Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2M5C
BMRB ID	:	19047
Title	:	Solution Structure of the Bacillus cereus Metallo-Beta-Lactamase BcII
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Deposited on	:	2013-02-20

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:

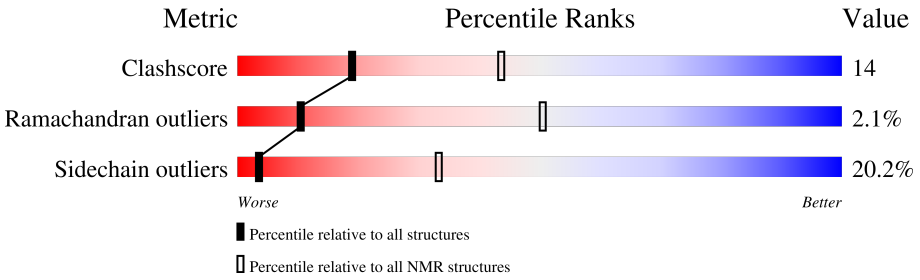
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 84%.

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	227	55% 32% · 10%

2 Ensemble composition and analysis

This entry contains 20 models. Model 7 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *lowest energy*.

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

Well-defined (core) protein residues			
Well-defined core	**Residue range (total)**	**Backbone RMSD (Å)**	**Medoid model**
1	A:8-A:32, A:39-A:173, A:184-A:227 (204)	0.27	7

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

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

The models can be grouped into 4 clusters and 5 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3590 atoms, of which 1830 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Beta-lactamase 2.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	227	3588	1113	1830	304	338	3	0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	2	2	2

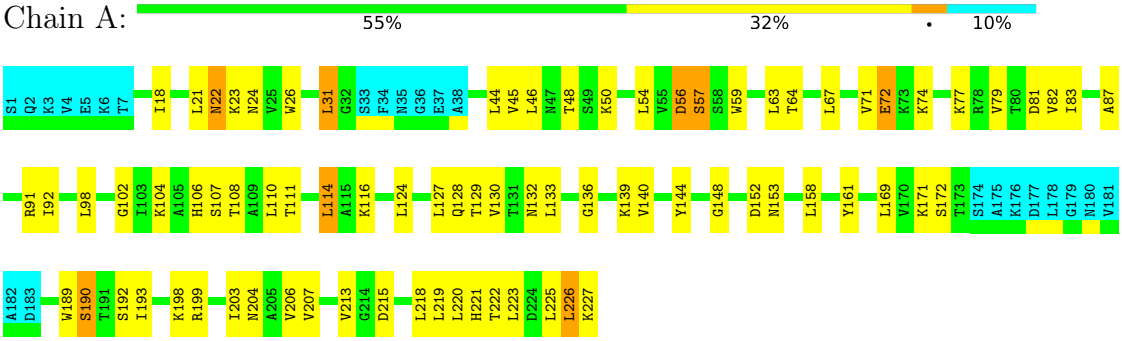
4 Residue-property plots

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: Beta-lactamase 2

Chain A:



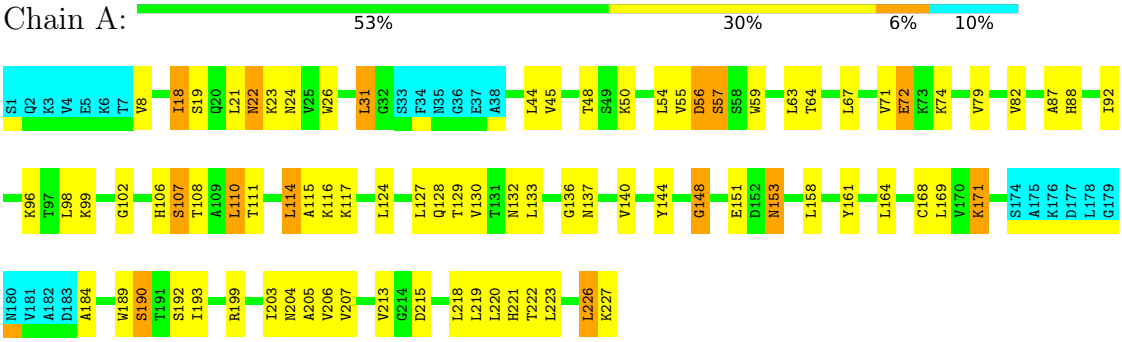
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Beta-lactamase 2

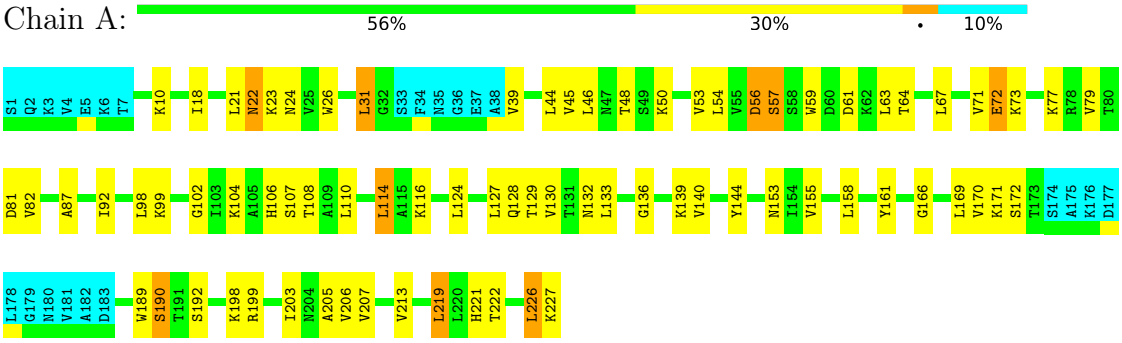
Chain A:



4.2.2 Score per residue for model 2

• Molecule 1: Beta-lactamase 2

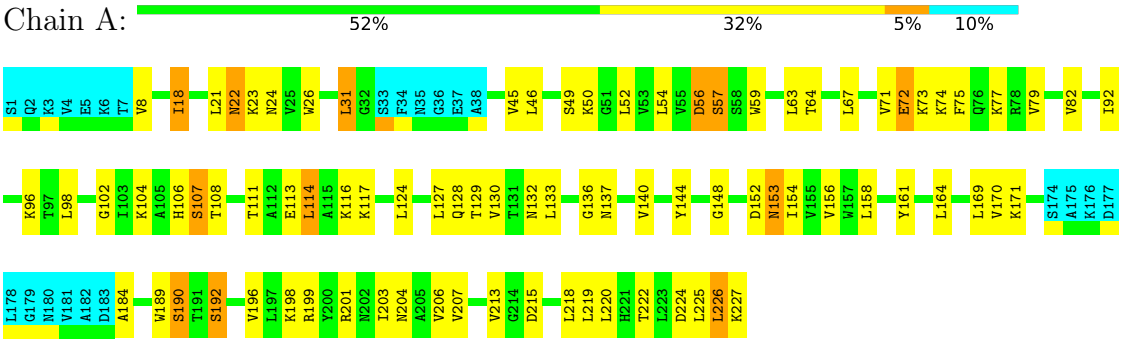
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: Beta-lactamase 2

