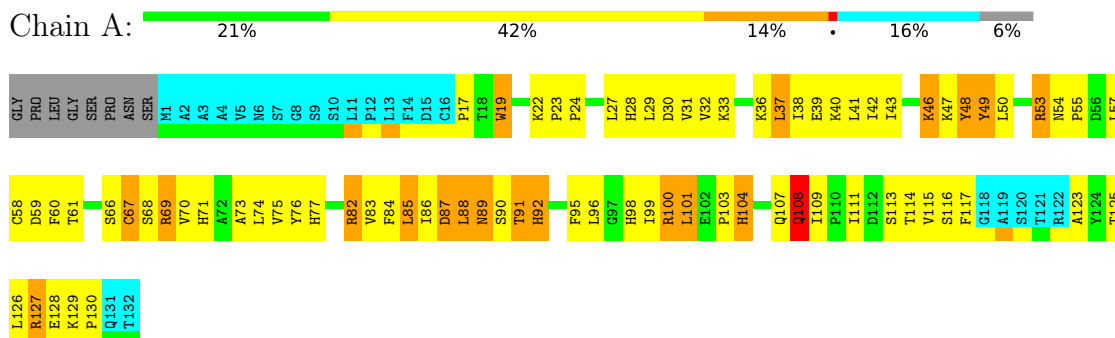
4.2.8 Score per residue for model 8

- Molecule 1: Nuclear inhibitor of protein phosphatase 1



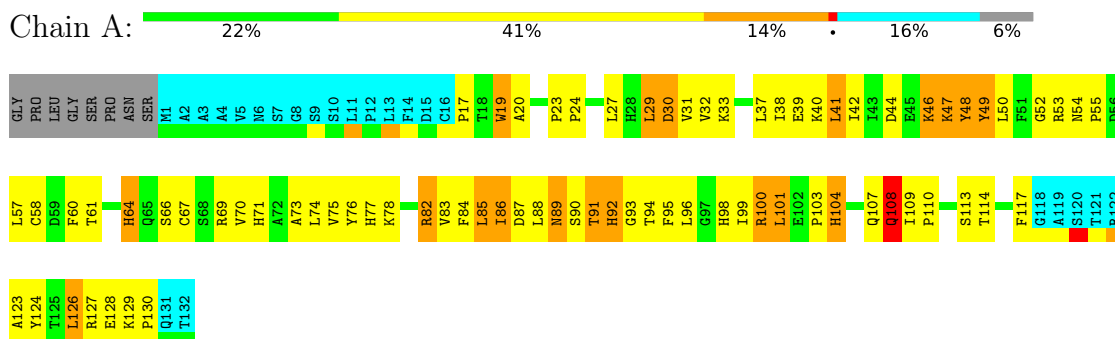
4.2.9 Score per residue for model 9

- Molecule 1: Nuclear inhibitor of protein phosphatase 1



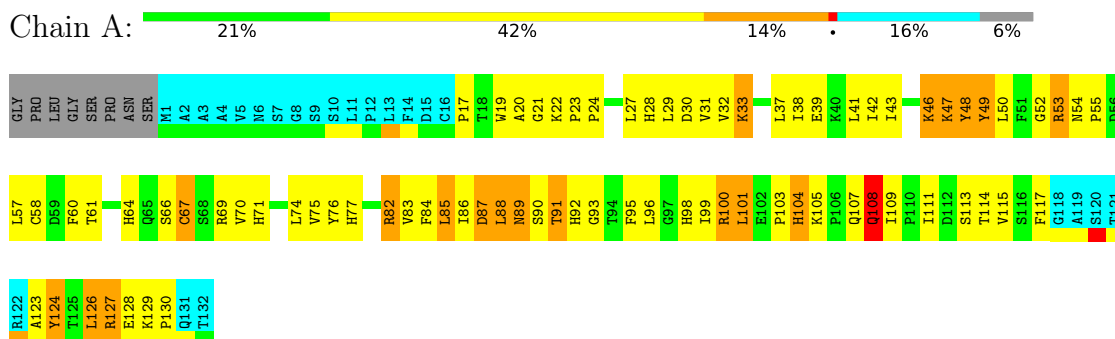
4.2.10 Score per residue for model 10

- Molecule 1: Nuclear inhibitor of protein phosphatase 1



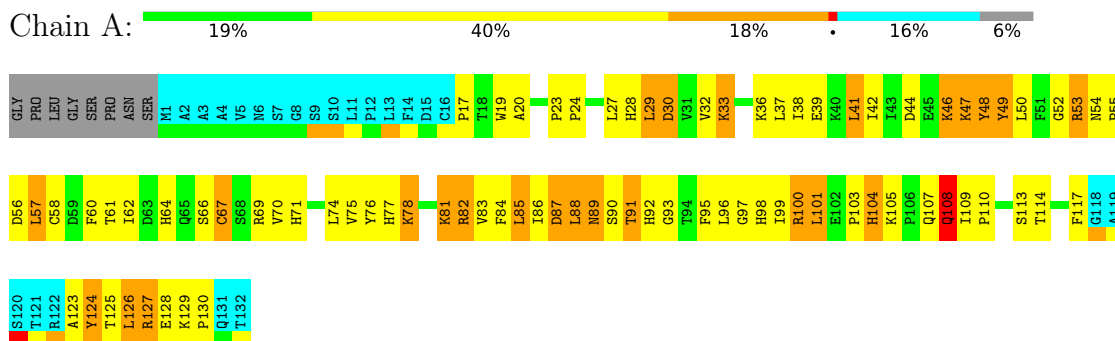
4.2.11 Score per residue for model 11

- Molecule 1: Nuclear inhibitor of protein phosphatase 1



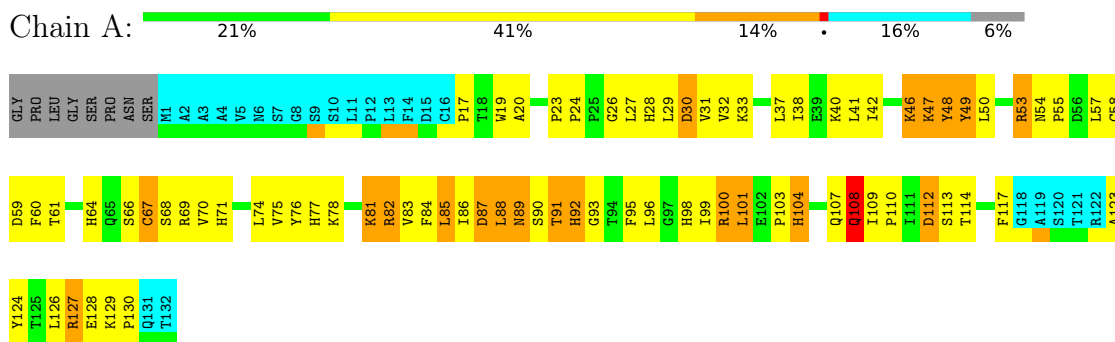
4.2.12 Score per residue for model 12

- Molecule 1: Nuclear inhibitor of protein phosphatase 1



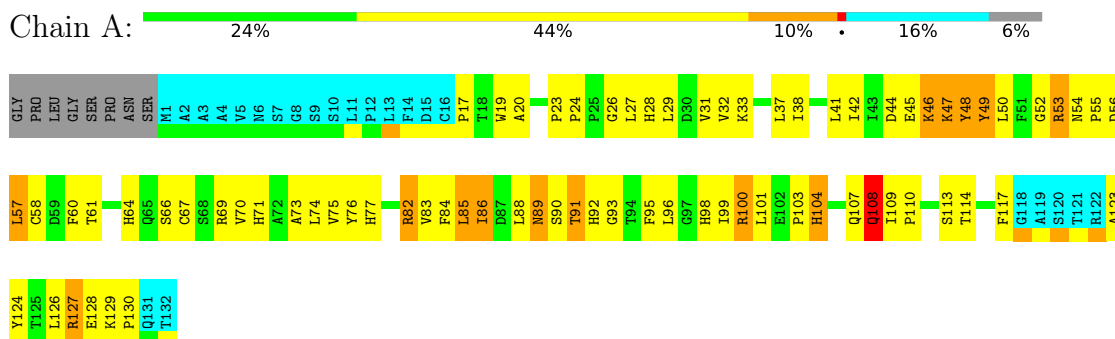
4.2.13 Score per residue for model 13

- Molecule 1: Nuclear inhibitor of protein phosphatase 1



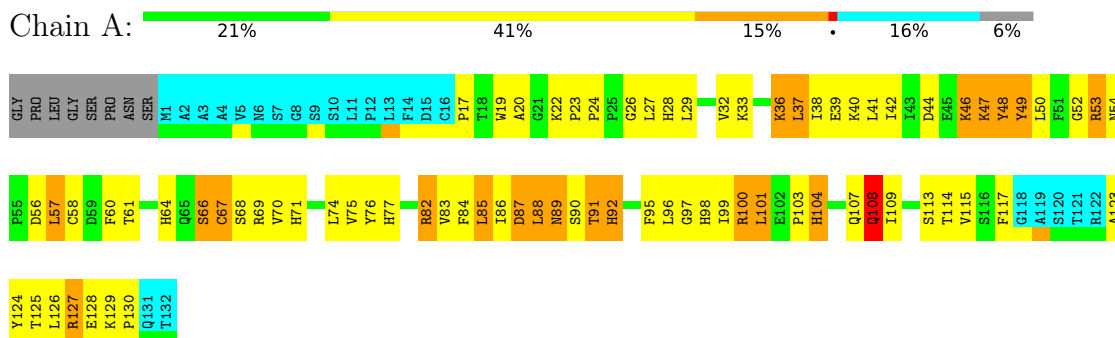
4.2.14 Score per residue for model 14

- Molecule 1: Nuclear inhibitor of protein phosphatase 1



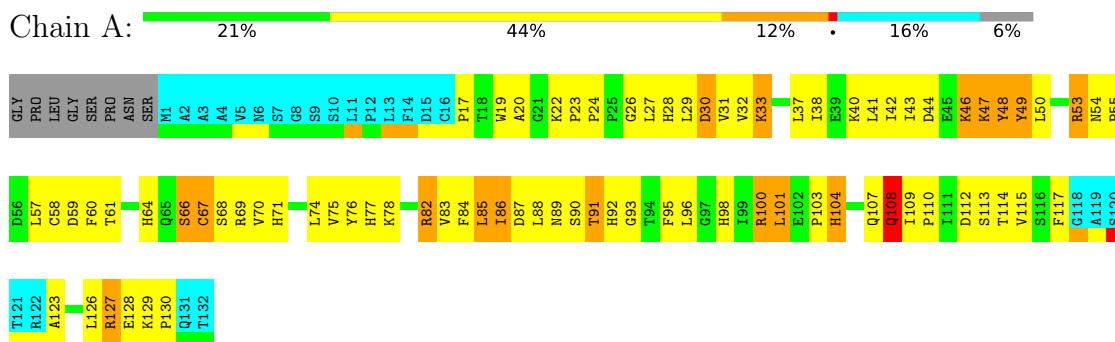
4.2.15 Score per residue for model 15

- Molecule 1: Nuclear inhibitor of protein phosphatase 1



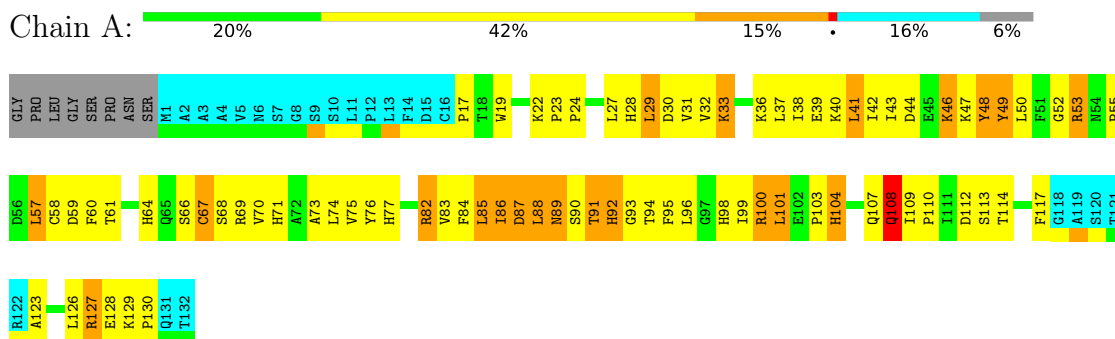
4.2.16 Score per residue for model 16

- Molecule 1: Nuclear inhibitor of protein phosphatase 1



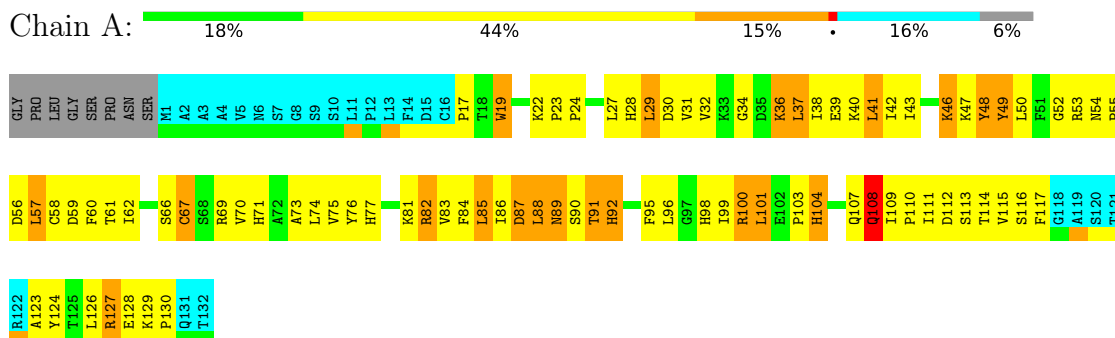
4.2.17 Score per residue for model 17

- Molecule 1: Nuclear inhibitor of protein phosphatase 1



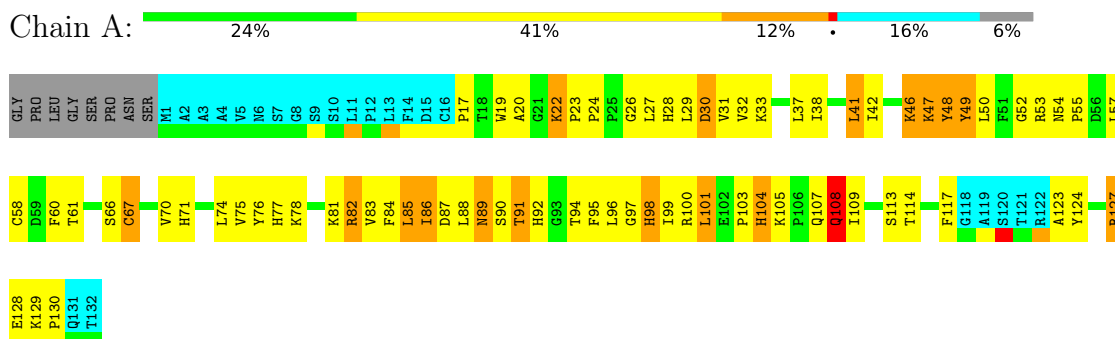
4.2.18 Score per residue for model 18

- Molecule 1: Nuclear inhibitor of protein phosphatase 1




4.2.19 Score per residue for model 19

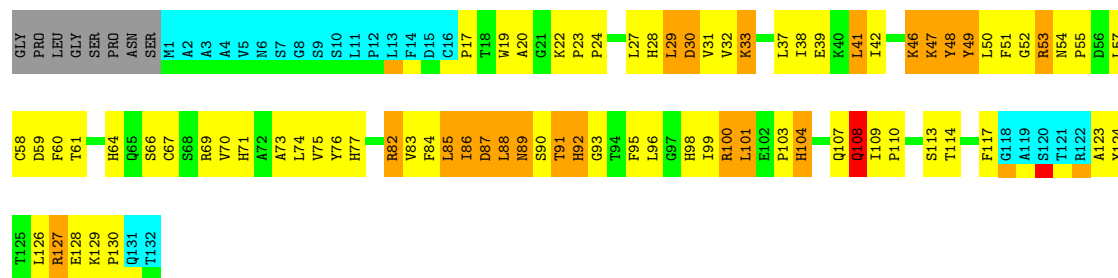
- Molecule 1: Nuclear inhibitor of protein phosphatase 1



4.2.20 Score per residue for model 20

- Molecule 1: Nuclear inhibitor of protein phosphatase 1

Chain A:  22% 40% 15% 16% 6%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *DGSA-distance geometry simulated annealing, 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
Sparky	refinement	3.110
CYANA	structure solution	2.1
CYANA	refinement	2.1

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	1692
Number of shifts mapped to atoms	1692
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

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	886	895	897	101±4
All	All	17720	17900	17940	2024

