Full wwPDB NMR Structure Validation Report (i)

Jun 6, 2023 – 08:36 pm BST

PDB ID	:	6TWR
BMRB ID	:	27893
Title	:	Structure of a constitutively active CAT-PRD1 mutant of the antiterminator LicT protein.
Authors	:	Demene, H.; Declerck, N.; Yinshan, Y.
Deposited on	:	2020-01-13

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:

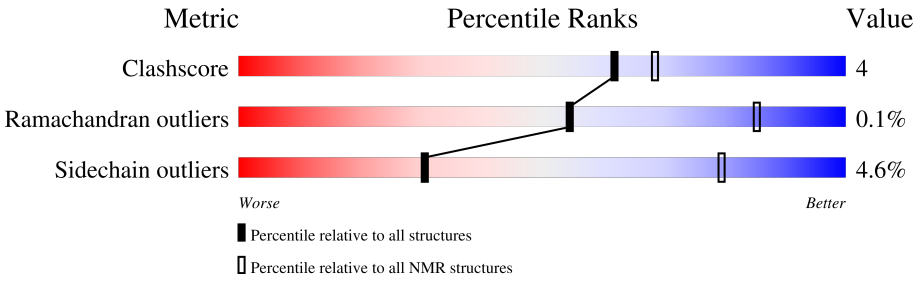
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment is 35%.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	175	87% 7% • •
1	B	175	86% 8% • •

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 4 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:1-A:165, B:1-B:165 (330)	1.10	4

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 4 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5456 atoms, of which 2774 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Beta-glucoside bgl operon antiterminator BglG family.

Mol	Chain	Residues	Atoms						Trace
1	A	169	Total	C	H	N	O	S	0
			2728	854	1387	224	258	5	
1	B	169	Total	C	H	N	O	S	0
			2728	854	1387	224	258	5	

There are 18 discrepancies between the modelled and reference sequences:

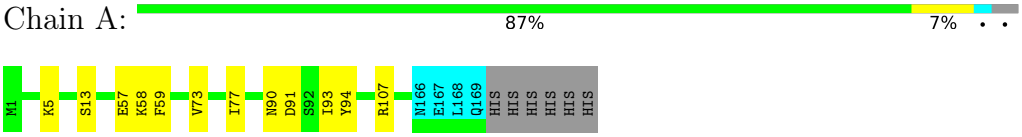
Chain	Residue	Modelled	Actual	Comment	Reference
A	99	ASN	ASP	conflict	UNP A0A063XFU4
A	168	LEU	-	expression tag	UNP A0A063XFU4
A	169	GLN	-	expression tag	UNP A0A063XFU4
A	170	HIS	-	expression tag	UNP A0A063XFU4
A	171	HIS	-	expression tag	UNP A0A063XFU4
A	172	HIS	-	expression tag	UNP A0A063XFU4
A	173	HIS	-	expression tag	UNP A0A063XFU4
A	174	HIS	-	expression tag	UNP A0A063XFU4
A	175	HIS	-	expression tag	UNP A0A063XFU4
B	99	ASN	ASP	engineered mutation	UNP A0A063XFU4
B	168	LEU	-	expression tag	UNP A0A063XFU4
B	169	GLN	-	expression tag	UNP A0A063XFU4
B	170	HIS	-	expression tag	UNP A0A063XFU4
B	171	HIS	-	expression tag	UNP A0A063XFU4
B	172	HIS	-	expression tag	UNP A0A063XFU4
B	173	HIS	-	expression tag	UNP A0A063XFU4
B	174	HIS	-	expression tag	UNP A0A063XFU4
B	175	HIS	-	expression tag	UNP A0A063XFU4

4 Residue-property plots (i)

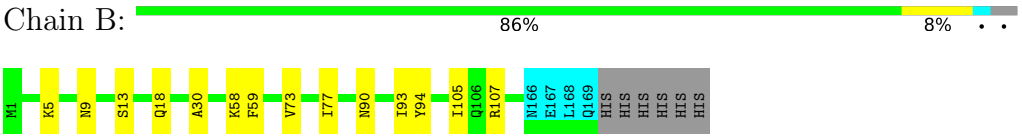
4.1 Average score per residue in the NMR ensemble

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: Beta-glucoside bgl operon antiterminator BglG family



• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

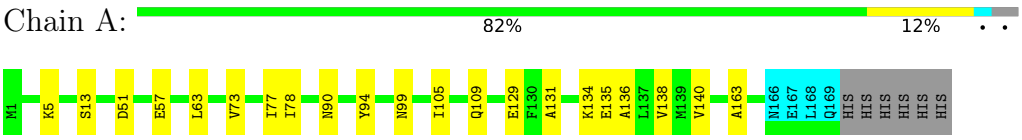


4.2 Scores per residue for each member of the ensemble

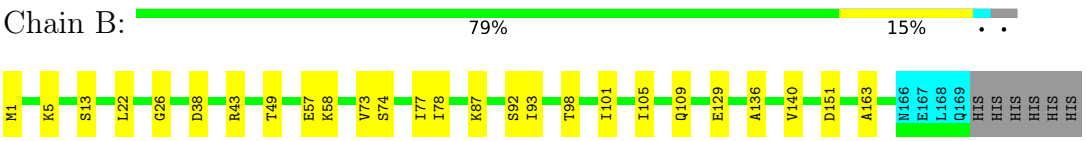
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family



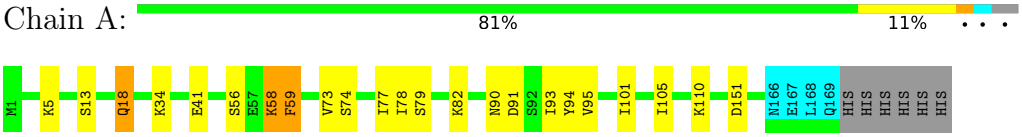
• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family



4.2.2 Score per residue for model 2

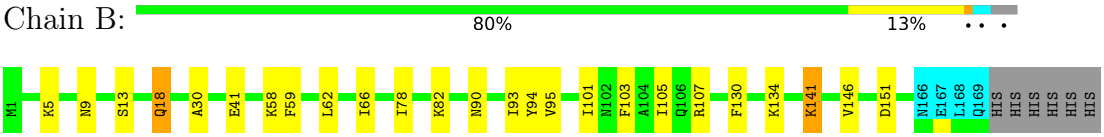
• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A:



• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

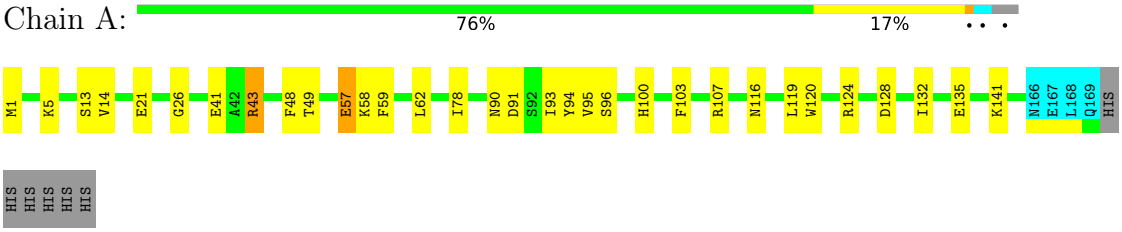
Chain B:



4.2.3 Score per residue for model 3

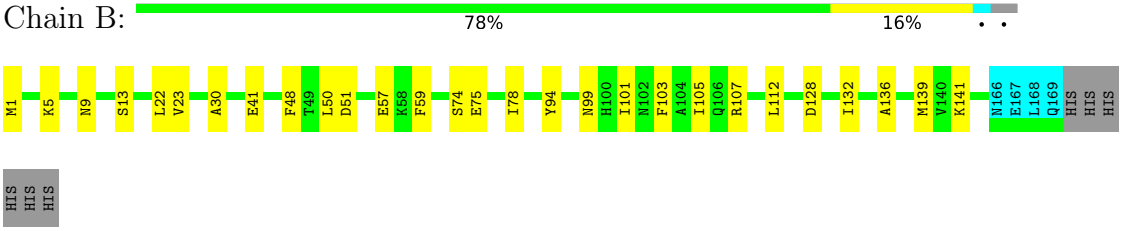
• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A:



• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

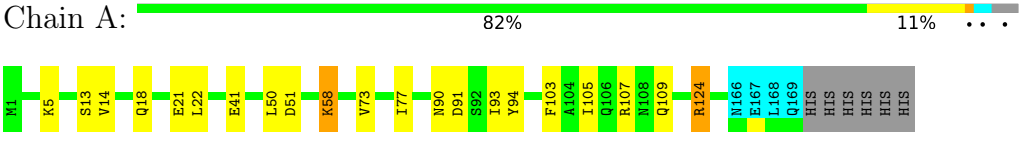
Chain B:



4.2.4 Score per residue for model 4 (medoid)

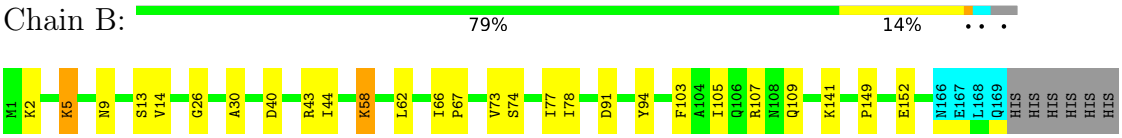
• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A:



• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

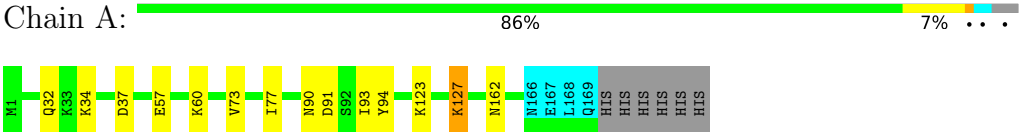
Chain B:



4.2.5 Score per residue for model 5

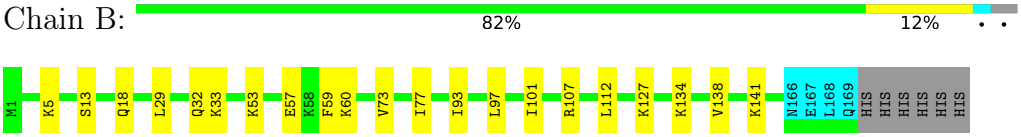
• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A:



• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

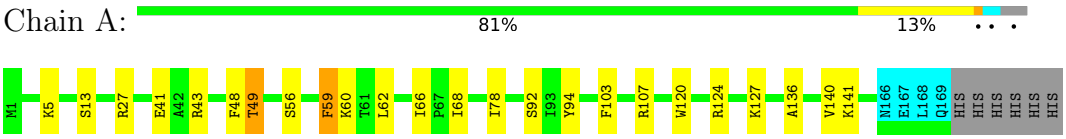
Chain B:



4.2.6 Score per residue for model 6

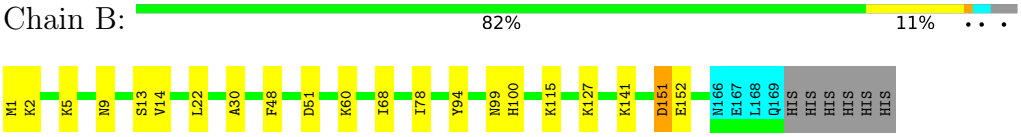
• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A:



• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

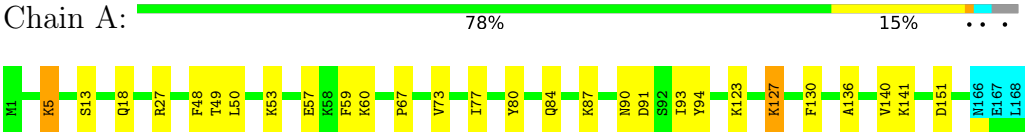
Chain B:



4.2.7 Score per residue for model 7

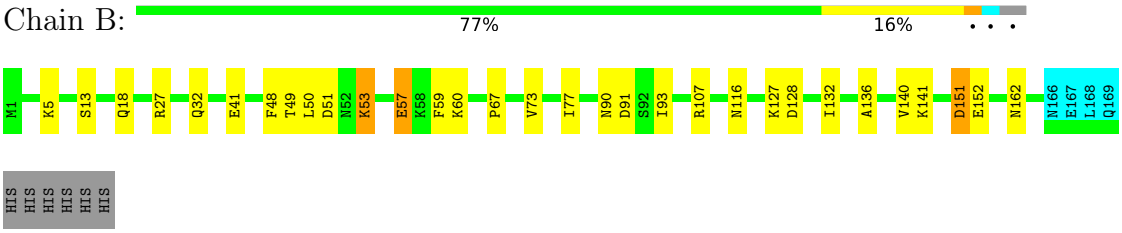
• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A:



• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

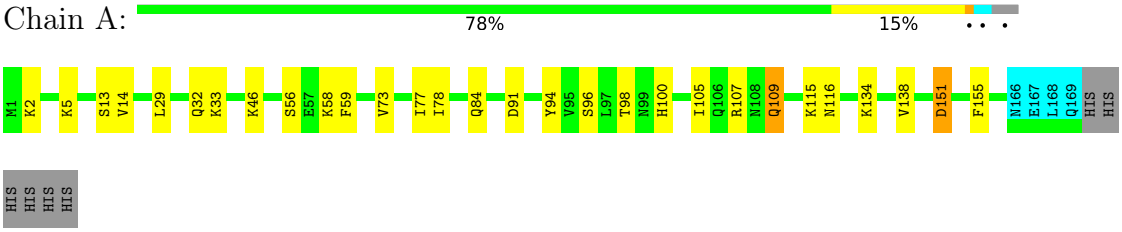
Chain B:



4.2.8 Score per residue for model 8

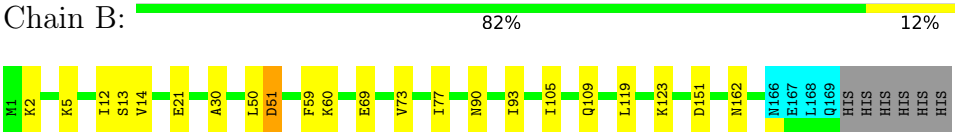
• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A:



• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

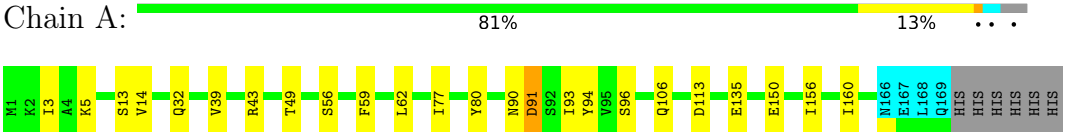
Chain B:



4.2.9 Score per residue for model 9

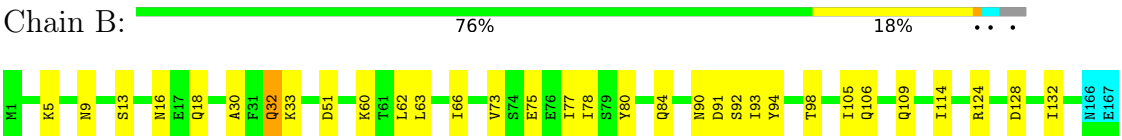
• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A:



• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

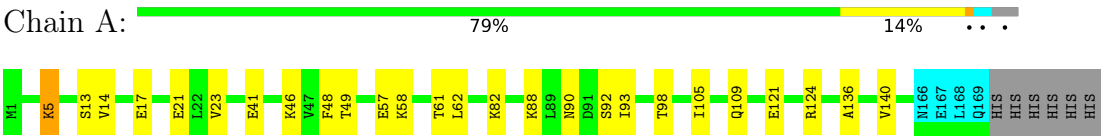
Chain B:



4.2.10 Score per residue for model 10

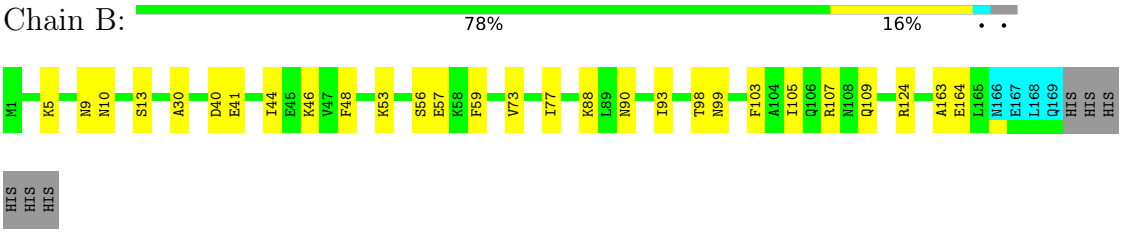
• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A:



• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

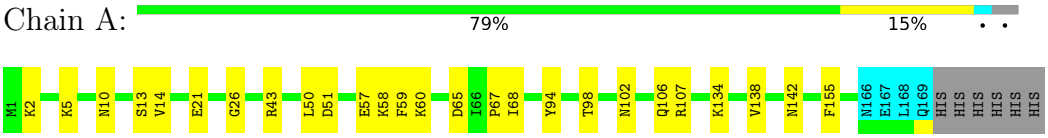
Chain B:



4.2.11 Score per residue for model 11

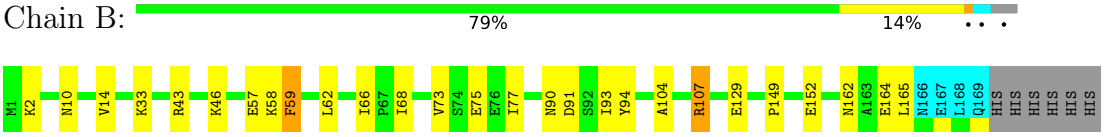
• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A:



• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

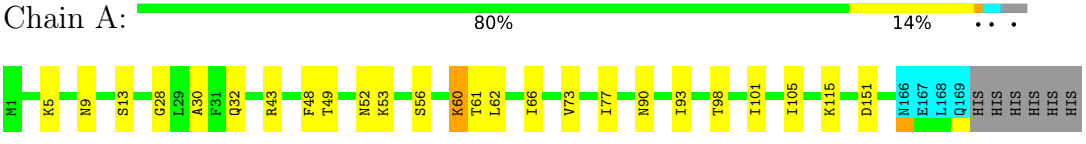
Chain B:



4.2.12 Score per residue for model 12

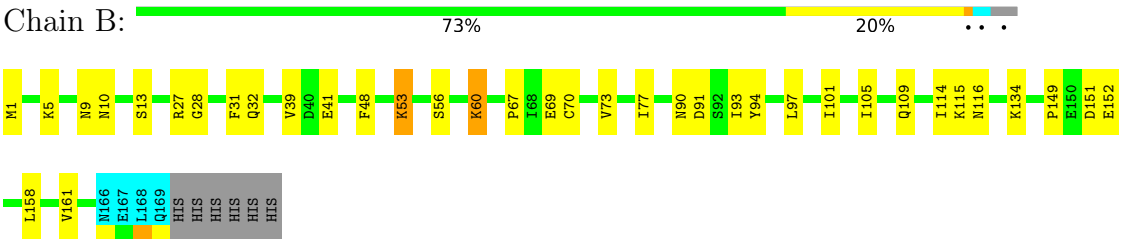
• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A:



• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

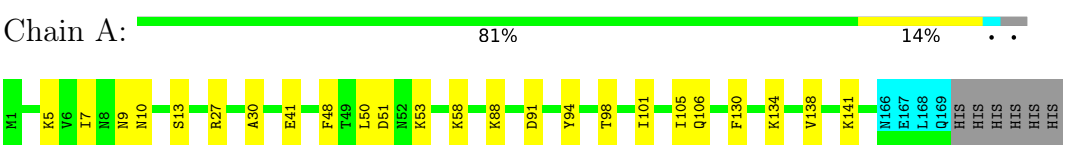
Chain B:



4.2.13 Score per residue for model 13

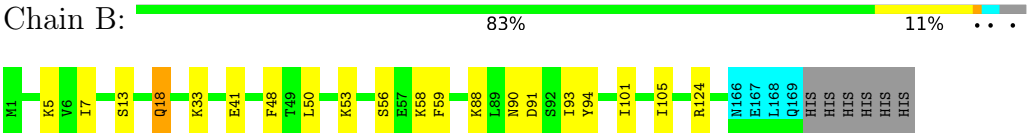
• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A:



• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

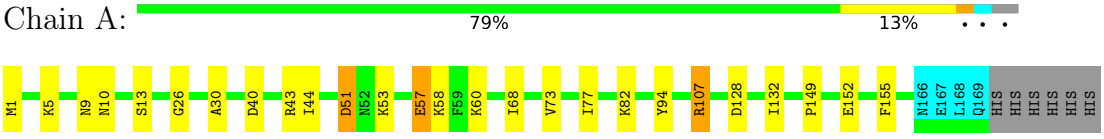
Chain B:



4.2.14 Score per residue for model 14

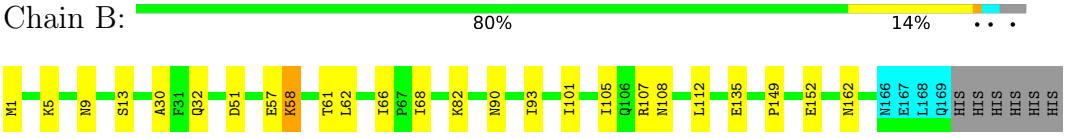
• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A:



• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

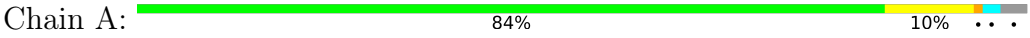
Chain B:



4.2.15 Score per residue for model 15

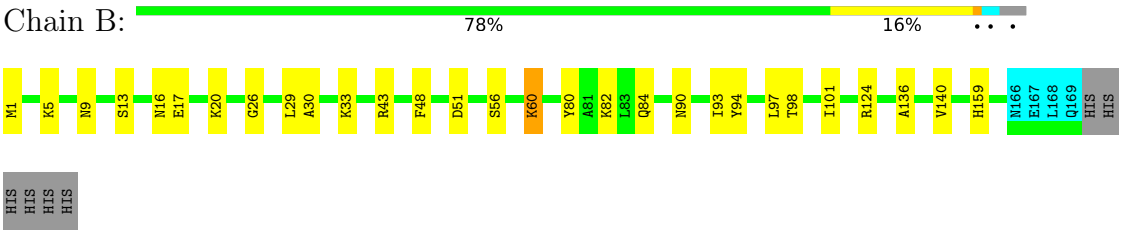
• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A:



• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

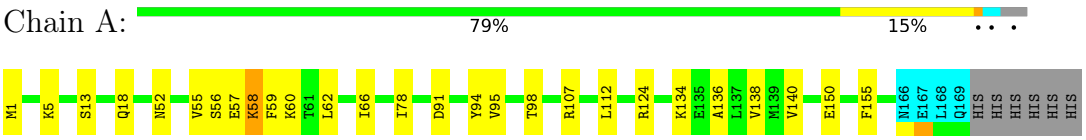
Chain B:



4.2.16 Score per residue for model 16

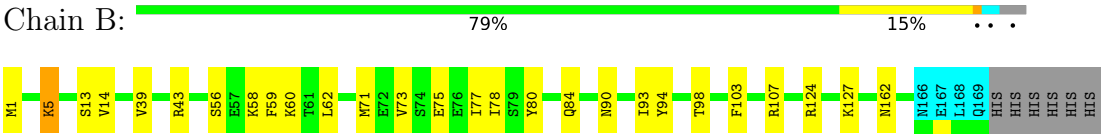
• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A:



• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

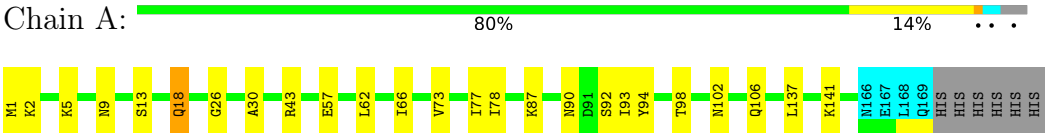
Chain B:



4.2.17 Score per residue for model 17

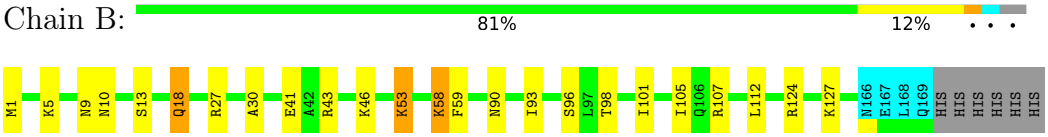
• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A:



• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

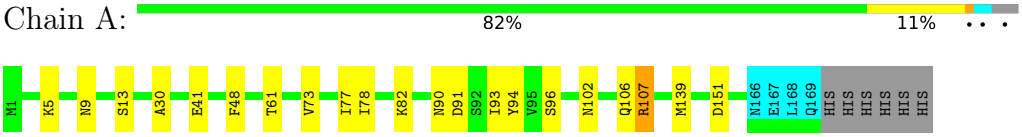
Chain B:



4.2.18 Score per residue for model 18

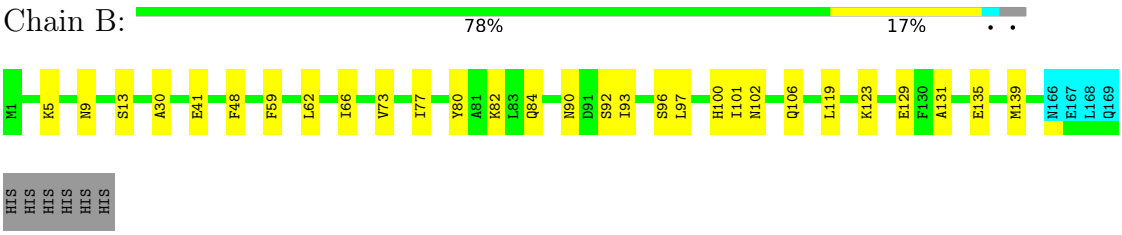
• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A:



• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

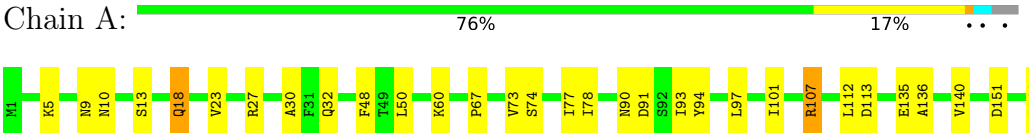
Chain B:



4.2.19 Score per residue for model 19

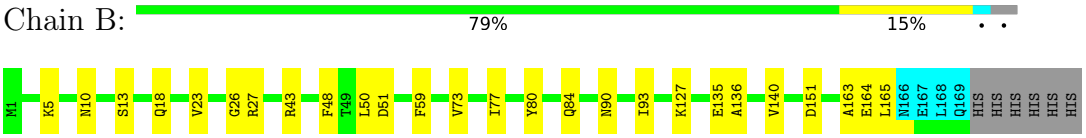
• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A:



• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

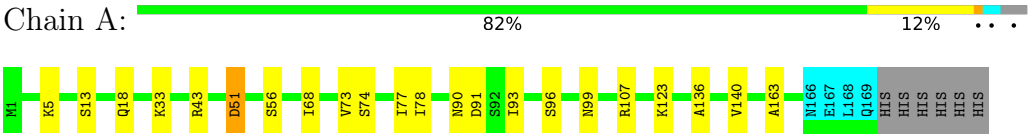
Chain B:



4.2.20 Score per residue for model 20

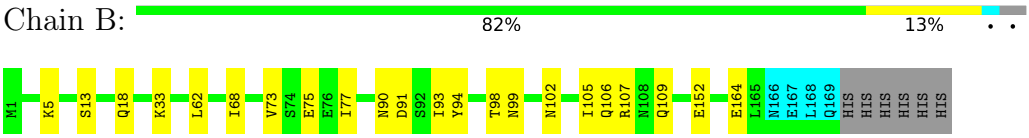
• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain A:



• Molecule 1: Beta-glucoside bgl operon antiterminator BglG family

Chain B:


82%
13%
M1
K5
S13
Q18
K33
L62
I68
V73
S74
E75
E76
I77
N90
D91
S92
I93
Y94
T98
N99
N102
I105
Q106
R107
N108
Q109
E152
E164
L165
N166
E167
L168
Q169
HIS
HIS
HIS
HIS
HIS
HIS

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: *structures with the least restraint violations*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CYANA	structure calculation	3.0
CNS	structure calculation	3.1
CNS	refinement	Xplor

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	1643
Number of shifts mapped to atoms	1643
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	35%

6 Model quality

6.1 Standard geometry

There are no covalent bond-length or bond-angle outliers.