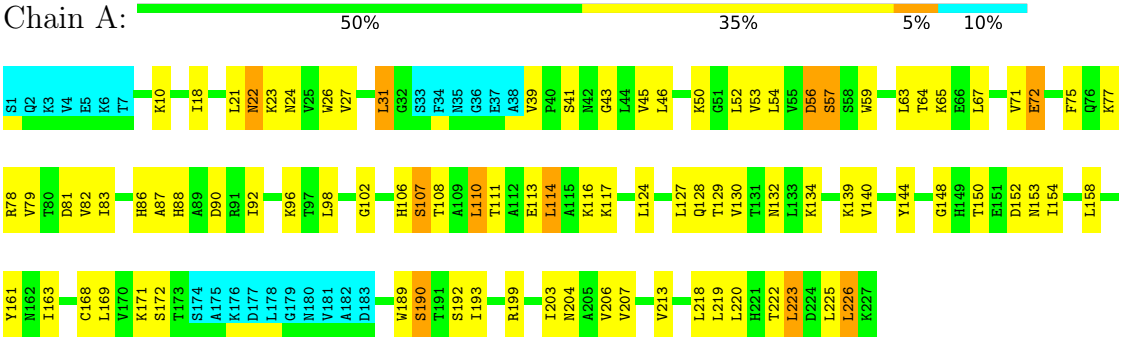
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: Beta-lactamase 2

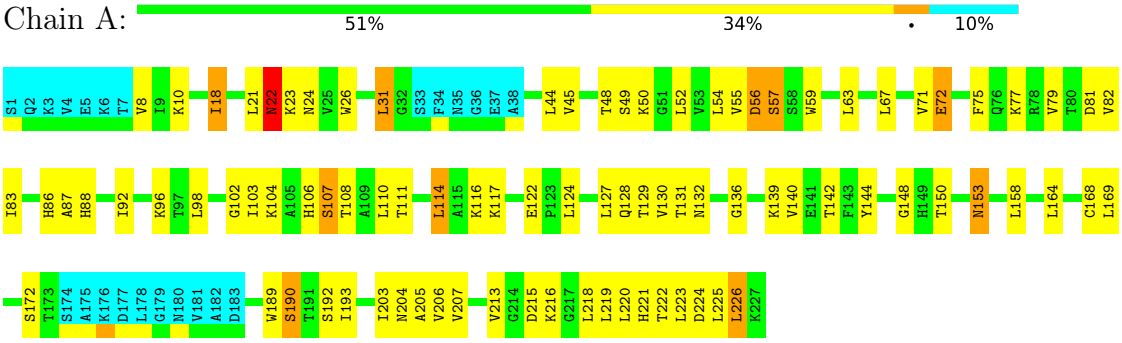
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: Beta-lactamase 2

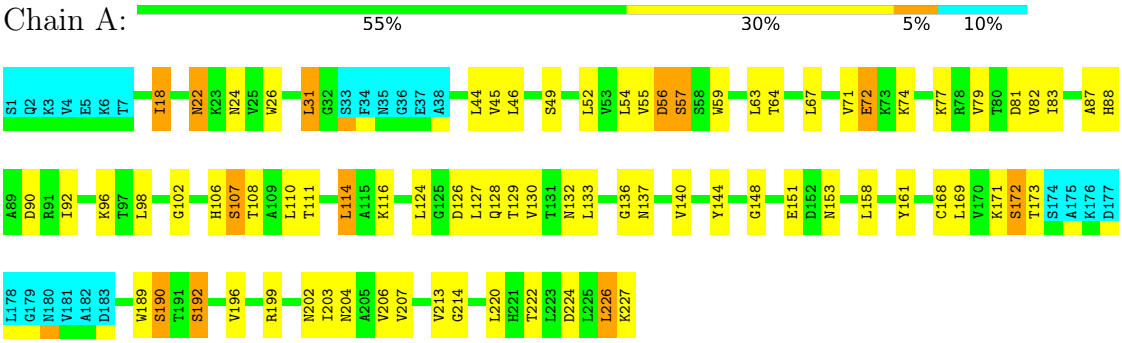
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: Beta-lactamase 2

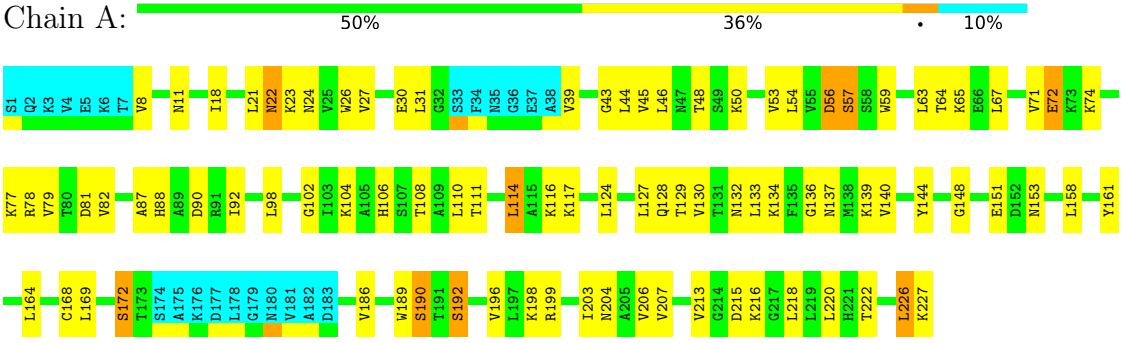
Chain A:



4.2.7 Score per residue for model 7 (medoid)

• Molecule 1: Beta-lactamase 2

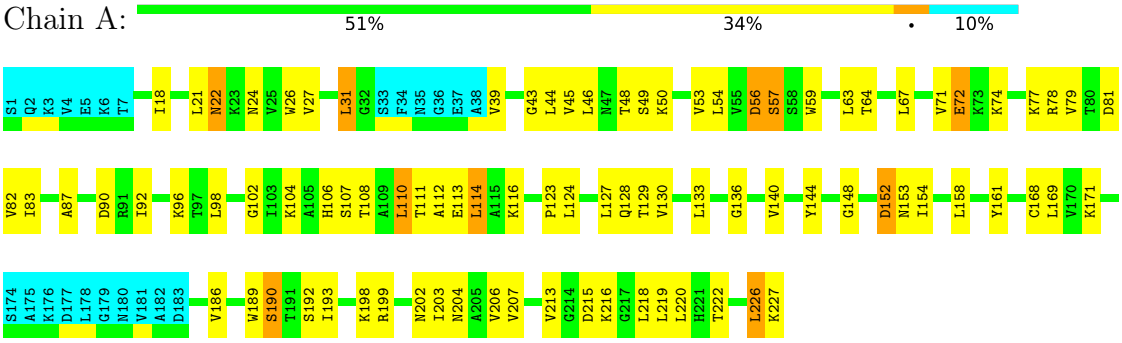
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: Beta-lactamase 2