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 57.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:91:THR:HG23	1:A:92:HIS:CD2	0.83	2.08	16	20
1:A:85:LEU:HD21	1:A:117:PHE:CE1	0.81	2.10	1	20
1:A:41:LEU:HD13	1:A:60:PHE:CE2	0.81	2.10	15	20
1:A:19:TRP:CE3	1:A:77:HIS:CD2	0.80	2.69	9	20
1:A:74:LEU:HD23	1:A:75:VAL:N	0.80	1.92	1	20
1:A:114:THR:CG2	1:A:123:ALA:HB1	0.79	2.08	1	10
1:A:101:LEU:HD13	1:A:107:GLN:HB3	0.76	1.55	4	14
1:A:96:LEU:HD11	1:A:113:SER:OG	0.76	1.81	15	19
1:A:101:LEU:HD23	1:A:101:LEU:N	0.75	1.95	6	13
1:A:33:LYS:HB3	1:A:38:ILE:HD11	0.75	1.56	3	16
1:A:74:LEU:HD11	1:A:83:VAL:HG11	0.74	1.59	8	20
1:A:87:ASP:OD1	1:A:101:LEU:HD12	0.72	1.83	15	5
1:A:87:ASP:OD2	1:A:101:LEU:HD12	0.72	1.85	8	8
1:A:114:THR:HG23	1:A:123:ALA:HB1	0.71	1.63	12	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LEU:C	1:A:42:ILE:HD12	0.69	2.07	14	20
1:A:100:ARG:C	1:A:101:LEU:HD23	0.69	2.08	2	13
1:A:41:LEU:HD13	1:A:60:PHE:CD2	0.68	2.23	9	20
1:A:53:ARG:HH21	1:A:69:ARG:NH1	0.68	1.87	10	3
1:A:40:LYS:O	1:A:41:LEU:HD23	0.67	1.87	3	13
1:A:108:GLN:O	1:A:109:ILE:HD13	0.67	1.89	9	20
1:A:53:ARG:HH21	1:A:69:ARG:HH11	0.67	1.31	10	3
1:A:37:LEU:HD11	1:A:39:GLU:O	0.66	1.91	9	15
1:A:74:LEU:HD21	1:A:83:VAL:HG13	0.66	1.68	8	13
1:A:27:LEU:HD13	1:A:76:TYR:CE1	0.65	2.27	15	11
1:A:31:VAL:O	1:A:37:LEU:HD22	0.65	1.92	10	17
1:A:30:ASP:HB3	1:A:37:LEU:HD21	0.64	1.68	18	15
1:A:85:LEU:HD21	1:A:117:PHE:CZ	0.64	2.27	9	15
1:A:48:TYR:C	1:A:48:TYR:CD1	0.64	2.71	2	3
1:A:115:VAL:HG23	1:A:116:SER:N	0.64	2.06	3	3
1:A:111:ILE:HD12	1:A:128:GLU:HB2	0.64	1.68	5	3
1:A:27:LEU:HD13	1:A:76:TYR:CE2	0.64	2.28	7	1
1:A:20:ALA:HB1	1:A:47:LYS:HG2	0.64	1.70	19	8
1:A:71:HIS:CE1	1:A:90:SER:HG	0.63	2.11	16	7
1:A:20:ALA:HB1	1:A:47:LYS:HB2	0.63	1.71	7	2
1:A:48:TYR:CD1	1:A:48:TYR:C	0.62	2.73	18	17
1:A:95:PHE:CD2	1:A:99:ILE:O	0.61	2.53	11	19
1:A:71:HIS:CE1	1:A:90:SER:OG	0.61	2.54	3	7
1:A:49:TYR:O	1:A:73:ALA:HB1	0.61	1.96	9	9
1:A:96:LEU:HD12	1:A:114:THR:O	0.61	1.95	19	8
1:A:29:LEU:HD13	1:A:30:ASP:N	0.60	2.11	5	8
1:A:17:PRO:CG	1:A:75:VAL:HG11	0.60	2.26	6	18
1:A:24:PRO:HD2	1:A:27:LEU:HD11	0.60	1.72	5	19
1:A:29:LEU:HD13	1:A:30:ASP:H	0.60	1.56	12	8
1:A:85:LEU:CD2	1:A:117:PHE:CE1	0.60	2.84	1	14
1:A:87:ASP:O	1:A:89:ASN:N	0.60	2.34	7	14
1:A:53:ARG:O	1:A:61:THR:HG22	0.60	1.96	1	20
1:A:84:PHE:CD2	1:A:108:GLN:N	0.60	2.70	15	20
1:A:29:LEU:HG	1:A:43:ILE:HG21	0.60	1.73	8	4
1:A:48:TYR:O	1:A:48:TYR:CD1	0.60	2.54	20	2
1:A:48:TYR:CD1	1:A:48:TYR:O	0.60	2.55	2	18
1:A:20:ALA:HB1	1:A:47:LYS:CG	0.59	2.27	13	14
1:A:71:HIS:CD2	1:A:117:PHE:CD2	0.59	2.90	8	18
1:A:74:LEU:HD23	1:A:74:LEU:C	0.58	2.18	15	13
1:A:91:THR:HG23	1:A:92:HIS:HD2	0.58	1.57	18	4
1:A:32:VAL:HB	1:A:123:ALA:HB3	0.58	1.75	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:103:PRO:O	1:A:104:HIS:CG	0.58	2.57	19	20
1:A:66:SER:OG	1:A:92:HIS:CE1	0.58	2.57	10	1
1:A:48:TYR:CG	1:A:48:TYR:O	0.57	2.56	3	12
1:A:42:ILE:HD12	1:A:42:ILE:N	0.57	2.14	1	20
1:A:129:LYS:CB	1:A:129:LYS:HZ3	0.57	2.11	12	4
1:A:84:PHE:CE2	1:A:108:GLN:N	0.57	2.73	14	17
1:A:85:LEU:C	1:A:85:LEU:HD12	0.57	2.20	19	12
1:A:48:TYR:O	1:A:48:TYR:CG	0.57	2.57	12	8
1:A:95:PHE:CG	1:A:99:ILE:O	0.56	2.58	19	12
1:A:98:HIS:O	1:A:98:HIS:CD2	0.56	2.58	16	17
1:A:50:LEU:HD23	1:A:70:VAL:CG1	0.56	2.31	7	17
1:A:27:LEU:HD23	1:A:128:GLU:HG3	0.56	1.77	7	6
1:A:74:LEU:HD11	1:A:83:VAL:CG1	0.55	2.31	16	14
1:A:23:PRO:CG	1:A:46:LYS:O	0.55	2.54	14	20
1:A:42:ILE:N	1:A:42:ILE:CD1	0.55	2.70	20	20
1:A:23:PRO:HA	1:A:76:TYR:CE2	0.54	2.37	18	7
1:A:126:LEU:O	1:A:126:LEU:HD13	0.54	2.02	20	17
1:A:50:LEU:HD13	1:A:58:CYS:HA	0.54	1.80	15	1
1:A:87:ASP:O	1:A:103:PRO:HA	0.54	2.03	13	16
1:A:46:LYS:HD3	1:A:49:TYR:CD2	0.54	2.38	9	20
1:A:66:SER:HG	1:A:92:HIS:CE1	0.54	2.21	10	1
1:A:46:LYS:HE2	1:A:49:TYR:CE2	0.54	2.38	16	20
1:A:103:PRO:O	1:A:104:HIS:CD2	0.54	2.61	14	20
1:A:95:PHE:CB	1:A:99:ILE:O	0.53	2.57	19	3
1:A:32:VAL:HG22	1:A:37:LEU:HD22	0.53	1.80	4	5
1:A:60:PHE:O	1:A:61:THR:HG23	0.53	2.04	12	15
1:A:101:LEU:HD22	1:A:107:GLN:HG2	0.52	1.81	5	7
1:A:117:PHE:CE1	1:A:124:TYR:CE2	0.52	2.97	18	8
1:A:29:LEU:HD12	1:A:41:LEU:HD12	0.52	1.80	20	7
1:A:83:VAL:O	1:A:109:ILE:N	0.52	2.43	13	20
1:A:50:LEU:HD23	1:A:70:VAL:HG13	0.52	1.81	7	18
1:A:23:PRO:CD	1:A:46:LYS:O	0.52	2.57	16	12
1:A:85:LEU:HD12	1:A:86:ILE:N	0.52	2.19	19	11
1:A:113:SER:OG	1:A:114:THR:N	0.52	2.43	15	20
1:A:32:VAL:HG13	1:A:36:LYS:C	0.52	2.25	15	7
1:A:88:LEU:O	1:A:89:ASN:C	0.52	2.49	3	20
1:A:87:ASP:OD2	1:A:87:ASP:N	0.51	2.44	18	8
1:A:46:LYS:NZ	1:A:49:TYR:CD2	0.51	2.78	10	14
1:A:115:VAL:CG2	1:A:116:SER:N	0.51	2.73	3	3
1:A:27:LEU:CD1	1:A:76:TYR:CE1	0.51	2.93	14	14
1:A:27:LEU:HB3	1:A:43:ILE:HD11	0.51	1.80	6	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:LEU:CD1	1:A:60:PHE:CE2	0.51	2.93	13	19
1:A:20:ALA:HB1	1:A:47:LYS:HG3	0.51	1.82	14	6
1:A:17:PRO:HG2	1:A:75:VAL:HG11	0.51	1.82	7	5
1:A:91:THR:CG2	1:A:92:HIS:CD2	0.51	2.92	18	11
1:A:95:PHE:CZ	1:A:100:ARG:HB3	0.51	2.41	9	16
1:A:33:LYS:HD2	1:A:38:ILE:HD11	0.51	1.82	10	2
1:A:17:PRO:HG3	1:A:19:TRP:CZ2	0.50	2.41	5	10
1:A:21:GLY:O	1:A:47:LYS:CB	0.50	2.59	4	7
1:A:89:ASN:N	1:A:89:ASN:ND2	0.50	2.60	11	13
1:A:97:GLY:O	1:A:98:HIS:ND1	0.50	2.44	19	1
1:A:103:PRO:O	1:A:104:HIS:CB	0.50	2.60	14	19
1:A:53:ARG:CD	1:A:67:CYS:SG	0.50	3.00	9	9
1:A:101:LEU:N	1:A:101:LEU:CD2	0.50	2.69	17	11
1:A:33:LYS:CB	1:A:38:ILE:HD11	0.50	2.36	12	8
1:A:53:ARG:NH2	1:A:69:ARG:NH1	0.50	2.60	10	1
1:A:37:LEU:C	1:A:37:LEU:HD13	0.49	2.27	13	10
1:A:41:LEU:HB3	1:A:60:PHE:CZ	0.49	2.42	6	16
1:A:33:LYS:CG	1:A:38:ILE:HD11	0.49	2.38	10	4
1:A:22:LYS:HZ1	1:A:47:LYS:HB3	0.49	1.67	19	1
1:A:46:LYS:HG2	1:A:49:TYR:CE1	0.49	2.42	1	6
1:A:33:LYS:NZ	1:A:36:LYS:NZ	0.49	2.60	15	1
1:A:77:HIS:CD2	1:A:84:PHE:CE1	0.49	3.00	8	19
1:A:46:LYS:CD	1:A:49:TYR:CD2	0.49	2.96	17	11
1:A:74:LEU:CD2	1:A:75:VAL:N	0.49	2.72	1	2
1:A:111:ILE:HD13	1:A:126:LEU:CD1	0.48	2.38	11	6
1:A:46:LYS:HZ3	1:A:49:TYR:HD2	0.48	1.48	8	12