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	B	0.0±0.0	0.1±0.3
1	A	0.0±0.0	0.3±0.5
All	All	0	9

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
1	A	43	ARG	Sidechain	5
1	A	107	ARG	Sidechain	2
1	B	43	ARG	Sidechain	2

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	1306	1356	1356	13±3
1	B	1306	1356	1356	14±4
All	All	52240	54240	54240	475

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:5:LYS:HB2	1:B:13:SER:HB2	0.69	1.63	2	5
1:A:5:LYS:HB2	1:A:13:SER:HB2	0.67	1.64	18	8
1:A:5:LYS:HB3	1:A:13:SER:HB2	0.66	1.68	17	11
1:B:5:LYS:HB3	1:B:13:SER:HB2	0.65	1.67	16	14
1:A:96:SER:HA	1:B:92:SER:OG	0.65	1.91	9	2
1:B:18:GLN:HE21	1:B:18:GLN:N	0.63	1.92	17	3
1:B:108:ASN:HA	1:B:112:LEU:O	0.62	1.93	14	1
1:B:116:ASN:H	1:B:151:ASP:HB2	0.61	1.55	12	1
1:A:155:PHE:HB3	1:B:162:ASN:ND2	0.60	2.10	8	4
1:A:18:GLN:HE21	1:A:18:GLN:N	0.59	1.94	19	2
1:B:91:ASP:HA	1:B:94:TYR:CD1	0.58	2.32	4	4
1:A:90:ASN:O	1:A:93:ILE:HG22	0.58	1.98	19	13
1:A:91:ASP:HA	1:A:94:TYR:CD1	0.58	2.34	9	3
1:A:5:LYS:HB2	1:A:13:SER:CB	0.57	2.29	18	6
1:A:116:ASN:H	1:A:151:ASP:HB2	0.57	1.60	8	1
1:A:62:LEU:O	1:A:66:ILE:HG12	0.57	2.00	17	1
1:A:48:PHE:CE1	1:B:50:LEU:HB2	0.56	2.36	19	2
1:B:1:MET:SD	1:B:39:VAL:HB	0.56	2.39	12	1
1:B:5:LYS:HB2	1:B:13:SER:CB	0.56	2.30	2	5
1:B:105:ILE:O	1:B:109:GLN:HG2	0.56	2.01	10	6
1:A:5:LYS:HB3	1:A:13:SER:CB	0.55	2.31	17	8
1:A:78:ILE:HG21	1:A:94:TYR:CZ	0.55	2.37	3	1
1:B:103:PHE:O	1:B:107:ARG:HG2	0.55	2.01	4	2
1:A:9:ASN:HA	1:A:30:ALA:HB3	0.55	1.79	18	6
1:A:14:VAL:HG11	1:A:39:VAL:HG22	0.54	1.78	9	1
1:B:5:LYS:HB3	1:B:13:SER:CB	0.54	2.33	16	12
1:A:48:PHE:CE2	1:B:50:LEU:HB2	0.53	2.38	3	2
1:B:80:TYR:O	1:B:84:GLN:HG2	0.53	2.03	9	5
1:B:90:ASN:O	1:B:93:ILE:HG22	0.53	2.02	8	15
1:A:18:GLN:OE1	1:B:67:PRO:HA	0.53	2.03	4	2
1:A:58:LYS:NZ	1:A:58:LYS:HA	0.53	2.18	2	2
1:A:10:ASN:OD1	1:A:27:ARG:HA	0.53	2.04	19	2
1:B:73:VAL:O	1:B:77:ILE:HG13	0.53	2.04	1	13
1:B:9:ASN:HA	1:B:30:ALA:HB3	0.53	1.80	2	10
1:B:27:ARG:O	1:B:43:ARG:HD3	0.52	2.05	17	1
1:B:74:SER:O	1:B:78:ILE:HG12	0.52	2.04	3	3
1:A:94:TYR:CZ	1:B:58:LYS:HG2	0.52	2.39	14	2
1:A:92:SER:HB2	1:B:99:ASN:CB	0.52	2.35	6	1
1:A:105:ILE:O	1:A:109:GLN:HG2	0.52	2.05	10	4
1:A:56:SER:HB3	1:A:59:PHE:HB2	0.52	1.82	2	3
1:A:62:LEU:O	1:A:66:ILE:HG13	0.52	2.04	16	3
1:A:92:SER:OG	1:B:96:SER:HA	0.51	2.05	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:102:ASN:O	1:B:106:GLN:HG2	0.51	2.05	18	2
1:A:123:LYS:O	1:A:127:LYS:HB3	0.51	2.05	7	2
1:A:50:LEU:HB2	1:B:48:PHE:CE2	0.51	2.41	19	2
1:A:73:VAL:O	1:A:77:ILE:HG13	0.51	2.06	8	13
1:B:56:SER:HB3	1:B:59:PHE:HB2	0.51	1.82	13	3
1:B:78:ILE:HB	1:B:94:TYR:CE2	0.51	2.40	9	1
1:A:90:ASN:HB3	1:A:163:ALA:HA	0.50	1.83	1	1
1:A:67:PRO:HA	1:B:18:GLN:OE1	0.50	2.07	7	2
1:A:120:TRP:O	1:A:124:ARG:HG2	0.50	2.05	3	2
1:B:101:ILE:O	1:B:105:ILE:HG12	0.50	2.06	13	4
1:A:107:ARG:NH1	1:A:113:ASP:HA	0.50	2.22	19	1
1:A:49:THR:O	1:B:48:PHE:HA	0.50	2.06	6	6
1:B:62:LEU:HD22	1:B:99:ASN:OD1	0.50	2.07	20	1
1:A:78:ILE:O	1:A:82:LYS:HG2	0.50	2.06	2	1
1:A:96:SER:O	1:A:100:HIS:HB2	0.50	2.07	8	2
1:B:5:LYS:CB	1:B:13:SER:HB2	0.50	2.37	1	2
1:A:3:ILE:HA	1:A:14:VAL:HG12	0.50	1.84	9	1
1:A:99:ASN:HB2	1:B:92:SER:OG	0.50	2.07	1	1
1:B:26:GLY:HA3	1:B:43:ARG:O	0.50	2.07	1	4
1:A:124:ARG:HA	1:A:124:ARG:NE	0.49	2.21	16	2
1:B:56:SER:O	1:B:60:LYS:HG2	0.49	2.07	15	1
1:B:62:LEU:O	1:B:66:ILE:HG12	0.49	2.07	18	2
1:B:53:LYS:O	1:B:57:GLU:HB3	0.49	2.08	7	1
1:A:107:ARG:HB3	1:A:112:LEU:O	0.49	2.06	16	2
1:A:101:ILE:O	1:A:105:ILE:HG12	0.49	2.08	2	3
1:A:110:LYS:O	1:A:110:LYS:HD3	0.49	2.08	2	1
1:A:52:ASN:O	1:A:56:SER:HB3	0.49	2.07	12	1
1:A:9:ASN:ND2	1:A:28:GLY:HA2	0.49	2.22	12	1
1:B:62:LEU:O	1:B:66:ILE:HG13	0.48	2.07	11	4
1:A:94:TYR:HB3	1:B:59:PHE:CE2	0.48	2.43	11	2
1:A:94:TYR:CE2	1:B:58:LYS:HG3	0.48	2.43	13	1
1:A:58:LYS:O	1:A:62:LEU:HG	0.48	2.08	10	2
1:A:48:PHE:HB3	1:B:48:PHE:HB3	0.48	1.85	3	7
1:B:60:LYS:CE	1:B:60:LYS:HA	0.48	2.38	12	1
1:A:162:ASN:HD22	1:B:159:HIS:CD2	0.48	2.27	15	1
1:B:58:LYS:HA	1:B:58:LYS:HE3	0.48	1.84	17	1
1:A:74:SER:O	1:A:78:ILE:HG12	0.48	2.09	20	3
1:A:2:LYS:O	1:A:14:VAL:HG23	0.48	2.08	8	2
1:B:40:ASP:O	1:B:44:ILE:HG13	0.48	2.08	10	2
1:B:58:LYS:NZ	1:B:58:LYS:HA	0.48	2.24	4	1
1:A:102:ASN:O	1:A:106:GLN:HG2	0.48	2.09	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:115:LYS:HA	1:B:151:ASP:OD1	0.48	2.09	12	1
1:A:51:ASP:OD1	1:A:56:SER:HB2	0.48	2.08	20	1
1:B:130:PHE:CE2	1:B:134:LYS:HE3	0.48	2.44	2	1
1:A:59:PHE:CE2	1:B:94:TYR:HB3	0.48	2.44	9	3
1:A:91:ASP:HB2	1:B:62:LEU:CB	0.47	2.39	16	1
1:B:149:PRO:HD2	1:B:152:GLU:OE1	0.47	2.09	12	4
1:B:69:GLU:O	1:B:73:VAL:HG23	0.47	2.09	12	2
1:B:10:ASN:OD1	1:B:27:ARG:HA	0.47	2.10	19	3
1:B:16:ASN:OD1	1:B:20:LYS:HB2	0.47	2.09	15	1
1:A:103:PHE:O	1:A:107:ARG:HG2	0.47	2.09	4	1
1:B:116:ASN:N	1:B:151:ASP:HB2	0.47	2.23	12	1
1:A:57:GLU:OE2	1:A:58:LYS:HG2	0.47	2.10	3	1
1:A:34:LYS:HG2	1:A:37:ASP:OD2	0.47	2.10	5	1
1:B:115:LYS:HG2	1:B:151:ASP:OD2	0.47	2.10	6	1
1:A:58:LYS:HG3	1:B:94:TYR:CZ	0.47	2.45	13	1
1:A:115:LYS:HA	1:A:151:ASP:OD2	0.46	2.10	8	1
1:A:62:LEU:HD11	1:B:91:ASP:O	0.46	2.10	9	1
1:A:51:ASP:OD1	1:A:60:LYS:HE2	0.46	2.10	11	1
1:A:94:TYR:CE2	1:B:58:LYS:HG2	0.46	2.46	1	1
1:B:2:LYS:O	1:B:14:VAL:HG23	0.46	2.11	11	4
1:B:158:LEU:O	1:B:161:VAL:HG22	0.46	2.10	12	1
1:A:93:ILE:HB	1:A:163:ALA:CB	0.46	2.40	20	1
1:B:87:LYS:HA	1:B:87:LYS:HE2	0.46	1.88	1	1
1:B:75:GLU:HA	1:B:94:TYR:CE2	0.46	2.45	9	1
1:A:48:PHE:CE1	1:B:23:VAL:HG23	0.46	2.46	19	1
1:B:51:ASP:OD2	1:B:60:LYS:HG3	0.46	2.10	8	1
1:A:26:GLY:HA3	1:A:43:ARG:O	0.46	2.10	11	4
1:A:59:PHE:CE1	1:B:95:VAL:HG22	0.46	2.46	2	1
1:B:78:ILE:O	1:B:82:LYS:HG2	0.46	2.11	2	1
1:A:124:ARG:O	1:A:124:ARG:HD3	0.46	2.10	4	1
1:A:78:ILE:CD1	1:A:94:TYR:HA	0.46	2.41	17	4
1:A:80:TYR:O	1:A:84:GLN:HG2	0.46	2.10	7	2
1:B:119:LEU:O	1:B:123:LYS:HG2	0.46	2.11	18	1
1:A:128:ASP:O	1:A:132:ILE:HG12	0.46	2.11	14	2
1:A:48:PHE:HA	1:B:49:THR:O	0.46	2.11	7	1
1:A:56:SER:HA	1:B:75:GLU:OE2	0.46	2.11	9	1
1:A:107:ARG:N	1:A:107:ARG:HE	0.46	2.09	14	1
1:A:5:LYS:CB	1:A:13:SER:HB2	0.45	2.40	4	2
1:A:103:PHE:O	1:A:107:ARG:HG3	0.45	2.10	3	2
1:B:32:GLN:O	1:B:33:LYS:HD2	0.45	2.10	9	1
1:A:107:ARG:HD3	1:A:112:LEU:O	0.45	2.10	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:136:ALA:O	1:A:140:VAL:HG23	0.45	2.11	7	7
1:B:93:ILE:HB	1:B:163:ALA:CB	0.45	2.41	19	2
1:A:58:LYS:HA	1:A:58:LYS:HE3	0.45	1.89	16	1
1:B:60:LYS:HA	1:B:60:LYS:HE3	0.45	1.87	12	1
1:A:49:THR:HG21	1:B:63:LEU:HD13	0.45	1.89	9	1
1:A:56:SER:O	1:A:60:LYS:HG2	0.45	2.12	12	1
1:B:128:ASP:O	1:B:132:ILE:HG12	0.45	2.12	9	3
1:B:100:HIS:NE2	1:B:152:GLU:HB3	0.45	2.26	6	1
1:B:103:PHE:O	1:B:107:ARG:HG3	0.45	2.12	16	2
1:A:21:GLU:O	1:A:50:LEU:HB2	0.44	2.13	11	2
1:B:97:LEU:O	1:B:101:ILE:HG12	0.44	2.11	12	4
1:A:56:SER:HA	1:B:75:GLU:OE1	0.44	2.12	9	2
1:A:77:ILE:O	1:A:80:TYR:HB3	0.44	2.12	9	1
1:A:95:VAL:HG22	1:B:59:PHE:CE1	0.44	2.48	2	2
1:B:134:LYS:O	1:B:138:VAL:HG23	0.44	2.12	5	1
1:B:78:ILE:CD1	1:B:94:TYR:HA	0.44	2.42	16	2
1:A:130:PHE:O	1:A:134:LYS:HB2	0.44	2.12	13	1
1:A:14:VAL:CG2	1:A:22:LEU:HB2	0.44	2.42	4	1
1:A:23:VAL:HG23	1:B:48:PHE:CE2	0.44	2.47	19	2
1:B:90:ASN:HB3	1:B:163:ALA:HA	0.44	1.89	10	1
1:A:14:VAL:O	1:A:21:GLU:HA	0.43	2.12	3	2
1:B:60:LYS:HB2	1:B:60:LYS:HZ2	0.43	1.72	9	1
1:B:107:ARG:HB3	1:B:112:LEU:O	0.43	2.12	5	2
1:B:71:MET:HA	1:B:98:THR:HG22	0.43	1.91	16	1
1:B:33:LYS:HA	1:B:33:LYS:HE2	0.43	1.90	20	1
1:B:136:ALA:O	1:B:140:VAL:HG23	0.43	2.14	7	4
1:A:78:ILE:HB	1:A:94:TYR:CZ	0.43	2.48	8	1
1:B:9:ASN:OD1	1:B:28:GLY:HA2	0.43	2.13	12	1
1:A:94:TYR:CZ	1:B:58:LYS:HG3	0.43	2.48	13	1
1:A:51:ASP:OD1	1:A:60:LYS:HG2	0.43	2.13	14	1
1:A:78:ILE:HG21	1:A:94:TYR:CE1	0.43	2.49	2	1
1:B:13:SER:HA	1:B:22:LEU:O	0.43	2.14	1	3
1:A:29:LEU:O	1:A:33:LYS:HD3	0.43	2.14	8	1
1:B:104:ALA:O	1:B:107:ARG:HG3	0.43	2.14	11	1
1:B:105:ILE:O	1:B:109:GLN:HG3	0.43	2.14	20	1
1:B:29:LEU:O	1:B:33:LYS:HD2	0.43	2.14	5	1
1:A:94:TYR:CZ	1:B:58:LYS:HB2	0.42	2.50	2	1
1:A:91:ASP:HA	1:A:94:TYR:CD2	0.42	2.49	7	3
1:A:7:ILE:CG2	1:B:7:ILE:HG21	0.42	2.43	13	1
1:A:116:ASN:O	1:A:119:LEU:HB2	0.42	2.15	3	1
1:A:149:PRO:HD2	1:A:152:GLU:OE1	0.42	2.13	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:LYS:O	1:A:123:LYS:HD3	0.42	2.14	20	1
1:A:78:ILE:HB	1:A:94:TYR:CE1	0.42	2.49	1	1
1:B:1:MET:O	1:B:38:ASP:HA	0.42	2.14	1	1
1:B:78:ILE:HG21	1:B:94:TYR:CE1	0.42	2.49	3	3
1:B:53:LYS:HA	1:B:56:SER:O	0.42	2.14	12	1
1:A:94:TYR:CE2	1:B:58:LYS:HB2	0.42	2.50	16	1
1:A:91:ASP:HB3	1:B:99:ASN:HD22	0.42	1.74	3	1
1:A:40:ASP:O	1:A:44:ILE:HG13	0.42	2.14	14	1
1:A:134:LYS:O	1:A:138:VAL:HG23	0.42	2.15	8	5
1:B:75:GLU:HA	1:B:94:TYR:CD2	0.42	2.49	9	1
1:A:92:SER:HB3	1:B:99:ASN:ND2	0.42	2.30	10	1
1:B:103:PHE:O	1:B:107:ARG:HB2	0.42	2.14	10	1
1:A:53:LYS:HE3	1:B:41:GLU:O	0.42	2.15	12	1
1:B:101:ILE:O	1:B:105:ILE:HG13	0.42	2.15	17	2
1:B:67:PRO:HD2	1:B:70:CYS:SG	0.42	2.54	12	1
1:B:131:ALA:O	1:B:135:GLU:HG2	0.42	2.14	18	1
1:A:91:ASP:HB2	1:B:62:LEU:HD21	0.42	1.92	20	1
1:A:91:ASP:HB2	1:B:62:LEU:CD1	0.42	2.45	2	1
1:B:107:ARG:HD2	1:B:152:GLU:OE1	0.42	2.15	7	1
1:A:5:LYS:O	1:A:13:SER:HB2	0.42	2.14	20	1
1:B:116:ASN:H	1:B:151:ASP:CB	0.41	2.28	7	1
1:A:93:ILE:HA	1:A:96:SER:OG	0.41	2.15	20	1
1:A:48:PHE:CE2	1:B:23:VAL:HG23	0.41	2.50	3	1
1:A:65:ASP:O	1:A:67:PRO:HD3	0.41	2.15	11	1
1:A:92:SER:HB2	1:B:99:ASN:HB3	0.41	1.92	6	1
1:B:21:GLU:O	1:B:50:LEU:HB2	0.41	2.16	8	1
1:A:50:LEU:HB2	1:B:48:PHE:CE1	0.41	2.51	7	2
1:B:9:ASN:OD1	1:B:31:PHE:HB2	0.41	2.16	12	1
1:A:91:ASP:OD2	1:A:95:VAL:HG23	0.41	2.16	16	1
1:A:63:LEU:HD13	1:B:49:THR:HG21	0.41	1.91	1	1
1:A:53:LYS:O	1:A:57:GLU:HB3	0.41	2.14	14	1
1:B:136:ALA:O	1:B:139:MET:HG2	0.41	2.16	3	1
1:B:14:VAL:HG11	1:B:39:VAL:HG21	0.41	1.93	16	1
1:A:33:LYS:HA	1:A:33:LYS:HE2	0.41	1.91	20	1
1:A:79:SER:HA	1:A:82:LYS:CE	0.41	2.45	2	1
1:B:141:LYS:HB2	1:B:146:VAL:O	0.41	2.16	2	1
1:A:52:ASN:ND2	1:A:55:VAL:HB	0.41	2.30	16	1
1:A:137:LEU:O	1:A:141:LYS:HG3	0.41	2.15	17	1
1:B:96:SER:O	1:B:100:HIS:HB2	0.41	2.16	18	1
1:B:119:LEU:O	1:B:123:LYS:HG3	0.40	2.16	8	1
1:A:150:GLU:H	1:A:150:GLU:CD	0.40	2.20	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:B:124:ARG:N	1:B:124:ARG:HD2	0.40	2.31	9	1
1:A:97:LEU:O	1:A:101:ILE:HG12	0.40	2.16	19	1
1:B:12:ILE:CG2	1:B:30:ALA:HB2	0.40	2.47	8	1
1:B:114:ILE:HG12	1:B:152:GLU:OE2	0.40	2.16	12	1
1:A:156:ILE:O	1:A:160:ILE:HG12	0.40	2.17	9	1
1:B:149:PRO:HB2	1:B:151:ASP:OD2	0.40	2.16	12	1
1:B:107:ARG:HG2	1:B:112:LEU:O	0.40	2.16	17	1
1:A:131:ALA:O	1:A:135:GLU:HG2	0.40	2.17	1	1
1:A:18:GLN:HE21	1:A:18:GLN:CA	0.40	2.30	2	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	164/175 (94%)	161±1 (98±1%)	3±1 (2±1%)	0±0 (0±0%)	54	85
1	B	164/175 (94%)	160±2 (98±1%)	3±2 (2±1%)	0±0 (0±0%)	54	85
All	All	6560/7000 (94%)	6421 (98%)	134 (2%)	5 (0%)	54	85

