Full wwPDB NMR Structure Validation Report (i)

Nov 11, 2026 – 12:24 PM JST

PDB ID	:	45SA / pdb_000045sa
BMRB ID	:	36876
Title	:	NMR structure of FgEC91
Authors	:	Kumeta, H.
Deposited on	:	2026-09-08

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

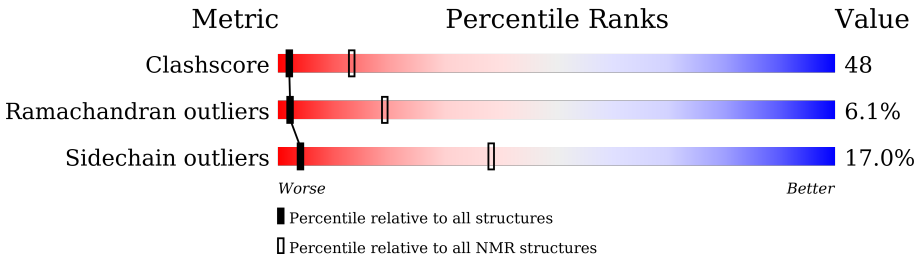
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4-5-2 with Phenix2.2
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.3.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	136	36% 49% 6% 10%

2 Ensemble composition and analysis

This entry contains 20 models. Model 19 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *target function*.

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:2-A:106, A:112-A:129 (123)	0.93	19

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

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

The models can be grouped into 4 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2024 atoms, of which 999 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Chromosome 3, complete genome.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	136	2024	640	999	179	199	7	0

There are 9 discrepancies between the modelled and reference sequences:

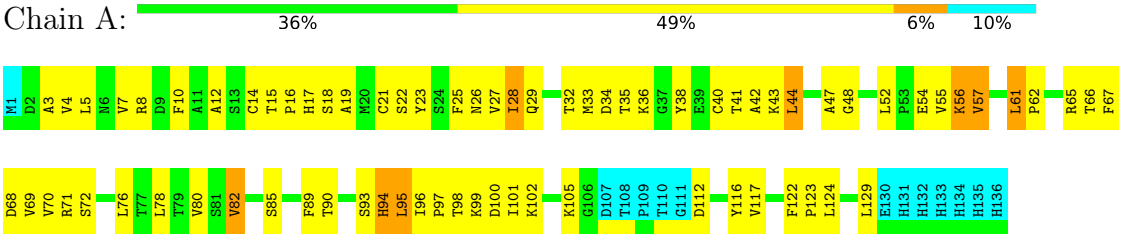
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP I1RLE5
A	129	LEU	-	expression tag	UNP I1RLE5
A	130	GLU	-	expression tag	UNP I1RLE5
A	131	HIS	-	expression tag	UNP I1RLE5
A	132	HIS	-	expression tag	UNP I1RLE5
A	133	HIS	-	expression tag	UNP I1RLE5
A	134	HIS	-	expression tag	UNP I1RLE5
A	135	HIS	-	expression tag	UNP I1RLE5
A	136	HIS	-	expression tag	UNP I1RLE5

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: Chromosome 3, complete genome

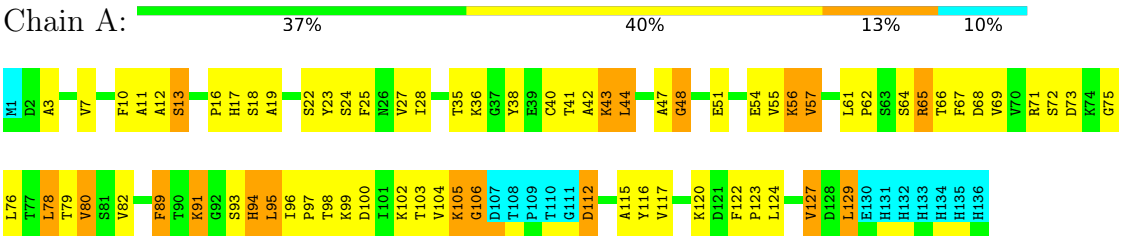


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

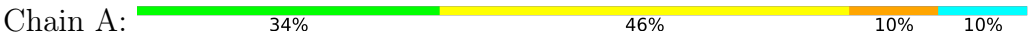
4.2.1 Score per residue for model 1

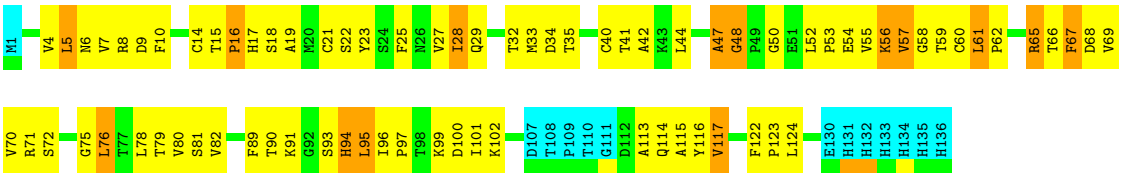
• Molecule 1: Chromosome 3, complete genome



4.2.2 Score per residue for model 2

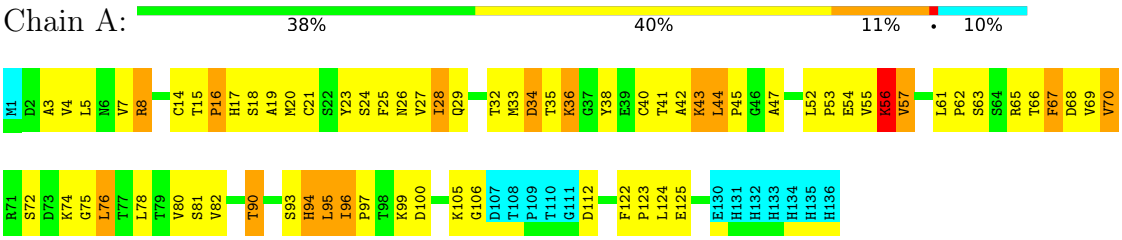
• Molecule 1: Chromosome 3, complete genome





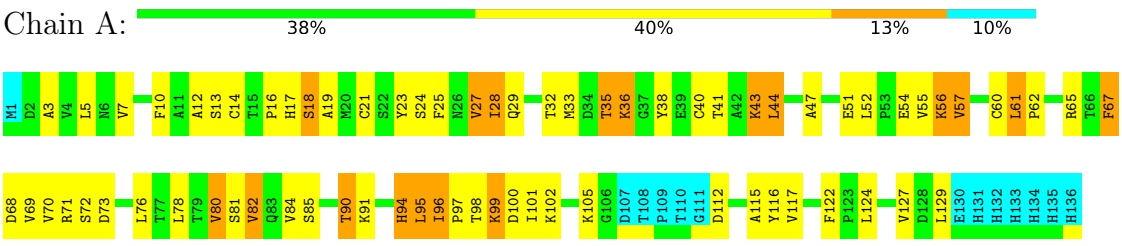
4.2.3 Score per residue for model 3

• Molecule 1: Chromosome 3, complete genome



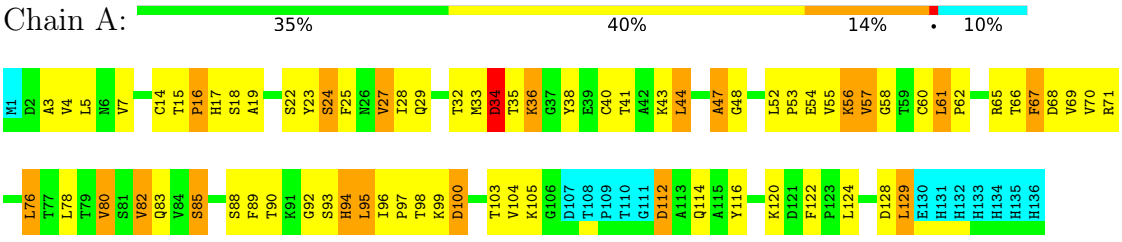
4.2.4 Score per residue for model 4

• Molecule 1: Chromosome 3, complete genome



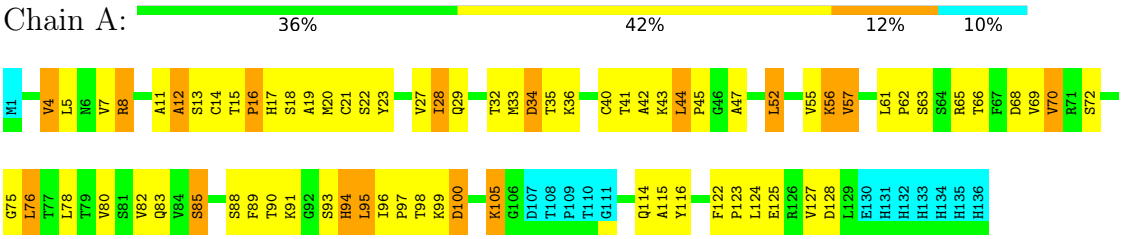
4.2.5 Score per residue for model 5

• Molecule 1: Chromosome 3, complete genome



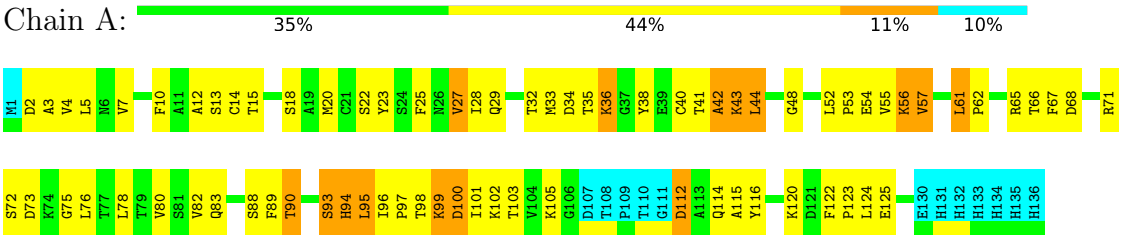
4.2.6 Score per residue for model 6

• Molecule 1: Chromosome 3, complete genome



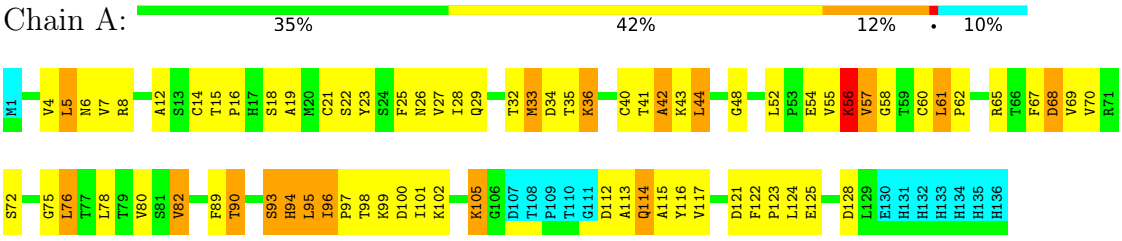
4.2.7 Score per residue for model 7

• Molecule 1: Chromosome 3, complete genome



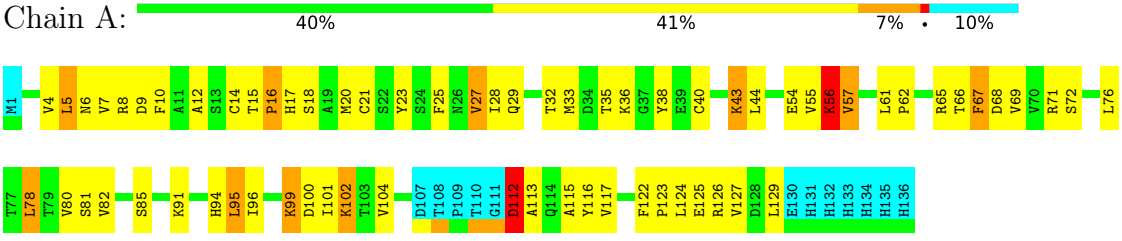
4.2.8 Score per residue for model 8

• Molecule 1: Chromosome 3, complete genome



4.2.9 Score per residue for model 9

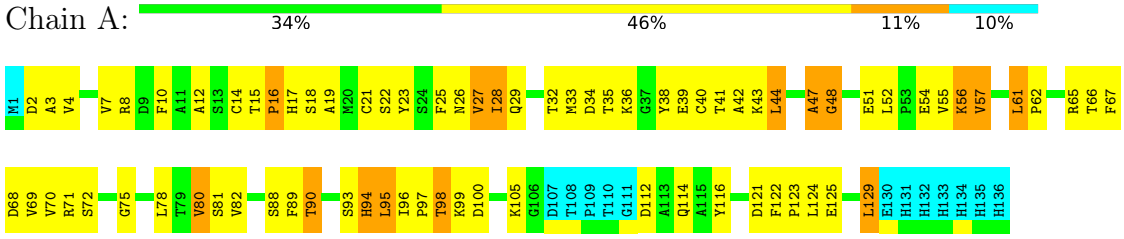
• Molecule 1: Chromosome 3, complete genome



4.2.10 Score per residue for model 10

• Molecule 1: Chromosome 3, complete genome

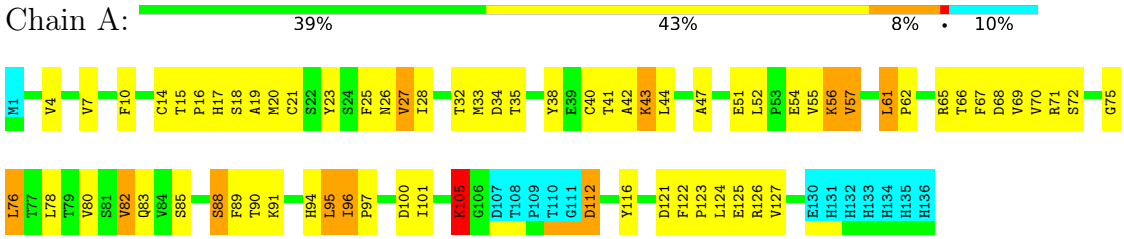
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Chromosome 3, complete genome

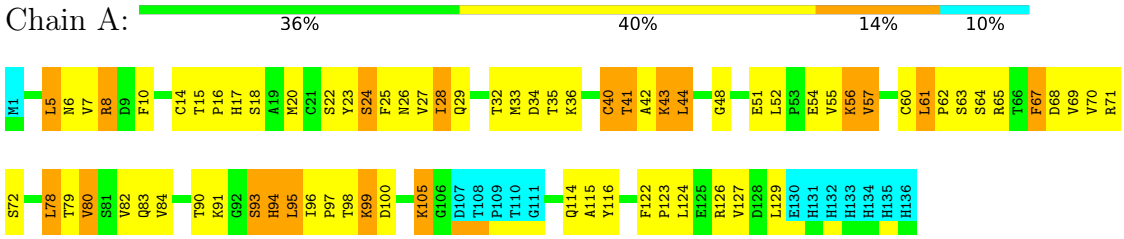
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Chromosome 3, complete genome