1:A:98:HIS:CD2	1:A:99:ILE:HG13	0.48	2.43	2	2
1:A:19:TRP:HB2	1:A:77:HIS:CE1	0.48	2.44	1	8
1:A:23:PRO:HB3	1:A:76:TYR:CE1	0.48	2.43	5	16
1:A:23:PRO:HB3	1:A:76:TYR:CD2	0.48	2.44	17	7
1:A:33:LYS:HG2	1:A:38:ILE:HD11	0.48	1.84	16	1
1:A:126:LEU:HD13	1:A:126:LEU:C	0.48	2.29	20	1
1:A:95:PHE:CA	1:A:99:ILE:O	0.48	2.62	19	8
1:A:24:PRO:CD	1:A:76:TYR:OH	0.48	2.61	19	2
1:A:29:LEU:N	1:A:41:LEU:O	0.48	2.47	6	20
1:A:39:GLU:OE2	1:A:41:LEU:HD21	0.47	2.09	11	2
1:A:28:HIS:CE1	1:A:127:ARG:HB3	0.47	2.44	7	19
1:A:23:PRO:HB3	1:A:76:TYR:CE2	0.47	2.44	17	7
1:A:83:VAL:HG12	1:A:84:PHE:N	0.47	2.23	5	13
1:A:95:PHE:CZ	1:A:100:ARG:CB	0.47	2.97	10	4
1:A:23:PRO:HB3	1:A:76:TYR:CD1	0.47	2.44	8	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:37:LEU:HD13	1:A:38:ILE:N	0.47	2.25	15	14
1:A:107:GLN:NE2	1:A:108:GLN:O	0.47	2.47	10	18
1:A:27:LEU:CD1	1:A:76:TYR:CE2	0.47	2.97	7	1
1:A:125:THR:HG22	1:A:127:ARG:NE	0.47	2.24	9	2
1:A:87:ASP:OD1	1:A:94:THR:N	0.47	2.48	19	2
1:A:32:VAL:O	1:A:123:ALA:N	0.47	2.48	1	18
1:A:71:HIS:NE2	1:A:90:SER:OG	0.47	2.48	16	7
1:A:46:LYS:HD3	1:A:49:TYR:CG	0.47	2.45	16	20
1:A:17:PRO:CB	1:A:19:TRP:NE1	0.46	2.78	2	17
1:A:110:PRO:O	1:A:113:SER:CB	0.46	2.63	17	11
1:A:115:VAL:HG22	1:A:124:TYR:HB2	0.46	1.86	18	2
1:A:96:LEU:C	1:A:114:THR:O	0.46	2.53	7	7
1:A:50:LEU:HD22	1:A:70:VAL:HG13	0.46	1.86	15	1
1:A:83:VAL:CG1	1:A:84:PHE:N	0.46	2.78	5	2
1:A:128:GLU:O	1:A:130:PRO:N	0.46	2.48	6	20
1:A:58:CYS:SG	1:A:70:VAL:HG13	0.46	2.50	16	4
1:A:70:VAL:HG12	1:A:88:LEU:HD12	0.46	1.86	14	2
1:A:46:LYS:CE	1:A:49:TYR:CE2	0.46	2.99	10	14
1:A:111:ILE:C	1:A:112:ASP:CG	0.46	2.74	4	1
1:A:33:LYS:CE	1:A:36:LYS:NZ	0.46	2.79	15	1
1:A:82:ARG:NH1	1:A:108:GLN:OE1	0.46	2.49	18	3
1:A:111:ILE:HD13	1:A:126:LEU:HD11	0.46	1.87	8	1
1:A:128:GLU:O	1:A:129:LYS:C	0.46	2.54	6	20
1:A:44:ASP:O	1:A:44:ASP:OD2	0.46	2.34	2	4
1:A:125:THR:HG22	1:A:127:ARG:CD	0.46	2.41	9	3
1:A:52:GLY:C	1:A:53:ARG:CG	0.45	2.85	1	13
1:A:46:LYS:CG	1:A:49:TYR:CZ	0.45	2.99	5	5
1:A:77:HIS:N	1:A:82:ARG:O	0.45	2.50	19	14
1:A:37:LEU:CD1	1:A:39:GLU:O	0.45	2.62	18	2
1:A:44:ASP:O	1:A:44:ASP:OD1	0.45	2.34	6	3
1:A:87:ASP:OD1	1:A:87:ASP:N	0.45	2.49	20	3
1:A:68:SER:O	1:A:69:ARG:C	0.45	2.55	7	9
1:A:90:SER:O	1:A:91:THR:C	0.45	2.55	18	17
1:A:91:THR:HG1	1:A:92:HIS:CD2	0.45	2.30	18	1
1:A:112:ASP:N	1:A:126:LEU:O	0.45	2.49	18	5
1:A:23:PRO:HB3	1:A:76:TYR:CZ	0.45	2.47	20	11
1:A:32:VAL:HG13	1:A:36:LYS:O	0.45	2.11	3	2
1:A:56:ASP:OD2	1:A:57:LEU:HD23	0.45	2.11	14	2
1:A:124:TYR:CD1	1:A:124:TYR:N	0.45	2.83	18	2
1:A:129:LYS:CB	1:A:129:LYS:NZ	0.45	2.79	12	2
1:A:115:VAL:HG13	1:A:124:TYR:O	0.45	2.12	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:75:VAL:O	1:A:84:PHE:N	0.44	2.50	19	6
1:A:56:ASP:OD1	1:A:57:LEU:HD23	0.44	2.11	15	3
1:A:102:GLU:OE1	1:A:105:LYS:NZ	0.44	2.48	2	1
1:A:74:LEU:CD2	1:A:83:VAL:HG13	0.44	2.40	18	5
1:A:26:GLY:O	1:A:129:LYS:N	0.44	2.51	15	1
1:A:33:LYS:CD	1:A:38:ILE:HD11	0.44	2.42	10	1
1:A:37:LEU:HD13	1:A:37:LEU:C	0.44	2.32	8	5
1:A:97:GLY:O	1:A:98:HIS:CG	0.44	2.71	19	1
1:A:108:GLN:HG3	1:A:109:ILE:N	0.44	2.28	5	12
1:A:66:SER:O	1:A:91:THR:HG21	0.44	2.13	3	2
1:A:57:LEU:HD12	1:A:69:ARG:HB3	0.44	1.89	17	1
1:A:123:ALA:O	1:A:125:THR:N	0.44	2.51	1	1
1:A:17:PRO:HB2	1:A:19:TRP:NE1	0.44	2.28	9	13
1:A:95:PHE:CE2	1:A:100:ARG:HB3	0.44	2.48	11	1
1:A:90:SER:OG	1:A:93:GLY:N	0.44	2.51	12	1
1:A:66:SER:HB3	1:A:92:HIS:CE1	0.44	2.47	3	1
1:A:29:LEU:HD13	1:A:30:ASP:O	0.44	2.12	6	3
1:A:27:LEU:O	1:A:44:ASP:OD2	0.43	2.37	6	3
1:A:19:TRP:O	1:A:78:LYS:N	0.43	2.52	7	4
1:A:27:LEU:O	1:A:44:ASP:OD1	0.43	2.36	2	3
1:A:23:PRO:HB3	1:A:76:TYR:CG	0.43	2.49	13	8
1:A:83:VAL:O	1:A:108:GLN:HA	0.43	2.14	6	18
1:A:74:LEU:O	1:A:75:VAL:CG2	0.43	2.67	1	2
1:A:95:PHE:HA	1:A:99:ILE:O	0.43	2.14	2	2
1:A:55:PRO:O	1:A:58:CYS:O	0.43	2.36	14	19
1:A:33:LYS:HE2	1:A:38:ILE:HD11	0.43	1.89	14	1
1:A:101:LEU:HD22	1:A:107:GLN:CB	0.43	2.44	19	1
1:A:17:PRO:CB	1:A:19:TRP:CE2	0.43	3.02	2	1
1:A:46:LYS:CE	1:A:49:TYR:CD2	0.43	3.01	15	12
1:A:42:ILE:CG2	1:A:45:GLU:OE1	0.42	2.68	5	1
1:A:27:LEU:HD23	1:A:128:GLU:CG	0.42	2.43	12	1
1:A:27:LEU:HD13	1:A:76:TYR:HE1	0.42	1.75	13	2
1:A:44:ASP:O	1:A:44:ASP:CG	0.42	2.56	14	1
1:A:62:ILE:HG21	1:A:67:CYS:SG	0.42	2.54	18	1
1:A:96:LEU:HD22	1:A:109:ILE:HD13	0.42	1.90	6	1
1:A:129:LYS:HZ3	1:A:129:LYS:HB3	0.42	1.73	8	1
1:A:97:GLY:N	1:A:114:THR:O	0.42	2.53	6	4
1:A:87:ASP:OD2	1:A:94:THR:CB	0.42	2.67	17	1
1:A:29:LEU:HD23	1:A:126:LEU:HA	0.42	1.92	8	2
1:A:17:PRO:HB2	1:A:19:TRP:CD1	0.41	2.50	9	9
1:A:19:TRP:CZ3	1:A:75:VAL:HG12	0.41	2.50	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:124:TYR:N	1:A:124:TYR:CD1	0.41	2.88	11	5
1:A:107:GLN:O	1:A:108:GLN:O	0.41	2.38	19	2
1:A:87:ASP:OD1	1:A:90:SER:CB	0.41	2.68	16	1
1:A:66:SER:O	1:A:67:CYS:O	0.41	2.39	1	6
1:A:123:ALA:O	1:A:124:TYR:C	0.41	2.57	1	3
1:A:60:PHE:O	1:A:61:THR:CG2	0.41	2.69	12	1
1:A:41:LEU:HB3	1:A:60:PHE:CE2	0.41	2.51	2	1
1:A:49:TYR:CE1	1:A:59:ASP:OD2	0.41	2.73	2	1
1:A:78:LYS:O	1:A:81:LYS:CD	0.41	2.68	13	2
1:A:74:LEU:CD1	1:A:83:VAL:CG1	0.41	2.98	16	1
1:A:29:LEU:C	1:A:30:ASP:OD1	0.41	2.59	9	3
1:A:56:ASP:C	1:A:57:LEU:HD23	0.41	2.36	18	1
1:A:50:LEU:O	1:A:51:PHE:CD2	0.41	2.74	20	1
1:A:74:LEU:C	1:A:75:VAL:HG23	0.41	2.36	1	1
1:A:30:ASP:OD2	1:A:125:THR:O	0.41	2.39	3	1
1:A:44:ASP:CG	1:A:44:ASP:O	0.41	2.60	16	1
1:A:53:ARG:O	1:A:55:PRO:HD3	0.41	2.16	1	4
1:A:74:LEU:HD21	1:A:83:VAL:CG1	0.41	2.44	18	1
1:A:17:PRO:CG	1:A:19:TRP:CE2	0.40	3.04	5	1
1:A:42:ILE:CG2	1:A:44:ASP:OD2	0.40	2.69	10	1
1:A:44:ASP:OD2	1:A:44:ASP:O	0.40	2.39	10	1
1:A:27:LEU:HD13	1:A:76:TYR:HE2	0.40	1.69	7	1
1:A:27:LEU:HD21	1:A:128:GLU:OE2	0.40	2.15	8	1
1:A:84:PHE:CZ	1:A:108:GLN:CB	0.40	3.05	16	1
1:A:32:VAL:CG1	1:A:36:LYS:O	0.40	2.70	3	1
1:A:98:HIS:CD2	1:A:98:HIS:O	0.40	2.74	11	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	109/140 (78%)	75±2 (69±2%)	30±2 (27±2%)	4±1 (4±1%)	5	33
All	All	2180/2800 (78%)	1503 (69%)	594 (27%)	83 (4%)	5	33