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

Mol	Chain	Res	Type	Models (Total)
1	B	93	ILE	1
1	A	27	ARG	1
1	B	53	LYS	1
1	A	165	LEU	1
1	B	165	LEU	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	145/155 (94%)	138±2 (95±1%)	7±2 (5±1%)	31 79
1	B	145/155 (94%)	138±3 (95±2%)	7±3 (5±2%)	30 79
All	All	5800/6200 (94%)	5532 (95%)	268 (5%)	31 79

All 83 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	57	GLU	9
1	B	51	ASP	8
1	B	57	GLU	7
1	A	41	GLU	7
1	A	59	PHE	7
1	B	41	GLU	7
1	A	98	THR	7
1	B	98	THR	6
1	B	151	ASP	6
1	A	58	LYS	6
1	A	151	ASP	6
1	B	18	GLN	6
1	B	141	LYS	6
1	B	1	MET	6
1	A	60	LYS	6
1	B	53	LYS	6
1	B	60	LYS	6
1	B	127	LYS	6
1	B	59	PHE	6
1	A	51	ASP	5
1	A	18	GLN	5
1	A	1	MET	5
1	A	32	GLN	5
1	B	32	GLN	5
1	B	124	ARG	5
1	A	107	ARG	5
1	A	141	LYS	4
1	B	58	LYS	4
1	A	68	ILE	4
1	B	68	ILE	4
1	A	61	THR	4
1	B	164	GLU	4
1	B	129	GLU	3
1	A	135	GLU	3

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Mol	Chain	Res	Type	Models (Total)
1	B	75	GLU	3
1	A	127	LYS	3
1	A	91	ASP	3
1	A	82	LYS	3
1	B	46	LYS	3
1	B	33	LYS	3
1	B	107	ARG	3
1	B	82	LYS	3
1	A	124	ARG	2
1	B	5	LYS	2
1	A	5	LYS	2
1	A	53	LYS	2
1	A	87	LYS	2
1	B	91	ASP	2
1	A	46	LYS	2
1	A	106	GLN	2
1	A	88	LYS	2
1	B	10	ASN	2
1	B	88	LYS	2
1	A	10	ASN	2
1	B	135	GLU	2
1	A	99	ASN	2
1	A	129	GLU	1
1	A	34	LYS	1
1	A	162	ASN	1
1	A	49	THR	1
1	A	27	ARG	1
1	A	130	PHE	1
1	B	27	ARG	1
1	B	162	ASN	1
1	A	84	GLN	1
1	A	109	GLN	1
1	A	113	ASP	1
1	B	16	ASN	1
1	B	106	GLN	1
1	A	17	GLU	1
1	A	121	GLU	1
1	A	142	ASN	1
1	A	115	LYS	1
1	B	134	LYS	1
1	B	61	THR	1
1	B	17	GLU	1

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Mol	Chain	Res	Type	Models (Total)
1	B	29	LEU	1
1	A	150	GLU	1
1	A	2	LYS	1
1	A	139	MET	1
1	B	139	MET	1
1	A	164	GLU	1
1	B	152	GLU	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 monosaccharides in this entry.

6.6 Ligand geometry

There are no ligands in this entry.

6.7 Other polymers

There are no such molecules in this entry.

6.8 Polymer linkage issues

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 35% for the well-defined parts and 35% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	1643
Number of shifts mapped to atoms	1643
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	167	-0.55 ± 0.08	Should be checked
$^{13}C_{\beta}$	57	-0.06 ± 0.19	None needed (< 0.5 ppm)
$^{13}C'$	160	-0.32 ± 0.08	None needed (< 0.5 ppm)
^{15}N	163	0.37 ± 0.23	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 35%, i.e. 1611 atoms were assigned a chemical shift out of a possible 4628. 0 out of 64 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	814/1660 (49%)	333/674 (49%)	322/660 (49%)	159/326 (49%)
Sidechain	741/2724 (27%)	585/1768 (33%)	156/860 (18%)	0/96 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	56/244 (23%)	56/120 (47%)	0/118 (0%)	0/6 (0%)
Overall	1611/4628 (35%)	974/2562 (38%)	478/1638 (29%)	159/428 (37%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 35%, i.e. 1643 atoms were assigned a chemical shift out of a possible 4742. 0 out of 66 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	830/1700 (49%)	340/690 (49%)	327/676 (48%)	163/334 (49%)
Sidechain	757/2798 (27%)	599/1814 (33%)	158/884 (18%)	0/100 (0%)
Aromatic	56/244 (23%)	56/120 (47%)	0/118 (0%)	0/6 (0%)
Overall	1643/4742 (35%)	995/2624 (38%)	485/1678 (29%)	163/440 (37%)

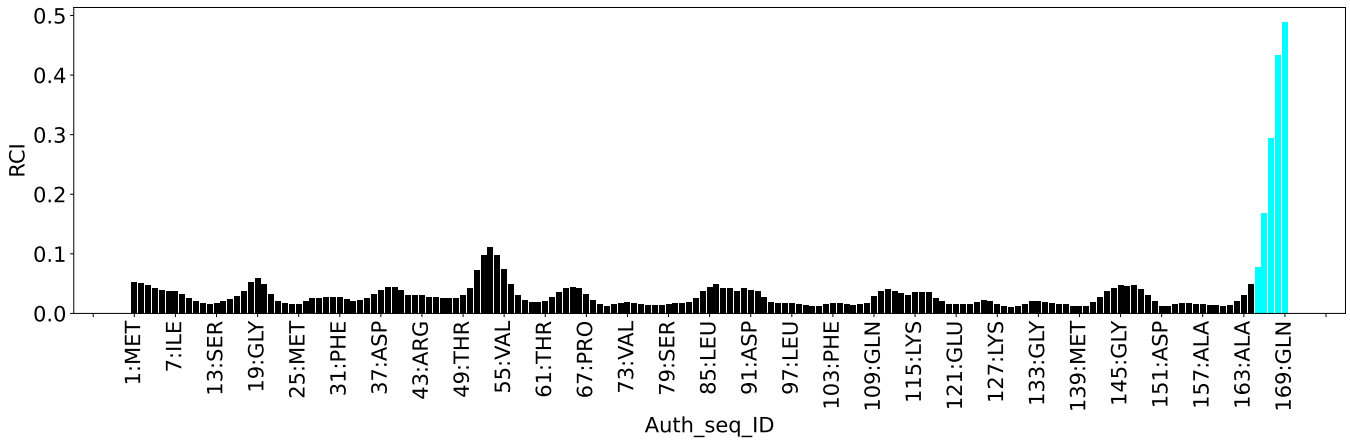
7.1.4 Statistically unusual chemical shifts (i)

There are no statistically unusual chemical shifts.