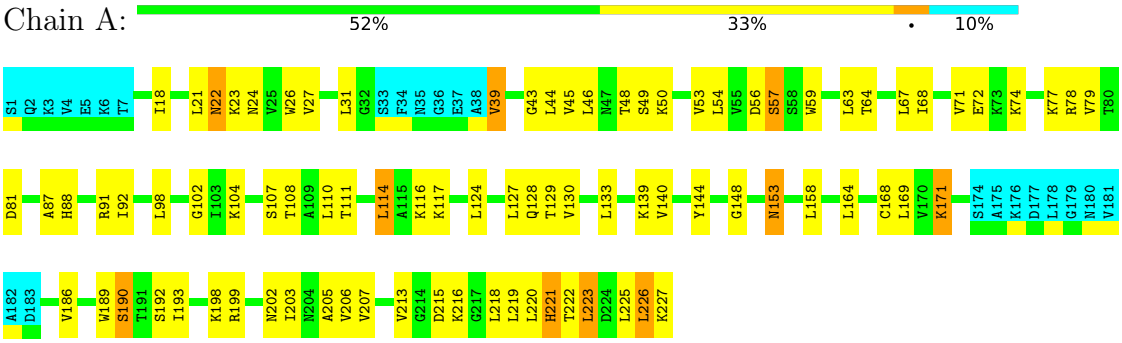
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: Beta-lactamase 2

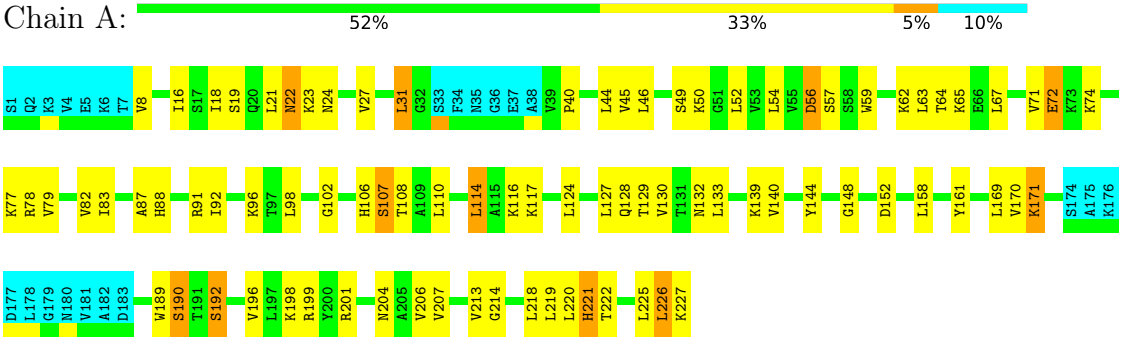
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: Beta-lactamase 2

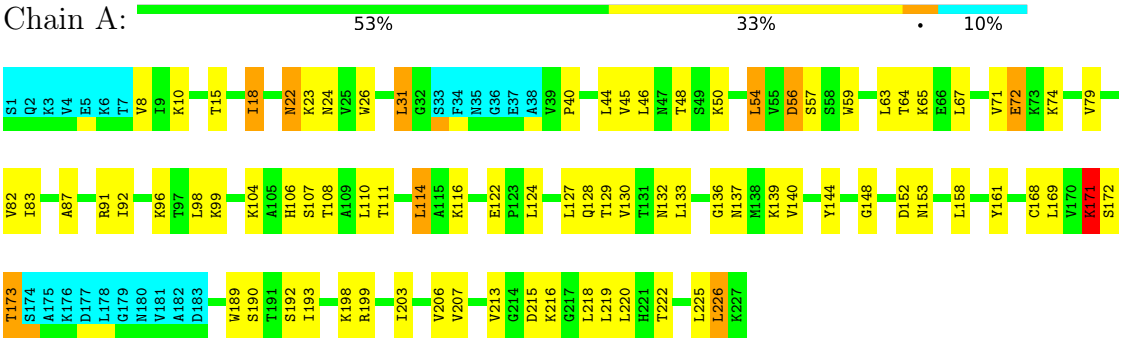
Chain A:



4.2.11 Score per residue for model 11

• Molecule 1: Beta-lactamase 2

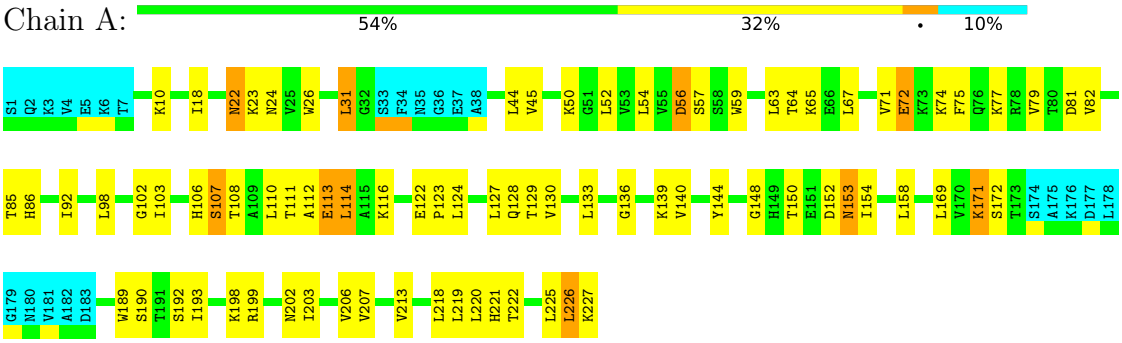
Chain A:



4.2.12 Score per residue for model 12

• Molecule 1: Beta-lactamase 2

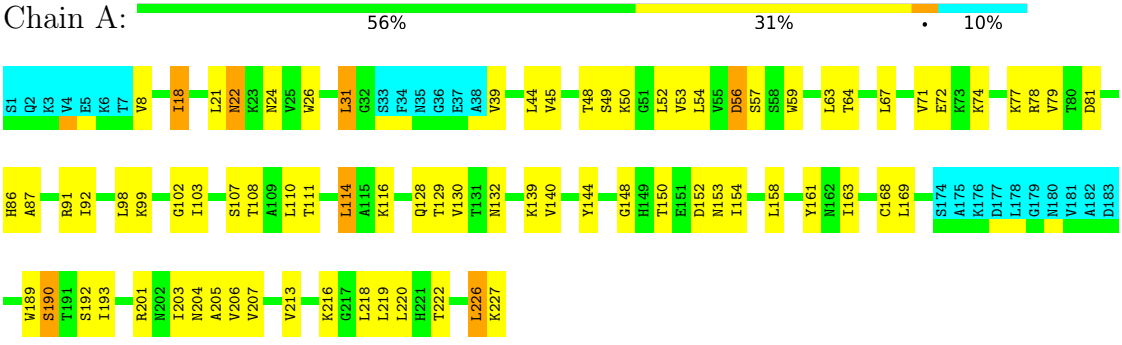
Chain A:



4.2.13 Score per residue for model 13

• Molecule 1: Beta-lactamase 2

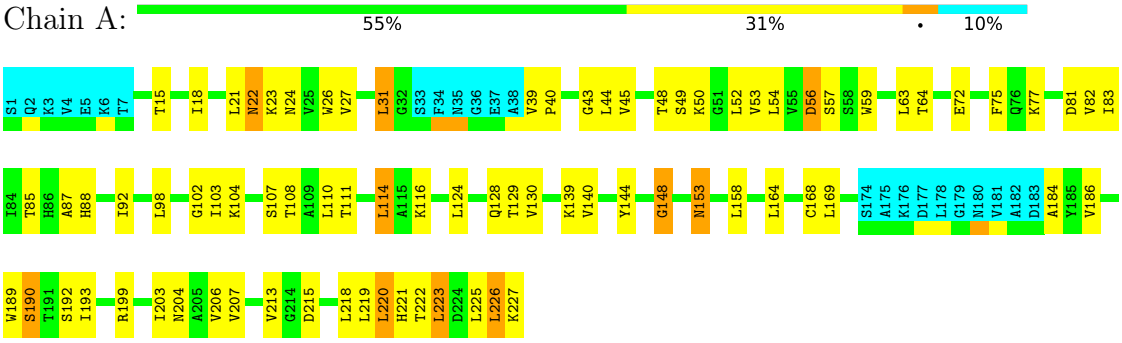
Chain A:



4.2.14 Score per residue for model 14

• Molecule 1: Beta-lactamase 2

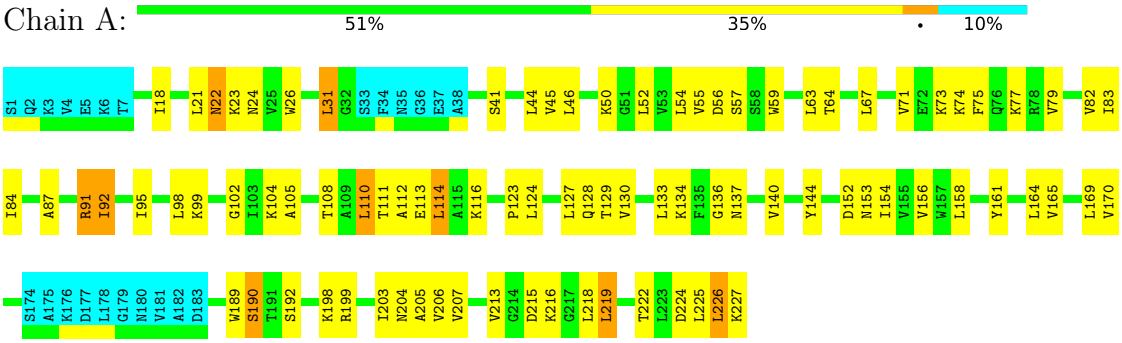
Chain A:



4.2.15 Score per residue for model 15

• Molecule 1: Beta-lactamase 2

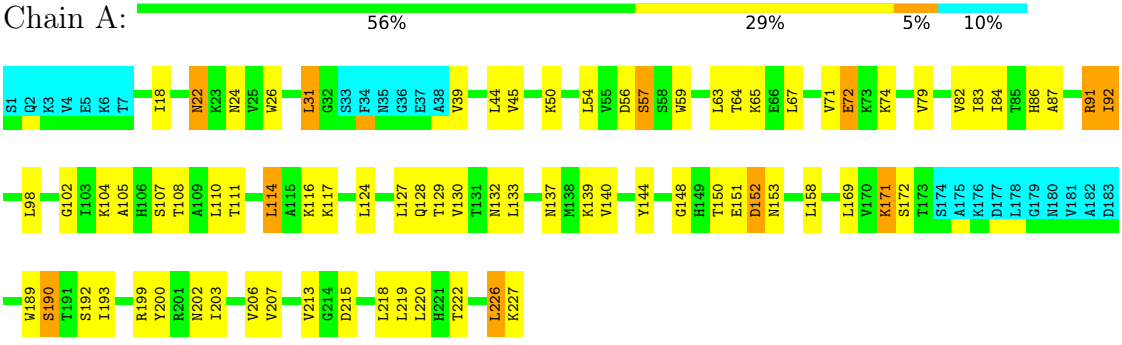
Chain A:



4.2.16 Score per residue for model 16

• Molecule 1: Beta-lactamase 2

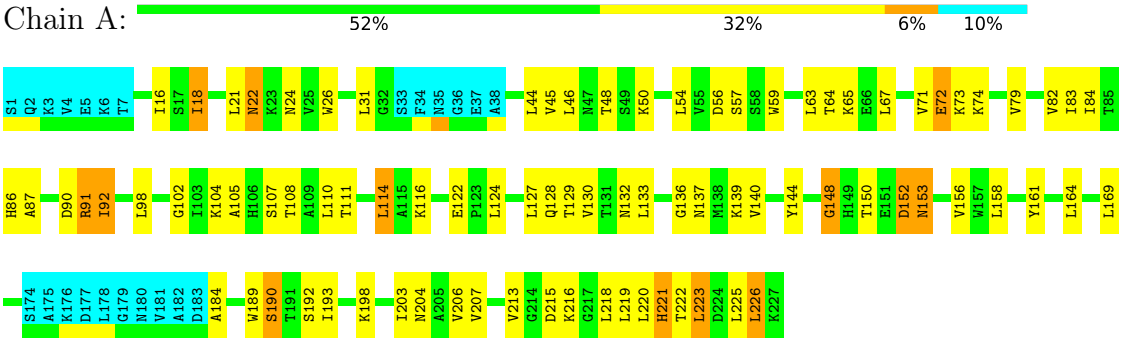
Chain A:



4.2.17 Score per residue for model 17

• Molecule 1: Beta-lactamase 2

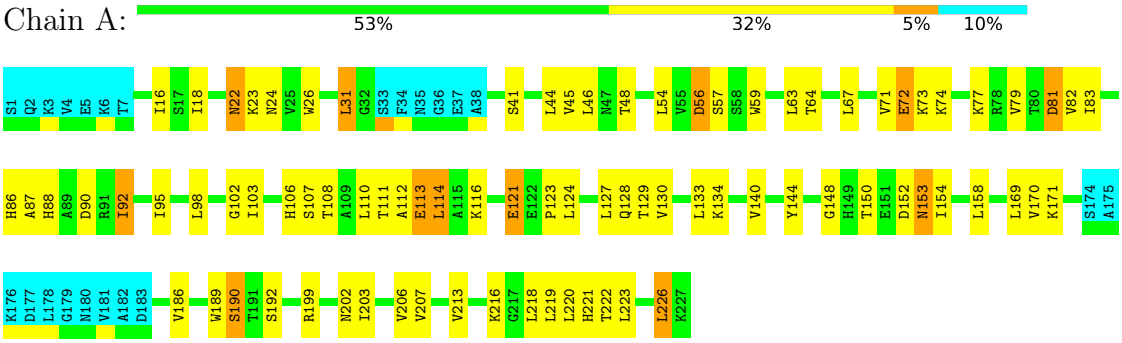
Chain A:



4.2.18 Score per residue for model 18

• Molecule 1: Beta-lactamase 2

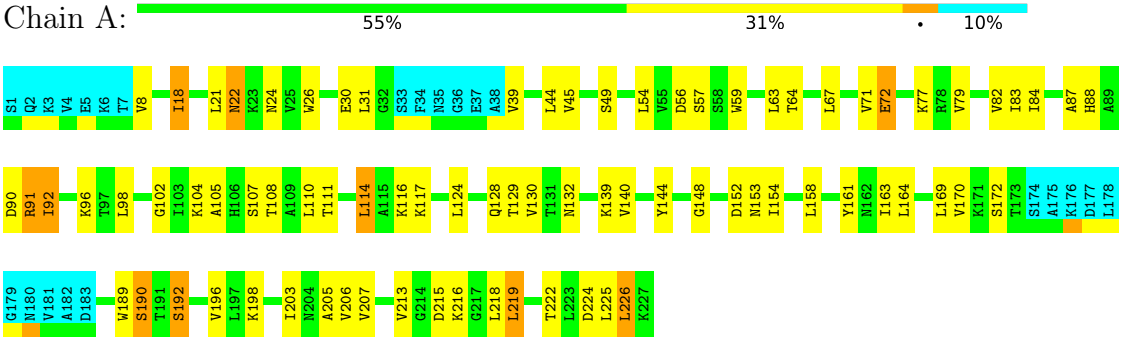
Chain A:



4.2.19 Score per residue for model 19

• Molecule 1: Beta-lactamase 2

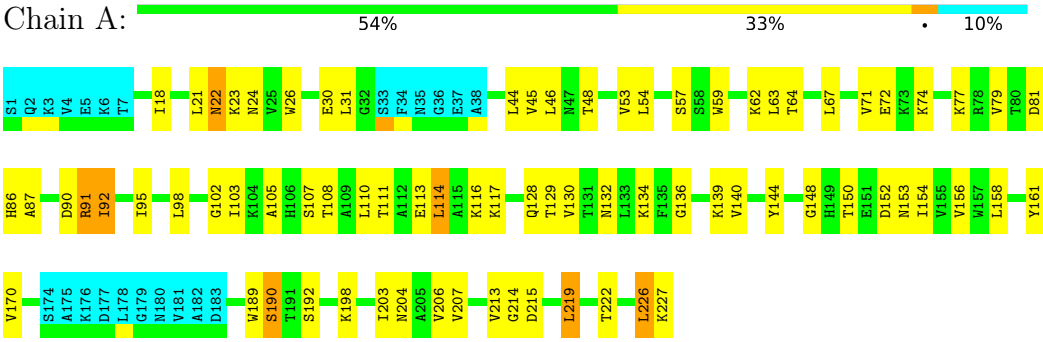
Chain A:



4.2.20 Score per residue for model 20

• Molecule 1: Beta-lactamase 2

Chain A:



5 Refinement protocol and experimental data overview

The models were refined using the following method: *simulated annealing, torsion angle dynamics.*

Of the 100 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CYANA	structure solution	
CYANA	refinement	
CANDID	structure solution	

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	2
Total number of shifts	4075
Number of shifts mapped to atoms	4075
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	84%

6 Model quality

6.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	1591	1666	1638	46±5
All	All	31860	33320	32760	926