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

Mol	Chain	Res	Type	Models (Total)
1	A	67	CYS	20
1	A	104	HIS	20
1	A	108	GLN	20
1	A	88	LEU	14
1	A	124	TYR	4
1	A	26	GLY	4
1	A	34	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	99/122 (81%)	75±2 (76±2%)	24±2 (24±2%)	2 27
All	All	1980/2440 (81%)	1509 (76%)	471 (24%)	2 27

All 39 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	46	LYS	20
1	A	47	LYS	20
1	A	48	TYR	20
1	A	49	TYR	20
1	A	57	LEU	20
1	A	82	ARG	20
1	A	85	LEU	20
1	A	86	ILE	20
1	A	91	THR	20
1	A	100	ARG	20
1	A	108	GLN	20
1	A	127	ARG	20
1	A	54	ASN	19
1	A	89	ASN	19
1	A	101	LEU	19
1	A	22	LYS	16
1	A	53	ARG	15

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Mol	Chain	Res	Type	Models (Total)
1	A	64	HIS	14
1	A	87	ASP	13
1	A	59	ASP	11
1	A	30	ASP	10
1	A	33	LYS	9
1	A	41	LEU	9
1	A	29	LEU	8
1	A	92	HIS	8
1	A	81	LYS	7
1	A	69	ARG	7
1	A	66	SER	6
1	A	112	ASP	6
1	A	126	LEU	6
1	A	115	VAL	6
1	A	19	TRP	5
1	A	37	LEU	4
1	A	105	LYS	4
1	A	45	GLU	3
1	A	98	HIS	3
1	A	36	LYS	2
1	A	56	ASP	1
1	A	78	LYS	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no 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](#)

The completeness of assignment taking into account all chemical shift lists is 93% for the well-defined parts and 93% 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 [i](#)

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	1692
Number of shifts mapped to atoms	1692
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	4

7.1.2 Chemical shift referencing [i](#)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	131	-0.29 ± 0.07	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	123	0.02 ± 0.10	None needed (< 0.5 ppm)
$^{13}\text{C}'$	118	0.29 ± 0.14	None needed (< 0.5 ppm)
^{15}N	122	-0.31 ± 0.52	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 93%, i.e. 1450 atoms were assigned a chemical shift out of a possible 1553. 0 out of 19 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	521/533 (98%)	213/215 (99%)	209/218 (96%)	99/100 (99%)
Sidechain	805/865 (93%)	540/564 (96%)	257/271 (95%)	8/30 (27%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	124/155 (80%)	65/79 (82%)	57/66 (86%)	2/10 (20%)
Overall	1450/1553 (93%)	818/858 (95%)	523/555 (94%)	109/140 (78%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 93%, i.e. 1687 atoms were assigned a chemical shift out of a possible 1818. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	621/648 (96%)	254/262 (97%)	249/264 (94%)	118/122 (97%)
Sidechain	932/1005 (93%)	626/657 (95%)	296/313 (95%)	10/35 (29%)
Aromatic	134/165 (81%)	70/84 (83%)	62/71 (87%)	2/10 (20%)
Overall	1687/1818 (93%)	950/1003 (95%)	607/648 (94%)	130/167 (78%)

7.1.4 Statistically unusual chemical shifts [i](#)

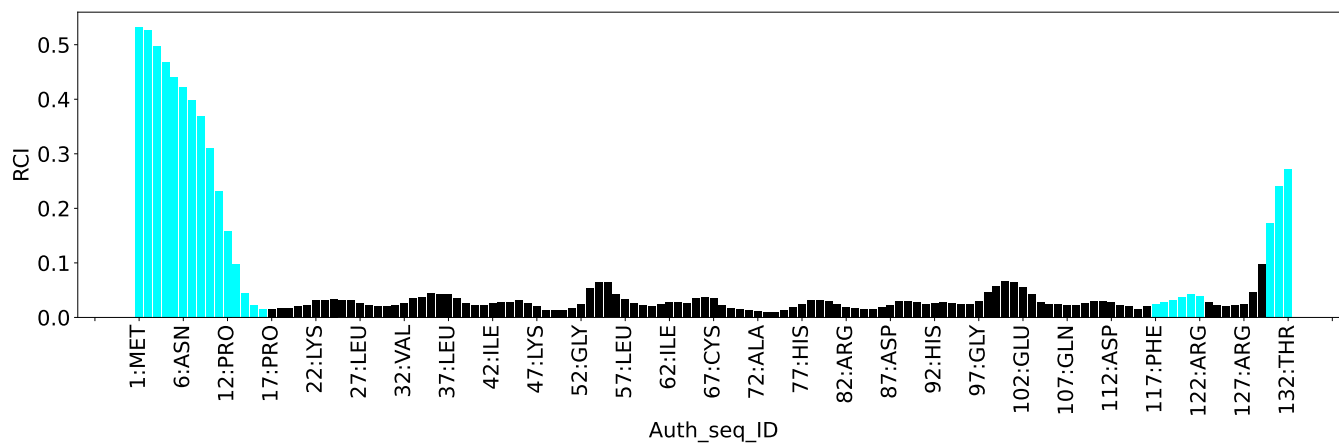
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	127	ARG	HB2	0.06	0.52 – 3.08	-6.8
1	A	17	PRO	HB2	-0.21	0.37 – 3.78	-6.7
1	A	68	SER	H	11.99	5.45 – 11.10	6.6
1	A	19	TRP	CE2	171.98	105.29 – 170.61	5.2

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:



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	3399
Intra-residue ($ i-j =0$)	751
Sequential ($ i-j =1$)	900
Medium range ($ i-j >1$ and $ i-j <5$)	389
Long range ($ i-j \geq 5$)	1359
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	24.3
Number of long range restraints per residue ¹	9.7

¹Long 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)	5.5	0.2
0.2-0.5 (Medium)	1.6	0.5
>0.5 (Large)	3.9	1.65

8.2.2 Average number of dihedral-angle violations per model

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

9 Distance violation analysis [i](#)

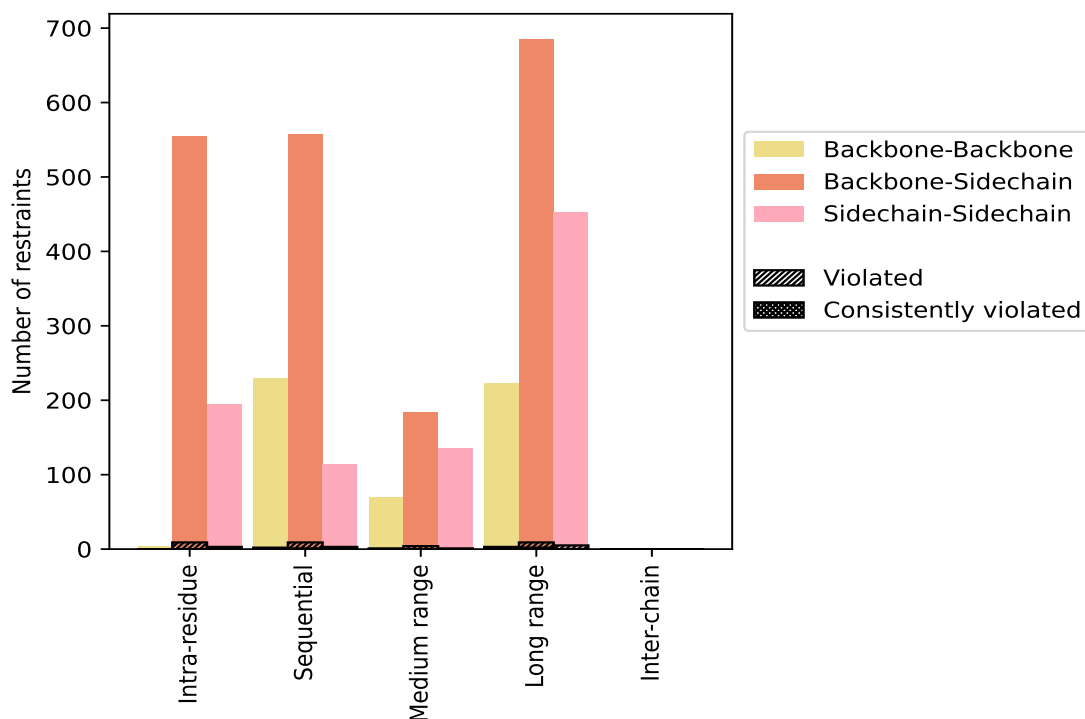
9.1 Summary of distance violations [i](#)

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.

Restrains type	Count	% ¹	Violated ³			Consistently Violated ⁴		
			Count	% ²	% ¹	Count	% ²	% ¹
Intra-residue ($i-j =0$)	751	22.1	12	1.6	0.4	0	0.0	0.0
Backbone-Backbone	3	0.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	554	16.3	9	1.6	0.3	0	0.0	0.0
Sidechain-Sidechain	194	5.7	3	1.5	0.1	0	0.0	0.0
Sequential ($i-j =1$)	900	26.5	14	1.6	0.4	1	0.1	0.0
Backbone-Backbone	229	6.7	2	0.9	0.1	0	0.0	0.0
Backbone-Sidechain	557	16.4	9	1.6	0.3	1	0.2	0.0
Sidechain-Sidechain	114	3.4	3	2.6	0.1	0	0.0	0.0
Medium range ($i-j >1$ & $i-j <5$)	389	11.4	6	1.5	0.2	0	0.0	0.0
Backbone-Backbone	70	2.1	1	1.4	0.0	0	0.0	0.0
Backbone-Sidechain	184	5.4	4	2.2	0.1	0	0.0	0.0
Sidechain-Sidechain	135	4.0	1	0.7	0.0	0	0.0	0.0
Long range ($i-j \geq 5$)	1359	40.0	17	1.3	0.5	4	0.3	0.1
Backbone-Backbone	222	6.5	3	1.4	0.1	2	0.9	0.1
Backbone-Sidechain	685	20.2	9	1.3	0.3	2	0.3	0.1
Sidechain-Sidechain	452	13.3	5	1.1	0.1	0	0.0	0.0
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	3399	100.0	49	1.4	1.4	5	0.1	0.1
Backbone-Backbone	524	15.4	6	1.1	0.2	2	0.4	0.1
Backbone-Sidechain	1980	58.3	31	1.6	0.9	3	0.2	0.1
Sidechain-Sidechain	895	26.3	12	1.3	0.4	0	0.0	0.0

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 [i](#)



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

9.2 Distance violation statistics for each model [i](#)

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	1	2	0	4	0	7	0.71	1.63	0.54	0.84
2	0	3	0	7	0	10	0.5	1.65	0.51	0.2
3	2	2	1	7	0	12	0.44	1.62	0.48	0.14
4	2	4	1	6	0	13	0.46	1.62	0.5	0.14
5	1	3	2	6	0	12	0.47	1.64	0.48	0.26
6	3	2	1	7	0	13	0.43	1.59	0.48	0.14
7	1	2	0	7	0	10	0.45	1.04	0.36	0.24
8	1	4	1	9	0	15	0.4	1.58	0.44	0.17
9	2	2	1	6	0	11	0.48	1.57	0.48	0.14
10	3	3	1	5	0	12	0.41	1.04	0.37	0.18
11	4	2	1	5	0	12	0.46	1.6	0.49	0.16