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	1679
Intra-residue (|i-j|=0)	411
Sequential (|i-j|=1)	595
Medium range (|i-j|>1 and |i-j|<5)	335
Long range (|i-j|≥5)	222
Inter-chain	52
Hydrogen bond restraints	64
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	4.8
Number of long range restraints per residue[1]	0.7

[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)	13.3	0.2
0.2-0.5 (Medium)	3.1	0.5
>0.5 (Large)	1.8	1.67

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)

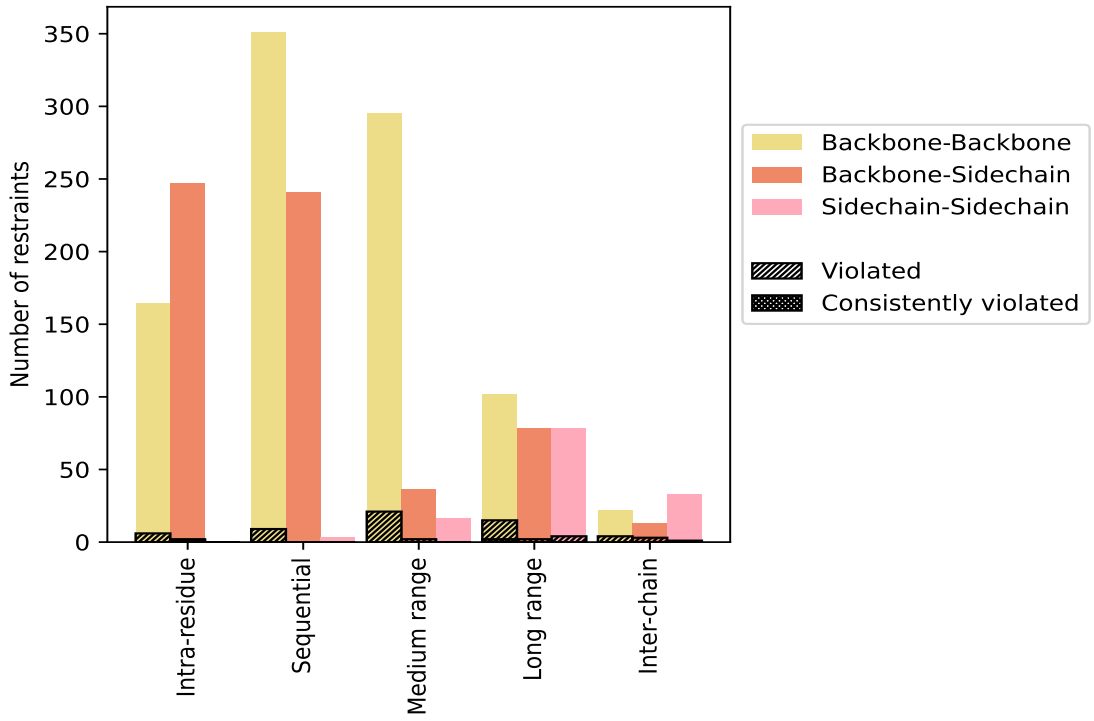
9.1 Summary of distance violations (i)

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)	411	24.5	8	1.9	0.5	1	0.2	0.1
Backbone-Backbone	164	9.8	6	3.7	0.4	0	0.0	0.0
Backbone-Sidechain	247	14.7	2	0.8	0.1	1	0.4	0.1
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	595	35.4	9	1.5	0.5	0	0.0	0.0
Backbone-Backbone	351	20.9	9	2.6	0.5	0	0.0	0.0
Backbone-Sidechain	241	14.4	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	3	0.2	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	335	20.0	21	6.3	1.3	0	0.0	0.0
Backbone-Backbone	283	16.9	19	6.7	1.1	0	0.0	0.0
Backbone-Sidechain	36	2.1	2	5.6	0.1	0	0.0	0.0
Sidechain-Sidechain	16	1.0	0	0.0	0.0	0	0.0	0.0
Long range (|i-j|≥5)	222	13.2	13	5.9	0.8	0	0.0	0.0
Backbone-Backbone	66	3.9	7	10.6	0.4	0	0.0	0.0
Backbone-Sidechain	78	4.6	2	2.6	0.1	0	0.0	0.0
Sidechain-Sidechain	78	4.6	4	5.1	0.2	0	0.0	0.0
Inter-chain	52	3.1	4	7.7	0.2	0	0.0	0.0
Backbone-Backbone	6	0.4	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	13	0.8	3	23.1	0.2	0	0.0	0.0
Sidechain-Sidechain	33	2.0	1	3.0	0.1	0	0.0	0.0
Hydrogen bond	64	3.8	14	21.9	0.8	2	3.1	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	1679	100.0	69	4.1	4.1	3	0.2	0.2
Backbone-Backbone	934	55.6	55	5.9	3.3	2	0.2	0.1
Backbone-Sidechain	615	36.6	9	1.5	0.5	1	0.2	0.1
Sidechain-Sidechain	130	7.7	5	3.8	0.3	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	1	1	6	9	3	20	0.25	1.0	0.23	0.16
2	2	6	9	8	4	29	0.17	0.53	0.08	0.14
3	1	0	8	8	0	17	0.27	0.78	0.22	0.18
4	1	0	5	10	4	20	0.17	0.35	0.06	0.16
5	2	3	0	7	2	14	0.28	1.09	0.28	0.18
6	2	2	8	7	1	20	0.18	0.56	0.1	0.15
7	1	0	6	7	0	14	0.26	0.86	0.22	0.16
8	1	1	3	7	3	15	0.2	0.47	0.09	0.19
9	1	1	3	8	4	17	0.27	1.15	0.28	0.17
10	1	2	4	8	2	17	0.35	1.67	0.41	0.15
11	2	1	2	9	2	16	0.23	0.68	0.15	0.18

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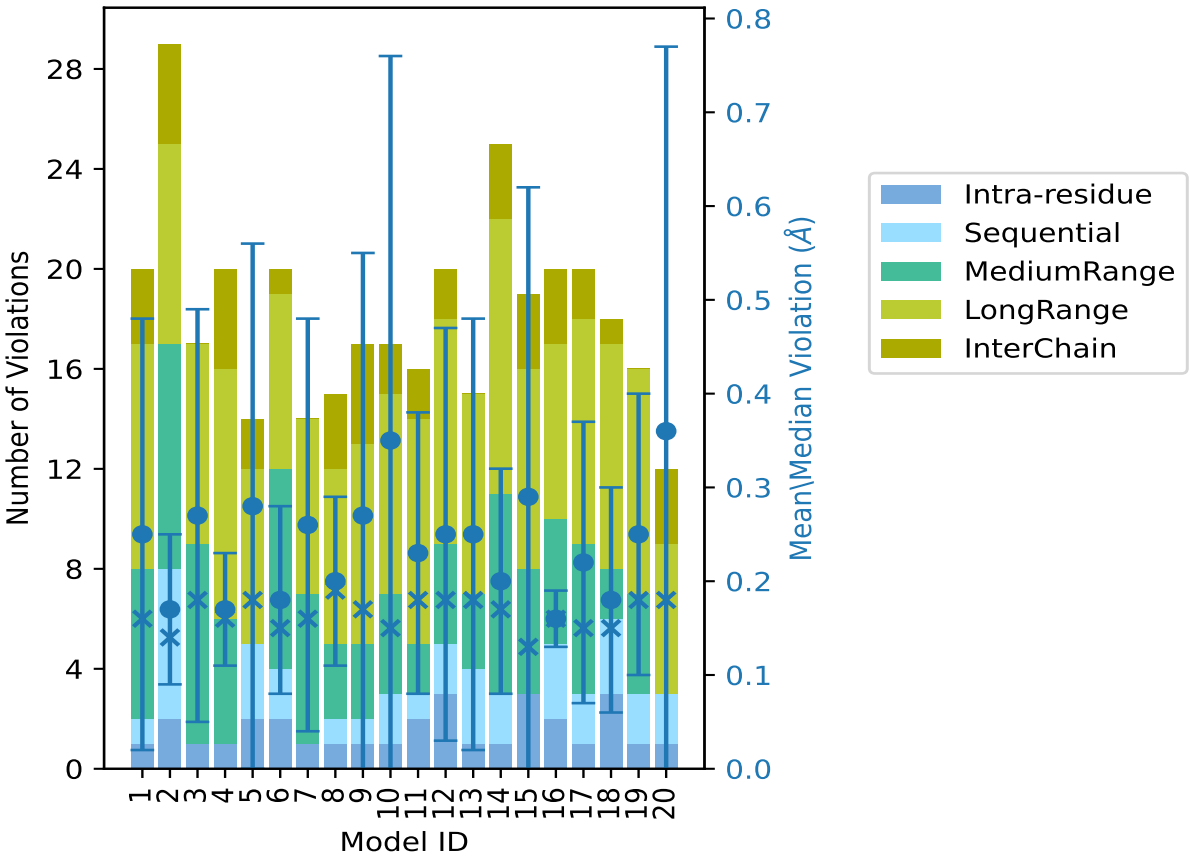
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	3	2	4	9	2	20	0.25	1.06	0.22	0.18
13	1	3	3	8	0	15	0.25	0.83	0.23	0.18
14	1	2	8	11	3	25	0.2	0.63	0.12	0.17
15	3	0	5	8	3	19	0.29	1.32	0.33	0.13
16	2	3	5	7	3	20	0.16	0.24	0.03	0.16
17	1	2	6	9	2	20	0.22	0.64	0.15	0.15
18	3	3	2	9	1	18	0.18	0.6	0.12	0.15
19	1	2	4	9	0	16	0.25	0.64	0.15	0.18
20	1	2	0	6	3	12	0.36	1.4	0.41	0.18

[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

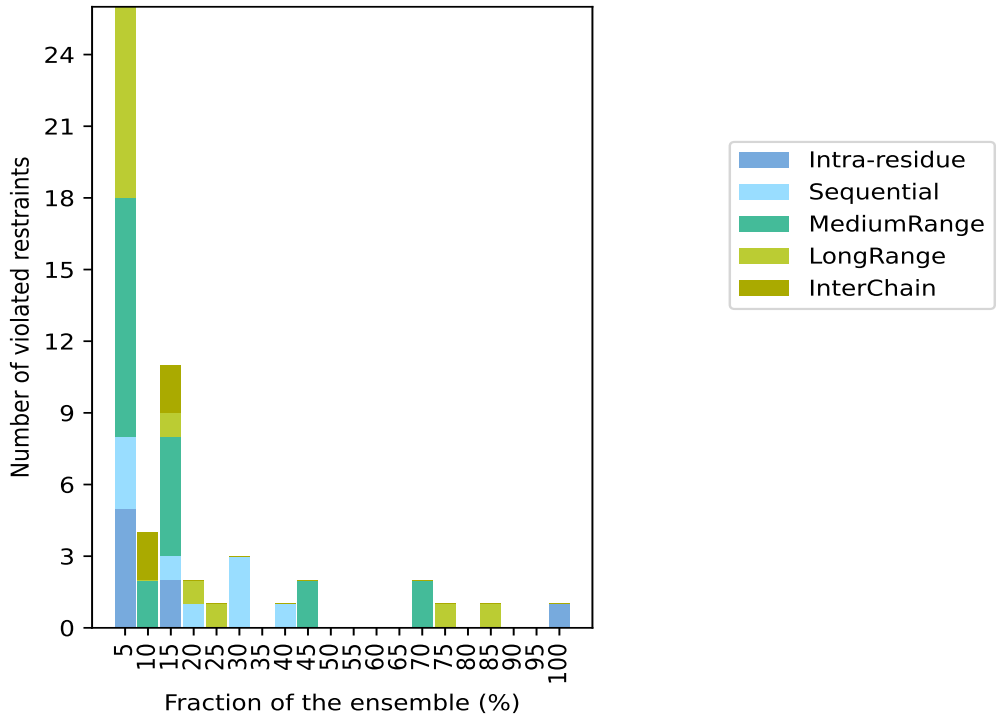
9.3 Distance violation statistics for the ensemble (i)

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, 1560(IR:403, SQ:586, MR:314, LR:209, IC:48) restraints are not violated in the ensemble.

Number of violated restraints						Fraction of the ensemble	
IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total	Count[6]	%
5	3	10	8	0	26	1	5.0
0	0	2	0	2	4	2	10.0
2	1	5	1	2	11	3	15.0
0	1	0	1	0	2	4	20.0
0	0	0	1	0	1	5	25.0
0	3	0	0	0	3	6	30.0
0	0	0	0	0	0	7	35.0
0	1	0	0	0	1	8	40.0
0	0	2	0	0	2	9	45.0
0	0	0	0	0	0	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	2	0	0	2	14	70.0
0	0	0	1	0	1	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	1	0	1	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
1	0	0	0	0	1	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

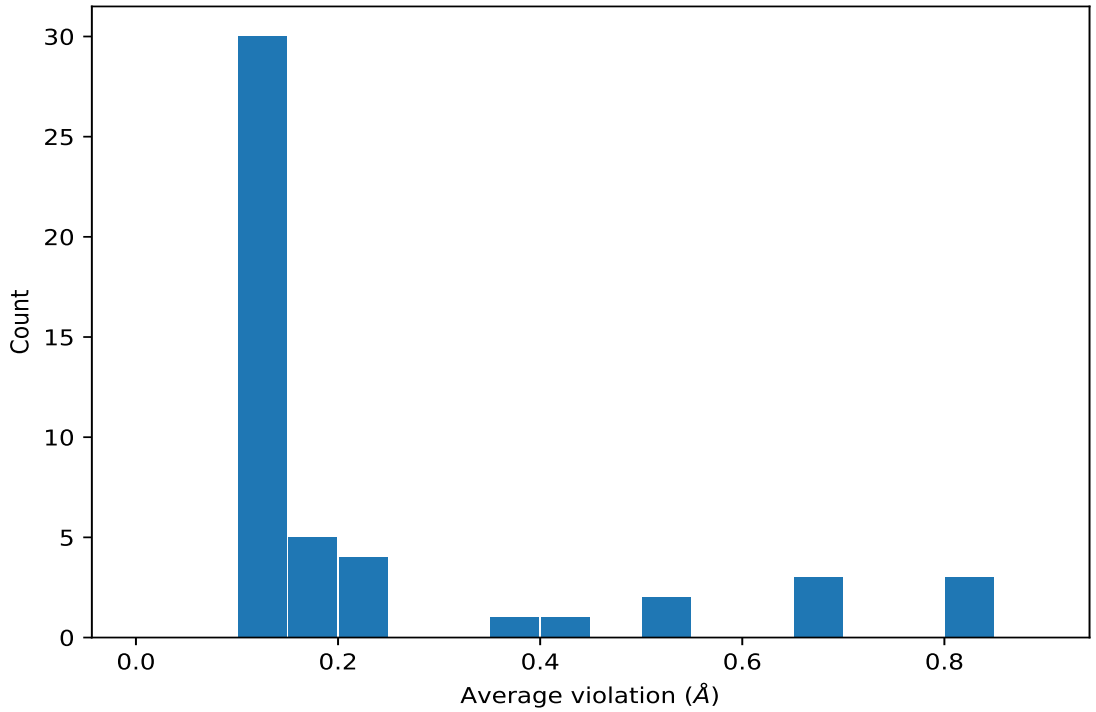
9.3.1 Bar graph : Distance violation statistics for the ensemble