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 14.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:207:VAL:HG22	1:A:213:VAL:HG12	0.91	1.41	16	13
1:A:84:ILE:HD11	1:A:105:ALA:HB1	0.88	1.42	15	5
1:A:207:VAL:HG22	1:A:213:VAL:HG22	0.88	1.45	1	5
1:A:21:LEU:HD21	1:A:213:VAL:HG21	0.86	1.48	5	5
1:A:222:THR:HG22	1:A:226:LEU:HD23	0.83	1.49	11	15
1:A:21:LEU:HD21	1:A:213:VAL:HG11	0.81	1.49	19	7
1:A:140:VAL:HG22	1:A:158:LEU:HD21	0.81	1.54	2	17
1:A:84:ILE:HD12	1:A:91:ARG:CZ	0.80	2.07	15	5
1:A:84:ILE:HG23	1:A:91:ARG:NE	0.78	1.94	17	5
1:A:87:ALA:HB2	1:A:114:LEU:HD13	0.76	1.56	20	16
1:A:129:THR:HG22	1:A:130:VAL:HG23	0.75	1.57	17	20
1:A:46:LEU:HD21	1:A:158:LEU:HD11	0.72	1.59	17	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:190:SER:CB	1:A:226:LEU:HD11	0.65	2.21	17	20
1:A:104:LYS:HE2	1:A:124:LEU:HD21	0.64	1.69	19	7
1:A:222:THR:HG22	1:A:226:LEU:CD2	0.64	2.23	18	17
1:A:87:ALA:CB	1:A:114:LEU:HD13	0.64	2.23	18	15
1:A:104:LYS:CE	1:A:124:LEU:HD21	0.63	2.24	19	5
1:A:190:SER:OG	1:A:223:LEU:HD23	0.63	1.93	17	3
1:A:221:HIS:CE1	1:A:225:LEU:HD11	0.63	2.28	9	4
1:A:207:VAL:HG22	1:A:213:VAL:HB	0.62	1.71	19	2
1:A:205:ALA:HB1	1:A:213:VAL:CG1	0.62	2.24	13	5
1:A:110:LEU:HD23	1:A:152:ASP:OD1	0.62	1.94	12	5
1:A:169:LEU:HD12	1:A:189:TRP:NE1	0.62	2.10	12	19
1:A:68:ILE:HG12	1:A:79:VAL:HG11	0.62	1.71	9	1
1:A:57:SER:HB3	1:A:98:LEU:HD11	0.62	1.72	15	16
1:A:44:LEU:HD21	1:A:158:LEU:HD12	0.61	1.72	20	13
1:A:190:SER:HB2	1:A:226:LEU:HD11	0.61	1.71	4	3
1:A:156:VAL:O	1:A:164:LEU:HD12	0.61	1.96	17	3
1:A:18:ILE:HG22	1:A:26:TRP:HB3	0.61	1.73	2	19
1:A:84:ILE:O	1:A:154:ILE:HD11	0.60	1.96	15	3
1:A:110:LEU:HD23	1:A:152:ASP:OD2	0.60	1.97	11	2
1:A:127:LEU:CD2	1:A:133:LEU:HD21	0.60	2.27	3	11
1:A:110:LEU:HD12	1:A:113:GLU:HG2	0.60	1.74	18	2
1:A:83:ILE:CD1	1:A:140:VAL:HG11	0.60	2.26	14	10
1:A:205:ALA:HB1	1:A:213:VAL:CG2	0.60	2.26	19	2
1:A:111:THR:HA	1:A:114:LEU:HD11	0.59	1.74	15	17
1:A:30:GLU:CD	1:A:67:LEU:HD22	0.59	2.18	20	3
1:A:72:GLU:OE2	1:A:79:VAL:HG23	0.59	1.97	12	10
1:A:57:SER:CB	1:A:98:LEU:HD11	0.59	2.27	17	19
1:A:190:SER:HB3	1:A:226:LEU:HD11	0.59	1.72	11	17
1:A:127:LEU:HD22	1:A:133:LEU:HD21	0.59	1.74	8	6
1:A:46:LEU:CD2	1:A:158:LEU:HD11	0.59	2.27	6	5
1:A:206:VAL:HB	1:A:218:LEU:HD12	0.58	1.75	19	17
1:A:72:GLU:OE1	1:A:79:VAL:HG23	0.58	1.98	4	5
1:A:153:ASN:OD1	1:A:169:LEU:HD13	0.58	1.98	9	8
1:A:140:VAL:HG22	1:A:158:LEU:CD2	0.58	2.27	2	15
1:A:110:LEU:HD22	1:A:113:GLU:OE1	0.58	1.98	15	1
1:A:45:VAL:HG13	1:A:54:LEU:CD2	0.58	2.29	2	20
1:A:207:VAL:HG22	1:A:213:VAL:CG1	0.58	2.28	7	13
1:A:104:LYS:HD3	1:A:124:LEU:HD21	0.58	1.73	15	1
1:A:131:THR:HG22	1:A:142:THR:OG1	0.58	1.99	5	1
1:A:203:ILE:HG21	1:A:206:VAL:HG22	0.57	1.76	3	16
1:A:152:ASP:O	1:A:154:ILE:HG23	0.57	1.98	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:54:LEU:O	1:A:82:VAL:HG13	0.57	1.99	5	14
1:A:129:THR:HG23	1:A:144:TYR:HB3	0.57	1.77	4	20
1:A:57:SER:OG	1:A:98:LEU:HD11	0.57	1.99	2	5
1:A:203:ILE:HG21	1:A:206:VAL:CG2	0.57	2.29	4	13
1:A:44:LEU:HD21	1:A:158:LEU:HD11	0.56	1.78	5	3
1:A:171:LYS:HG2	1:A:222:THR:HG23	0.56	1.78	16	5
1:A:110:LEU:HD12	1:A:152:ASP:HB3	0.56	1.76	8	1
1:A:84:ILE:CD1	1:A:105:ALA:HB1	0.55	2.29	17	4
1:A:84:ILE:HD11	1:A:105:ALA:CB	0.55	2.29	17	4
1:A:55:VAL:HG12	1:A:56:ASP:OD1	0.55	2.02	6	3
1:A:207:VAL:CG2	1:A:213:VAL:HG12	0.55	2.29	8	8
1:A:207:VAL:HG22	1:A:213:VAL:CG2	0.55	2.27	13	5
1:A:98:LEU:HA	1:A:103:ILE:HD13	0.54	1.78	13	5
1:A:81:ASP:N	1:A:103:ILE:HG23	0.54	2.17	14	3
1:A:192:SER:O	1:A:196:VAL:HG23	0.54	2.02	10	5
1:A:226:LEU:HD12	1:A:226:LEU:O	0.54	2.03	12	19
1:A:106:HIS:HA	1:A:124:LEU:HD12	0.54	1.79	5	12
1:A:53:VAL:HG13	1:A:81:ASP:CB	0.54	2.32	14	2
1:A:44:LEU:HD21	1:A:158:LEU:CD1	0.54	2.33	5	9
1:A:31:LEU:HD12	1:A:40:PRO:HB3	0.54	1.80	14	3
1:A:107:SER:CA	1:A:127:LEU:HD12	0.54	2.33	6	9
1:A:83:ILE:HD13	1:A:140:VAL:HG11	0.53	1.79	14	6
1:A:59:TRP:HB2	1:A:63:LEU:HD12	0.53	1.80	5	20
1:A:164:LEU:HD22	1:A:203:ILE:HD13	0.53	1.79	15	8
1:A:45:VAL:HG22	1:A:54:LEU:HD23	0.52	1.80	16	7
1:A:171:LYS:HE3	1:A:225:LEU:HD11	0.52	1.80	11	1
1:A:205:ALA:HB1	1:A:213:VAL:HG11	0.52	1.79	5	3
1:A:52:LEU:HB3	1:A:79:VAL:HG22	0.52	1.81	15	7
1:A:21:LEU:HG	1:A:27:VAL:HG23	0.52	1.80	10	2
1:A:53:VAL:HG13	1:A:81:ASP:O	0.52	2.05	20	6
1:A:104:LYS:HE3	1:A:124:LEU:HD21	0.52	1.80	7	3
1:A:56:ASP:OD2	1:A:85:THR:HG23	0.51	2.05	14	1
1:A:45:VAL:HG13	1:A:54:LEU:HD23	0.51	1.82	5	12
1:A:91:ARG:HH22	1:A:95:ILE:HD12	0.51	1.65	20	2
1:A:193:ILE:HG21	1:A:219:LEU:O	0.51	2.06	8	11
1:A:144:TYR:CD1	1:A:154:ILE:HG22	0.50	2.41	12	3
1:A:107:SER:HA	1:A:127:LEU:HD12	0.50	1.84	6	4
1:A:164:LEU:HD22	1:A:203:ILE:CD1	0.50	2.37	14	8
1:A:54:LEU:HD11	1:A:79:VAL:HG21	0.50	1.83	20	6
1:A:67:LEU:O	1:A:71:VAL:HG22	0.49	2.06	5	18
1:A:53:VAL:HG13	1:A:81:ASP:HB2	0.49	1.84	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:52:LEU:HD11	1:A:75:PHE:HB2	0.49	1.83	14	6
1:A:27:VAL:HG13	1:A:43:GLY:O	0.49	2.08	14	5
1:A:16:ILE:HD13	1:A:67:LEU:HB2	0.49	1.85	10	2
1:A:104:LYS:HB3	1:A:124:LEU:HD11	0.49	1.83	8	6
1:A:91:ARG:HH21	1:A:92:ILE:HG22	0.49	1.65	16	5
1:A:57:SER:OG	1:A:98:LEU:HD21	0.49	2.07	16	2
1:A:92:ILE:O	1:A:95:ILE:HG22	0.49	2.08	18	1
1:A:171:LYS:HD3	1:A:222:THR:HG23	0.49	1.84	10	1
1:A:222:THR:O	1:A:226:LEU:HD23	0.48	2.08	7	2
1:A:107:SER:OG	1:A:111:THR:HG21	0.48	2.08	6	2
1:A:27:VAL:HG21	1:A:213:VAL:CG2	0.48	2.39	9	1
1:A:170:VAL:HG13	1:A:219:LEU:HA	0.48	1.85	10	7
1:A:21:LEU:HD13	1:A:163:ILE:HD13	0.48	1.84	19	3
1:A:67:LEU:O	1:A:67:LEU:HD12	0.47	2.09	17	5
1:A:22:ASN:N	1:A:22:ASN:ND2	0.47	2.63	18	20
1:A:148:GLY:O	1:A:184:ALA:HB1	0.47	2.09	3	4
1:A:106:HIS:CA	1:A:124:LEU:HD12	0.47	2.39	5	1
1:A:54:LEU:O	1:A:82:VAL:HG22	0.47	2.09	19	4
1:A:84:ILE:HG23	1:A:91:ARG:HE	0.47	1.68	20	1
1:A:111:THR:HG23	1:A:152:ASP:OD1	0.46	2.11	15	2
1:A:86:HIS:HB2	1:A:150:THR:HG21	0.46	1.87	12	8
1:A:222:THR:C	1:A:226:LEU:HD23	0.46	2.31	13	7
1:A:91:ARG:NH2	1:A:95:ILE:HD12	0.46	2.25	20	1
1:A:110:LEU:HD12	1:A:113:GLU:CG	0.46	2.41	12	1
1:A:106:HIS:CG	1:A:124:LEU:HD12	0.46	2.46	6	2
1:A:171:LYS:CE	1:A:225:LEU:HD11	0.46	2.40	11	1
1:A:207:VAL:CG2	1:A:213:VAL:HG22	0.45	2.34	15	3
1:A:207:VAL:HG13	1:A:213:VAL:HG12	0.45	1.87	10	3
1:A:127:LEU:HD21	1:A:133:LEU:HD21	0.45	1.88	2	2
1:A:55:VAL:HG11	1:A:165:VAL:HG11	0.45	1.88	15	1
1:A:52:LEU:HD13	1:A:77:LYS:HB2	0.45	1.89	13	1
1:A:30:GLU:OE2	1:A:67:LEU:HD22	0.45	2.12	19	1
1:A:15:THR:HG23	1:A:31:LEU:HB3	0.45	1.89	14	2
1:A:114:LEU:HD23	1:A:151:GLU:HB3	0.45	1.89	1	4
1:A:112:ALA:HB2	1:A:123:PRO:HG2	0.45	1.89	18	4
1:A:110:LEU:HD21	1:A:151:GLU:HG2	0.44	1.88	7	2
1:A:110:LEU:HD23	1:A:152:ASP:CG	0.44	2.32	12	1
1:A:169:LEU:HD12	1:A:189:TRP:HE1	0.44	1.72	18	3
1:A:54:LEU:CD1	1:A:79:VAL:HG21	0.43	2.44	2	4
1:A:46:LEU:HD21	1:A:158:LEU:HD21	0.43	1.89	4	1
1:A:200:TYR:O	1:A:203:ILE:HD11	0.43	2.14	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:95:ILE:HG12	1:A:121:GLU:CG	0.42	2.44	18	1
1:A:171:LYS:HG3	1:A:225:LEU:HD12	0.42	1.91	3	2
1:A:203:ILE:HG21	1:A:206:VAL:HG23	0.42	1.91	4	1
1:A:18:ILE:CD1	1:A:71:VAL:HG12	0.42	2.45	7	3
1:A:67:LEU:O	1:A:71:VAL:HG13	0.42	2.15	20	2
1:A:52:LEU:HD11	1:A:75:PHE:CB	0.42	2.44	12	2
1:A:114:LEU:HD12	1:A:115:ALA:N	0.41	2.30	1	1
1:A:190:SER:OG	1:A:226:LEU:HD11	0.41	2.15	5	1
1:A:16:ILE:HG21	1:A:67:LEU:HD13	0.41	1.91	17	1
1:A:110:LEU:HD22	1:A:113:GLU:CD	0.41	2.35	4	1
1:A:39:VAL:HG12	1:A:59:TRP:CZ2	0.41	2.50	19	1
1:A:155:VAL:HG12	1:A:166:GLY:HA2	0.41	1.92	2	1
1:A:111:THR:HG23	1:A:152:ASP:OD2	0.40	2.16	19	1
1:A:220:LEU:HA	1:A:223:LEU:HD12	0.40	1.93	14	1
1:A:139:LYS:O	1:A:158:LEU:HD23	0.40	2.16	9	1
1:A:53:VAL:HG22	1:A:81:ASP:HB2	0.40	1.94	14	1
1:A:83:ILE:HG21	1:A:156:VAL:HG22	0.40	1.91	20	1
1:A:81:ASP:O	1:A:82:VAL:HG23	0.40	2.16	14	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	203/227 (89%)	175±3 (86±1%)	24±3 (12±1%)	4±1 (2±1%)	10	50
All	All	4060/4540 (89%)	3499 (86%)	476 (12%)	85 (2%)	10	50