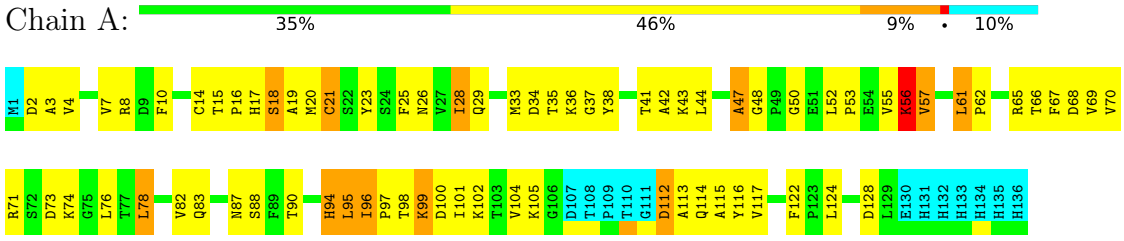
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Chromosome 3, complete genome

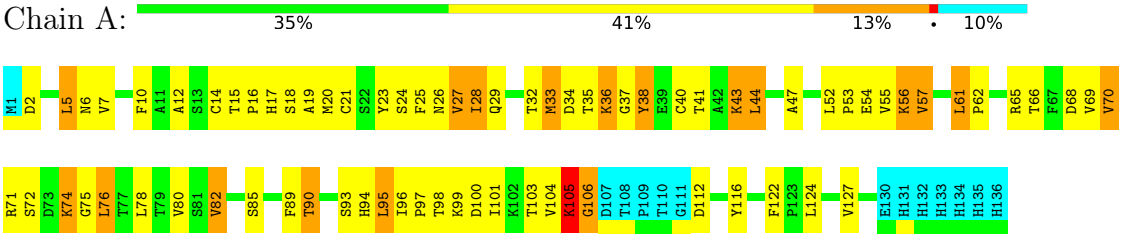
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Chromosome 3, complete genome

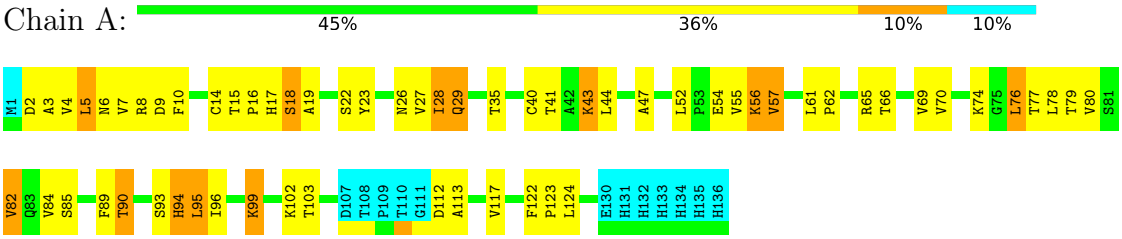
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Chromosome 3, complete genome

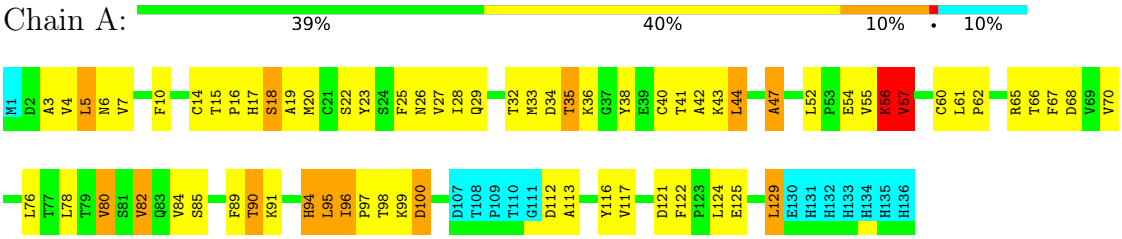
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Chromosome 3, complete genome

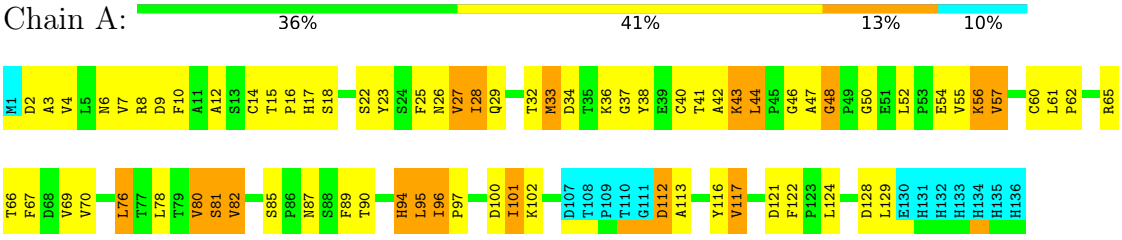
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Chromosome 3, complete genome

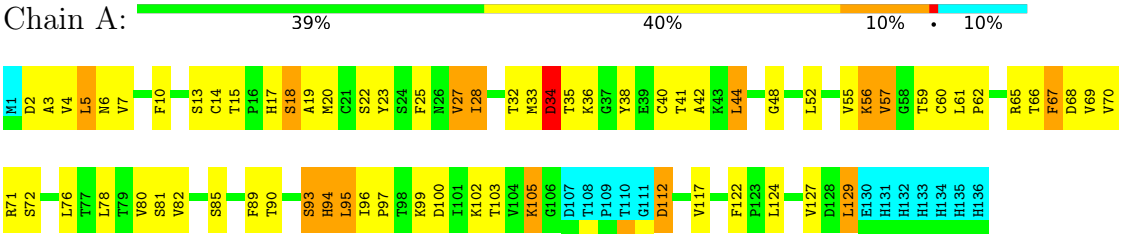
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Chromosome 3, complete genome

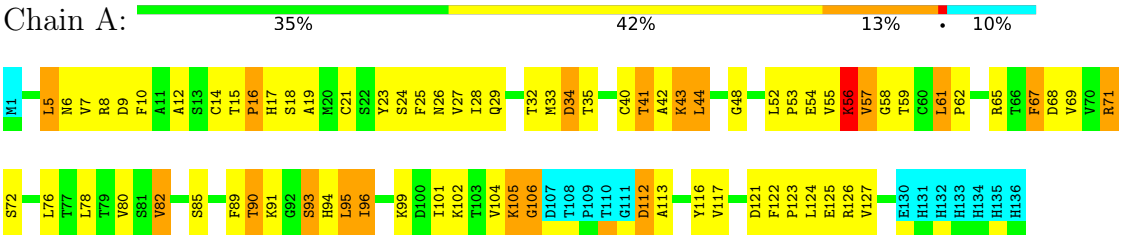
Chain A:



4.2.19 Score per residue for model 19 (medoid)

• Molecule 1: Chromosome 3, complete genome

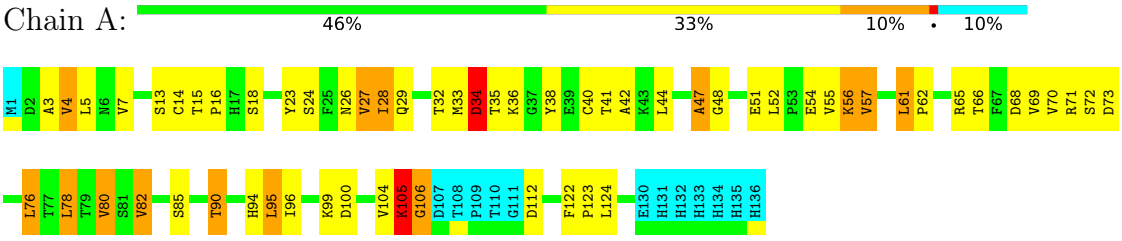
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Chromosome 3, complete genome

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing*.

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
CYANA	structure calculation	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	1540
Number of shifts mapped to atoms	1540
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

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	915	912	912	88±7
All	All	18300	18240	18240	1763