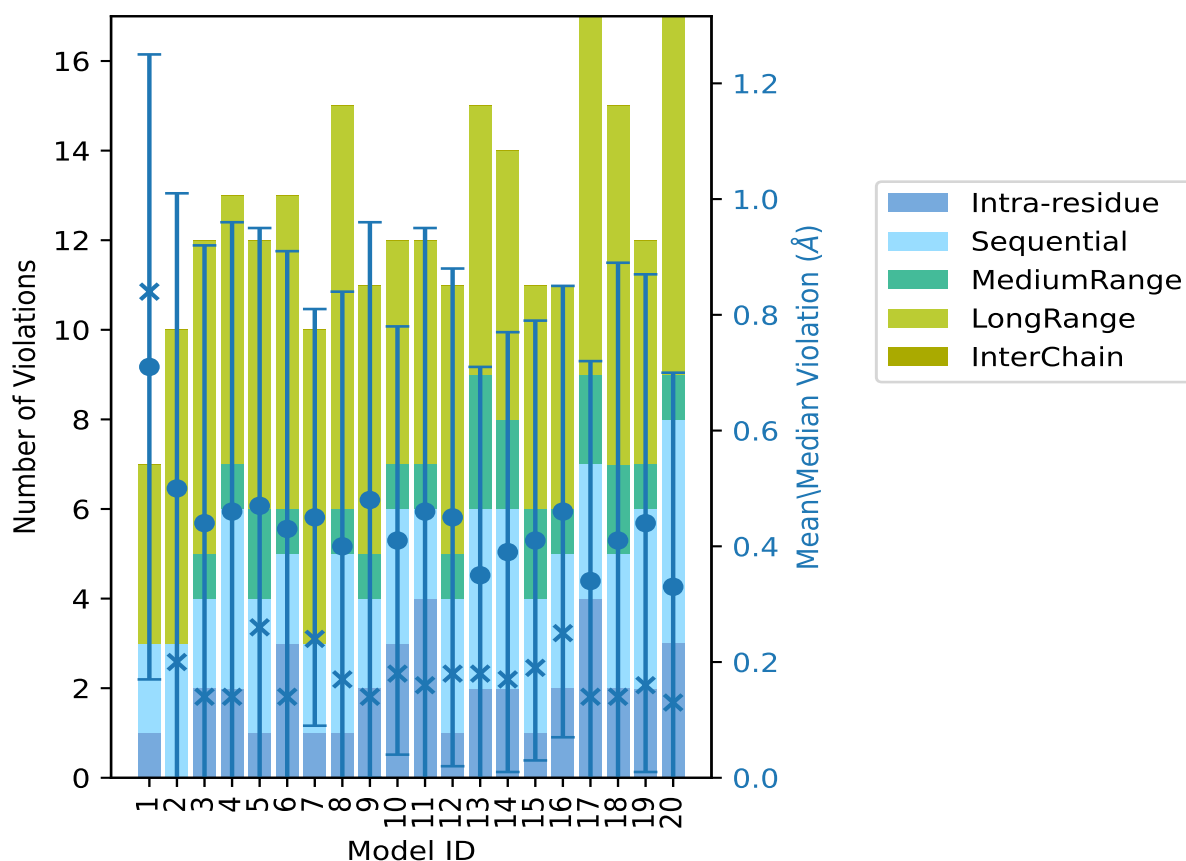
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Model ID	Number of violations					Total	Mean (Å)	Max (Å)	SD ⁶ (Å)	Median (Å)
	IR ¹	SQ ²	MR ³	LR ⁴	IC ⁵					
12	1	3	1	6	0	11	0.45	1.34	0.43	0.18
13	2	4	3	6	0	15	0.35	1.18	0.36	0.18
14	2	4	2	6	0	14	0.39	1.18	0.38	0.17
15	1	3	2	5	0	11	0.41	1.15	0.38	0.19
16	2	3	1	5	0	11	0.46	1.18	0.39	0.25
17	4	3	2	8	0	17	0.34	1.31	0.38	0.14
18	2	3	2	8	0	15	0.41	1.64	0.48	0.14
19	2	4	1	5	0	12	0.44	1.32	0.43	0.16
20	3	5	1	8	0	17	0.33	1.21	0.37	0.13

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

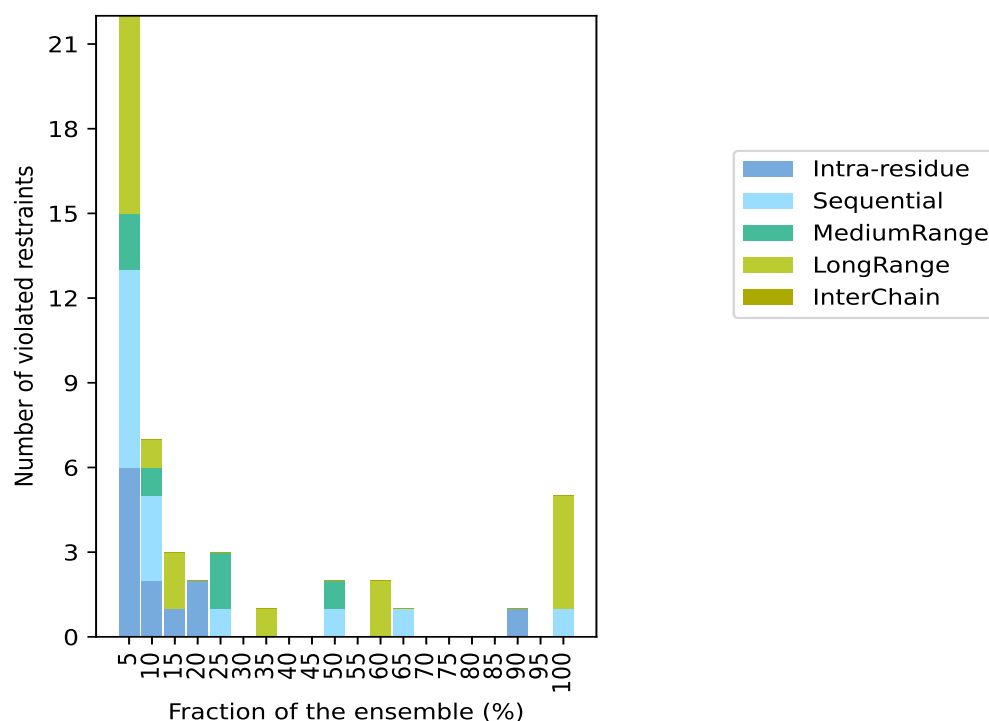
9.3 Distance violation statistics for the ensemble

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, 3350(IR:739, SQ:886, MR:383, LR:1342, 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	%
6	7	2	7	0	22	1	5.0
2	3	1	1	0	7	2	10.0
1	0	0	2	0	3	3	15.0
2	0	0	0	0	2	4	20.0
0	1	2	0	0	3	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	1	0	1	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	1	1	0	0	2	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	2	0	2	12	60.0
0	1	0	0	0	1	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
1	0	0	0	0	1	18	90.0
0	0	0	0	0	0	19	95.0
0	1	0	4	0	5	20	100.0

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

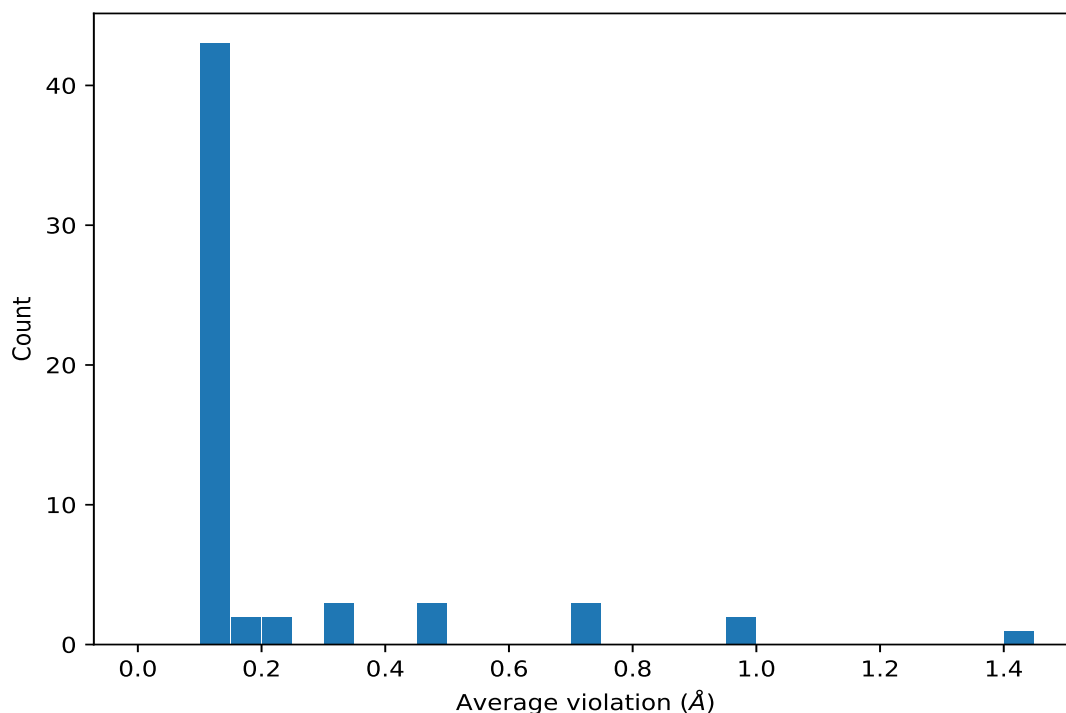
9.3.1 Bar graph : Distance violation statistics for the ensemble [i](#)



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 violation for each restraint sorted by number of violated models and the mean 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)
(1,1270)	1:21:A:GLY:HA2	1:78:A:LYS:HA	20	1.4	0.22	1.46
(1,992)	1:52:A:GLY:HA2	1:70:A:VAL:HB	20	0.98	0.03	0.98
(1,2451)	1:21:A:GLY:HA2	1:78:A:LYS:H	20	0.97	0.07	0.96
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB1	20	0.72	0.16	0.74
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB2	20	0.72	0.16	0.74
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB3	20	0.72	0.16	0.74
(1,990)	1:52:A:GLY:HA2	1:53:A:ARG:HB2	20	0.23	0.02	0.24
(1,1580)	1:107:A:GLN:H	1:107:A:GLN:HE21	18	0.12	0.0	0.12
(1,1369)	1:60:A:PHE:HB3	1:61:A:THR:HB	13	0.1	0.0	0.1
(1,856)	1:94:A:THR:HG21	1:101:A:LEU:HB3	12	0.13	0.02	0.14
(1,856)	1:94:A:THR:HG22	1:101:A:LEU:HB3	12	0.13	0.02	0.14
(1,856)	1:94:A:THR:HG23	1:101:A:LEU:HB3	12	0.13	0.02	0.14
(1,1303)	1:52:A:GLY:HA2	1:61:A:THR:HA	12	0.13	0.02	0.14
(1,973)	1:21:A:GLY:HA3	1:22:A:LYS:HA	10	0.2	0.02	0.2
(1,633)	1:67:A:CYS:HB2	1:71:A:HIS:HE1	10	0.13	0.03	0.12
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD11	7	0.11	0.01	0.11