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 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)
(1,6)	1:A:5:LYS:O	1:A:13:SER:N	20	0.21	0.03	0.2
(1,14)	1:A:14:VAL:O	1:A:22:LEU:N	20	0.2	0.04	0.2
(2,832)	1:A:161:VAL:H	1:A:161:VAL:HB	20	0.18	0.01	0.18
(1,20)	1:A:23:VAL:O	1:A:48:PHE:N	19	0.19	0.02	0.19
(1,12)	1:A:14:VAL:N	1:A:22:LEU:O	18	0.15	0.02	0.15
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG21	17	0.83	0.35	0.7
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG22	17	0.83	0.35	0.7
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG23	17	0.83	0.35	0.7
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG21	15	0.65	0.31	0.54
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG22	15	0.65	0.31	0.54
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG23	15	0.65	0.31	0.54
(1,25)	1:A:56:SER:H	1:A:53:LYS:HA	14	0.42	0.17	0.45
(2,1459)	1:A:85:LEU:HA	1:A:87:LYS:H	14	0.21	0.04	0.22
(1,43)	1:A:51:ASP:H	1:B:47:VAL:O	14	0.15	0.03	0.16
(1,18)	1:A:23:VAL:N	1:A:48:PHE:O	14	0.13	0.02	0.14
(1,22)	1:A:25:MET:N	1:A:46:LYS:O	12	0.14	0.01	0.13

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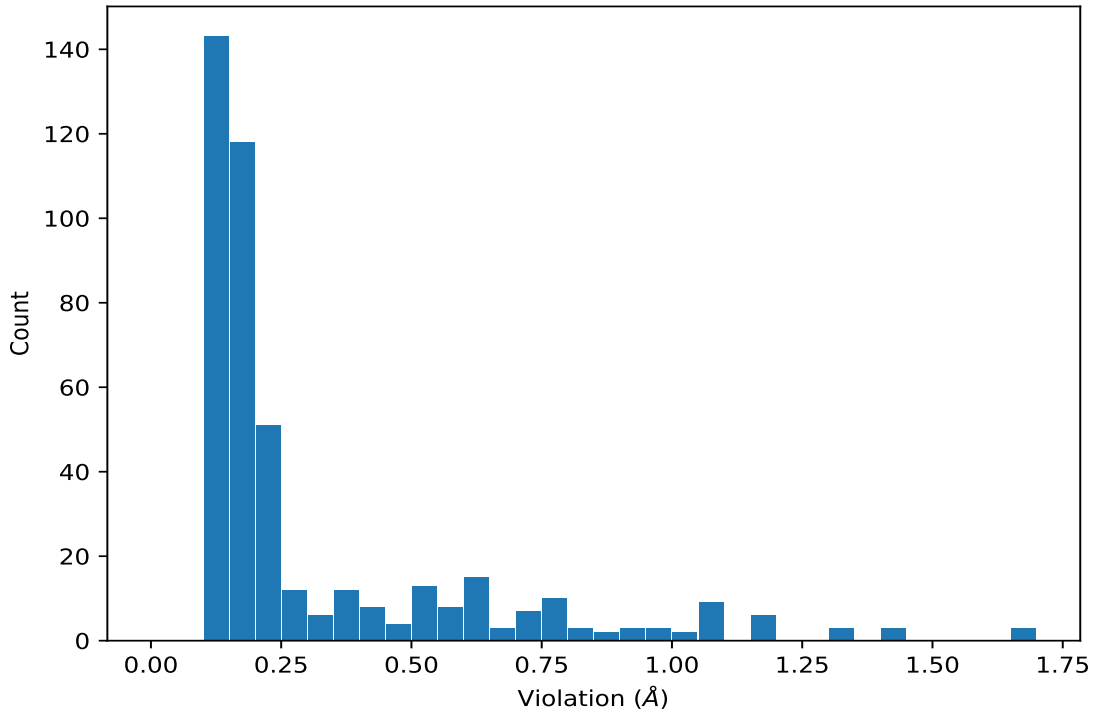
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,26)	1:A:53:LYS:HA	1:A:56:SER:HB2	9	0.53	0.24	0.4
(1,26)	1:A:53:LYS:HA	1:A:56:SER:HB3	9	0.53	0.24	0.4
(2,547)	1:A:56:SER:H	1:A:54:ASP:HA	9	0.14	0.02	0.14
(1,42)	1:A:49:THR:O	1:B:49:THR:N	9	0.14	0.03	0.13
(2,854)	1:A:65:ASP:HA	1:A:66:ILE:H	8	0.2	0.06	0.22
(1,40)	1:A:49:THR:N	1:B:49:THR:O	8	0.15	0.02	0.16
(1,16)	1:A:16:ASN:N	1:A:20:LYS:O	8	0.14	0.02	0.13
(1,24)	1:A:16:ASN:N	1:A:20:LYS:O	8	0.14	0.02	0.13
(2,198)	1:A:53:LYS:HA	1:A:54:ASP:H	6	0.16	0.02	0.16
(1,28)	1:A:52:ASN:HA	1:A:53:LYS:H	6	0.15	0.03	0.14
(1,4)	1:A:5:LYS:N	1:A:13:SER:O	6	0.13	0.01	0.13
(2,903)	1:A:117:ALA:HA	1:A:118:LEU:H	6	0.12	0.01	0.11
(2,336)	1:A:5:LYS:H	1:A:13:SER:H	5	0.11	0.0	0.11
(1,33)	1:A:82:LYS:HA	1:A:87:LYS:H	4	0.36	0.06	0.36
(2,177)	1:A:32:GLN:HA	1:A:33:LYS:H	4	0.15	0.04	0.14
(2,1414)	1:A:91:ASP:HA	1:A:95:VAL:H	3	0.17	0.05	0.17
(2,1275)	1:A:98:THR:HA	1:A:101:ILE:H	3	0.17	0.02	0.17
(2,329)	1:A:52:ASN:H	1:A:53:LYS:H	3	0.15	0.02	0.15
(2,1462)	1:A:59:PHE:HE2	1:B:75:GLU:HA	3	0.14	0.01	0.14
(2,409)	1:A:10:ASN:HA	1:A:30:ALA:H	3	0.14	0.02	0.13
(2,1444)	1:A:155:PHE:HE1	1:A:152:GLU:HA	3	0.14	0.02	0.15
(1,10)	1:A:12:ILE:O	1:A:24:VAL:N	3	0.13	0.01	0.13
(2,1421)	1:A:117:ALA:HA	1:A:120:TRP:H	3	0.12	0.02	0.11
(2,1466)	1:A:59:PHE:HD2	1:B:75:GLU:HA	3	0.12	0.0	0.12
(2,53)	1:A:55:VAL:H	1:A:55:VAL:HA	3	0.12	0.01	0.11
(2,1259)	1:A:94:TYR:HA	1:A:97:LEU:H	3	0.11	0.0	0.11
(2,663)	1:A:144:THR:H	1:A:144:THR:HA	3	0.11	0.0	0.11
(2,1255)	1:A:93:ILE:HA	1:A:96:SER:H	2	0.15	0.02	0.15
(2,1467)	1:A:59:PHE:HD1	1:B:63:LEU:HD21	2	0.15	0.0	0.15
(2,1467)	1:A:59:PHE:HD1	1:B:63:LEU:HD22	2	0.15	0.0	0.15
(2,1467)	1:A:59:PHE:HD1	1:B:63:LEU:HD23	2	0.15	0.0	0.15
(2,1343)	1:A:135:GLU:HA	1:A:139:MET:H	2	0.12	0.0	0.12
(2,1461)	1:A:59:PHE:HE2	1:B:95:VAL:HA	2	0.12	0.0	0.12

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

The following table 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)
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG21	10	1.67
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG22	10	1.67
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG23	10	1.67
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG21	20	1.4
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG22	20	1.4
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG23	20	1.4
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG21	15	1.32
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG22	15	1.32
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG23	15	1.32
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG21	9	1.15
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG22	9	1.15
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG23	9	1.15
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG21	20	1.15
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG22	20	1.15
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG23	20	1.15
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG21	5	1.09

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG22	5	1.09
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG23	5	1.09
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG21	12	1.06
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG22	12	1.06
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG23	12	1.06
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG21	10	1.05
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG22	10	1.05
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG23	10	1.05
(1,26)	1:A:53:LYS:HA	1:A:56:SER:HB2	1	1.0
(1,26)	1:A:53:LYS:HA	1:A:56:SER:HB3	1	1.0
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG21	15	0.98
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG22	15	0.98
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG23	15	0.98
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG21	9	0.91
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG22	9	0.91
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG23	9	0.91
(1,26)	1:A:53:LYS:HA	1:A:56:SER:HB2	7	0.86
(1,26)	1:A:53:LYS:HA	1:A:56:SER:HB3	7	0.86
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG21	13	0.83
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG22	13	0.83
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG23	13	0.83
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG21	13	0.79
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG22	13	0.79
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG23	13	0.79
(1,29)	1:A:51:ASP:HB2	1:A:60:LYS:HD2	3	0.78
(1,29)	1:A:51:ASP:HB2	1:A:60:LYS:HD3	3	0.78
(1,29)	1:A:51:ASP:HB3	1:A:60:LYS:HD2	3	0.78
(1,29)	1:A:51:ASP:HB3	1:A:60:LYS:HD3	3	0.78
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG21	5	0.76
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG22	5	0.76
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG23	5	0.76
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG21	1	0.72
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG22	1	0.72
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG23	1	0.72
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG21	3	0.7
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG22	3	0.7
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG23	3	0.7
(1,25)	1:A:56:SER:H	1:A:53:LYS:HA	3	0.7
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG21	11	0.68
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG22	11	0.68
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG23	11	0.68
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG21	17	0.64

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG22	17	0.64
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG23	17	0.64
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG21	19	0.64
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG22	19	0.64
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG23	19	0.64
(1,25)	1:A:56:SER:H	1:A:53:LYS:HA	15	0.64
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG21	14	0.63
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG22	14	0.63
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG23	14	0.63
(1,26)	1:A:53:LYS:HA	1:A:56:SER:HB2	10	0.62
(1,26)	1:A:53:LYS:HA	1:A:56:SER:HB3	10	0.62
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG21	18	0.6
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG22	18	0.6
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG23	18	0.6
(1,25)	1:A:56:SER:H	1:A:53:LYS:HA	7	0.57
(1,25)	1:A:56:SER:H	1:A:53:LYS:HA	10	0.57
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG21	12	0.56
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG22	12	0.56
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG23	12	0.56
(1,26)	1:A:53:LYS:HA	1:A:56:SER:HB2	12	0.56
(1,26)	1:A:53:LYS:HA	1:A:56:SER:HB3	12	0.56
(1,25)	1:A:56:SER:H	1:A:53:LYS:HA	6	0.56
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG21	1	0.54
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG22	1	0.54
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG23	1	0.54
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG21	2	0.53
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG22	2	0.53
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG23	2	0.53
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG21	17	0.52
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG22	17	0.52
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG23	17	0.52
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG21	7	0.52
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG22	7	0.52
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG23	7	0.52
(1,25)	1:A:56:SER:H	1:A:53:LYS:HA	17	0.5
(1,25)	1:A:56:SER:H	1:A:53:LYS:HA	8	0.47
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG21	14	0.46
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG22	14	0.46
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG23	14	0.46
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG21	11	0.43
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG22	11	0.43
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG23	11	0.43