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 48.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:94:HIS:CE1	1:A:96:ILE:HD11	1.08	1.84	6	20
1:A:5:LEU:HD11	1:A:27:VAL:HG23	1.01	1.27	9	1
1:A:67:PHE:CE2	1:A:80:VAL:HG22	1.00	1.90	7	1
1:A:67:PHE:CE2	1:A:78:LEU:HD11	0.96	1.96	12	2
1:A:96:ILE:HG22	1:A:100:ASP:OD2	0.89	1.65	16	2
1:A:70:VAL:O	1:A:76:LEU:HD23	0.88	1.67	2	7
1:A:122:PHE:CE1	1:A:124:LEU:HD11	0.87	2.04	2	7
1:A:23:TYR:CE1	1:A:55:VAL:HG22	0.87	2.05	3	10
1:A:95:LEU:HD13	1:A:95:LEU:O	0.87	1.70	15	10
1:A:23:TYR:CZ	1:A:52:LEU:HD23	0.87	2.04	10	3
1:A:65:ARG:NH2	1:A:82:VAL:HG13	0.86	1.85	9	2
1:A:65:ARG:HH11	1:A:82:VAL:HG13	0.86	1.27	7	1
1:A:28:ILE:HD11	1:A:34:ASP:CG	0.85	1.95	14	1
1:A:95:LEU:HD22	1:A:96:ILE:N	0.85	1.87	5	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:ARG:NH1	1:A:82:VAL:HG12	0.84	1.88	16	1
1:A:71:ARG:NH1	1:A:101:ILE:HG21	0.84	1.88	7	3
1:A:76:LEU:HD13	1:A:116:TYR:OH	0.84	1.73	6	3
1:A:122:PHE:CE2	1:A:124:LEU:HD11	0.84	2.07	19	7
1:A:27:VAL:HG21	1:A:65:ARG:HH11	0.83	1.31	18	1
1:A:70:VAL:O	1:A:76:LEU:HD13	0.83	1.73	8	2
1:A:7:VAL:HG11	1:A:122:PHE:CE2	0.83	2.07	14	1
1:A:43:LYS:C	1:A:44:LEU:HD23	0.82	1.98	12	7
1:A:71:ARG:HH11	1:A:76:LEU:HD12	0.82	1.32	1	1
1:A:55:VAL:HG11	1:A:67:PHE:CE1	0.82	2.08	2	4
1:A:23:TYR:CE2	1:A:55:VAL:HG22	0.82	2.09	1	9
1:A:28:ILE:HD12	1:A:35:THR:O	0.82	1.74	6	14
1:A:5:LEU:HD12	1:A:7:VAL:HG23	0.81	1.53	8	6
1:A:68:ASP:O	1:A:78:LEU:HD12	0.81	1.76	5	11
1:A:76:LEU:HD22	1:A:116:TYR:OH	0.80	1.75	7	2
1:A:23:TYR:O	1:A:41:THR:HG23	0.80	1.76	4	8
1:A:44:LEU:HD12	1:A:47:ALA:CB	0.80	2.05	4	3
1:A:57:VAL:HG13	1:A:68:ASP:OD1	0.80	1.76	16	1
1:A:94:HIS:CD2	1:A:122:PHE:CE2	0.79	2.70	17	9
1:A:94:HIS:CD2	1:A:122:PHE:CE1	0.79	2.71	4	11
1:A:71:ARG:HH11	1:A:101:ILE:HG21	0.79	1.38	7	1
1:A:25:PHE:CZ	1:A:67:PHE:CD1	0.79	2.71	18	3
1:A:55:VAL:HG11	1:A:67:PHE:CE2	0.78	2.13	5	3
1:A:76:LEU:HD13	1:A:116:TYR:CZ	0.77	2.14	2	1
1:A:28:ILE:HD11	1:A:34:ASP:OD2	0.77	1.78	11	3
1:A:5:LEU:HD13	1:A:6:ASN:N	0.77	1.94	14	8
1:A:44:LEU:HB3	1:A:47:ALA:HB3	0.76	1.56	15	5
1:A:25:PHE:CE1	1:A:67:PHE:CE1	0.76	2.73	18	1
1:A:95:LEU:C	1:A:95:LEU:HD13	0.76	2.06	11	16
1:A:68:ASP:OD1	1:A:70:VAL:HG23	0.76	1.80	8	1
1:A:57:VAL:HG23	1:A:68:ASP:OD1	0.76	1.80	4	1
1:A:25:PHE:CZ	1:A:67:PHE:CE1	0.76	2.73	10	1
1:A:7:VAL:HG22	1:A:26:ASN:O	0.75	1.81	16	7
1:A:68:ASP:OD2	1:A:70:VAL:HG23	0.75	1.81	10	1
1:A:103:THR:HG23	1:A:112:ASP:OD1	0.75	1.81	5	1
1:A:96:ILE:HD13	1:A:116:TYR:CE1	0.75	2.17	7	2
1:A:127:VAL:HG12	1:A:129:LEU:CD2	0.74	2.11	18	1
1:A:11:ALA:HB3	1:A:24:SER:OG	0.74	1.82	1	1
1:A:28:ILE:HD11	1:A:35:THR:HA	0.74	1.58	19	2
1:A:94:HIS:CD2	1:A:122:PHE:CZ	0.74	2.76	16	11
1:A:44:LEU:N	1:A:44:LEU:HD23	0.73	1.98	17	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:23:TYR:OH	1:A:52:LEU:HD23	0.73	1.84	18	3
1:A:67:PHE:CZ	1:A:78:LEU:HD11	0.73	2.17	12	2
1:A:61:LEU:N	1:A:61:LEU:HD22	0.73	1.99	4	2
1:A:35:THR:HG21	1:A:38:TYR:OH	0.73	1.83	7	2
1:A:95:LEU:HD13	1:A:95:LEU:C	0.73	2.07	2	4
1:A:20:MET:HE1	1:A:43:LYS:HB3	0.73	1.61	16	1
1:A:26:ASN:O	1:A:27:VAL:HG23	0.73	1.82	14	4
1:A:95:LEU:HD13	1:A:96:ILE:N	0.72	1.99	8	8
1:A:65:ARG:NH1	1:A:82:VAL:HG13	0.72	1.99	7	1
1:A:94:HIS:HA	1:A:124:LEU:HD22	0.72	1.61	11	5
1:A:95:LEU:HD22	1:A:96:ILE:H	0.72	1.44	1	15
1:A:12:ALA:HB1	1:A:52:LEU:HD21	0.72	1.60	10	1
1:A:14:CYS:HB2	1:A:52:LEU:HD13	0.71	1.62	13	6
1:A:96:ILE:HG21	1:A:116:TYR:CE1	0.71	2.19	5	4
1:A:67:PHE:CD2	1:A:78:LEU:HD11	0.71	2.20	4	1
1:A:43:LYS:C	1:A:44:LEU:HD12	0.71	2.09	11	2
1:A:76:LEU:HD12	1:A:96:ILE:HD12	0.71	1.63	18	3
1:A:44:LEU:HD13	1:A:56:LYS:HD3	0.71	1.61	16	1
1:A:67:PHE:CE2	1:A:80:VAL:CG2	0.70	2.75	16	2
1:A:94:HIS:CE1	1:A:96:ILE:CD1	0.70	2.75	19	19
1:A:44:LEU:HD23	1:A:44:LEU:N	0.69	2.01	4	5
1:A:96:ILE:HD13	1:A:116:TYR:CE2	0.69	2.22	14	4
1:A:15:THR:HG22	1:A:113:ALA:HB1	0.69	1.63	16	5
1:A:57:VAL:HG13	1:A:68:ASP:CG	0.69	2.11	16	1
1:A:27:VAL:HG21	1:A:65:ARG:NH1	0.69	2.02	18	2
1:A:23:TYR:CE2	1:A:55:VAL:CG2	0.69	2.75	1	5
1:A:96:ILE:HD13	1:A:116:TYR:CZ	0.69	2.23	7	4
1:A:23:TYR:CE1	1:A:55:VAL:CG2	0.69	2.75	12	7
1:A:78:LEU:HD22	1:A:94:HIS:HB3	0.69	1.64	17	13
1:A:44:LEU:HD21	1:A:56:LYS:HG3	0.69	1.63	13	1
1:A:67:PHE:CD1	1:A:78:LEU:HD21	0.69	2.22	16	1
1:A:12:ALA:HB3	1:A:116:TYR:CD1	0.68	2.24	9	5
1:A:55:VAL:O	1:A:55:VAL:HG12	0.68	1.89	10	20
1:A:23:TYR:OH	1:A:52:LEU:HD22	0.68	1.89	8	3
1:A:13:SER:HA	1:A:52:LEU:HD11	0.68	1.64	6	2
1:A:5:LEU:HD13	1:A:6:ASN:H	0.67	1.50	15	8
1:A:23:TYR:CE2	1:A:69:VAL:HG21	0.67	2.23	9	7
1:A:69:VAL:HG13	1:A:76:LEU:HD11	0.67	1.66	15	1
1:A:20:MET:HE2	1:A:21:CYS:O	0.67	1.87	13	1
1:A:96:ILE:HG22	1:A:100:ASP:CG	0.67	2.14	16	1
1:A:76:LEU:HD13	1:A:77:THR:H	0.67	1.49	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:PHE:CE1	1:A:67:PHE:CD1	0.67	2.82	18	1
1:A:65:ARG:O	1:A:66:THR:HG23	0.66	1.90	17	15
1:A:25:PHE:CE1	1:A:67:PHE:CE2	0.66	2.84	4	3
1:A:23:TYR:CE1	1:A:69:VAL:HG21	0.66	2.26	1	7
1:A:57:VAL:HG12	1:A:67:PHE:O	0.66	1.90	10	1
1:A:5:LEU:CD1	1:A:7:VAL:HG23	0.66	2.21	16	1
1:A:100:ASP:C	1:A:101:ILE:HD13	0.66	2.14	17	1
1:A:129:LEU:HD12	1:A:129:LEU:N	0.66	2.05	1	1
1:A:55:VAL:CG1	1:A:67:PHE:CE1	0.66	2.79	2	2
1:A:67:PHE:CE1	1:A:80:VAL:CG1	0.66	2.79	17	2
1:A:67:PHE:CD2	1:A:67:PHE:C	0.65	2.75	18	3
1:A:94:HIS:NE2	1:A:122:PHE:CZ	0.65	2.65	13	11
1:A:57:VAL:HG22	1:A:67:PHE:O	0.65	1.91	8	1
1:A:67:PHE:CE1	1:A:80:VAL:HG12	0.65	2.27	10	2
1:A:28:ILE:HD11	1:A:34:ASP:OD1	0.65	1.91	10	4
1:A:7:VAL:HG21	1:A:124:LEU:CD1	0.65	2.22	20	3
1:A:8:ARG:HH11	1:A:26:ASN:HB3	0.65	1.52	17	1
1:A:65:ARG:HG2	1:A:82:VAL:HG22	0.65	1.67	9	2
1:A:25:PHE:CZ	1:A:67:PHE:CD2	0.65	2.84	19	3
1:A:88:SER:C	1:A:89:PHE:CD2	0.65	2.75	11	4
1:A:65:ARG:CZ	1:A:82:VAL:HG22	0.65	2.22	14	1
1:A:67:PHE:CD1	1:A:68:ASP:N	0.64	2.65	19	2
1:A:123:PRO:C	1:A:124:LEU:HD12	0.64	2.16	3	9
1:A:7:VAL:CG1	1:A:122:PHE:CE2	0.64	2.80	14	4
1:A:122:PHE:CE2	1:A:124:LEU:HD21	0.64	2.27	11	2
1:A:71:ARG:NH1	1:A:76:LEU:HD12	0.64	2.07	1	1
1:A:14:CYS:O	1:A:15:THR:HG23	0.64	1.93	6	15
1:A:33:MET:O	1:A:35:THR:HG23	0.64	1.93	12	2
1:A:3:ALA:HB1	1:A:124:LEU:C	0.63	2.17	20	9
1:A:38:TYR:CD2	1:A:38:TYR:C	0.63	2.76	14	1
1:A:23:TYR:CZ	1:A:55:VAL:HG22	0.63	2.29	6	4
1:A:20:MET:HE1	1:A:43:LYS:HB2	0.63	1.70	13	1
1:A:8:ARG:HH11	1:A:26:ASN:CB	0.63	2.07	17	1
1:A:12:ALA:HB3	1:A:116:TYR:CE1	0.63	2.29	9	3
1:A:65:ARG:HH11	1:A:82:VAL:HG12	0.63	1.51	16	1
1:A:27:VAL:HG11	1:A:65:ARG:NE	0.63	2.08	18	1
1:A:65:ARG:HH11	1:A:82:VAL:CG1	0.62	2.06	7	1
1:A:23:TYR:CZ	1:A:55:VAL:CG2	0.62	2.82	6	16
1:A:76:LEU:HB3	1:A:96:ILE:HD12	0.62	1.69	15	1
1:A:44:LEU:HD21	1:A:56:LYS:HG2	0.62	1.71	20	1
1:A:28:ILE:HD11	1:A:35:THR:C	0.62	2.20	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:ARG:HH11	1:A:114:GLN:HE22	0.62	1.35	5	2
1:A:67:PHE:C	1:A:67:PHE:CD1	0.62	2.75	2	3
1:A:4:VAL:HG13	1:A:4:VAL:O	0.62	1.95	13	7
1:A:67:PHE:HD2	1:A:78:LEU:HD11	0.62	1.54	4	1
1:A:67:PHE:CE2	1:A:80:VAL:HG21	0.62	2.30	16	1
1:A:102:LYS:CD	1:A:117:VAL:HG11	0.62	2.24	15	1
1:A:5:LEU:HD21	1:A:29:GLN:CD	0.62	2.20	3	1
1:A:4:VAL:O	1:A:5:LEU:HD22	0.61	1.94	20	1
1:A:44:LEU:HD12	1:A:47:ALA:HB1	0.61	1.72	16	2
1:A:35:THR:HG21	1:A:38:TYR:CZ	0.61	2.29	7	1
1:A:38:TYR:CD1	1:A:65:ARG:NE	0.61	2.68	20	1
1:A:76:LEU:HD13	1:A:77:THR:N	0.61	2.08	15	1
1:A:10:PHE:CD1	1:A:122:PHE:CE2	0.61	2.88	14	4
1:A:96:ILE:CG2	1:A:101:ILE:HD11	0.61	2.25	7	6
1:A:65:ARG:HD3	1:A:82:VAL:HG13	0.61	1.71	15	1
1:A:33:MET:HE1	1:A:82:VAL:HG12	0.61	1.72	18	1
1:A:25:PHE:CZ	1:A:40:CYS:CB	0.61	2.84	17	4
1:A:27:VAL:O	1:A:27:VAL:HG13	0.61	1.96	1	6
1:A:89:PHE:CD1	1:A:89:PHE:N	0.61	2.68	1	2
1:A:122:PHE:CE1	1:A:124:LEU:CD1	0.61	2.82	2	5
1:A:67:PHE:CD1	1:A:67:PHE:C	0.60	2.79	12	2
1:A:27:VAL:HG11	1:A:65:ARG:CZ	0.60	2.27	18	1
1:A:6:ASN:HB3	1:A:28:ILE:HG23	0.60	1.73	9	1
1:A:43:LYS:H	1:A:43:LYS:NZ	0.60	1.93	7	1
1:A:66:THR:O	1:A:67:PHE:CD2	0.60	2.55	16	2
1:A:100:ASP:OD1	1:A:116:TYR:CE2	0.60	2.55	16	1
1:A:5:LEU:HD23	1:A:6:ASN:H	0.60	1.57	18	1
1:A:60:CYS:SG	1:A:67:PHE:CD2	0.60	2.94	18	1
1:A:67:PHE:CE2	1:A:78:LEU:HD21	0.60	2.32	12	2
1:A:40:CYS:SG	1:A:67:PHE:CZ	0.60	2.95	9	2
1:A:15:THR:HG22	1:A:113:ALA:CB	0.60	2.26	19	2
1:A:40:CYS:SG	1:A:67:PHE:CE1	0.60	2.95	2	4
1:A:76:LEU:HD13	1:A:96:ILE:HD12	0.59	1.74	13	3
1:A:40:CYS:SG	1:A:67:PHE:CE2	0.59	2.95	3	4
1:A:23:TYR:CE1	1:A:52:LEU:HD23	0.59	2.31	10	2
1:A:40:CYS:SG	1:A:67:PHE:CD2	0.59	2.95	11	3
1:A:55:VAL:CG1	1:A:67:PHE:CZ	0.59	2.86	8	1
1:A:100:ASP:OD2	1:A:116:TYR:CE2	0.59	2.55	13	1
1:A:122:PHE:CE2	1:A:124:LEU:CD1	0.59	2.85	15	4
1:A:25:PHE:CZ	1:A:67:PHE:CZ	0.59	2.89	10	1
1:A:25:PHE:CD1	1:A:25:PHE:O	0.59	2.55	14	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:122:PHE:CE1	1:A:124:LEU:HD21	0.59	2.32	10	2
1:A:42:ALA:CB	1:A:55:VAL:HG13	0.59	2.28	16	1
1:A:28:ILE:HD11	1:A:35:THR:CA	0.59	2.27	1	2
1:A:23:TYR:CZ	1:A:52:LEU:HD22	0.59	2.32	8	6
1:A:44:LEU:HD11	1:A:53:PRO:CG	0.59	2.28	7	2
1:A:60:CYS:C	1:A:61:LEU:HD13	0.59	2.22	8	2
1:A:5:LEU:HD22	1:A:29:GLN:HG2	0.59	1.74	8	3
1:A:7:VAL:HG11	1:A:122:PHE:CZ	0.59	2.32	14	9
1:A:17:HIS:CG	1:A:18:SER:N	0.59	2.70	12	3
1:A:82:VAL:HG13	1:A:84:VAL:HG13	0.58	1.74	4	1
1:A:12:ALA:HB3	1:A:116:TYR:CD2	0.58	2.34	1	2
1:A:65:ARG:NE	1:A:82:VAL:HG22	0.58	2.14	17	2
1:A:78:LEU:HD23	1:A:80:VAL:HG23	0.58	1.75	7	2
1:A:127:VAL:HG12	1:A:129:LEU:HD22	0.58	1.76	18	1
1:A:25:PHE:CE1	1:A:67:PHE:CZ	0.58	2.92	10	2
1:A:44:LEU:HD21	1:A:56:LYS:CG	0.58	2.29	13	1
1:A:60:CYS:SG	1:A:67:PHE:CD1	0.58	2.97	2	1
1:A:27:VAL:HG11	1:A:65:ARG:HH12	0.58	1.58	3	2
1:A:43:LYS:H	1:A:43:LYS:HZ3	0.58	1.42	7	1
1:A:33:MET:HE1	1:A:82:VAL:CG1	0.58	2.29	18	1
1:A:90:THR:HG21	1:A:126:ARG:NH2	0.58	2.13	11	1
1:A:69:VAL:HG13	1:A:76:LEU:HD21	0.57	1.75	5	1
1:A:38:TYR:CE1	1:A:65:ARG:NH2	0.57	2.72	7	1
1:A:52:LEU:CD1	1:A:116:TYR:CE1	0.57	2.87	8	1
1:A:25:PHE:CE1	1:A:67:PHE:CD2	0.57	2.92	19	1
1:A:47:ALA:HB1	1:A:56:LYS:HE3	0.57	1.76	3	1
1:A:61:LEU:HD22	1:A:61:LEU:H	0.57	1.59	4	1
1:A:101:ILE:HD13	1:A:101:ILE:N	0.57	2.13	17	1
1:A:10:PHE:C	1:A:10:PHE:CD1	0.57	2.82	13	1
1:A:7:VAL:HG12	1:A:7:VAL:O	0.57	1.98	11	7
1:A:89:PHE:CD1	1:A:89:PHE:O	0.57	2.56	14	1
1:A:55:VAL:HG11	1:A:67:PHE:CZ	0.57	2.35	5	3
1:A:71:ARG:NH1	1:A:114:GLN:HE22	0.57	1.98	10	1