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Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD12	7	0.11	0.01	0.11
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD13	7	0.11	0.01	0.11
(1,2203)	1:67:A:CYS:H	1:71:A:HIS:HE1	5	0.11	0.01	0.11
(1,2133)	1:64:A:HIS:H	1:66:A:SER:H	5	0.11	0.01	0.11
(1,191)	1:62:A:ILE:HG21	1:63:A:ASP:H	5	0.11	0.01	0.11
(1,191)	1:62:A:ILE:HG22	1:63:A:ASP:H	5	0.11	0.01	0.11
(1,191)	1:62:A:ILE:HG23	1:63:A:ASP:H	5	0.11	0.01	0.11
(1,3056)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	4	0.14	0.01	0.14
(1,3056)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	4	0.14	0.01	0.14
(1,3056)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	4	0.14	0.01	0.14
(1,3056)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	4	0.14	0.01	0.14
(1,1752)	1:29:A:LEU:H	1:29:A:LEU:HG	4	0.12	0.01	0.12
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD11	3	0.12	0.01	0.11
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD12	3	0.12	0.01	0.11
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD13	3	0.12	0.01	0.11
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD21	3	0.12	0.01	0.11
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD22	3	0.12	0.01	0.11
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD23	3	0.12	0.01	0.11
(1,1818)	1:89:A:ASN:H	1:89:A:ASN:HB2	3	0.1	0.0	0.1
(1,3086)	1:50:A:LEU:HD11	1:70:A:VAL:H	3	0.1	0.0	0.1
(1,3086)	1:50:A:LEU:HD12	1:70:A:VAL:H	3	0.1	0.0	0.1
(1,3086)	1:50:A:LEU:HD13	1:70:A:VAL:H	3	0.1	0.0	0.1
(1,3086)	1:50:A:LEU:HD21	1:70:A:VAL:H	3	0.1	0.0	0.1
(1,3086)	1:50:A:LEU:HD22	1:70:A:VAL:H	3	0.1	0.0	0.1
(1,3086)	1:50:A:LEU:HD23	1:70:A:VAL:H	3	0.1	0.0	0.1
(1,301)	1:121:A:THR:HA	1:121:A:THR:HG21	2	0.46	0.0	0.46
(1,301)	1:121:A:THR:HA	1:121:A:THR:HG22	2	0.46	0.0	0.46
(1,301)	1:121:A:THR:HA	1:121:A:THR:HG23	2	0.46	0.0	0.46
(1,2366)	1:10:A:SER:HB2	1:11:A:LEU:H	2	0.3	0.01	0.3
(1,2366)	1:10:A:SER:HB3	1:11:A:LEU:H	2	0.3	0.01	0.3
(1,2367)	1:10:A:SER:HA	1:11:A:LEU:H	2	0.3	0.01	0.3
(1,3337)	1:105:A:LYS:HA	1:105:A:LYS:HD2	2	0.16	0.01	0.16
(1,3337)	1:105:A:LYS:HA	1:105:A:LYS:HD3	2	0.16	0.01	0.16
(1,2905)	1:22:A:LYS:HG2	1:23:A:PRO:HA	2	0.12	0.02	0.12
(1,2905)	1:22:A:LYS:HG3	1:23:A:PRO:HA	2	0.12	0.02	0.12
(1,547)	1:24:A:PRO:HG2	1:27:A:LEU:H	2	0.11	0.01	0.11
(1,547)	1:24:A:PRO:HG3	1:27:A:LEU:H	2	0.11	0.01	0.11
(1,2897)	1:20:A:ALA:HB1	1:47:A:LYS:HE2	2	0.11	0.01	0.11
(1,2897)	1:20:A:ALA:HB1	1:47:A:LYS:HE3	2	0.11	0.01	0.11
(1,2897)	1:20:A:ALA:HB2	1:47:A:LYS:HE2	2	0.11	0.01	0.11
(1,2897)	1:20:A:ALA:HB2	1:47:A:LYS:HE3	2	0.11	0.01	0.11
(1,2897)	1:20:A:ALA:HB3	1:47:A:LYS:HE2	2	0.11	0.01	0.11

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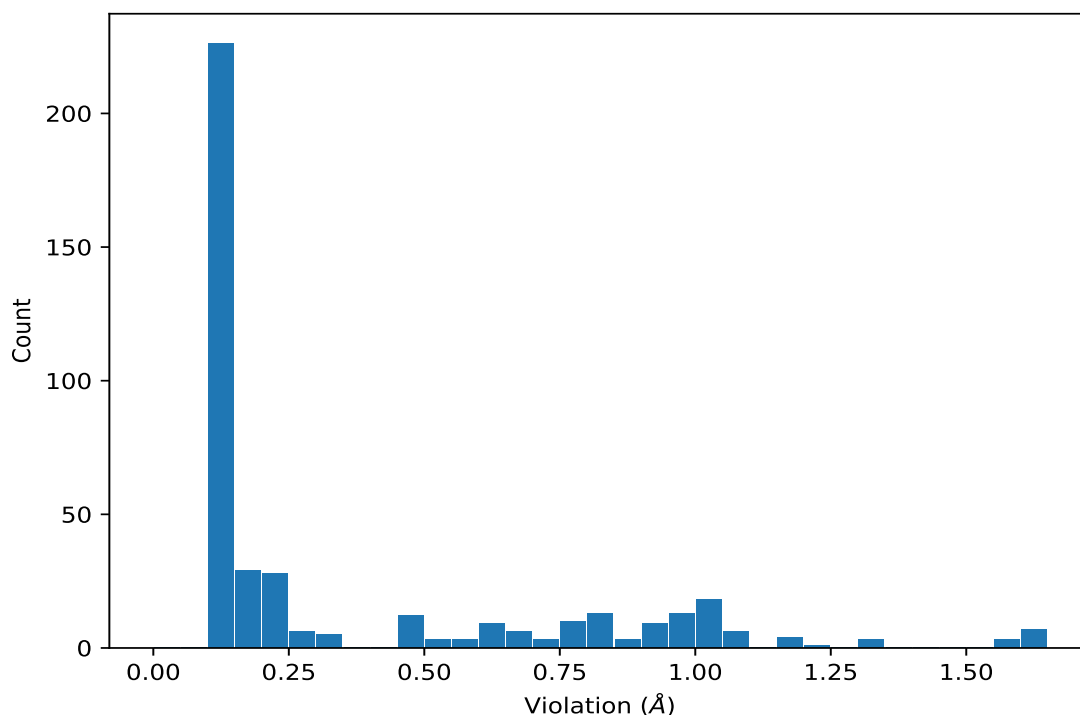
Key	Atom-1	Atom-2	Models ¹	Mean (Å)	SD ¹ (Å)	Median (Å)
(1,2897)	1:20:A:ALA:HB3	1:47:A:LYS:HE3	2	0.11	0.01	0.11

¹Number of violated models, ²Standard 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 lists the absolute value of the violation for each restraint in the ensemble sorted by its 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)
(1,1270)	1:21:A:GLY:HA2	1:78:A:LYS:HA	2	1.65
(1,1270)	1:21:A:GLY:HA2	1:78:A:LYS:HA	5	1.64
(1,1270)	1:21:A:GLY:HA2	1:78:A:LYS:HA	18	1.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1270)	1:21:A:GLY:HA2	1:78:A:LYS:HA	1	1.63
(1,1270)	1:21:A:GLY:HA2	1:78:A:LYS:HA	3	1.62
(1,1270)	1:21:A:GLY:HA2	1:78:A:LYS:HA	4	1.62
(1,1270)	1:21:A:GLY:HA2	1:78:A:LYS:HA	11	1.6
(1,1270)	1:21:A:GLY:HA2	1:78:A:LYS:HA	6	1.59
(1,1270)	1:21:A:GLY:HA2	1:78:A:LYS:HA	8	1.58
(1,1270)	1:21:A:GLY:HA2	1:78:A:LYS:HA	9	1.57
(1,1270)	1:21:A:GLY:HA2	1:78:A:LYS:HA	12	1.34
(1,1270)	1:21:A:GLY:HA2	1:78:A:LYS:HA	19	1.32
(1,1270)	1:21:A:GLY:HA2	1:78:A:LYS:HA	17	1.31
(1,1270)	1:21:A:GLY:HA2	1:78:A:LYS:HA	20	1.21
(1,1270)	1:21:A:GLY:HA2	1:78:A:LYS:HA	13	1.18
(1,1270)	1:21:A:GLY:HA2	1:78:A:LYS:HA	14	1.18
(1,1270)	1:21:A:GLY:HA2	1:78:A:LYS:HA	16	1.18
(1,1270)	1:21:A:GLY:HA2	1:78:A:LYS:HA	15	1.15
(1,2451)	1:21:A:GLY:HA2	1:78:A:LYS:H	1	1.07
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB1	4	1.07
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB2	4	1.07
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB3	4	1.07
(1,2451)	1:21:A:GLY:HA2	1:78:A:LYS:H	5	1.06
(1,2451)	1:21:A:GLY:HA2	1:78:A:LYS:H	3	1.05
(1,2451)	1:21:A:GLY:HA2	1:78:A:LYS:H	2	1.04
(1,2451)	1:21:A:GLY:HA2	1:78:A:LYS:H	4	1.04
(1,1270)	1:21:A:GLY:HA2	1:78:A:LYS:HA	7	1.04
(1,1270)	1:21:A:GLY:HA2	1:78:A:LYS:HA	10	1.04
(1,992)	1:52:A:GLY:HA2	1:70:A:VAL:HB	19	1.04
(1,2451)	1:21:A:GLY:HA2	1:78:A:LYS:H	17	1.02
(1,992)	1:52:A:GLY:HA2	1:70:A:VAL:HB	11	1.02
(1,992)	1:52:A:GLY:HA2	1:70:A:VAL:HB	14	1.02
(1,2451)	1:21:A:GLY:HA2	1:78:A:LYS:H	11	1.01
(1,992)	1:52:A:GLY:HA2	1:70:A:VAL:HB	6	1.01
(1,992)	1:52:A:GLY:HA2	1:70:A:VAL:HB	8	1.01
(1,2451)	1:21:A:GLY:HA2	1:78:A:LYS:H	8	1.0
(1,2451)	1:21:A:GLY:HA2	1:78:A:LYS:H	18	1.0
(1,992)	1:52:A:GLY:HA2	1:70:A:VAL:HB	4	1.0
(1,992)	1:52:A:GLY:HA2	1:70:A:VAL:HB	18	1.0
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB1	18	1.0
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB2	18	1.0
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB3	18	1.0
(1,992)	1:52:A:GLY:HA2	1:70:A:VAL:HB	5	0.99
(1,992)	1:52:A:GLY:HA2	1:70:A:VAL:HB	20	0.99
(1,992)	1:52:A:GLY:HA2	1:70:A:VAL:HB	1	0.98

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,992)	1:52:A:GLY:HA2	1:70:A:VAL:HB	3	0.98
(1,2451)	1:21:A:GLY:HA2	1:78:A:LYS:H	6	0.97
(1,992)	1:52:A:GLY:HA2	1:70:A:VAL:HB	2	0.97
(1,992)	1:52:A:GLY:HA2	1:70:A:VAL:HB	10	0.97
(1,2451)	1:21:A:GLY:HA2	1:78:A:LYS:H	19	0.96
(1,2451)	1:21:A:GLY:HA2	1:78:A:LYS:H	12	0.95
(1,2451)	1:21:A:GLY:HA2	1:78:A:LYS:H	13	0.95
(1,992)	1:52:A:GLY:HA2	1:70:A:VAL:HB	9	0.95
(1,992)	1:52:A:GLY:HA2	1:70:A:VAL:HB	16	0.95
(1,992)	1:52:A:GLY:HA2	1:70:A:VAL:HB	17	0.95
(1,2451)	1:21:A:GLY:HA2	1:78:A:LYS:H	14	0.94
(1,2451)	1:21:A:GLY:HA2	1:78:A:LYS:H	16	0.94
(1,2451)	1:21:A:GLY:HA2	1:78:A:LYS:H	20	0.94
(1,992)	1:52:A:GLY:HA2	1:70:A:VAL:HB	13	0.94
(1,2451)	1:21:A:GLY:HA2	1:78:A:LYS:H	9	0.93
(1,992)	1:52:A:GLY:HA2	1:70:A:VAL:HB	7	0.93
(1,992)	1:52:A:GLY:HA2	1:70:A:VAL:HB	15	0.93
(1,992)	1:52:A:GLY:HA2	1:70:A:VAL:HB	12	0.92
(1,2451)	1:21:A:GLY:HA2	1:78:A:LYS:H	15	0.91
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB1	10	0.85
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB2	10	0.85
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB3	10	0.85
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB1	1	0.84
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB2	1	0.84
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB3	1	0.84
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB1	9	0.84
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB2	9	0.84
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB3	9	0.84
(1,2451)	1:21:A:GLY:HA2	1:78:A:LYS:H	10	0.83
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB1	6	0.82
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB2	6	0.82
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB3	6	0.82
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB1	19	0.81
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB2	19	0.81
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB3	19	0.81
(1,2451)	1:21:A:GLY:HA2	1:78:A:LYS:H	7	0.79
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB1	7	0.79
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB2	7	0.79
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB3	7	0.79
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB1	11	0.79
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB2	11	0.79
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB3	11	0.79