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,33)	1:A:82:LYS:HA	1:A:87:LYS:H	11	0.43
(1,25)	1:A:56:SER:H	1:A:53:LYS:HA	1	0.43
(1,25)	1:A:56:SER:H	1:A:53:LYS:HA	19	0.43
(1,26)	1:A:53:LYS:HA	1:A:56:SER:HB2	15	0.4
(1,26)	1:A:53:LYS:HA	1:A:56:SER:HB3	15	0.4
(1,26)	1:A:53:LYS:HA	1:A:56:SER:HB2	19	0.39
(1,26)	1:A:53:LYS:HA	1:A:56:SER:HB3	19	0.39
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG21	19	0.38
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG22	19	0.38
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG23	19	0.38
(1,33)	1:A:82:LYS:HA	1:A:87:LYS:H	19	0.37
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG21	18	0.35
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG22	18	0.35
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG23	18	0.35
(1,33)	1:A:82:LYS:HA	1:A:87:LYS:H	8	0.35
(1,26)	1:A:53:LYS:HA	1:A:56:SER:HB2	4	0.35
(1,26)	1:A:53:LYS:HA	1:A:56:SER:HB3	4	0.35
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG21	3	0.34
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG22	3	0.34
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG23	3	0.34
(1,25)	1:A:56:SER:H	1:A:53:LYS:HA	4	0.33
(1,26)	1:A:53:LYS:HA	1:A:56:SER:HB2	17	0.3
(1,26)	1:A:53:LYS:HA	1:A:56:SER:HB3	17	0.3
(2,854)	1:A:65:ASP:HA	1:A:66:ILE:H	14	0.28
(2,854)	1:A:65:ASP:HA	1:A:66:ILE:H	20	0.27
(2,1459)	1:A:85:LEU:HA	1:A:87:LYS:H	10	0.27
(1,6)	1:A:5:LYS:O	1:A:13:SER:N	20	0.27
(1,33)	1:A:82:LYS:HA	1:A:87:LYS:H	2	0.27
(1,14)	1:A:14:VAL:O	1:A:22:LEU:N	7	0.27
(1,14)	1:A:14:VAL:O	1:A:22:LEU:N	8	0.27
(2,854)	1:A:65:ASP:HA	1:A:66:ILE:H	5	0.25
(1,6)	1:A:5:LYS:O	1:A:13:SER:N	15	0.25
(1,26)	1:A:53:LYS:HA	1:A:56:SER:HB2	13	0.25
(1,26)	1:A:53:LYS:HA	1:A:56:SER:HB3	13	0.25
(1,14)	1:A:14:VAL:O	1:A:22:LEU:N	17	0.25
(2,1459)	1:A:85:LEU:HA	1:A:87:LYS:H	2	0.24
(2,1459)	1:A:85:LEU:HA	1:A:87:LYS:H	9	0.24
(2,1459)	1:A:85:LEU:HA	1:A:87:LYS:H	11	0.24
(2,1459)	1:A:85:LEU:HA	1:A:87:LYS:H	14	0.24
(2,1459)	1:A:85:LEU:HA	1:A:87:LYS:H	16	0.24
(2,1414)	1:A:91:ASP:HA	1:A:95:VAL:H	14	0.24
(1,6)	1:A:5:LYS:O	1:A:13:SER:N	5	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6)	1:A:5:LYS:O	1:A:13:SER:N	11	0.24
(1,14)	1:A:14:VAL:O	1:A:22:LEU:N	14	0.24
(2,854)	1:A:65:ASP:HA	1:A:66:ILE:H	2	0.23
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG21	7	0.23
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG22	7	0.23
(2,1465)	1:A:59:PHE:HE1	1:A:95:VAL:HG23	7	0.23
(1,6)	1:A:5:LYS:O	1:A:13:SER:N	3	0.23
(1,6)	1:A:5:LYS:O	1:A:13:SER:N	14	0.23
(1,30)	1:A:51:ASP:HB2	1:A:60:LYS:HG2	6	0.23
(1,30)	1:A:51:ASP:HB2	1:A:60:LYS:HG3	6	0.23
(1,30)	1:A:51:ASP:HB3	1:A:60:LYS:HG2	6	0.23
(1,30)	1:A:51:ASP:HB3	1:A:60:LYS:HG3	6	0.23
(1,25)	1:A:56:SER:H	1:A:53:LYS:HA	14	0.23
(1,20)	1:A:23:VAL:O	1:A:48:PHE:N	8	0.23
(1,20)	1:A:23:VAL:O	1:A:48:PHE:N	17	0.23
(2,177)	1:A:32:GLN:HA	1:A:33:LYS:H	17	0.22
(2,1459)	1:A:85:LEU:HA	1:A:87:LYS:H	3	0.22
(2,1459)	1:A:85:LEU:HA	1:A:87:LYS:H	6	0.22
(1,6)	1:A:5:LYS:O	1:A:13:SER:N	2	0.22
(1,20)	1:A:23:VAL:O	1:A:48:PHE:N	4	0.22
(1,20)	1:A:23:VAL:O	1:A:48:PHE:N	5	0.22
(1,20)	1:A:23:VAL:O	1:A:48:PHE:N	6	0.22
(1,14)	1:A:14:VAL:O	1:A:22:LEU:N	3	0.22
(1,14)	1:A:14:VAL:O	1:A:22:LEU:N	18	0.22
(2,854)	1:A:65:ASP:HA	1:A:66:ILE:H	12	0.21
(2,1459)	1:A:85:LEU:HA	1:A:87:LYS:H	4	0.21
(2,1459)	1:A:85:LEU:HA	1:A:87:LYS:H	12	0.21
(1,6)	1:A:5:LYS:O	1:A:13:SER:N	6	0.21
(1,6)	1:A:5:LYS:O	1:A:13:SER:N	8	0.21
(1,20)	1:A:23:VAL:O	1:A:48:PHE:N	11	0.21
(1,14)	1:A:14:VAL:O	1:A:22:LEU:N	13	0.21
(1,14)	1:A:14:VAL:O	1:A:22:LEU:N	20	0.21
(2,1459)	1:A:85:LEU:HA	1:A:87:LYS:H	8	0.2
(2,1454)	1:A:116:ASN:HA	1:A:151:ASP:HA	8	0.2
(1,6)	1:A:5:LYS:O	1:A:13:SER:N	13	0.2
(1,6)	1:A:5:LYS:O	1:A:13:SER:N	17	0.2
(1,6)	1:A:5:LYS:O	1:A:13:SER:N	19	0.2
(1,28)	1:A:52:ASN:HA	1:A:53:LYS:H	16	0.2
(1,25)	1:A:56:SER:H	1:A:53:LYS:HA	2	0.2
(1,20)	1:A:23:VAL:O	1:A:48:PHE:N	1	0.2
(1,14)	1:A:14:VAL:O	1:A:22:LEU:N	2	0.2
(1,14)	1:A:14:VAL:O	1:A:22:LEU:N	9	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,14)	1:A:14:VAL:O	1:A:22:LEU:N	11	0.2
(1,14)	1:A:14:VAL:O	1:A:22:LEU:N	19	0.2
(2,832)	1:A:161:VAL:H	1:A:161:VAL:HB	3	0.19
(2,832)	1:A:161:VAL:H	1:A:161:VAL:HB	6	0.19
(2,832)	1:A:161:VAL:H	1:A:161:VAL:HB	11	0.19
(2,832)	1:A:161:VAL:H	1:A:161:VAL:HB	15	0.19
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG21	4	0.19
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG22	4	0.19
(2,1464)	1:A:59:PHE:HD1	1:A:95:VAL:HG23	4	0.19
(2,1459)	1:A:85:LEU:HA	1:A:87:LYS:H	19	0.19
(2,1275)	1:A:98:THR:HA	1:A:101:ILE:H	14	0.19
(1,6)	1:A:5:LYS:O	1:A:13:SER:N	4	0.19
(1,6)	1:A:5:LYS:O	1:A:13:SER:N	12	0.19
(1,6)	1:A:5:LYS:O	1:A:13:SER:N	16	0.19
(1,43)	1:A:51:ASP:H	1:B:47:VAL:O	8	0.19
(1,40)	1:A:49:THR:N	1:B:49:THR:O	16	0.19
(1,28)	1:A:52:ASN:HA	1:A:53:LYS:H	13	0.19
(1,20)	1:A:23:VAL:O	1:A:48:PHE:N	9	0.19
(1,20)	1:A:23:VAL:O	1:A:48:PHE:N	13	0.19
(1,20)	1:A:23:VAL:O	1:A:48:PHE:N	15	0.19
(1,14)	1:A:14:VAL:O	1:A:22:LEU:N	5	0.19
(1,12)	1:A:14:VAL:N	1:A:22:LEU:O	1	0.19
(1,12)	1:A:14:VAL:N	1:A:22:LEU:O	12	0.19
(2,832)	1:A:161:VAL:H	1:A:161:VAL:HB	1	0.18
(2,832)	1:A:161:VAL:H	1:A:161:VAL:HB	2	0.18
(2,832)	1:A:161:VAL:H	1:A:161:VAL:HB	4	0.18
(2,832)	1:A:161:VAL:H	1:A:161:VAL:HB	5	0.18
(2,832)	1:A:161:VAL:H	1:A:161:VAL:HB	9	0.18
(2,832)	1:A:161:VAL:H	1:A:161:VAL:HB	10	0.18
(2,832)	1:A:161:VAL:H	1:A:161:VAL:HB	12	0.18
(2,832)	1:A:161:VAL:H	1:A:161:VAL:HB	13	0.18
(2,832)	1:A:161:VAL:H	1:A:161:VAL:HB	14	0.18
(2,832)	1:A:161:VAL:H	1:A:161:VAL:HB	17	0.18
(2,832)	1:A:161:VAL:H	1:A:161:VAL:HB	18	0.18
(2,832)	1:A:161:VAL:H	1:A:161:VAL:HB	19	0.18
(2,832)	1:A:161:VAL:H	1:A:161:VAL:HB	20	0.18
(2,547)	1:A:56:SER:H	1:A:54:ASP:HA	3	0.18
(2,198)	1:A:53:LYS:HA	1:A:54:ASP:H	5	0.18
(1,6)	1:A:5:LYS:O	1:A:13:SER:N	7	0.18
(1,6)	1:A:5:LYS:O	1:A:13:SER:N	9	0.18
(1,43)	1:A:51:ASP:H	1:B:47:VAL:O	1	0.18
(1,43)	1:A:51:ASP:H	1:B:47:VAL:O	9	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,43)	1:A:51:ASP:H	1:B:47:VAL:O	14	0.18
(1,43)	1:A:51:ASP:H	1:B:47:VAL:O	18	0.18
(1,20)	1:A:23:VAL:O	1:A:48:PHE:N	2	0.18
(1,20)	1:A:23:VAL:O	1:A:48:PHE:N	10	0.18
(1,20)	1:A:23:VAL:O	1:A:48:PHE:N	12	0.18
(1,20)	1:A:23:VAL:O	1:A:48:PHE:N	14	0.18
(1,20)	1:A:23:VAL:O	1:A:48:PHE:N	16	0.18
(1,20)	1:A:23:VAL:O	1:A:48:PHE:N	19	0.18
(1,20)	1:A:23:VAL:O	1:A:48:PHE:N	20	0.18
(1,14)	1:A:14:VAL:O	1:A:22:LEU:N	6	0.18
(1,14)	1:A:14:VAL:O	1:A:22:LEU:N	10	0.18
(1,14)	1:A:14:VAL:O	1:A:22:LEU:N	12	0.18
(1,12)	1:A:14:VAL:N	1:A:22:LEU:O	3	0.18
(2,854)	1:A:65:ASP:HA	1:A:66:ILE:H	6	0.17
(2,832)	1:A:161:VAL:H	1:A:161:VAL:HB	7	0.17
(2,832)	1:A:161:VAL:H	1:A:161:VAL:HB	8	0.17
(2,832)	1:A:161:VAL:H	1:A:161:VAL:HB	16	0.17
(2,329)	1:A:52:ASN:H	1:A:53:LYS:H	12	0.17
(2,198)	1:A:53:LYS:HA	1:A:54:ASP:H	20	0.17
(2,1414)	1:A:91:ASP:HA	1:A:95:VAL:H	18	0.17
(2,1275)	1:A:98:THR:HA	1:A:101:ILE:H	16	0.17
(1,6)	1:A:5:LYS:O	1:A:13:SER:N	1	0.17
(1,43)	1:A:51:ASP:H	1:B:47:VAL:O	2	0.17
(1,42)	1:A:49:THR:O	1:B:49:THR:N	4	0.17
(1,42)	1:A:49:THR:O	1:B:49:THR:N	9	0.17
(1,42)	1:A:49:THR:O	1:B:49:THR:N	16	0.17
(1,25)	1:A:56:SER:H	1:A:53:LYS:HA	11	0.17
(1,24)	1:A:16:ASN:N	1:A:20:LYS:O	12	0.17
(1,18)	1:A:23:VAL:N	1:A:48:PHE:O	14	0.17
(1,16)	1:A:16:ASN:N	1:A:20:LYS:O	12	0.17
(1,14)	1:A:14:VAL:O	1:A:22:LEU:N	16	0.17
(1,12)	1:A:14:VAL:N	1:A:22:LEU:O	9	0.17
(1,12)	1:A:14:VAL:N	1:A:22:LEU:O	20	0.17
(2,547)	1:A:56:SER:H	1:A:54:ASP:HA	6	0.16
(2,547)	1:A:56:SER:H	1:A:54:ASP:HA	9	0.16
(2,409)	1:A:10:ASN:HA	1:A:30:ALA:H	4	0.16
(2,198)	1:A:53:LYS:HA	1:A:54:ASP:H	16	0.16
(2,1462)	1:A:59:PHE:HE2	1:B:75:GLU:HA	9	0.16
(2,1255)	1:A:93:ILE:HA	1:A:96:SER:H	16	0.16
(1,6)	1:A:5:LYS:O	1:A:13:SER:N	18	0.16
(1,43)	1:A:51:ASP:H	1:B:47:VAL:O	16	0.16
(1,40)	1:A:49:THR:N	1:B:49:THR:O	1	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,40)	1:A:49:THR:N	1:B:49:THR:O	4	0.16
(1,40)	1:A:49:THR:N	1:B:49:THR:O	14	0.16
(1,24)	1:A:16:ASN:N	1:A:20:LYS:O	15	0.16