1:A:100:ASP:OD1	1:A:116:TYR:CD2	0.57	2.57	16	1
1:A:41:THR:HG22	1:A:43:LYS:CE	0.56	2.30	15	1
1:A:44:LEU:HD11	1:A:53:PRO:CB	0.56	2.30	2	2
1:A:67:PHE:CZ	1:A:69:VAL:HG23	0.56	2.35	19	2
1:A:103:THR:HG22	1:A:112:ASP:CG	0.56	2.25	14	1
1:A:25:PHE:CE2	1:A:67:PHE:CD2	0.56	2.93	2	2
1:A:79:THR:HG23	1:A:91:LYS:CE	0.56	2.31	1	1
1:A:90:THR:HG21	1:A:126:ARG:CZ	0.56	2.30	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:67:PHE:CZ	1:A:80:VAL:HG21	0.56	2.35	16	1
1:A:3:ALA:HB1	1:A:124:LEU:O	0.56	2.01	13	5
1:A:96:ILE:HG21	1:A:116:TYR:HE1	0.56	1.60	13	3
1:A:78:LEU:HD23	1:A:80:VAL:CG1	0.56	2.31	1	3
1:A:40:CYS:SG	1:A:67:PHE:CD1	0.56	2.98	8	2
1:A:91:LYS:NZ	1:A:129:LEU:HD21	0.55	2.16	1	1
1:A:80:VAL:HG22	1:A:92:GLY:HA3	0.55	1.76	5	1
1:A:65:ARG:HH21	1:A:82:VAL:HG22	0.55	1.61	20	1
1:A:23:TYR:HE1	1:A:69:VAL:HG21	0.55	1.59	10	4
1:A:5:LEU:HD12	1:A:124:LEU:HB2	0.55	1.79	5	1
1:A:96:ILE:HG22	1:A:101:ILE:HD11	0.55	1.77	9	5
1:A:95:LEU:C	1:A:95:LEU:CD1	0.55	2.80	6	20
1:A:96:ILE:HD13	1:A:116:TYR:OH	0.55	2.01	1	3
1:A:94:HIS:NE2	1:A:96:ILE:CG1	0.55	2.70	2	7
1:A:40:CYS:SG	1:A:67:PHE:CG	0.55	3.00	8	1
1:A:7:VAL:HG11	1:A:122:PHE:CE1	0.55	2.37	15	1
1:A:5:LEU:HD11	1:A:29:GLN:HG2	0.55	1.79	4	2
1:A:23:TYR:CD2	1:A:42:ALA:HB3	0.55	2.36	6	1
1:A:102:LYS:CB	1:A:117:VAL:HG21	0.54	2.33	1	2
1:A:41:THR:HG22	1:A:43:LYS:HE3	0.54	1.80	15	1
1:A:12:ALA:C	1:A:52:LEU:HD21	0.54	2.27	17	1
1:A:33:MET:SD	1:A:82:VAL:HG11	0.54	2.43	18	1
1:A:5:LEU:HD11	1:A:27:VAL:HG13	0.54	1.79	19	1
1:A:97:PRO:CG	1:A:99:LYS:NZ	0.54	2.70	1	1
1:A:96:ILE:HG21	1:A:116:TYR:CE2	0.54	2.37	8	1
1:A:25:PHE:CD1	1:A:25:PHE:C	0.54	2.86	14	4
1:A:61:LEU:HD12	1:A:62:PRO:HA	0.54	1.80	7	7
1:A:102:LYS:HD3	1:A:117:VAL:HG11	0.54	1.80	15	1
1:A:103:THR:HG22	1:A:112:ASP:HB2	0.54	1.80	1	1
1:A:67:PHE:CD1	1:A:80:VAL:HG12	0.54	2.37	17	2
1:A:90:THR:CB	1:A:126:ARG:NH1	0.54	2.70	11	1
1:A:7:VAL:CG2	1:A:124:LEU:HD13	0.54	2.33	2	6
1:A:44:LEU:HD11	1:A:53:PRO:HB2	0.54	1.78	2	2
1:A:65:ARG:HH11	1:A:80:VAL:HG21	0.54	1.62	12	2
1:A:67:PHE:CG	1:A:68:ASP:N	0.54	2.75	12	2
1:A:8:ARG:HH11	1:A:26:ASN:CG	0.54	2.10	17	1
1:A:50:GLY:O	1:A:113:ALA:HB1	0.54	2.03	2	2
1:A:65:ARG:NH2	1:A:82:VAL:HG22	0.54	2.18	20	1
1:A:82:VAL:HB	1:A:90:THR:HG22	0.53	1.81	20	5
1:A:65:ARG:HH21	1:A:82:VAL:HG13	0.53	1.61	6	2
1:A:7:VAL:HG21	1:A:124:LEU:HD12	0.53	1.80	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:8:ARG:NH2	1:A:28:ILE:HG21	0.53	2.18	3	3
1:A:129:LEU:H	1:A:129:LEU:HD23	0.53	1.62	17	1
1:A:25:PHE:CZ	1:A:40:CYS:HB3	0.53	2.38	17	4
1:A:12:ALA:O	1:A:116:TYR:CD1	0.53	2.62	9	1
1:A:5:LEU:CD2	1:A:29:GLN:CD	0.53	2.82	3	1
1:A:25:PHE:CZ	1:A:65:ARG:CZ	0.52	2.92	2	1
1:A:5:LEU:HD23	1:A:6:ASN:N	0.52	2.19	18	1
1:A:44:LEU:N	1:A:44:LEU:CD2	0.52	2.70	17	9
1:A:76:LEU:HD13	1:A:116:TYR:CE2	0.52	2.39	2	1
1:A:23:TYR:HE2	1:A:69:VAL:HG21	0.52	1.61	9	4
1:A:23:TYR:CZ	1:A:52:LEU:HD12	0.52	2.39	12	2
1:A:44:LEU:HD23	1:A:47:ALA:CB	0.52	2.34	13	1
1:A:99:LYS:CB	1:A:99:LYS:NZ	0.52	2.73	15	1
1:A:129:LEU:HD12	1:A:129:LEU:H	0.52	1.63	1	1
1:A:70:VAL:C	1:A:76:LEU:HD23	0.52	2.29	2	4
1:A:69:VAL:HG22	1:A:78:LEU:HD12	0.52	1.82	17	1
1:A:101:ILE:HG23	1:A:114:GLN:NE2	0.52	2.19	8	1
1:A:61:LEU:HA	1:A:62:PRO:C	0.52	2.30	19	20
1:A:91:LYS:HB2	1:A:129:LEU:HD23	0.52	1.81	4	1
1:A:93:SER:OG	1:A:127:VAL:HG22	0.52	2.05	1	1
1:A:27:VAL:HG11	1:A:65:ARG:NH1	0.52	2.19	11	2
1:A:38:TYR:CD1	1:A:65:ARG:CD	0.51	2.93	11	2
1:A:102:LYS:HB2	1:A:117:VAL:HG21	0.51	1.81	8	3
1:A:25:PHE:CZ	1:A:40:CYS:HB2	0.51	2.40	10	2
1:A:60:CYS:SG	1:A:67:PHE:CE2	0.51	3.03	18	1
1:A:32:THR:HG23	1:A:34:ASP:H	0.51	1.65	19	1
1:A:25:PHE:C	1:A:25:PHE:CD2	0.51	2.88	19	2
1:A:60:CYS:C	1:A:61:LEU:HD22	0.51	2.30	17	1
1:A:122:PHE:CD2	1:A:124:LEU:HD11	0.51	2.40	19	1
1:A:55:VAL:CG1	1:A:67:PHE:CE2	0.51	2.92	5	1
1:A:12:ALA:HB1	1:A:52:LEU:CD2	0.51	2.33	10	1
1:A:65:ARG:CD	1:A:82:VAL:HG13	0.51	2.36	15	1
1:A:35:THR:HG22	1:A:36:LYS:N	0.51	2.20	16	4
1:A:10:PHE:CD1	1:A:122:PHE:CZ	0.51	2.99	11	2
1:A:93:SER:OG	1:A:127:VAL:HG21	0.51	2.06	12	1
1:A:76:LEU:O	1:A:95:LEU:HD23	0.51	2.06	15	1
1:A:67:PHE:CE1	1:A:78:LEU:HD21	0.51	2.41	16	1
1:A:13:SER:HB3	1:A:115:ALA:HB1	0.50	1.82	7	3
1:A:52:LEU:HD13	1:A:116:TYR:CE1	0.50	2.41	8	1
1:A:65:ARG:O	1:A:66:THR:CG2	0.50	2.60	17	12
1:A:38:TYR:CD1	1:A:65:ARG:HD3	0.50	2.41	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:71:ARG:HH11	1:A:76:LEU:CD1	0.50	2.14	1	1
1:A:3:ALA:CB	1:A:124:LEU:O	0.50	2.60	5	3
1:A:67:PHE:CZ	1:A:80:VAL:HG22	0.50	2.36	7	1
1:A:65:ARG:CZ	1:A:82:VAL:HG12	0.50	2.37	16	1
1:A:94:HIS:HE1	1:A:96:ILE:HD11	0.50	1.58	14	6
1:A:60:CYS:O	1:A:61:LEU:HD13	0.50	2.06	8	1
1:A:103:THR:HG23	1:A:112:ASP:CG	0.50	2.31	5	1
1:A:90:THR:HG21	1:A:126:ARG:NH1	0.50	2.22	11	1
1:A:8:ARG:NH1	1:A:26:ASN:CG	0.50	2.70	17	1
1:A:7:VAL:HG21	1:A:124:LEU:CD2	0.50	2.36	19	1
1:A:27:VAL:O	1:A:27:VAL:CG1	0.50	2.60	7	7
1:A:12:ALA:HB3	1:A:116:TYR:HD1	0.50	1.67	19	5
1:A:100:ASP:CG	1:A:116:TYR:CE2	0.50	2.90	13	1
1:A:29:GLN:CG	1:A:34:ASP:OD2	0.50	2.60	19	1
1:A:40:CYS:HB3	1:A:67:PHE:CE2	0.50	2.41	5	1
1:A:55:VAL:O	1:A:55:VAL:CG1	0.50	2.60	11	11
1:A:14:CYS:O	1:A:15:THR:CG2	0.50	2.60	3	15
1:A:26:ASN:O	1:A:27:VAL:CG2	0.50	2.60	8	7
1:A:10:PHE:CD2	1:A:10:PHE:C	0.50	2.90	4	4
1:A:65:ARG:CG	1:A:81:SER:O	0.50	2.60	10	1
1:A:50:GLY:O	1:A:113:ALA:CB	0.50	2.60	2	3
1:A:89:PHE:N	1:A:89:PHE:CD2	0.50	2.80	5	3
1:A:22:SER:O	1:A:23:TYR:CD2	0.50	2.65	6	1
1:A:123:PRO:O	1:A:124:LEU:HD23	0.50	2.07	11	4
1:A:41:THR:CG2	1:A:42:ALA:N	0.50	2.75	19	3
1:A:68:ASP:O	1:A:78:LEU:CD1	0.49	2.60	1	7
1:A:20:MET:HE3	1:A:45:PRO:CB	0.49	2.37	6	1
1:A:20:MET:HE3	1:A:45:PRO:HG3	0.49	1.84	3	1
1:A:35:THR:HG22	1:A:36:LYS:H	0.49	1.68	4	4
1:A:43:LYS:C	1:A:44:LEU:CD2	0.49	2.80	12	4
1:A:93:SER:OG	1:A:127:VAL:CG2	0.49	2.60	1	3
1:A:99:LYS:CG	1:A:100:ASP:N	0.49	2.76	16	15
1:A:105:LYS:O	1:A:105:LYS:CG	0.49	2.60	14	11
1:A:8:ARG:NH2	1:A:28:ILE:CG2	0.49	2.76	3	1
1:A:7:VAL:CG1	1:A:122:PHE:CE1	0.49	2.95	15	2
1:A:32:THR:CG2	1:A:33:MET:N	0.49	2.76	18	6
1:A:7:VAL:O	1:A:121:ASP:CB	0.49	2.60	10	1
1:A:100:ASP:OD1	1:A:116:TYR:CD1	0.49	2.65	11	1
1:A:51:GLU:OE1	1:A:71:ARG:CD	0.49	2.60	1	1
1:A:64:SER:HB3	1:A:65:ARG:HH11	0.49	1.68	1	1
1:A:25:PHE:CE2	1:A:40:CYS:HB3	0.49	2.42	10	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:5:LEU:HD23	1:A:124:LEU:HB2	0.49	1.83	4	1
1:A:38:TYR:CZ	1:A:65:ARG:NE	0.49	2.81	5	1
1:A:65:ARG:CG	1:A:82:VAL:HG22	0.49	2.38	6	1
1:A:17:HIS:CD2	1:A:18:SER:N	0.49	2.81	18	2
1:A:69:VAL:HG12	1:A:69:VAL:O	0.49	2.06	4	3
1:A:91:LYS:O	1:A:127:VAL:HG12	0.49	2.07	4	2
1:A:7:VAL:C	1:A:8:ARG:CG	0.49	2.85	15	2
1:A:65:ARG:CB	1:A:81:SER:O	0.49	2.61	10	1
1:A:42:ALA:O	1:A:44:LEU:CD2	0.49	2.61	7	1
1:A:90:THR:HG22	1:A:90:THR:O	0.49	2.06	15	1
1:A:65:ARG:HH11	1:A:82:VAL:HG22	0.48	1.68	8	1
1:A:10:PHE:CE2	1:A:116:TYR:CZ	0.48	3.01	12	2
1:A:67:PHE:CE1	1:A:80:VAL:HB	0.48	2.43	16	1
1:A:43:LYS:N	1:A:43:LYS:CD	0.48	2.76	14	2
1:A:129:LEU:N	1:A:129:LEU:CD1	0.48	2.76	1	1
1:A:26:ASN:C	1:A:27:VAL:HG23	0.48	2.33	3	6
1:A:38:TYR:CE1	1:A:65:ARG:HD3	0.48	2.44	14	1
1:A:91:LYS:C	1:A:127:VAL:CG1	0.48	2.86	4	1
1:A:28:ILE:CD1	1:A:35:THR:O	0.48	2.61	9	6
1:A:122:PHE:C	1:A:122:PHE:CD2	0.48	2.91	13	4
1:A:28:ILE:CG1	1:A:35:THR:O	0.48	2.61	7	2
1:A:39:GLU:O	1:A:61:LEU:HD23	0.48	2.08	10	1
1:A:88:SER:O	1:A:89:PHE:CD2	0.48	2.66	11	1
1:A:67:PHE:CE2	1:A:78:LEU:CD1	0.48	2.86	12	1
1:A:12:ALA:HB3	1:A:116:TYR:HD2	0.48	1.66	1	2
1:A:83:GLN:HG3	1:A:89:PHE:CE1	0.48	2.43	11	2
1:A:102:LYS:CG	1:A:103:THR:N	0.48	2.76	15	1
1:A:91:LYS:O	1:A:127:VAL:CG1	0.48	2.61	11	4
1:A:33:MET:CE	1:A:82:VAL:CG1	0.48	2.91	18	1
1:A:10:PHE:CE1	1:A:94:HIS:CE1	0.48	3.02	4	9
1:A:28:ILE:CG1	1:A:29:GLN:N	0.48	2.77	10	7
1:A:60:CYS:SG	1:A:67:PHE:CE1	0.48	3.07	2	1
1:A:25:PHE:CZ	1:A:67:PHE:CE2	0.48	3.02	4	1
1:A:10:PHE:CD2	1:A:122:PHE:CE1	0.48	3.01	7	1
1:A:116:TYR:C	1:A:116:TYR:CD1	0.48	2.92	16	1
1:A:10:PHE:CE2	1:A:116:TYR:CE2	0.48	3.02	10	1
1:A:51:GLU:OE2	1:A:71:ARG:CZ	0.48	2.62	10	1
1:A:67:PHE:CD2	1:A:78:LEU:HD21	0.48	2.44	19	1
1:A:25:PHE:CE1	1:A:65:ARG:NH1	0.48	2.82	2	1
1:A:44:LEU:HB2	1:A:47:ALA:HB2	0.48	1.85	4	1
1:A:129:LEU:HD22	1:A:129:LEU:N	0.47	2.24	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:65:ARG:NH1	1:A:82:VAL:HG22	0.47	2.23	14	1
1:A:14:CYS:C	1:A:15:THR:CG2	0.47	2.87	15	1
1:A:65:ARG:HD2	1:A:82:VAL:HG13	0.47	1.86	17	2
1:A:97:PRO:C	1:A:99:LYS:N	0.47	2.71	10	13
1:A:103:THR:HG22	1:A:112:ASP:CB	0.47	2.40	1	2
1:A:10:PHE:CD1	1:A:122:PHE:CE1	0.47	3.01	11	2
1:A:100:ASP:OD1	1:A:116:TYR:CE1	0.47	2.67	11	1
1:A:69:VAL:HG13	1:A:76:LEU:HD22	0.47	1.85	13	1
1:A:84:VAL:HG23	1:A:85:SER:N	0.47	2.24	15	1
1:A:62:PRO:HG2	1:A:65:ARG:HH11	0.47	1.69	6	1
1:A:62:PRO:C	1:A:64:SER:N	0.47	2.72	12	1
1:A:7:VAL:HG13	1:A:26:ASN:O	0.47	2.10	14	1
1:A:42:ALA:O	1:A:44:LEU:HD23	0.47	2.10	2	1
1:A:38:TYR:CE1	1:A:65:ARG:HD2	0.47	2.44	11	1
1:A:6:ASN:CG	1:A:8:ARG:NH2	0.47	2.73	12	1
1:A:80:VAL:HG22	1:A:92:GLY:CA	0.47	2.40	5	1
1:A:100:ASP:O	1:A:117:VAL:HG22	0.47	2.09	9	1
1:A:71:ARG:HA	1:A:76:LEU:HD23	0.47	1.87	9	2
1:A:54:GLU:O	1:A:55:VAL:C	0.47	2.58	16	17
1:A:122:PHE:C	1:A:122:PHE:CD1	0.47	2.93	12	4
1:A:23:TYR:CE1	1:A:52:LEU:CD2	0.47	2.97	10	1
1:A:67:PHE:CZ	1:A:80:VAL:CG1	0.47	2.98	10	1
1:A:25:PHE:CD2	1:A:25:PHE:O	0.47	2.68	19	1
1:A:38:TYR:CE2	1:A:62:PRO:HG3	0.46	2.45	3	1
1:A:89:PHE:CD2	1:A:89:PHE:N	0.46	2.82	6	4
1:A:10:PHE:CD2	1:A:116:TYR:CE2	0.46	3.03	10	1
1:A:14:CYS:HB2	1:A:52:LEU:HD23	0.46	1.86	5	2
1:A:71:ARG:HH11	1:A:114:GLN:NE2	0.46	2.04	5	1
1:A:76:LEU:CD1	1:A:116:TYR:OH	0.46	2.63	9	1
1:A:44:LEU:CB	1:A:47:ALA:HB3	0.46	2.35	15	1
1:A:102:LYS:CB	1:A:117:VAL:CG2	0.46	2.93	1	3
1:A:7:VAL:HG22	1:A:27:VAL:HG22	0.46	1.88	3	2
1:A:47:ALA:HB3	1:A:53:PRO:HB3	0.46	1.87	14	2
1:A:68:ASP:CG	1:A:69:VAL:N	0.46	2.73	8	1
1:A:25:PHE:CE1	1:A:40:CYS:HB3	0.46	2.45	11	4
1:A:71:ARG:CG	1:A:72:SER:N	0.46	2.78	12	6
1:A:25:PHE:CZ	1:A:65:ARG:NH1	0.46	2.83	2	1
1:A:78:LEU:CD2	1:A:80:VAL:HG12	0.46	2.41	5	1
1:A:5:LEU:HD22	1:A:29:GLN:CG	0.46	2.40	8	1
1:A:6:ASN:CB	1:A:28:ILE:O	0.46	2.64	9	1
1:A:38:TYR:CD1	1:A:62:PRO:HG3	0.46	2.45	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:LEU:CD2	1:A:62:PRO:HA	0.46	2.41	9	1