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB1	20	0.76
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB2	20	0.76
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB3	20	0.76
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB1	12	0.71
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB2	12	0.71
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB3	12	0.71
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB1	17	0.69
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB2	17	0.69
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB3	17	0.69
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB1	16	0.66
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB2	16	0.66
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB3	16	0.66
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB1	8	0.63
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB2	8	0.63
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB3	8	0.63
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB1	14	0.63
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB2	14	0.63
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB3	14	0.63
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB1	13	0.6
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB2	13	0.6
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB3	13	0.6
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB1	5	0.55
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB2	5	0.55
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB3	5	0.55
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB1	2	0.5
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB2	2	0.5
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB3	2	0.5
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB1	3	0.48
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB2	3	0.48
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB3	3	0.48
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB1	15	0.47
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB2	15	0.47
(1,247)	1:34:A:GLY:HA3	1:123:A:ALA:HB3	15	0.47
(1,301)	1:121:A:THR:HA	1:121:A:THR:HG21	14	0.46
(1,301)	1:121:A:THR:HA	1:121:A:THR:HG22	14	0.46
(1,301)	1:121:A:THR:HA	1:121:A:THR:HG23	14	0.46
(1,301)	1:121:A:THR:HA	1:121:A:THR:HG21	16	0.46
(1,301)	1:121:A:THR:HA	1:121:A:THR:HG22	16	0.46
(1,301)	1:121:A:THR:HA	1:121:A:THR:HG23	16	0.46
(1,2367)	1:10:A:SER:HA	1:11:A:LEU:H	8	0.31
(1,2366)	1:10:A:SER:HB2	1:11:A:LEU:H	5	0.31
(1,2366)	1:10:A:SER:HB3	1:11:A:LEU:H	5	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2366)	1:10:A:SER:HB2	1:11:A:LEU:H	8	0.3
(1,2366)	1:10:A:SER:HB3	1:11:A:LEU:H	8	0.3
(1,2367)	1:10:A:SER:HA	1:11:A:LEU:H	5	0.29
(1,990)	1:52:A:GLY:HA2	1:53:A:ARG:HB2	9	0.26
(1,990)	1:52:A:GLY:HA2	1:53:A:ARG:HB2	3	0.25
(1,990)	1:52:A:GLY:HA2	1:53:A:ARG:HB2	7	0.25
(1,990)	1:52:A:GLY:HA2	1:53:A:ARG:HB2	13	0.25
(1,990)	1:52:A:GLY:HA2	1:53:A:ARG:HB2	16	0.25
(1,990)	1:52:A:GLY:HA2	1:53:A:ARG:HB2	1	0.24
(1,990)	1:52:A:GLY:HA2	1:53:A:ARG:HB2	2	0.24
(1,990)	1:52:A:GLY:HA2	1:53:A:ARG:HB2	5	0.24
(1,990)	1:52:A:GLY:HA2	1:53:A:ARG:HB2	12	0.24
(1,990)	1:52:A:GLY:HA2	1:53:A:ARG:HB2	15	0.24
(1,990)	1:52:A:GLY:HA2	1:53:A:ARG:HB2	17	0.24
(1,973)	1:21:A:GLY:HA3	1:22:A:LYS:HA	10	0.24
(1,990)	1:52:A:GLY:HA2	1:53:A:ARG:HB2	4	0.23
(1,990)	1:52:A:GLY:HA2	1:53:A:ARG:HB2	11	0.23
(1,3343)	1:105:A:LYS:HG2	1:106:A:PRO:HD3	13	0.22
(1,3343)	1:105:A:LYS:HG3	1:106:A:PRO:HD3	13	0.22
(1,990)	1:52:A:GLY:HA2	1:53:A:ARG:HB2	6	0.22
(1,990)	1:52:A:GLY:HA2	1:53:A:ARG:HB2	14	0.22
(1,990)	1:52:A:GLY:HA2	1:53:A:ARG:HB2	18	0.22
(1,990)	1:52:A:GLY:HA2	1:53:A:ARG:HB2	20	0.22
(1,973)	1:21:A:GLY:HA3	1:22:A:LYS:HA	7	0.22
(1,973)	1:21:A:GLY:HA3	1:22:A:LYS:HA	17	0.22
(1,3342)	1:105:A:LYS:HG2	1:105:A:LYS:HE2	20	0.21
(1,3342)	1:105:A:LYS:HG2	1:105:A:LYS:HE3	20	0.21
(1,3342)	1:105:A:LYS:HG3	1:105:A:LYS:HE2	20	0.21
(1,3342)	1:105:A:LYS:HG3	1:105:A:LYS:HE3	20	0.21
(1,2859)	1:11:A:LEU:HB2	1:11:A:LEU:HG	4	0.21
(1,2859)	1:11:A:LEU:HB3	1:11:A:LEU:HG	4	0.21
(1,990)	1:52:A:GLY:HA2	1:53:A:ARG:HB2	19	0.21
(1,990)	1:52:A:GLY:HA2	1:53:A:ARG:HB2	10	0.2
(1,973)	1:21:A:GLY:HA3	1:22:A:LYS:HA	14	0.2
(1,973)	1:21:A:GLY:HA3	1:22:A:LYS:HA	16	0.2
(1,633)	1:67:A:CYS:HB2	1:71:A:HIS:HE1	8	0.2
(1,973)	1:21:A:GLY:HA3	1:22:A:LYS:HA	13	0.19
(1,973)	1:21:A:GLY:HA3	1:22:A:LYS:HA	15	0.19
(1,973)	1:21:A:GLY:HA3	1:22:A:LYS:HA	19	0.19
(1,2210)	1:102:A:GLU:H	1:105:A:LYS:HE2	13	0.18
(1,2210)	1:102:A:GLU:H	1:105:A:LYS:HE3	13	0.18
(1,973)	1:21:A:GLY:HA3	1:22:A:LYS:HA	12	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,973)	1:21:A:GLY:HA3	1:22:A:LYS:HA	20	0.18
(1,3337)	1:105:A:LYS:HA	1:105:A:LYS:HD2	10	0.17
(1,3337)	1:105:A:LYS:HA	1:105:A:LYS:HD3	10	0.17
(1,3336)	1:105:A:LYS:H	1:105:A:LYS:HD2	11	0.17
(1,3336)	1:105:A:LYS:H	1:105:A:LYS:HD3	11	0.17
(1,3061)	1:47:A:LYS:HD2	1:48:A:TYR:H	17	0.17
(1,3061)	1:47:A:LYS:HD3	1:48:A:TYR:H	17	0.17
(1,990)	1:52:A:GLY:HA2	1:53:A:ARG:HB2	8	0.17
(1,856)	1:94:A:THR:HG21	1:101:A:LEU:HB3	17	0.17
(1,856)	1:94:A:THR:HG22	1:101:A:LEU:HB3	17	0.17
(1,856)	1:94:A:THR:HG23	1:101:A:LEU:HB3	17	0.17
(1,633)	1:67:A:CYS:HB2	1:71:A:HIS:HE1	18	0.17
(1,3337)	1:105:A:LYS:HA	1:105:A:LYS:HD2	20	0.15
(1,3337)	1:105:A:LYS:HA	1:105:A:LYS:HD3	20	0.15
(1,3056)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	10	0.15
(1,3056)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	10	0.15
(1,3056)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	10	0.15
(1,3056)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	10	0.15
(1,1303)	1:52:A:GLY:HA2	1:61:A:THR:HA	2	0.15
(1,1303)	1:52:A:GLY:HA2	1:61:A:THR:HA	3	0.15
(1,856)	1:94:A:THR:HG21	1:101:A:LEU:HB3	7	0.15
(1,856)	1:94:A:THR:HG22	1:101:A:LEU:HB3	7	0.15
(1,856)	1:94:A:THR:HG23	1:101:A:LEU:HB3	7	0.15
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD11	19	0.14
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD12	19	0.14
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD13	19	0.14
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD21	19	0.14
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD22	19	0.14
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD23	19	0.14
(1,3056)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	17	0.14
(1,3056)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	17	0.14
(1,3056)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	17	0.14
(1,3056)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	17	0.14
(1,2905)	1:22:A:LYS:HG2	1:23:A:PRO:HA	4	0.14
(1,2905)	1:22:A:LYS:HG3	1:23:A:PRO:HA	4	0.14
(1,1752)	1:29:A:LEU:H	1:29:A:LEU:HG	11	0.14
(1,1303)	1:52:A:GLY:HA2	1:61:A:THR:HA	9	0.14
(1,1303)	1:52:A:GLY:HA2	1:61:A:THR:HA	13	0.14
(1,1303)	1:52:A:GLY:HA2	1:61:A:THR:HA	14	0.14
(1,1303)	1:52:A:GLY:HA2	1:61:A:THR:HA	17	0.14
(1,1303)	1:52:A:GLY:HA2	1:61:A:THR:HA	18	0.14
(1,856)	1:94:A:THR:HG21	1:101:A:LEU:HB3	4	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,856)	1:94:A:THR:HG22	1:101:A:LEU:HB3	4	0.14
(1,856)	1:94:A:THR:HG23	1:101:A:LEU:HB3	4	0.14
(1,856)	1:94:A:THR:HG21	1:101:A:LEU:HB3	6	0.14
(1,856)	1:94:A:THR:HG22	1:101:A:LEU:HB3	6	0.14
(1,856)	1:94:A:THR:HG23	1:101:A:LEU:HB3	6	0.14
(1,856)	1:94:A:THR:HG21	1:101:A:LEU:HB3	9	0.14
(1,856)	1:94:A:THR:HG22	1:101:A:LEU:HB3	9	0.14
(1,856)	1:94:A:THR:HG23	1:101:A:LEU:HB3	9	0.14
(1,856)	1:94:A:THR:HG21	1:101:A:LEU:HB3	12	0.14
(1,856)	1:94:A:THR:HG22	1:101:A:LEU:HB3	12	0.14
(1,856)	1:94:A:THR:HG23	1:101:A:LEU:HB3	12	0.14
(1,856)	1:94:A:THR:HG21	1:101:A:LEU:HB3	13	0.14
(1,856)	1:94:A:THR:HG22	1:101:A:LEU:HB3	13	0.14
(1,856)	1:94:A:THR:HG23	1:101:A:LEU:HB3	13	0.14
(1,856)	1:94:A:THR:HG21	1:101:A:LEU:HB3	18	0.14
(1,856)	1:94:A:THR:HG22	1:101:A:LEU:HB3	18	0.14
(1,856)	1:94:A:THR:HG23	1:101:A:LEU:HB3	18	0.14
(1,633)	1:67:A:CYS:HB2	1:71:A:HIS:HE1	6	0.14
(1,3056)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	18	0.13
(1,3056)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	18	0.13
(1,3056)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	18	0.13
(1,3056)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	18	0.13
(1,2203)	1:67:A:CYS:H	1:71:A:HIS:HE1	15	0.13
(1,922)	1:105:A:LYS:HA	1:105:A:LYS:HE2	19	0.13
(1,922)	1:105:A:LYS:HA	1:105:A:LYS:HE3	19	0.13
(1,633)	1:67:A:CYS:HB2	1:71:A:HIS:HE1	4	0.13
(1,633)	1:67:A:CYS:HB2	1:71:A:HIS:HE1	20	0.13
(1,191)	1:62:A:ILE:HG21	1:63:A:ASP:H	19	0.13
(1,191)	1:62:A:ILE:HG22	1:63:A:ASP:H	19	0.13
(1,191)	1:62:A:ILE:HG23	1:63:A:ASP:H	19	0.13
(1,3359)	1:112:A:ASP:HB2	1:113:A:SER:H	4	0.12
(1,3359)	1:112:A:ASP:HB3	1:113:A:SER:H	4	0.12
(1,3056)	1:47:A:LYS:HB2	1:47:A:LYS:HE2	6	0.12
(1,3056)	1:47:A:LYS:HB2	1:47:A:LYS:HE3	6	0.12
(1,3056)	1:47:A:LYS:HB3	1:47:A:LYS:HE2	6	0.12
(1,3056)	1:47:A:LYS:HB3	1:47:A:LYS:HE3	6	0.12
(1,2897)	1:20:A:ALA:HB1	1:47:A:LYS:HE2	18	0.12
(1,2897)	1:20:A:ALA:HB1	1:47:A:LYS:HE3	18	0.12
(1,2897)	1:20:A:ALA:HB2	1:47:A:LYS:HE2	18	0.12
(1,2897)	1:20:A:ALA:HB2	1:47:A:LYS:HE3	18	0.12
(1,2897)	1:20:A:ALA:HB3	1:47:A:LYS:HE2	18	0.12
(1,2897)	1:20:A:ALA:HB3	1:47:A:LYS:HE3	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2203)	1:67:A:CYS:H	1:71:A:HIS:HE1	9	0.12
(1,2133)	1:64:A:HIS:H	1:66:A:SER:H	15	0.12
(1,2133)	1:64:A:HIS:H	1:66:A:SER:H	17	0.12
(1,2057)	1:94:A:THR:H	1:95:A:PHE:HB2	2	0.12
(1,2057)	1:94:A:THR:H	1:95:A:PHE:HB3	2	0.12
(1,1752)	1:29:A:LEU:H	1:29:A:LEU:HG	3	0.12
(1,1752)	1:29:A:LEU:H	1:29:A:LEU:HG	13	0.12
(1,1752)	1:29:A:LEU:H	1:29:A:LEU:HG	19	0.12
(1,1580)	1:107:A:GLN:H	1:107:A:GLN:HE21	3	0.12
(1,1580)	1:107:A:GLN:H	1:107:A:GLN:HE21	5	0.12
(1,1580)	1:107:A:GLN:H	1:107:A:GLN:HE21	6	0.12
(1,1580)	1:107:A:GLN:H	1:107:A:GLN:HE21	7	0.12
(1,1580)	1:107:A:GLN:H	1:107:A:GLN:HE21	8	0.12
(1,1580)	1:107:A:GLN:H	1:107:A:GLN:HE21	9	0.12
(1,1580)	1:107:A:GLN:H	1:107:A:GLN:HE21	10	0.12
(1,1580)	1:107:A:GLN:H	1:107:A:GLN:HE21	12	0.12
(1,1580)	1:107:A:GLN:H	1:107:A:GLN:HE21	17	0.12
(1,1580)	1:107:A:GLN:H	1:107:A:GLN:HE21	18	0.12
(1,1303)	1:52:A:GLY:HA2	1:61:A:THR:HA	5	0.12
(1,1303)	1:52:A:GLY:HA2	1:61:A:THR:HA	7	0.12
(1,856)	1:94:A:THR:HG21	1:101:A:LEU:HB3	8	0.12
(1,856)	1:94:A:THR:HG22	1:101:A:LEU:HB3	8	0.12
(1,856)	1:94:A:THR:HG23	1:101:A:LEU:HB3	8	0.12
(1,633)	1:67:A:CYS:HB2	1:71:A:HIS:HE1	14	0.12
(1,547)	1:24:A:PRO:HG2	1:27:A:LEU:H	14	0.12
(1,547)	1:24:A:PRO:HG3	1:27:A:LEU:H	14	0.12
(1,512)	1:88:A:LEU:HD11	1:89:A:ASN:H	16	0.12
(1,512)	1:88:A:LEU:HD12	1:89:A:ASN:H	16	0.12
(1,512)	1:88:A:LEU:HD13	1:89:A:ASN:H	16	0.12
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD11	3	0.12
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD12	3	0.12
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD13	3	0.12
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD11	8	0.12
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD12	8	0.12
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD13	8	0.12
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD11	3	0.11
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD12	3	0.11
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD13	3	0.11
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD21	3	0.11
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD22	3	0.11
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD23	3	0.11
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD11	10	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD12	10	0.11
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD13	10	0.11
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD21	10	0.11
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD22	10	0.11
(1,3080)	1:50:A:LEU:HB3	1:88:A:LEU:HD23	10	0.11
(1,2905)	1:22:A:LYS:HG2	1:23:A:PRO:HA	1	0.11
(1,2905)	1:22:A:LYS:HG3	1:23:A:PRO:HA	1	0.11
(1,2712)	1:48:A:TYR:HA	1:48:A:TYR:HE1	17	0.11
(1,2712)	1:48:A:TYR:HA	1:48:A:TYR:HE2	17	0.11
(1,2694)	1:71:A:HIS:HE2	1:90:A:SER:H	6	0.11
(1,2384)	1:84:A:PHE:HB2	1:109:A:ILE:H	7	0.11
(1,2203)	1:67:A:CYS:H	1:71:A:HIS:HE1	3	0.11
(1,2203)	1:67:A:CYS:H	1:71:A:HIS:HE1	5	0.11
(1,2133)	1:64:A:HIS:H	1:66:A:SER:H	5	0.11
(1,2133)	1:64:A:HIS:H	1:66:A:SER:H	16	0.11
(1,2055)	1:94:A:THR:H	1:101:A:LEU:HB3	20	0.11
(1,1818)	1:89:A:ASN:H	1:89:A:ASN:HB2	9	0.11
(1,1580)	1:107:A:GLN:H	1:107:A:GLN:HE21	1	0.11
(1,1580)	1:107:A:GLN:H	1:107:A:GLN:HE21	4	0.11
(1,1580)	1:107:A:GLN:H	1:107:A:GLN:HE21	11	0.11
(1,1580)	1:107:A:GLN:H	1:107:A:GLN:HE21	13	0.11
(1,1580)	1:107:A:GLN:H	1:107:A:GLN:HE21	14	0.11
(1,1580)	1:107:A:GLN:H	1:107:A:GLN:HE21	15	0.11
(1,1580)	1:107:A:GLN:H	1:107:A:GLN:HE21	16	0.11
(1,1580)	1:107:A:GLN:H	1:107:A:GLN:HE21	20	0.11
(1,1369)	1:60:A:PHE:HB3	1:61:A:THR:HB	2	0.11
(1,1369)	1:60:A:PHE:HB3	1:61:A:THR:HB	3	0.11
(1,1369)	1:60:A:PHE:HB3	1:61:A:THR:HB	8	0.11
(1,1369)	1:60:A:PHE:HB3	1:61:A:THR:HB	10	0.11
(1,1369)	1:60:A:PHE:HB3	1:61:A:THR:HB	19	0.11
(1,1369)	1:60:A:PHE:HB3	1:61:A:THR:HB	20	0.11
(1,1303)	1:52:A:GLY:HA2	1:61:A:THR:HA	15	0.11
(1,1303)	1:52:A:GLY:HA2	1:61:A:THR:HA	20	0.11
(1,856)	1:94:A:THR:HG21	1:101:A:LEU:HB3	11	0.11
(1,856)	1:94:A:THR:HG22	1:101:A:LEU:HB3	11	0.11
(1,856)	1:94:A:THR:HG23	1:101:A:LEU:HB3	11	0.11
(1,856)	1:94:A:THR:HG21	1:101:A:LEU:HB3	20	0.11
(1,856)	1:94:A:THR:HG22	1:101:A:LEU:HB3	20	0.11
(1,856)	1:94:A:THR:HG23	1:101:A:LEU:HB3	20	0.11
(1,748)	1:22:A:LYS:H	1:78:A:LYS:HB2	12	0.11
(1,665)	1:57:A:LEU:H	1:58:A:CYS:HB3	15	0.11
(1,382)	1:72:A:ALA:HB1	1:94:A:THR:HB	17	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,382)	1:72:A:ALA:HB2	1:94:A:THR:HB	17	0.11
(1,382)	1:72:A:ALA:HB3	1:94:A:THR:HB	17	0.11
(1,191)	1:62:A:ILE:HG21	1:63:A:ASP:H	6	0.11
(1,191)	1:62:A:ILE:HG22	1:63:A:ASP:H	6	0.11
(1,191)	1:62:A:ILE:HG23	1:63:A:ASP:H	6	0.11
(1,191)	1:62:A:ILE:HG21	1:63:A:ASP:H	20	0.11
(1,191)	1:62:A:ILE:HG22	1:63:A:ASP:H	20	0.11
(1,191)	1:62:A:ILE:HG23	1:63:A:ASP:H	20	0.11
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD11	14	0.11
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD12	14	0.11
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD13	14	0.11
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD11	18	0.11
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD12	18	0.11
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD13	18	0.11
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD11	20	0.11
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD12	20	0.11
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD13	20	0.11
(1,3345)	1:105:A:LYS:HD2	1:106:A:PRO:HD2	20	0.1
(1,3345)	1:105:A:LYS:HD3	1:106:A:PRO:HD2	20	0.1
(1,3329)	1:102:A:GLU:HG2	1:105:A:LYS:H	18	0.1
(1,3329)	1:102:A:GLU:HG3	1:105:A:LYS:H	18	0.1
(1,3086)	1:50:A:LEU:HD11	1:70:A:VAL:H	2	0.1
(1,3086)	1:50:A:LEU:HD12	1:70:A:VAL:H	2	0.1
(1,3086)	1:50:A:LEU:HD13	1:70:A:VAL:H	2	0.1
(1,3086)	1:50:A:LEU:HD21	1:70:A:VAL:H	2	0.1
(1,3086)	1:50:A:LEU:HD22	1:70:A:VAL:H	2	0.1
(1,3086)	1:50:A:LEU:HD23	1:70:A:VAL:H	2	0.1
(1,3086)	1:50:A:LEU:HD11	1:70:A:VAL:H	16	0.1
(1,3086)	1:50:A:LEU:HD12	1:70:A:VAL:H	16	0.1
(1,3086)	1:50:A:LEU:HD13	1:70:A:VAL:H	16	0.1
(1,3086)	1:50:A:LEU:HD21	1:70:A:VAL:H	16	0.1
(1,3086)	1:50:A:LEU:HD22	1:70:A:VAL:H	16	0.1
(1,3086)	1:50:A:LEU:HD23	1:70:A:VAL:H	16	0.1
(1,3086)	1:50:A:LEU:HD11	1:70:A:VAL:H	17	0.1
(1,3086)	1:50:A:LEU:HD12	1:70:A:VAL:H	17	0.1
(1,3086)	1:50:A:LEU:HD13	1:70:A:VAL:H	17	0.1
(1,3086)	1:50:A:LEU:HD21	1:70:A:VAL:H	17	0.1
(1,3086)	1:50:A:LEU:HD22	1:70:A:VAL:H	17	0.1
(1,3086)	1:50:A:LEU:HD23	1:70:A:VAL:H	17	0.1
(1,2897)	1:20:A:ALA:HB1	1:47:A:LYS:HE2	6	0.1
(1,2897)	1:20:A:ALA:HB1	1:47:A:LYS:HE3	6	0.1
(1,2897)	1:20:A:ALA:HB2	1:47:A:LYS:HE2	6	0.1