(1,22)	1:A:25:MET:N	1:A:46:LYS:O	4	0.16
(1,18)	1:A:23:VAL:N	1:A:48:PHE:O	12	0.16
(1,16)	1:A:16:ASN:N	1:A:20:LYS:O	15	0.16
(1,14)	1:A:14:VAL:O	1:A:22:LEU:N	4	0.16
(1,12)	1:A:14:VAL:N	1:A:22:LEU:O	6	0.16
(2,547)	1:A:56:SER:H	1:A:54:ASP:HA	8	0.15
(2,329)	1:A:52:ASN:H	1:A:53:LYS:H	10	0.15
(2,198)	1:A:53:LYS:HA	1:A:54:ASP:H	18	0.15
(2,1467)	1:A:59:PHE:HD1	1:B:63:LEU:HD21	12	0.15
(2,1467)	1:A:59:PHE:HD1	1:B:63:LEU:HD22	12	0.15
(2,1467)	1:A:59:PHE:HD1	1:B:63:LEU:HD23	12	0.15
(2,1444)	1:A:155:PHE:HE1	1:A:152:GLU:HA	3	0.15
(2,1444)	1:A:155:PHE:HE1	1:A:152:GLU:HA	13	0.15
(2,1421)	1:A:117:ALA:HA	1:A:120:TRP:H	3	0.15
(2,1275)	1:A:98:THR:HA	1:A:101:ILE:H	1	0.15
(1,6)	1:A:5:LYS:O	1:A:13:SER:N	10	0.15
(1,43)	1:A:51:ASP:H	1:B:47:VAL:O	4	0.15
(1,43)	1:A:51:ASP:H	1:B:47:VAL:O	17	0.15
(1,40)	1:A:49:THR:N	1:B:49:THR:O	9	0.15
(1,4)	1:A:5:LYS:N	1:A:13:SER:O	19	0.15
(1,25)	1:A:56:SER:H	1:A:53:LYS:HA	9	0.15
(1,24)	1:A:16:ASN:N	1:A:20:LYS:O	2	0.15
(1,22)	1:A:25:MET:N	1:A:46:LYS:O	1	0.15
(1,22)	1:A:25:MET:N	1:A:46:LYS:O	8	0.15
(1,22)	1:A:25:MET:N	1:A:46:LYS:O	14	0.15
(1,20)	1:A:23:VAL:O	1:A:48:PHE:N	18	0.15
(1,18)	1:A:23:VAL:N	1:A:48:PHE:O	16	0.15
(1,16)	1:A:16:ASN:N	1:A:20:LYS:O	2	0.15
(1,12)	1:A:14:VAL:N	1:A:22:LEU:O	7	0.15
(1,12)	1:A:14:VAL:N	1:A:22:LEU:O	10	0.15
(1,12)	1:A:14:VAL:N	1:A:22:LEU:O	14	0.15
(1,12)	1:A:14:VAL:N	1:A:22:LEU:O	17	0.15
(1,12)	1:A:14:VAL:N	1:A:22:LEU:O	19	0.15
(2,547)	1:A:56:SER:H	1:A:54:ASP:HA	14	0.14
(2,198)	1:A:53:LYS:HA	1:A:54:ASP:H	19	0.14
(2,177)	1:A:32:GLN:HA	1:A:33:LYS:H	2	0.14
(2,1467)	1:A:59:PHE:HD1	1:B:63:LEU:HD21	2	0.14
(2,1467)	1:A:59:PHE:HD1	1:B:63:LEU:HD22	2	0.14
(2,1467)	1:A:59:PHE:HD1	1:B:63:LEU:HD23	2	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,1462)	1:A:59:PHE:HE2	1:B:75:GLU:HA	2	0.14
(1,43)	1:A:51:ASP:H	1:B:47:VAL:O	11	0.14
(1,43)	1:A:51:ASP:H	1:B:47:VAL:O	20	0.14
(1,40)	1:A:49:THR:N	1:B:49:THR:O	5	0.14
(1,28)	1:A:52:ASN:HA	1:A:53:LYS:H	18	0.14
(1,22)	1:A:25:MET:N	1:A:46:LYS:O	17	0.14
(1,20)	1:A:23:VAL:O	1:A:48:PHE:N	3	0.14
(1,18)	1:A:23:VAL:N	1:A:48:PHE:O	1	0.14
(1,18)	1:A:23:VAL:N	1:A:48:PHE:O	4	0.14
(1,18)	1:A:23:VAL:N	1:A:48:PHE:O	9	0.14
(1,18)	1:A:23:VAL:N	1:A:48:PHE:O	11	0.14
(1,14)	1:A:14:VAL:O	1:A:22:LEU:N	1	0.14
(1,12)	1:A:14:VAL:N	1:A:22:LEU:O	5	0.14
(1,12)	1:A:14:VAL:N	1:A:22:LEU:O	16	0.14
(1,10)	1:A:12:ILE:O	1:A:24:VAL:N	17	0.14
(2,903)	1:A:117:ALA:HA	1:A:118:LEU:H	9	0.13
(2,684)	1:A:166:ASN:H	1:A:166:ASN:HA	2	0.13
(2,547)	1:A:56:SER:H	1:A:54:ASP:HA	16	0.13
(2,53)	1:A:55:VAL:H	1:A:55:VAL:HA	12	0.13
(2,409)	1:A:10:ASN:HA	1:A:30:ALA:H	14	0.13
(2,329)	1:A:52:ASN:H	1:A:53:LYS:H	16	0.13
(2,198)	1:A:53:LYS:HA	1:A:54:ASP:H	2	0.13
(2,177)	1:A:32:GLN:HA	1:A:33:LYS:H	19	0.13
(2,1466)	1:A:59:PHE:HD2	1:B:75:GLU:HA	20	0.13
(2,1462)	1:A:59:PHE:HE2	1:B:75:GLU:HA	15	0.13
(2,1459)	1:A:85:LEU:HA	1:A:87:LYS:H	7	0.13
(2,1455)	1:A:151:ASP:H	1:A:115:LYS:HA	12	0.13
(2,1375)	1:A:152:GLU:HA	1:A:156:ILE:H	2	0.13
(2,1255)	1:A:93:ILE:HA	1:A:96:SER:H	2	0.13
(2,107)	1:A:29:LEU:H	1:A:29:LEU:HG	11	0.13
(1,42)	1:A:49:THR:O	1:B:49:THR:N	11	0.13
(1,42)	1:A:49:THR:O	1:B:49:THR:N	17	0.13
(1,40)	1:A:49:THR:N	1:B:49:THR:O	8	0.13
(1,4)	1:A:5:LYS:N	1:A:13:SER:O	4	0.13
(1,4)	1:A:5:LYS:N	1:A:13:SER:O	6	0.13
(1,4)	1:A:5:LYS:N	1:A:13:SER:O	10	0.13
(1,4)	1:A:5:LYS:N	1:A:13:SER:O	18	0.13
(1,28)	1:A:52:ASN:HA	1:A:53:LYS:H	2	0.13
(1,24)	1:A:16:ASN:N	1:A:20:LYS:O	1	0.13
(1,24)	1:A:16:ASN:N	1:A:20:LYS:O	6	0.13
(1,24)	1:A:16:ASN:N	1:A:20:LYS:O	17	0.13
(1,22)	1:A:25:MET:N	1:A:46:LYS:O	2	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,22)	1:A:25:MET:N	1:A:46:LYS:O	5	0.13
(1,22)	1:A:25:MET:N	1:A:46:LYS:O	11	0.13
(1,22)	1:A:25:MET:N	1:A:46:LYS:O	15	0.13
(1,18)	1:A:23:VAL:N	1:A:48:PHE:O	2	0.13
(1,18)	1:A:23:VAL:N	1:A:48:PHE:O	17	0.13
(1,16)	1:A:16:ASN:N	1:A:20:LYS:O	1	0.13
(1,16)	1:A:16:ASN:N	1:A:20:LYS:O	6	0.13
(1,16)	1:A:16:ASN:N	1:A:20:LYS:O	17	0.13
(1,12)	1:A:14:VAL:N	1:A:22:LEU:O	4	0.13
(1,12)	1:A:14:VAL:N	1:A:22:LEU:O	13	0.13
(1,12)	1:A:14:VAL:N	1:A:22:LEU:O	18	0.13
(1,10)	1:A:12:ILE:O	1:A:24:VAL:N	16	0.13
(4,31)	1:A:51:ASP:O	1:B:47:VAL:H	6	0.12
(2,903)	1:A:117:ALA:HA	1:A:118:LEU:H	11	0.12
(2,879)	1:A:90:ASN:HA	1:A:91:ASP:H	6	0.12
(2,854)	1:A:65:ASP:HA	1:A:66:ILE:H	17	0.12
(2,468)	1:A:10:ASN:HA	1:A:27:ARG:HA	14	0.12
(2,433)	1:A:15:VAL:HA	1:A:20:LYS:H	6	0.12
(2,409)	1:A:10:ASN:HA	1:A:30:ALA:H	18	0.12
(2,336)	1:A:5:LYS:H	1:A:13:SER:H	2	0.12
(2,1466)	1:A:59:PHE:HD2	1:B:75:GLU:HA	4	0.12
(2,1466)	1:A:59:PHE:HD2	1:B:75:GLU:HA	12	0.12
(2,1461)	1:A:59:PHE:HE2	1:B:95:VAL:HA	15	0.12
(2,1459)	1:A:85:LEU:HA	1:A:87:LYS:H	18	0.12
(2,1447)	1:A:155:PHE:HE1	1:A:116:ASN:HA	13	0.12
(2,1399)	1:A:158:LEU:HA	1:A:162:ASN:H	19	0.12
(2,1383)	1:A:154:GLY:HA2	1:A:158:LEU:H	6	0.12
(2,1343)	1:A:135:GLU:HA	1:A:139:MET:H	2	0.12
(2,1294)	1:A:102:ASN:HA	1:A:106:GLN:H	2	0.12
(2,1259)	1:A:94:TYR:HA	1:A:97:LEU:H	7	0.12
(2,1219)	1:A:73:VAL:HA	1:A:76:GLU:H	6	0.12
(2,1135)	1:A:126:TYR:H	1:A:127:LYS:H	10	0.12
(1,42)	1:A:49:THR:O	1:B:49:THR:N	14	0.12
(1,40)	1:A:49:THR:N	1:B:49:THR:O	10	0.12
(1,28)	1:A:52:ASN:HA	1:A:53:LYS:H	5	0.12
(1,22)	1:A:25:MET:N	1:A:46:LYS:O	7	0.12
(1,22)	1:A:25:MET:N	1:A:46:LYS:O	16	0.12
(1,18)	1:A:23:VAL:N	1:A:48:PHE:O	7	0.12
(1,18)	1:A:23:VAL:N	1:A:48:PHE:O	8	0.12
(1,14)	1:A:14:VAL:O	1:A:22:LEU:N	15	0.12
(1,12)	1:A:14:VAL:N	1:A:22:LEU:O	15	0.12
(2,951)	1:A:165:LEU:HA	1:A:166:ASN:H	2	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,903)	1:A:117:ALA:HA	1:A:118:LEU:H	2	0.11
(2,903)	1:A:117:ALA:HA	1:A:118:LEU:H	8	0.11
(2,903)	1:A:117:ALA:HA	1:A:118:LEU:H	13	0.11
(2,903)	1:A:117:ALA:HA	1:A:118:LEU:H	18	0.11
(2,854)	1:A:65:ASP:HA	1:A:66:ILE:H	1	0.11
(2,663)	1:A:144:THR:H	1:A:144:THR:HA	12	0.11
(2,663)	1:A:144:THR:H	1:A:144:THR:HA	15	0.11
(2,663)	1:A:144:THR:H	1:A:144:THR:HA	18	0.11
(2,607)	1:A:85:LEU:H	1:A:85:LEU:HA	16	0.11
(2,588)	1:A:65:ASP:H	1:A:65:ASP:HA	18	0.11
(2,547)	1:A:56:SER:H	1:A:54:ASP:HA	1	0.11
(2,547)	1:A:56:SER:H	1:A:54:ASP:HA	13	0.11
(2,547)	1:A:56:SER:H	1:A:54:ASP:HA	15	0.11
(2,53)	1:A:55:VAL:H	1:A:55:VAL:HA	5	0.11
(2,53)	1:A:55:VAL:H	1:A:55:VAL:HA	15	0.11
(2,442)	1:A:3:ILE:HA	1:A:5:LYS:H	10	0.11
(2,336)	1:A:5:LYS:H	1:A:13:SER:H	1	0.11
(2,336)	1:A:5:LYS:H	1:A:13:SER:H	4	0.11
(2,336)	1:A:5:LYS:H	1:A:13:SER:H	18	0.11
(2,336)	1:A:5:LYS:H	1:A:13:SER:H	19	0.11
(2,32)	1:A:33:LYS:H	1:A:33:LYS:HA	6	0.11
(2,177)	1:A:32:GLN:HA	1:A:33:LYS:H	13	0.11
(2,1461)	1:A:59:PHE:HE2	1:B:95:VAL:HA	20	0.11
(2,1444)	1:A:155:PHE:HE1	1:A:152:GLU:HA	16	0.11
(2,1432)	1:A:80:TYR:HD2	1:A:132:ILE:HA	9	0.11
(2,1421)	1:A:117:ALA:HA	1:A:120:TRP:H	7	0.11
(2,1421)	1:A:117:ALA:HA	1:A:120:TRP:H	17	0.11
(2,1414)	1:A:91:ASP:HA	1:A:95:VAL:H	17	0.11
(2,1371)	1:A:151:ASP:HA	1:A:155:PHE:H	3	0.11
(2,1343)	1:A:135:GLU:HA	1:A:139:MET:H	6	0.11
(2,1266)	1:A:95:VAL:HA	1:A:99:ASN:H	14	0.11
(2,1259)	1:A:94:TYR:HA	1:A:97:LEU:H	2	0.11
(2,1259)	1:A:94:TYR:HA	1:A:97:LEU:H	3	0.11
(2,1238)	1:A:77:ILE:HA	1:A:81:ALA:H	3	0.11
(2,1215)	1:A:72:GLU:HA	1:A:75:GLU:H	7	0.11
(1,43)	1:A:51:ASP:H	1:B:47:VAL:O	5	0.11
(1,43)	1:A:51:ASP:H	1:B:47:VAL:O	10	0.11
(1,43)	1:A:51:ASP:H	1:B:47:VAL:O	15	0.11
(1,42)	1:A:49:THR:O	1:B:49:THR:N	1	0.11
(1,42)	1:A:49:THR:O	1:B:49:THR:N	2	0.11
(1,42)	1:A:49:THR:O	1:B:49:THR:N	8	0.11
(1,4)	1:A:5:LYS:N	1:A:13:SER:O	13	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,28)	1:A:52:ASN:HA	1:A:53:LYS:H	14	0.11
(1,24)	1:A:16:ASN:N	1:A:20:LYS:O	4	0.11
(1,24)	1:A:16:ASN:N	1:A:20:LYS:O	14	0.11
(1,22)	1:A:25:MET:N	1:A:46:LYS:O	12	0.11
(1,18)	1:A:23:VAL:N	1:A:48:PHE:O	3	0.11
(1,18)	1:A:23:VAL:N	1:A:48:PHE:O	10	0.11
(1,18)	1:A:23:VAL:N	1:A:48:PHE:O	15	0.11
(1,16)	1:A:16:ASN:N	1:A:20:LYS:O	4	0.11
(1,16)	1:A:16:ASN:N	1:A:20:LYS:O	14	0.11
(1,12)	1:A:14:VAL:N	1:A:22:LEU:O	11	0.11
(1,10)	1:A:12:ILE:O	1:A:24:VAL:N	14	0.11

10 Dihedral-angle violation analysis (i)

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