1:A:25:PHE:CE2	1:A:40:CYS:HB2	0.46	2.45	1	1
1:A:32:THR:HG23	1:A:33:MET:N	0.46	2.26	5	10
1:A:61:LEU:N	1:A:61:LEU:CD2	0.46	2.70	4	2
1:A:91:LYS:C	1:A:127:VAL:HG12	0.46	2.35	4	1
1:A:65:ARG:NH1	1:A:82:VAL:CG1	0.46	2.70	16	1
1:A:33:MET:SD	1:A:82:VAL:CG1	0.46	3.04	18	1
1:A:41:THR:HG22	1:A:42:ALA:N	0.46	2.26	8	2
1:A:7:VAL:O	1:A:7:VAL:HG12	0.46	2.10	16	1
1:A:55:VAL:O	1:A:56:LYS:C	0.46	2.59	16	18
1:A:14:CYS:C	1:A:15:THR:HG23	0.46	2.36	7	13
1:A:62:PRO:O	1:A:65:ARG:N	0.46	2.49	12	1
1:A:40:CYS:SG	1:A:41:THR:N	0.45	2.90	2	2
1:A:94:HIS:O	1:A:94:HIS:CG	0.45	2.70	7	12
1:A:57:VAL:CG1	1:A:67:PHE:O	0.45	2.63	10	1
1:A:102:LYS:HD2	1:A:117:VAL:HG11	0.45	1.88	15	1
1:A:68:ASP:OD1	1:A:69:VAL:N	0.45	2.49	3	3
1:A:68:ASP:O	1:A:78:LEU:CG	0.45	2.65	11	2
1:A:82:VAL:O	1:A:84:VAL:HG13	0.45	2.11	12	1
1:A:40:CYS:C	1:A:41:THR:OG1	0.45	2.60	20	12
1:A:41:THR:HG22	1:A:42:ALA:H	0.45	1.71	6	3
1:A:38:TYR:CE1	1:A:62:PRO:HG3	0.45	2.47	9	1
1:A:5:LEU:HD22	1:A:7:VAL:HG23	0.45	1.89	18	1
1:A:56:LYS:O	1:A:57:VAL:C	0.45	2.59	18	18
1:A:51:GLU:O	1:A:52:LEU:C	0.45	2.60	4	2
1:A:17:HIS:O	1:A:18:SER:C	0.45	2.60	1	8
1:A:18:SER:O	1:A:19:ALA:C	0.45	2.60	10	13
1:A:55:VAL:O	1:A:57:VAL:N	0.45	2.50	15	11
1:A:125:GLU:CG	1:A:126:ARG:N	0.45	2.80	19	3
1:A:72:SER:N	1:A:75:GLY:O	0.45	2.50	14	8
1:A:129:LEU:HD22	1:A:129:LEU:H	0.45	1.71	5	1
1:A:41:THR:O	1:A:42:ALA:HB2	0.45	2.12	12	2
1:A:22:SER:OG	1:A:23:TYR:N	0.45	2.50	1	1
1:A:72:SER:OG	1:A:73:ASP:N	0.45	2.50	20	3
1:A:8:ARG:O	1:A:9:ASP:C	0.45	2.60	17	5
1:A:55:VAL:HG23	1:A:69:VAL:HB	0.45	1.89	13	3
1:A:32:THR:C	1:A:34:ASP:N	0.45	2.74	8	2
1:A:2:ASP:N	1:A:125:GLU:OE1	0.45	2.50	10	1
1:A:82:VAL:O	1:A:90:THR:N	0.45	2.50	10	1
1:A:7:VAL:HG21	1:A:124:LEU:HD11	0.45	1.86	20	2
1:A:67:PHE:C	1:A:68:ASP:OD2	0.45	2.60	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:GLN:OE1	1:A:115:ALA:N	0.45	2.50	13	5
1:A:19:ALA:C	1:A:20:MET:CG	0.45	2.90	6	1
1:A:41:THR:OG1	1:A:42:ALA:N	0.45	2.50	11	2
1:A:61:LEU:CD1	1:A:62:PRO:HA	0.45	2.42	19	7
1:A:33:MET:O	1:A:35:THR:N	0.45	2.50	19	5
1:A:93:SER:O	1:A:125:GLU:N	0.45	2.50	6	4
1:A:38:TYR:CD2	1:A:62:PRO:CD	0.45	3.00	4	1
1:A:115:ALA:O	1:A:117:VAL:HG13	0.45	2.12	9	1
1:A:35:THR:C	1:A:37:GLY:N	0.45	2.74	14	1
1:A:70:VAL:O	1:A:77:THR:N	0.45	2.50	15	1
1:A:46:GLY:O	1:A:47:ALA:C	0.45	2.60	17	1
1:A:2:ASP:OD1	1:A:2:ASP:C	0.45	2.60	18	1
1:A:34:ASP:OD1	1:A:34:ASP:N	0.45	2.50	20	1
1:A:47:ALA:O	1:A:48:GLY:C	0.45	2.60	17	4
1:A:33:MET:O	1:A:34:ASP:C	0.45	2.59	12	3
1:A:3:ALA:N	1:A:125:GLU:OE1	0.45	2.50	10	1
1:A:57:VAL:CG1	1:A:68:ASP:OD1	0.45	2.61	16	1
1:A:29:GLN:O	1:A:34:ASP:N	0.44	2.50	3	2
1:A:28:ILE:CG1	1:A:34:ASP:OD2	0.44	2.65	20	1
1:A:16:PRO:O	1:A:17:HIS:C	0.44	2.60	5	7
1:A:68:ASP:OD1	1:A:68:ASP:C	0.44	2.60	11	1
1:A:36:LYS:CD	1:A:37:GLY:O	0.44	2.66	14	1
1:A:4:VAL:O	1:A:4:VAL:CG1	0.44	2.64	17	2
1:A:5:LEU:CD1	1:A:29:GLN:CG	0.44	2.95	20	1
1:A:104:VAL:O	1:A:106:GLY:N	0.44	2.50	14	4
1:A:79:THR:HG22	1:A:91:LYS:HE3	0.44	1.89	12	1
1:A:32:THR:OG1	1:A:33:MET:N	0.44	2.50	19	2
1:A:103:THR:CG2	1:A:112:ASP:CG	0.44	2.90	5	2
1:A:82:VAL:N	1:A:90:THR:O	0.44	2.50	8	2
1:A:91:LYS:O	1:A:127:VAL:N	0.44	2.50	9	1
1:A:99:LYS:CD	1:A:99:LYS:C	0.44	2.90	9	1
1:A:7:VAL:CG2	1:A:124:LEU:HD12	0.44	2.42	11	1
1:A:79:THR:CG2	1:A:91:LYS:CE	0.44	2.96	12	1
1:A:97:PRO:O	1:A:98:THR:C	0.44	2.60	10	11
1:A:22:SER:O	1:A:23:TYR:CG	0.44	2.71	6	1
1:A:65:ARG:HG3	1:A:82:VAL:HG22	0.44	1.90	6	1
1:A:97:PRO:O	1:A:100:ASP:N	0.44	2.50	7	4
1:A:32:THR:O	1:A:33:MET:C	0.44	2.61	14	2
1:A:8:ARG:O	1:A:26:ASN:N	0.44	2.50	10	1
1:A:34:ASP:CG	1:A:34:ASP:O	0.44	2.60	12	1
1:A:51:GLU:OE1	1:A:71:ARG:NH2	0.44	2.50	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:41:THR:HG22	1:A:43:LYS:NZ	0.44	2.27	15	1
1:A:3:ALA:CB	1:A:124:LEU:C	0.43	2.90	5	2
1:A:112:ASP:OD2	1:A:112:ASP:N	0.43	2.50	14	2
1:A:97:PRO:O	1:A:99:LYS:N	0.43	2.51	10	8
1:A:65:ARG:HE	1:A:82:VAL:HG13	0.43	1.73	7	1
1:A:25:PHE:O	1:A:25:PHE:CD2	0.43	2.71	8	1
1:A:122:PHE:CD2	1:A:124:LEU:CD1	0.43	3.01	19	1
1:A:23:TYR:HD2	1:A:42:ALA:HB3	0.43	1.73	20	1
1:A:65:ARG:NH1	1:A:80:VAL:CG2	0.43	2.82	4	1
1:A:4:VAL:HG22	1:A:4:VAL:O	0.43	2.14	6	1
1:A:23:TYR:CE1	1:A:52:LEU:HD22	0.43	2.49	16	1
1:A:84:VAL:HG13	1:A:90:THR:HB	0.43	1.90	16	1
1:A:9:ASP:CG	1:A:9:ASP:O	0.43	2.61	17	1
1:A:65:ARG:NH1	1:A:80:VAL:HG21	0.43	2.28	4	1
1:A:47:ALA:HB1	1:A:53:PRO:HB3	0.43	1.90	5	1
1:A:93:SER:N	1:A:125:GLU:O	0.43	2.50	7	1
1:A:62:PRO:O	1:A:63:SER:C	0.43	2.60	12	1
1:A:116:TYR:C	1:A:117:VAL:CG1	0.43	2.91	17	2
1:A:26:ASN:C	1:A:27:VAL:CG2	0.43	2.91	12	3
1:A:33:MET:O	1:A:34:ASP:CG	0.43	2.60	13	2
1:A:44:LEU:HD12	1:A:47:ALA:HB2	0.43	1.88	16	1
1:A:29:GLN:CD	1:A:34:ASP:OD2	0.43	2.62	19	1
1:A:65:ARG:CD	1:A:66:THR:N	0.43	2.82	2	1
1:A:65:ARG:HH21	1:A:82:VAL:HG12	0.43	1.72	5	1
1:A:67:PHE:CD1	1:A:78:LEU:HD11	0.43	2.49	5	2
1:A:2:ASP:O	1:A:3:ALA:C	0.43	2.62	18	3
1:A:83:GLN:NE2	1:A:85:SER:O	0.43	2.52	6	2
1:A:93:SER:OG	1:A:125:GLU:CG	0.43	2.67	19	1
1:A:13:SER:CB	1:A:115:ALA:HB1	0.43	2.43	1	1
1:A:38:TYR:CD1	1:A:38:TYR:N	0.43	2.84	1	1
1:A:57:VAL:HG12	1:A:58:GLY:N	0.43	2.28	8	1
1:A:65:ARG:NH1	1:A:83:GLN:O	0.43	2.52	13	1
1:A:69:VAL:HA	1:A:78:LEU:HD12	0.43	1.91	13	1
1:A:67:PHE:CZ	1:A:80:VAL:CG2	0.43	2.99	16	1
1:A:25:PHE:CD2	1:A:25:PHE:C	0.43	2.97	8	1
1:A:114:GLN:OE1	1:A:114:GLN:C	0.43	2.62	8	1
1:A:29:GLN:CB	1:A:32:THR:CG2	0.43	2.97	9	1
1:A:27:VAL:HG12	1:A:38:TYR:HB2	0.43	1.90	4	1
1:A:70:VAL:O	1:A:76:LEU:CD2	0.43	2.60	13	2
1:A:83:GLN:HG3	1:A:89:PHE:CD1	0.43	2.49	6	1
1:A:35:THR:O	1:A:36:LYS:C	0.43	2.62	7	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:25:PHE:CE2	1:A:67:PHE:CE2	0.43	3.07	13	1
1:A:12:ALA:O	1:A:116:TYR:CD2	0.42	2.72	7	2
1:A:68:ASP:C	1:A:68:ASP:OD2	0.42	2.61	2	1
1:A:27:VAL:HG13	1:A:38:TYR:CD1	0.42	2.49	5	1
1:A:96:ILE:CD1	1:A:116:TYR:CZ	0.42	3.01	7	1
1:A:38:TYR:CG	1:A:62:PRO:HD3	0.42	2.49	16	1
1:A:35:THR:HG22	1:A:36:LYS:HD2	0.42	1.91	3	1
1:A:99:LYS:NZ	1:A:99:LYS:CB	0.42	2.83	4	1
1:A:18:SER:OG	1:A:19:ALA:N	0.42	2.51	18	1
1:A:23:TYR:CD1	1:A:55:VAL:HG22	0.42	2.48	5	1
1:A:4:VAL:N	1:A:124:LEU:O	0.42	2.51	10	2
1:A:95:LEU:C	1:A:95:LEU:HD22	0.42	2.40	15	1
1:A:61:LEU:CG	1:A:62:PRO:HA	0.42	2.45	20	7
1:A:32:THR:O	1:A:34:ASP:N	0.42	2.52	8	2
1:A:70:VAL:CG1	1:A:71:ARG:N	0.42	2.81	10	2
1:A:27:VAL:HG11	1:A:65:ARG:HH22	0.42	1.75	15	1
1:A:3:ALA:HB2	1:A:125:GLU:OE1	0.42	2.14	16	1
1:A:42:ALA:HB2	1:A:55:VAL:HG13	0.42	1.91	16	1
1:A:60:CYS:SG	1:A:61:LEU:N	0.42	2.92	16	1
1:A:3:ALA:CA	1:A:124:LEU:O	0.42	2.67	13	1
1:A:94:HIS:NE2	1:A:96:ILE:CD1	0.42	2.83	13	1
1:A:67:PHE:CE1	1:A:80:VAL:HG11	0.42	2.47	17	1
1:A:102:LYS:HB2	1:A:117:VAL:CG2	0.42	2.45	4	3
1:A:102:LYS:CB	1:A:117:VAL:HG11	0.42	2.45	2	2
1:A:13:SER:OG	1:A:115:ALA:CB	0.42	2.68	6	1
1:A:94:HIS:NE2	1:A:96:ILE:HD11	0.42	2.24	6	1
1:A:87:ASN:OD1	1:A:87:ASN:N	0.42	2.52	13	2
1:A:23:TYR:O	1:A:41:THR:CB	0.42	2.68	16	1
1:A:116:TYR:CD1	1:A:117:VAL:N	0.42	2.88	16	1
1:A:71:ARG:HD3	1:A:76:LEU:CD2	0.42	2.45	19	1
1:A:7:VAL:HG12	1:A:122:PHE:CE2	0.42	2.50	1	2
1:A:70:VAL:C	1:A:76:LEU:HD13	0.42	2.39	11	1
1:A:58:GLY:C	1:A:59:THR:OG1	0.42	2.61	19	1
1:A:122:PHE:CD1	1:A:124:LEU:HD11	0.42	2.50	3	1
1:A:71:ARG:NH1	1:A:114:GLN:OE1	0.42	2.53	7	1
1:A:102:LYS:CE	1:A:117:VAL:HG21	0.42	2.44	13	1
1:A:74:LYS:HZ1	1:A:74:LYS:HA	0.42	1.75	14	1
1:A:76:LEU:CB	1:A:96:ILE:HD12	0.42	2.42	15	1
1:A:67:PHE:CD1	1:A:80:VAL:HB	0.42	2.49	16	1
1:A:73:ASP:C	1:A:75:GLY:N	0.41	2.77	1	1
1:A:68:ASP:C	1:A:78:LEU:HD12	0.41	2.37	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:10:PHE:CG	1:A:122:PHE:CE1	0.41	3.07	7	1
1:A:62:PRO:O	1:A:64:SER:N	0.41	2.53	12	1
1:A:65:ARG:C	1:A:66:THR:HG23	0.41	2.41	9	10
1:A:38:TYR:CE2	1:A:65:ARG:HD2	0.41	2.50	16	1
1:A:57:VAL:CG1	1:A:68:ASP:OD2	0.41	2.68	16	1
1:A:61:LEU:O	1:A:65:ARG:NH2	0.41	2.53	19	1
1:A:94:HIS:CE1	1:A:96:ILE:CG1	0.41	3.03	20	1
1:A:82:VAL:CG1	1:A:90:THR:HB	0.41	2.45	4	1
1:A:69:VAL:O	1:A:69:VAL:HG12	0.41	2.16	11	3
1:A:11:ALA:O	1:A:12:ALA:HB2	0.41	2.15	6	1
1:A:20:MET:HE2	1:A:43:LYS:HB2	0.41	1.91	3	1
1:A:84:VAL:CG2	1:A:85:SER:N	0.41	2.83	15	1
1:A:8:ARG:C	1:A:10:PHE:N	0.41	2.75	17	1
1:A:23:TYR:CD1	1:A:42:ALA:HB3	0.41	2.50	18	1
1:A:79:THR:HG23	1:A:91:LYS:HE2	0.41	1.93	1	1
1:A:78:LEU:CD2	1:A:80:VAL:CG1	0.41	2.98	5	1
1:A:96:ILE:CD1	1:A:116:TYR:OH	0.41	2.68	8	1
1:A:68:ASP:OD1	1:A:68:ASP:N	0.41	2.53	18	1
1:A:91:LYS:O	1:A:127:VAL:HG13	0.41	2.16	19	2
1:A:44:LEU:CD1	1:A:53:PRO:HB2	0.41	2.45	19	1
1:A:57:VAL:CG1	1:A:58:GLY:N	0.41	2.84	2	2
1:A:26:ASN:ND2	1:A:37:GLY:O	0.41	2.54	17	1
1:A:71:ARG:NH2	1:A:72:SER:O	0.41	2.53	1	1
1:A:59:THR:O	1:A:60:CYS:SG	0.41	2.79	18	2
1:A:25:PHE:O	1:A:25:PHE:CG	0.41	2.74	5	1
1:A:65:ARG:HH11	1:A:82:VAL:CG2	0.41	2.27	8	1
1:A:38:TYR:CD1	1:A:65:ARG:HD2	0.41	2.50	11	1
1:A:126:ARG:CZ	1:A:126:ARG:CB	0.41	2.99	12	1
1:A:5:LEU:CD1	1:A:29:GLN:HG2	0.41	2.46	20	1
1:A:122:PHE:HE1	1:A:124:LEU:HD21	0.41	1.73	20	1
1:A:44:LEU:HD22	1:A:53:PRO:CB	0.41	2.46	13	1
1:A:122:PHE:CD2	1:A:122:PHE:O	0.41	2.74	13	1
1:A:81:SER:O	1:A:81:SER:OG	0.41	2.39	17	1
1:A:71:ARG:CD	1:A:72:SER:O	0.41	2.69	18	1
1:A:56:LYS:O	1:A:57:VAL:O	0.40	2.40	1	5
1:A:7:VAL:CG2	1:A:124:LEU:CD1	0.40	2.99	2	3
1:A:56:LYS:C	1:A:57:VAL:O	0.40	2.65	8	1
1:A:10:PHE:CE1	1:A:122:PHE:CZ	0.40	3.09	11	1
1:A:97:PRO:O	1:A:100:ASP:OD2	0.40	2.40	11	1
1:A:28:ILE:CD1	1:A:36:LYS:N	0.40	2.85	1	1
1:A:79:THR:HG23	1:A:91:LYS:HE3	0.40	1.93	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:LEU:HD23	1:A:63:SER:N	0.40	2.32	3	1
1:A:38:TYR:N	1:A:38:TYR:CD2	0.40	2.87	13	1
1:A:48:GLY:C	1:A:51:GLU:O	0.40	2.64	20	1
1:A:54:GLU:O	1:A:68:ASP:OD1	0.40	2.40	3	1
1:A:44:LEU:CD1	1:A:53:PRO:CB	0.40	2.99	7	1
1:A:36:LYS:CG	1:A:37:GLY:N	0.40	2.85	13	1
1:A:40:CYS:C	1:A:41:THR:HG1	0.40	2.24	18	1
1:A:29:GLN:O	1:A:32:THR:HG22	0.40	2.16	20	1
1:A:7:VAL:O	1:A:120:LYS:O	0.40	2.40	1	1
1:A:80:VAL:CG1	1:A:82:VAL:HG23	0.40	2.46	6	1
1:A:60:CYS:HB2	1:A:67:PHE:CE2	0.40	2.52	8	1
1:A:89:PHE:O	1:A:89:PHE:CG	0.40	2.74	8	1
1:A:91:LYS:O	1:A:127:VAL:O	0.40	2.40	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	123/136 (90%)	96±4 (78±3%)	20±4 (16±3%)	7±1 (6±1%)	2	19
All	All	2460/2720 (90%)	1914 (78%)	397 (16%)	149 (6%)	2	19