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2897)	1:20:A:ALA:HB2	1:47:A:LYS:HE3	6	0.1
(1,2897)	1:20:A:ALA:HB3	1:47:A:LYS:HE2	6	0.1
(1,2897)	1:20:A:ALA:HB3	1:47:A:LYS:HE3	6	0.1
(1,2203)	1:67:A:CYS:H	1:71:A:HIS:HE1	17	0.1
(1,2133)	1:64:A:HIS:H	1:66:A:SER:H	13	0.1
(1,1818)	1:89:A:ASN:H	1:89:A:ASN:HB2	6	0.1
(1,1818)	1:89:A:ASN:H	1:89:A:ASN:HB2	11	0.1
(1,1471)	1:62:A:ILE:HB	1:120:A:SER:H	8	0.1
(1,1369)	1:60:A:PHE:HB3	1:61:A:THR:HB	4	0.1
(1,1369)	1:60:A:PHE:HB3	1:61:A:THR:HB	9	0.1
(1,1369)	1:60:A:PHE:HB3	1:61:A:THR:HB	11	0.1
(1,1369)	1:60:A:PHE:HB3	1:61:A:THR:HB	12	0.1
(1,1369)	1:60:A:PHE:HB3	1:61:A:THR:HB	13	0.1
(1,1369)	1:60:A:PHE:HB3	1:61:A:THR:HB	14	0.1
(1,1369)	1:60:A:PHE:HB3	1:61:A:THR:HB	18	0.1
(1,1303)	1:52:A:GLY:HA2	1:61:A:THR:HA	8	0.1
(1,1247)	1:47:A:LYS:HA	1:47:A:LYS:HE3	17	0.1
(1,856)	1:94:A:THR:HG21	1:101:A:LEU:HB3	2	0.1
(1,856)	1:94:A:THR:HG22	1:101:A:LEU:HB3	2	0.1
(1,856)	1:94:A:THR:HG23	1:101:A:LEU:HB3	2	0.1
(1,633)	1:67:A:CYS:HB2	1:71:A:HIS:HE1	10	0.1
(1,633)	1:67:A:CYS:HB2	1:71:A:HIS:HE1	11	0.1
(1,633)	1:67:A:CYS:HB2	1:71:A:HIS:HE1	12	0.1
(1,633)	1:67:A:CYS:HB2	1:71:A:HIS:HE1	19	0.1
(1,630)	1:62:A:ILE:HG12	1:67:A:CYS:HB2	8	0.1
(1,547)	1:24:A:PRO:HG2	1:27:A:LEU:H	13	0.1
(1,547)	1:24:A:PRO:HG3	1:27:A:LEU:H	13	0.1
(1,191)	1:62:A:ILE:HG21	1:63:A:ASP:H	14	0.1
(1,191)	1:62:A:ILE:HG22	1:63:A:ASP:H	14	0.1
(1,191)	1:62:A:ILE:HG23	1:63:A:ASP:H	14	0.1
(1,191)	1:62:A:ILE:HG21	1:63:A:ASP:H	18	0.1
(1,191)	1:62:A:ILE:HG22	1:63:A:ASP:H	18	0.1
(1,191)	1:62:A:ILE:HG23	1:63:A:ASP:H	18	0.1
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD11	4	0.1
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD12	4	0.1
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD13	4	0.1
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD11	5	0.1
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD12	5	0.1
(1,49)	1:52:A:GLY:HA3	1:62:A:ILE:HD13	5	0.1

10 Dihedral-angle violation analysis

No dihedral-angle restraints found