All 20 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	56	LYS	20
1	A	57	VAL	20
1	A	16	PRO	17
1	A	112	ASP	13
1	A	48	GLY	11
1	A	27	VAL	11
1	A	105	LYS	10
1	A	18	SER	10
1	A	24	SER	7

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Mol	Chain	Res	Type	Models (Total)
1	A	34	ASP	7
1	A	47	ALA	6
1	A	106	GLY	5
1	A	42	ALA	3
1	A	35	THR	2
1	A	33	MET	2
1	A	12	ALA	1
1	A	98	THR	1
1	A	101	ILE	1
1	A	83	GLN	1
1	A	38	TYR	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	105/117 (90%)	87±4 (83±3%)	18±4 (17±3%)	4 38
All	All	2100/2340 (90%)	1743 (83%)	357 (17%)	4 38

All 66 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	95	LEU	20
1	A	80	VAL	17
1	A	90	THR	17
1	A	43	LYS	15
1	A	94	HIS	15
1	A	44	LEU	14
1	A	28	ILE	13
1	A	61	LEU	12
1	A	82	VAL	12
1	A	21	CYS	11
1	A	85	SER	11
1	A	22	SER	10
1	A	76	LEU	10
1	A	93	SER	10

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Mol	Chain	Res	Type	Models (Total)
1	A	36	LYS	10
1	A	5	LEU	9
1	A	67	PHE	8
1	A	96	ILE	8
1	A	70	VAL	7
1	A	99	LYS	7
1	A	129	LEU	6
1	A	81	SER	6
1	A	4	VAL	6
1	A	56	LYS	6
1	A	105	LYS	6
1	A	20	MET	6
1	A	78	LEU	5
1	A	112	ASP	5
1	A	128	ASP	5
1	A	121	ASP	5
1	A	8	ARG	4
1	A	74	LYS	4
1	A	100	ASP	4
1	A	91	LYS	3
1	A	34	ASP	3
1	A	104	VAL	3
1	A	13	SER	2
1	A	65	ARG	2
1	A	127	VAL	2
1	A	79	THR	2
1	A	117	VAL	2
1	A	24	SER	2
1	A	60	CYS	2
1	A	88	SER	2
1	A	120	LYS	2
1	A	2	ASP	2
1	A	73	ASP	2
1	A	102	LYS	2
1	A	41	THR	2
1	A	29	GLN	2
1	A	89	PHE	1
1	A	52	LEU	1
1	A	63	SER	1
1	A	68	ASP	1
1	A	114	GLN	1
1	A	40	CYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	38	TYR	1
1	A	57	VAL	1
1	A	6	ASN	1
1	A	17	HIS	1
1	A	33	MET	1
1	A	101	ILE	1
1	A	103	THR	1
1	A	71	ARG	1
1	A	72	SER	1
1	A	27	VAL	1

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 oligosaccharides 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 93% for the well-defined parts and 89% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *starch_output*

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	1540
Number of shifts mapped to atoms	1540
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	6

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	131	-0.29 ± 0.11	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	120	0.03 ± 0.08	None needed (< 0.5 ppm)
$^{13}C'$	115	0.10 ± 0.14	None needed (< 0.5 ppm)
^{15}N	117	0.19 ± 0.31	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 93%, i.e. 1463 atoms were assigned a chemical shift out of a possible 1569. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	578/605 (96%)	234/246 (95%)	233/246 (95%)	111/113 (98%)
Sidechain	828/873 (95%)	558/571 (98%)	261/275 (95%)	9/27 (33%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	57/91 (63%)	36/45 (80%)	21/44 (48%)	0/2 (0%)
Overall	1463/1569 (93%)	828/862 (96%)	515/565 (91%)	120/142 (85%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 89%, i.e. 1539 atoms were assigned a chemical shift out of a possible 1735. 0 out of 22 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	611/669 (91%)	248/272 (91%)	246/272 (90%)	117/125 (94%)
Sidechain	871/933 (93%)	587/610 (96%)	275/296 (93%)	9/27 (33%)
Aromatic	57/133 (43%)	36/69 (52%)	21/56 (38%)	0/8 (0%)
Overall	1539/1735 (89%)	871/951 (92%)	542/624 (87%)	126/160 (79%)

7.1.4 Statistically unusual chemical shifts (i)

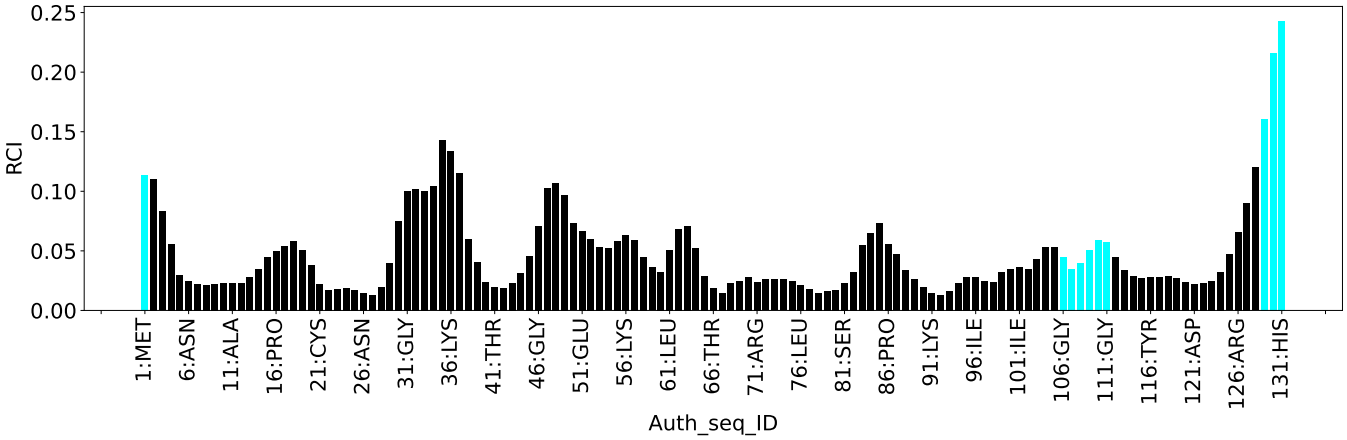
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	79	THR	HG1	6.15	0.08 – 2.19	23.8
1	A	71	ARG	CZ	184.66	141.81 – 177.93	6.9
1	A	126	ARG	CZ	184.63	141.81 – 177.93	6.8
1	A	8	ARG	CZ	184.49	141.81 – 177.93	6.8
1	A	40	CYS	HB2	0.40	0.81 – 5.11	-6.0
1	A	58	GLY	HA2	1.83	2.15 – 5.77	-5.9

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
0.25
0.20
0.15
0.10
0.05
0.00
1:MET
6:ASN
11:ALA
16:PRO
21:CYS
26:ASN
31:GLY
36:LYS
41:THR
46:GLY
51:GLU
56:LYS
61:LEU
66:THR
71:ARG
76:LEU
81:SER
86:PRO
91:LYS
96:ILE
101:ILE
106:GLY
111:GLY
116:TYR
121:ASP
126:ARG
131:HIS
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	2298
Intra-residue (|i-j|=0)	476
Sequential (|i-j|=1)	576
Medium range (|i-j|>1 and |i-j|<5)	213
Long range (|i-j|≥5)	1033
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	195
Number of unmapped restraints	0
Number of restraints per residue	18.3
Number of long range restraints per residue[1]	7.6

[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)	0.5	0.2
0.2-0.5 (Medium)	1.1	0.49
>0.5 (Large)	1.4	1.2

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)

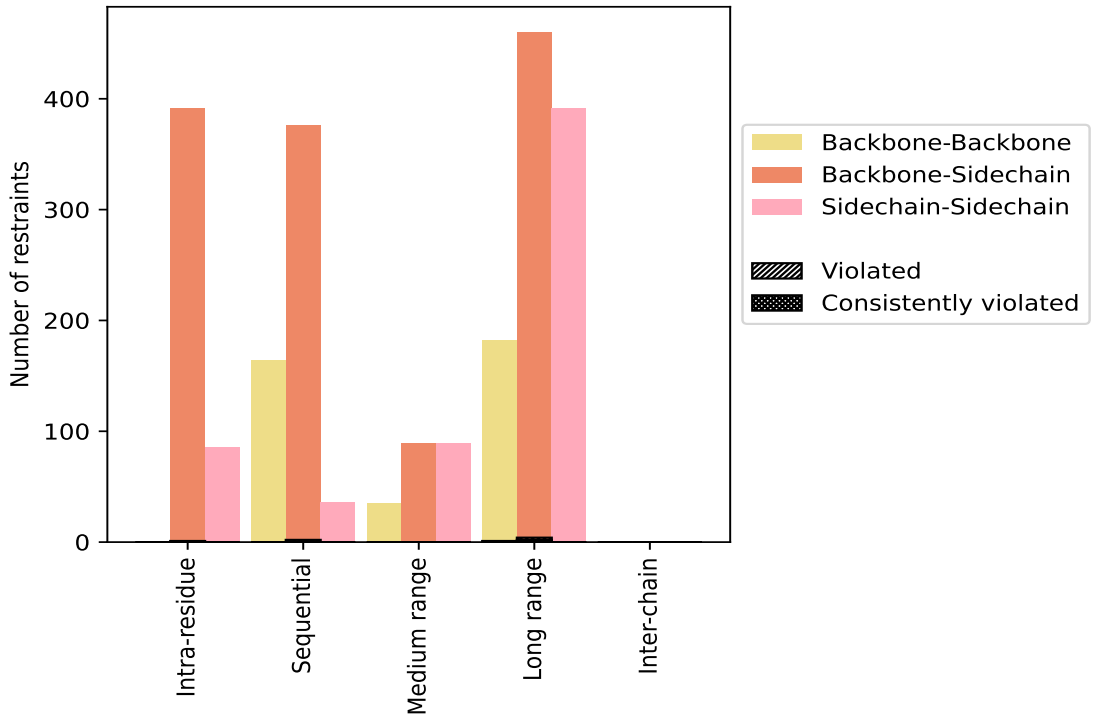
9.1 Summary of distance violations (i)

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)	476	20.7	1	0.2	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	391	17.0	1	0.3	0.0	0	0.0	0.0
Sidechain-Sidechain	85	3.7	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	576	25.1	2	0.3	0.1	0	0.0	0.0
Backbone-Backbone	164	7.1	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	376	16.4	2	0.5	0.1	0	0.0	0.0
Sidechain-Sidechain	36	1.6	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	213	9.3	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	35	1.5	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	89	3.9	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	89	3.9	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	1033	45.0	5	0.5	0.2	2	0.2	0.1
Backbone-Backbone	182	7.9	1	0.5	0.0	0	0.0	0.0
Backbone-Sidechain	460	20.0	4	0.9	0.2	2	0.4	0.1
Sidechain-Sidechain	391	17.0	0	0.0	0.0	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	2298	100.0	8	0.3	0.3	2	0.1	0.1
Backbone-Backbone	381	16.6	1	0.3	0.0	0	0.0	0.0
Backbone-Sidechain	1316	57.3	7	0.5	0.3	2	0.2	0.1
Sidechain-Sidechain	601	26.2	0	0.0	0.0	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



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	1	0	3	0	4	0.35	0.68	0.22	0.31
2	0	0	0	2	0	2	0.72	1.08	0.36	0.72
3	0	0	0	3	0	3	0.35	0.51	0.12	0.34
4	0	0	0	3	0	3	0.56	0.7	0.1	0.51
5	0	1	0	3	0	4	0.63	1.17	0.37	0.59
6	0	0	0	4	0	4	0.62	1.2	0.38	0.58
7	0	0	0	3	0	3	0.44	0.51	0.05	0.41
8	0	0	0	2	0	2	0.43	0.51	0.08	0.43
9	0	1	0	2	0	3	0.54	1.01	0.35	0.44
10	0	0	0	2	0	2	0.64	0.91	0.26	0.64

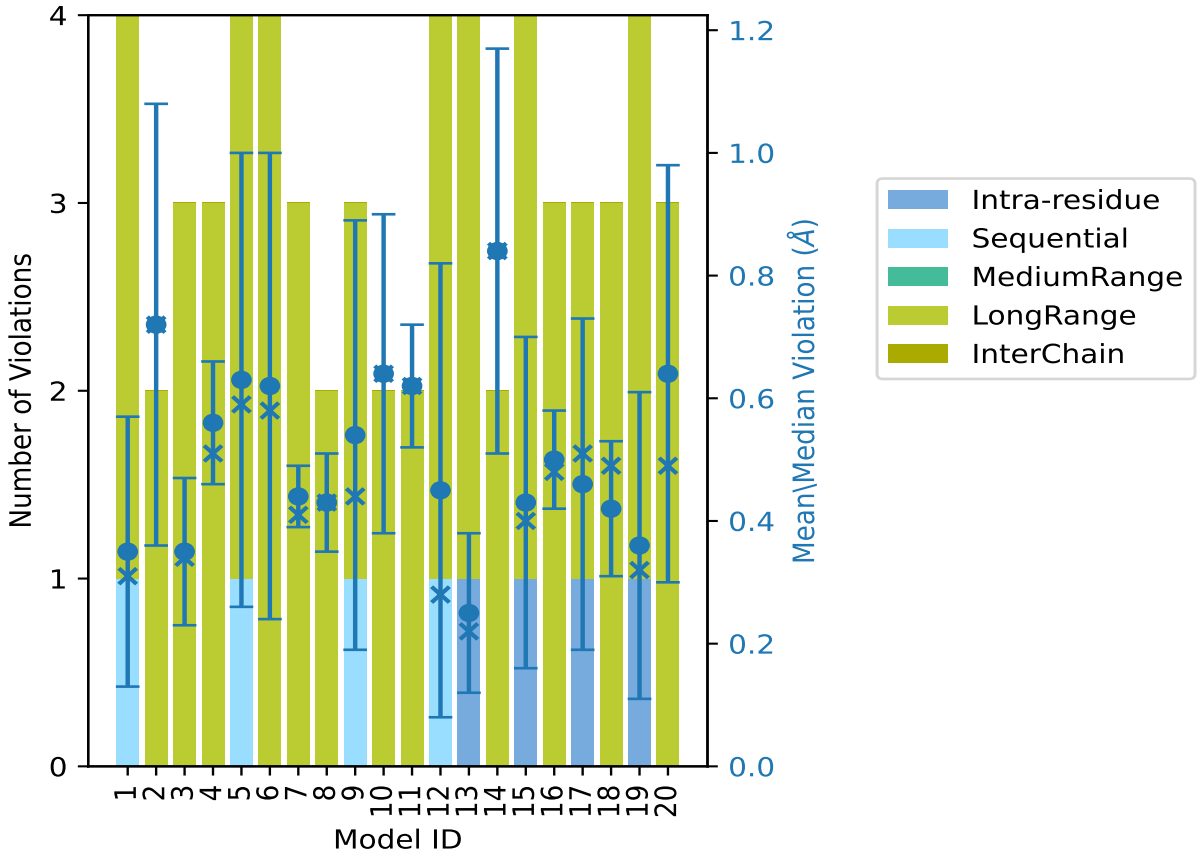
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
11	0	0	0	2	0	2	0.62	0.72	0.1	0.62
12	0	1	0	3	0	4	0.45	1.08	0.37	0.28
13	1	0	0	3	0	4	0.25	0.44	0.13	0.22
14	0	0	0	2	0	2	0.84	1.17	0.33	0.84
15	1	0	0	3	0	4	0.43	0.83	0.27	0.4
16	0	0	0	3	0	3	0.5	0.61	0.08	0.48
17	1	0	0	2	0	3	0.46	0.77	0.27	0.51
18	0	0	0	3	0	3	0.42	0.51	0.11	0.49
19	1	0	0	3	0	4	0.36	0.69	0.25	0.32
20	0	0	0	3	0	3	0.64	1.12	0.34	0.49

[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

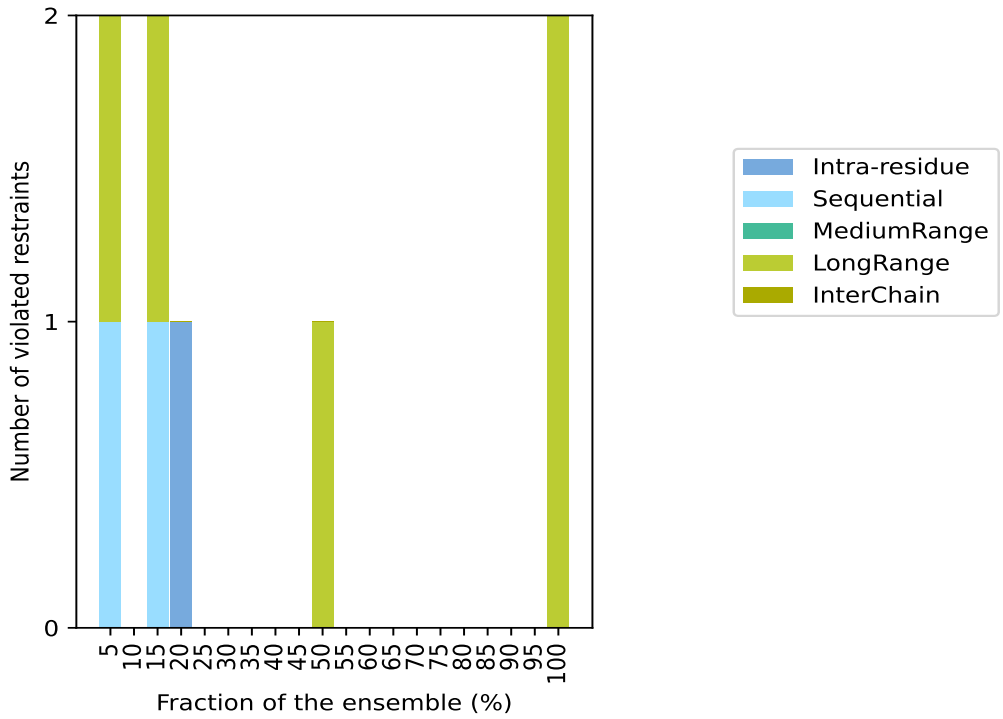
9.3 Distance violation statistics for the ensemble (i)

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, 2290(IR:475, SQ:574, MR:213, LR:1028, 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]	%
0	1	0	1	0	2	1	5.0
0	0	0	0	0	0	2	10.0
0	1	0	1	0	2	3	15.0
1	0	0	0	0	1	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	1	0	1	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	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
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	2	0	2	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

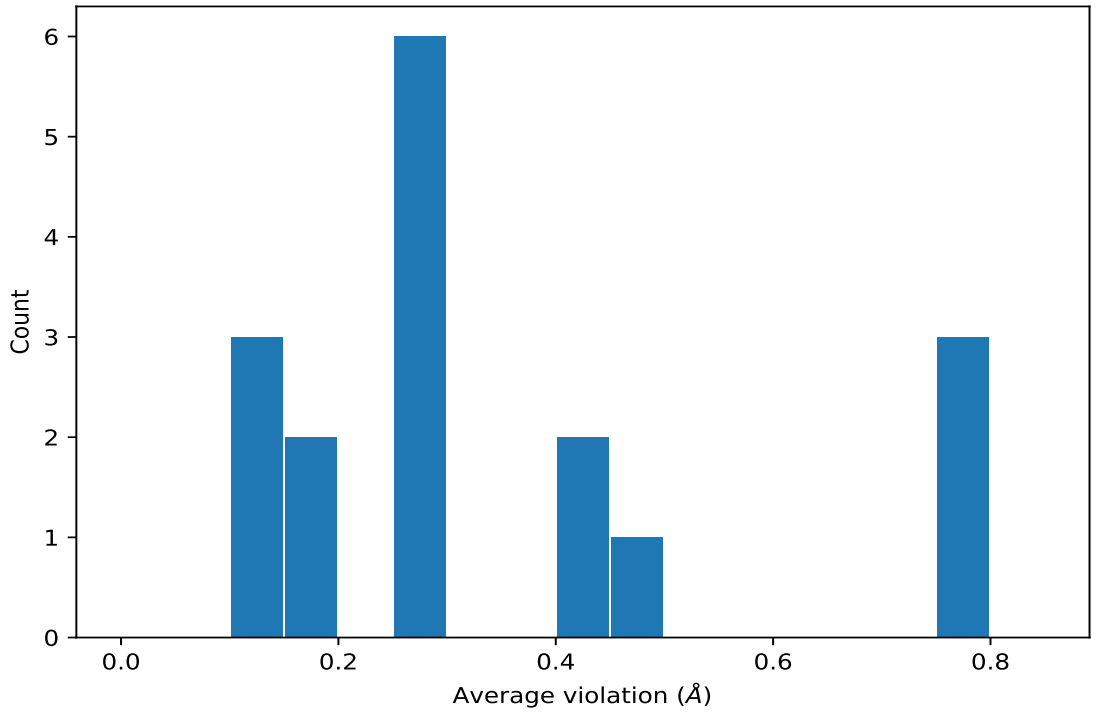
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 (i)

The following table provides the mean and the standard deviation of theviolation 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)
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD11	20	0.78	0.29	0.74
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD12	20	0.78	0.29	0.74
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD13	20	0.78	0.29	0.74
(1,1077)	1:75:A:GLY:HA3	1:101:A:ILE:HG13	20	0.45	0.08	0.51
(1,1592)	1:92:A:GLY:HA3	1:126:A:ARG:HG2	10	0.4	0.21	0.31
(1,1592)	1:92:A:GLY:HA3	1:126:A:ARG:HG3	10	0.4	0.21	0.31
(1,883)	1:110:A:THR:HA	1:110:A:THR:HG21	4	0.1	0.0	0.1
(1,883)	1:110:A:THR:HA	1:110:A:THR:HG22	4	0.1	0.0	0.1
(1,883)	1:110:A:THR:HA	1:110:A:THR:HG23	4	0.1	0.0	0.1
(1,1548)	1:80:A:VAL:HG11	1:92:A:GLY:HA2	3	0.27	0.11	0.28
(1,1548)	1:80:A:VAL:HG12	1:92:A:GLY:HA2	3	0.27	0.11	0.28
(1,1548)	1:80:A:VAL:HG13	1:92:A:GLY:HA2	3	0.27	0.11	0.28
(1,1548)	1:80:A:VAL:HG21	1:92:A:GLY:HA2	3	0.27	0.11	0.28
(1,1548)	1:80:A:VAL:HG22	1:92:A:GLY:HA2	3	0.27	0.11	0.28
(1,1548)	1:80:A:VAL:HG23	1:92:A:GLY:HA2	3	0.27	0.11	0.28
(1,1516)	1:74:A:LYS:HB2	1:75:A:GLY:HA2	3	0.15	0.03	0.16

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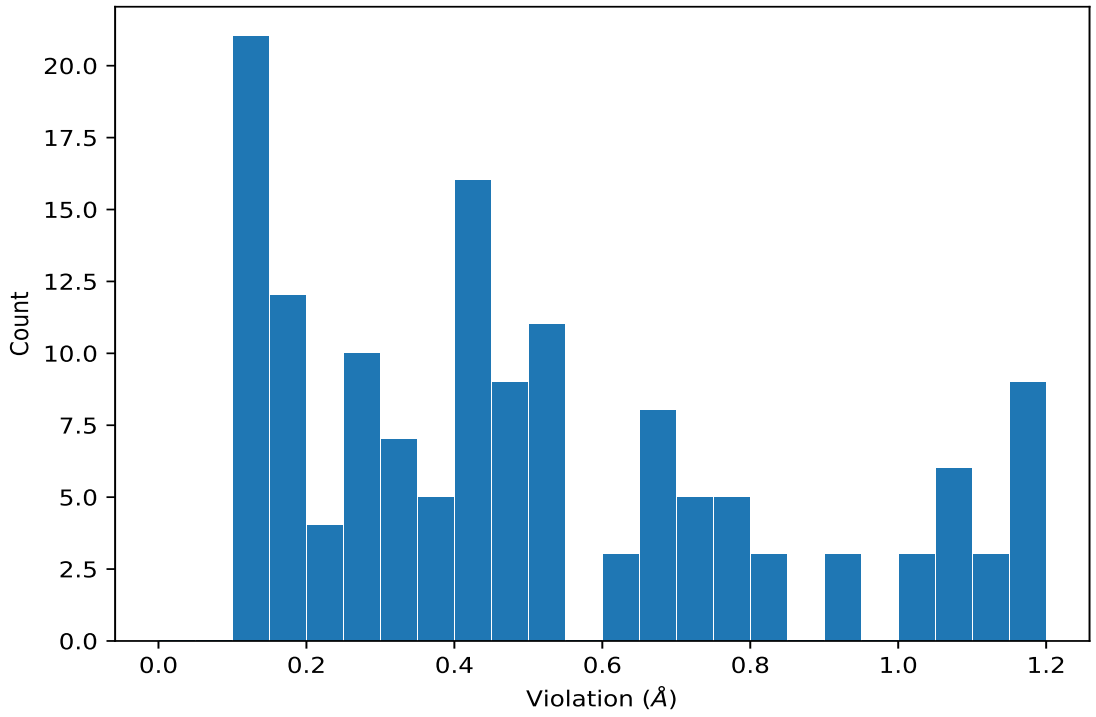
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1516)	1:74:A:LYS:HB3	1:75:A:GLY:HA2	3	0.15	0.03	0.16

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

9.5 All violated distance restraints

9.5.1 Histogram : Distribution of distance violations

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

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)
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD11	6	1.2
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD12	6	1.2
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD13	6	1.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD11	5	1.17
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD12	5	1.17
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD13	5	1.17
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD11	14	1.17
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD12	14	1.17
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD13	14	1.17
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD11	20	1.12
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD12	20	1.12
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD13	20	1.12
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD11	2	1.08
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD12	2	1.08
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD13	2	1.08
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD11	12	1.08
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD12	12	1.08
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD13	12	1.08
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD11	9	1.01
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD12	9	1.01
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD13	9	1.01
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD11	10	0.91
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD12	10	0.91
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD13	10	0.91
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD11	15	0.83
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD12	15	0.83
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD13	15	0.83
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD11	17	0.77
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD12	17	0.77
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD13	17	0.77
(1,1592)	1:92:A:GLY:HA3	1:126:A:ARG:HG2	5	0.75
(1,1592)	1:92:A:GLY:HA3	1:126:A:ARG:HG3	5	0.75
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD11	11	0.72
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD12	11	0.72
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD13	11	0.72
(1,1592)	1:92:A:GLY:HA3	1:126:A:ARG:HG2	4	0.7
(1,1592)	1:92:A:GLY:HA3	1:126:A:ARG:HG3	4	0.7
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD11	19	0.69
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD12	19	0.69
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD13	19	0.69
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD11	1	0.68
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD12	1	0.68
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD13	1	0.68
(1,1592)	1:92:A:GLY:HA3	1:126:A:ARG:HG2	6	0.65
(1,1592)	1:92:A:GLY:HA3	1:126:A:ARG:HG3	6	0.65

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD11	16	0.61
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD12	16	0.61
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD13	16	0.61
(1,1077)	1:75:A:GLY:HA3	1:101:A:ILE:HG13	3	0.51
(1,1077)	1:75:A:GLY:HA3	1:101:A:ILE:HG13	4	0.51
(1,1077)	1:75:A:GLY:HA3	1:101:A:ILE:HG13	6	0.51
(1,1077)	1:75:A:GLY:HA3	1:101:A:ILE:HG13	7	0.51
(1,1077)	1:75:A:GLY:HA3	1:101:A:ILE:HG13	8	0.51
(1,1077)	1:75:A:GLY:HA3	1:101:A:ILE:HG13	11	0.51
(1,1077)	1:75:A:GLY:HA3	1:101:A:ILE:HG13	14	0.51
(1,1077)	1:75:A:GLY:HA3	1:101:A:ILE:HG13	15	0.51
(1,1077)	1:75:A:GLY:HA3	1:101:A:ILE:HG13	17	0.51
(1,1077)	1:75:A:GLY:HA3	1:101:A:ILE:HG13	18	0.51
(1,1077)	1:75:A:GLY:HA3	1:101:A:ILE:HG13	19	0.51
(1,1077)	1:75:A:GLY:HA3	1:101:A:ILE:HG13	20	0.49
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD11	18	0.49
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD12	18	0.49
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD13	18	0.49
(1,1592)	1:92:A:GLY:HA3	1:126:A:ARG:HG2	16	0.48
(1,1592)	1:92:A:GLY:HA3	1:126:A:ARG:HG3	16	0.48
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD11	4	0.46
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD12	4	0.46
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD13	4	0.46
(1,1077)	1:75:A:GLY:HA3	1:101:A:ILE:HG13	9	0.44
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD11	13	0.44
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD12	13	0.44
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD13	13	0.44
(1,1077)	1:75:A:GLY:HA3	1:101:A:ILE:HG13	5	0.43
(1,1077)	1:75:A:GLY:HA3	1:101:A:ILE:HG13	1	0.42
(1,1077)	1:75:A:GLY:HA3	1:101:A:ILE:HG13	16	0.42
(1,1548)	1:80:A:VAL:HG11	1:92:A:GLY:HA2	7	0.41
(1,1548)	1:80:A:VAL:HG12	1:92:A:GLY:HA2	7	0.41
(1,1548)	1:80:A:VAL:HG13	1:92:A:GLY:HA2	7	0.41
(1,1548)	1:80:A:VAL:HG21	1:92:A:GLY:HA2	7	0.41
(1,1548)	1:80:A:VAL:HG22	1:92:A:GLY:HA2	7	0.41
(1,1548)	1:80:A:VAL:HG23	1:92:A:GLY:HA2	7	0.41
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD11	7	0.4
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD12	7	0.4
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD13	7	0.4
(1,1077)	1:75:A:GLY:HA3	1:101:A:ILE:HG13	10	0.38
(1,1077)	1:75:A:GLY:HA3	1:101:A:ILE:HG13	2	0.36
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD11	8	0.35

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD12	8	0.35
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD13	8	0.35
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD11	3	0.34
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD12	3	0.34
(1,977)	1:75:A:GLY:HA2	1:95:A:LEU:HD13	3	0.34
(1,1592)	1:92:A:GLY:HA3	1:126:A:ARG:HG2	20	0.32
(1,1592)	1:92:A:GLY:HA3	1:126:A:ARG:HG3	20	0.32
(1,1592)	1:92:A:GLY:HA3	1:126:A:ARG:HG2	12	0.3
(1,1592)	1:92:A:GLY:HA3	1:126:A:ARG:HG3	12	0.3
(1,1548)	1:80:A:VAL:HG11	1:92:A:GLY:HA2	15	0.28
(1,1548)	1:80:A:VAL:HG12	1:92:A:GLY:HA2	15	0.28
(1,1548)	1:80:A:VAL:HG13	1:92:A:GLY:HA2	15	0.28
(1,1548)	1:80:A:VAL:HG21	1:92:A:GLY:HA2	15	0.28
(1,1548)	1:80:A:VAL:HG22	1:92:A:GLY:HA2	15	0.28
(1,1548)	1:80:A:VAL:HG23	1:92:A:GLY:HA2	15	0.28
(1,1592)	1:92:A:GLY:HA3	1:126:A:ARG:HG2	18	0.27
(1,1592)	1:92:A:GLY:HA3	1:126:A:ARG:HG3	18	0.27
(1,1077)	1:75:A:GLY:HA3	1:101:A:ILE:HG13	13	0.27
(1,1077)	1:75:A:GLY:HA3	1:101:A:ILE:HG13	12	0.25
(1,1592)	1:92:A:GLY:HA3	1:126:A:ARG:HG2	3	0.21
(1,1592)	1:92:A:GLY:HA3	1:126:A:ARG:HG3	3	0.21
(1,1592)	1:92:A:GLY:HA3	1:126:A:ARG:HG2	1	0.2
(1,1592)	1:92:A:GLY:HA3	1:126:A:ARG:HG3	1	0.2
(1,1516)	1:74:A:LYS:HB2	1:75:A:GLY:HA2	9	0.18
(1,1516)	1:74:A:LYS:HB3	1:75:A:GLY:HA2	9	0.18
(1,1592)	1:92:A:GLY:HA3	1:126:A:ARG:HG2	13	0.17
(1,1592)	1:92:A:GLY:HA3	1:126:A:ARG:HG3	13	0.17
(1,1520)	1:75:A:GLY:HA3	1:76:A:LEU:HD11	5	0.17
(1,1520)	1:75:A:GLY:HA3	1:76:A:LEU:HD12	5	0.17
(1,1520)	1:75:A:GLY:HA3	1:76:A:LEU:HD13	5	0.17
(1,1520)	1:75:A:GLY:HA3	1:76:A:LEU:HD21	5	0.17
(1,1520)	1:75:A:GLY:HA3	1:76:A:LEU:HD22	5	0.17
(1,1520)	1:75:A:GLY:HA3	1:76:A:LEU:HD23	5	0.17
(1,1516)	1:74:A:LYS:HB2	1:75:A:GLY:HA2	12	0.16
(1,1516)	1:74:A:LYS:HB3	1:75:A:GLY:HA2	12	0.16
(1,601)	1:92:A:GLY:HA3	1:127:A:VAL:H	19	0.14
(1,1548)	1:80:A:VAL:HG11	1:92:A:GLY:HA2	6	0.13
(1,1548)	1:80:A:VAL:HG12	1:92:A:GLY:HA2	6	0.13
(1,1548)	1:80:A:VAL:HG13	1:92:A:GLY:HA2	6	0.13
(1,1548)	1:80:A:VAL:HG21	1:92:A:GLY:HA2	6	0.13
(1,1548)	1:80:A:VAL:HG22	1:92:A:GLY:HA2	6	0.13
(1,1548)	1:80:A:VAL:HG23	1:92:A:GLY:HA2	6	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1516)	1:74:A:LYS:HB2	1:75:A:GLY:HA2	1	0.11
(1,1516)	1:74:A:LYS:HB3	1:75:A:GLY:HA2	1	0.11
(1,883)	1:110:A:THR:HA	1:110:A:THR:HG21	17	0.11
(1,883)	1:110:A:THR:HA	1:110:A:THR:HG22	17	0.11
(1,883)	1:110:A:THR:HA	1:110:A:THR:HG23	17	0.11
(1,883)	1:110:A:THR:HA	1:110:A:THR:HG21	13	0.1
(1,883)	1:110:A:THR:HA	1:110:A:THR:HG22	13	0.1
(1,883)	1:110:A:THR:HA	1:110:A:THR:HG23	13	0.1
(1,883)	1:110:A:THR:HA	1:110:A:THR:HG21	15	0.1
(1,883)	1:110:A:THR:HA	1:110:A:THR:HG22	15	0.1
(1,883)	1:110:A:THR:HA	1:110:A:THR:HG23	15	0.1
(1,883)	1:110:A:THR:HA	1:110:A:THR:HG21	19	0.1
(1,883)	1:110:A:THR:HA	1:110:A:THR:HG22	19	0.1
(1,883)	1:110:A:THR:HA	1:110:A:THR:HG23	19	0.1

10 Dihedral-angle violation analysis

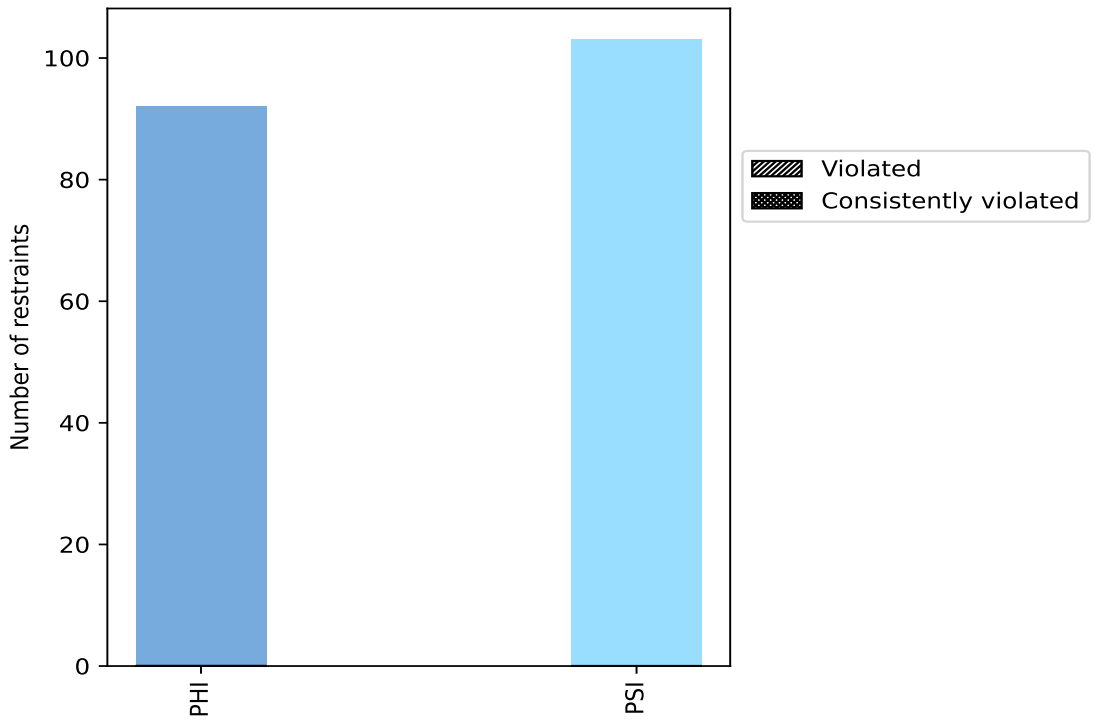
10.1 Summary of dihedral-angle violations

The following table provides the summary of dihedral-angle violations in different dihedral-angle types. Violations less than 1° are not included in the calculation.

Angle type	Count	%[1]	Violated[3]			Consistently Violated[4]		
			Count	%[2]	%[1]	Count	%[2]	%[1]
PHI	92	47.2	0	0.0	0.0	0	0.0	0.0
PSI	103	52.8	0	0.0	0.0	0	0.0	0.0
Total	195	100.0	0	0.0	0.0	0	0.0	0.0

[1] percentage calculated with respect to total number of dihedral-angle restraints, [2] percentage calculated with respect to number of restraints in a particular dihedral-angle type, [3] violated in at least one model, [4] violated in all the models

10.1.1 Bar chart : Distribution of dihedral-angles and violations



Violated and consistently violated restraints are shown using different hatch patterns in their respective categories

10.2 Dihedral-angle violation statistics for each model

No violations found

10.3 Dihedral-angle violation statistics for the ensemble

No violations found

10.4 Most violated dihedral-angle restraints in the ensemble

No violations found

10.5 All violated dihedral-angle restraints

No violations found