All 11 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	102	GLY	19
1	A	148	GLY	17
1	A	56	ASP	15
1	A	136	GLY	12

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Mol	Chain	Res	Type	Models (Total)
1	A	8	VAL	8
1	A	202	ASN	6
1	A	214	GLY	3
1	A	171	LYS	2
1	A	57	SER	1
1	A	22	ASN	1
1	A	11	ASN	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	178/196 (91%)	142±3 (80±2%)	36±3 (20±2%)	3 33
All	All	3560/3920 (91%)	2842 (80%)	718 (20%)	3 33

All 70 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	22	ASN	20
1	A	24	ASN	20
1	A	92	ILE	20
1	A	108	THR	20
1	A	114	LEU	20
1	A	116	LYS	20
1	A	128	GLN	20
1	A	192	SER	20
1	A	226	LEU	20
1	A	64	THR	19
1	A	72	GLU	19
1	A	153	ASN	19
1	A	190	SER	18
1	A	50	LYS	16
1	A	107	SER	16
1	A	220	LEU	16
1	A	31	LEU	15
1	A	74	LYS	15

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Mol	Chain	Res	Type	Models (Total)
1	A	199	ARG	15
1	A	77	LYS	15
1	A	23	LYS	14
1	A	132	ASN	14
1	A	161	TYR	14
1	A	227	LYS	14
1	A	56	ASP	14
1	A	204	ASN	13
1	A	215	ASP	13
1	A	139	LYS	13
1	A	48	THR	12
1	A	198	LYS	12
1	A	110	LEU	11
1	A	88	HIS	10
1	A	117	LYS	10
1	A	168	CYS	10
1	A	216	LYS	10
1	A	18	ILE	9
1	A	96	LYS	9
1	A	57	SER	9
1	A	49	SER	9
1	A	91	ARG	9
1	A	137	ASN	8
1	A	221	HIS	8
1	A	172	SER	8
1	A	90	ASP	8
1	A	171	LYS	7
1	A	223	LEU	7
1	A	65	LYS	7
1	A	78	ARG	6
1	A	99	LYS	5
1	A	10	LYS	5
1	A	39	VAL	5
1	A	73	LYS	5
1	A	113	GLU	5
1	A	224	ASP	5
1	A	134	LYS	5
1	A	219	LEU	4
1	A	122	GLU	4
1	A	201	ARG	3
1	A	41	SER	3
1	A	81	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	A	152	ASP	3
1	A	19	SER	2
1	A	173	THR	2
1	A	62	LYS	2
1	A	61	ASP	1
1	A	154	ILE	1
1	A	126	ASP	1
1	A	54	LEU	1
1	A	85	THR	1
1	A	121	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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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 84% for the well-defined parts and 83% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping

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

Total number of shifts	2293
Number of shifts mapped to atoms	2293
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	15

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	202	-0.63 ± 0.13	Should be checked
$^{13}C_{\beta}$	202	-0.17 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	0	—	None (insufficient data)

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 75%, i.e. 2111 atoms were assigned a chemical shift out of a possible 2807. 0 out of 45 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	596/1028 (58%)	412/421 (98%)	184/408 (45%)	0/199 (0%)
Sidechain	1395/1602 (87%)	970/1045 (93%)	425/504 (84%)	0/53 (0%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	120/177 (68%)	71/87 (82%)	49/74 (66%)	0/16 (0%)
Overall	2111/2807 (75%)	1453/1553 (94%)	658/986 (67%)	0/268 (0%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 74%, i.e. 2286 atoms were assigned a chemical shift out of a possible 3082. 0 out of 48 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	655/1145 (57%)	453/469 (97%)	202/454 (44%)	0/222 (0%)
Sidechain	1503/1750 (86%)	1046/1139 (92%)	457/552 (83%)	0/59 (0%)
Aromatic	128/187 (68%)	76/92 (83%)	52/79 (66%)	0/16 (0%)
Overall	2286/3082 (74%)	1575/1700 (93%)	711/1085 (66%)	0/297 (0%)

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.

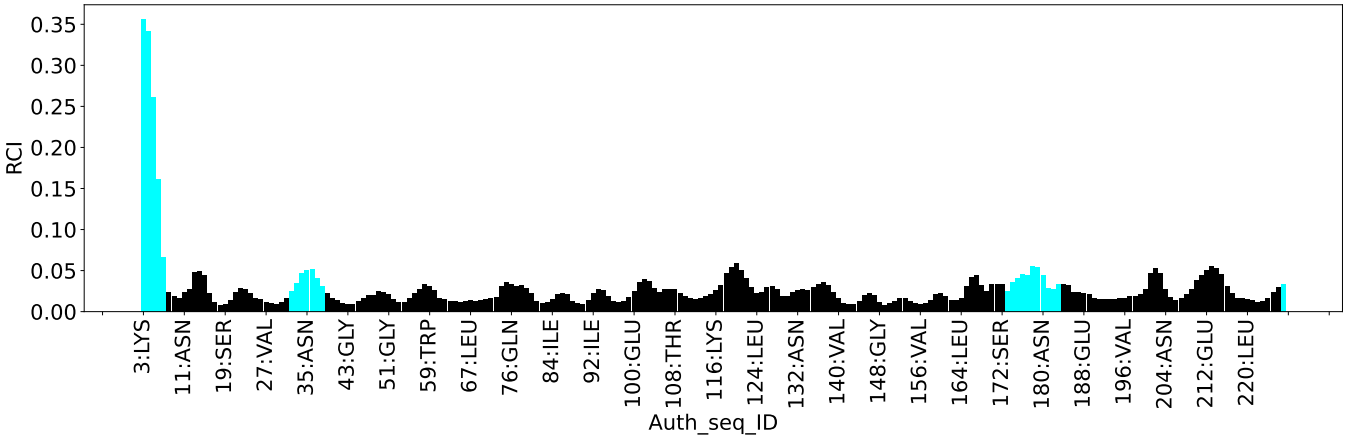
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	108	THR	HG1	6.69	0.08 – 2.19	26.3
1	A	80	THR	HG1	6.26	0.08 – 2.19	24.3
1	A	48	THR	HG1	5.65	0.08 – 2.19	21.4
1	A	222	THR	HG1	5.32	0.08 – 2.19	19.8
1	A	29	THR	HG1	4.78	0.08 – 2.19	17.2
1	A	200	TYR	CD2	116.27	125.28 – 140.14	-11.1
1	A	90	ASP	HB3	0.40	1.32 – 4.00	-8.4
1	A	20	GLN	HB3	-0.07	0.71 – 3.33	-8.0
1	A	199	ARG	HD2	1.35	1.97 – 4.26	-7.7
1	A	199	ARG	HD3	1.23	1.81 – 4.39	-7.3
1	A	199	ARG	HG3	-0.25	0.15 – 2.94	-6.4
1	A	147	LYS	HD3	0.28	0.54 – 2.65	-6.3
1	A	90	ASP	HA	2.75	3.04 – 6.12	-5.9
1	A	32	GLY	HA3	1.88	2.08 – 5.71	-5.6
1	A	75	PHE	HZ	4.82	4.94 – 9.06	-5.3

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:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_2*

7.2.1 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	1782
Number of shifts mapped to atoms	1782
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	12

7.2.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	0	—	None (insufficient data)
$^{13}C_{\beta}$	0	—	None (insufficient data)
$^{13}C'$	0	—	None (insufficient data)

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Nucleus	# values	Correction ± precision, *ppm*	Suggested action
^{15}N	211	0.50 ± 0.22	None needed (< 0.5 ppm)

7.2.3 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 58%, i.e. 1635 atoms were assigned a chemical shift out of a possible 2807. 0 out of 45 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	607/1028 (59%)	414/421 (98%)	0/408 (0%)	193/199 (97%)
Sidechain	974/1602 (61%)	957/1045 (92%)	0/504 (0%)	17/53 (32%)
Aromatic	54/177 (31%)	50/87 (57%)	0/74 (0%)	4/16 (25%)
Overall	1635/2807 (58%)	1421/1553 (92%)	0/986 (0%)	214/268 (80%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 58%, i.e. 1775 atoms were assigned a chemical shift out of a possible 3082. 0 out of 48 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	665/1145 (58%)	454/469 (97%)	0/454 (0%)	211/222 (95%)
Sidechain	1054/1750 (60%)	1034/1139 (91%)	0/552 (0%)	20/59 (34%)
Aromatic	56/187 (30%)	52/92 (57%)	0/79 (0%)	4/16 (25%)
Overall	1775/3082 (58%)	1540/1700 (91%)	0/1085 (0%)	235/297 (79%)

7.2.4 Statistically unusual chemical shifts

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
2	A	108	THR	HG1	6.72	0.08 – 2.19	26.4
2	A	80	THR	HG1	6.28	0.08 – 2.19	24.4
2	A	48	THR	HG1	5.66	0.08 – 2.19	21.4
2	A	222	THR	HG1	5.32	0.08 – 2.19	19.8
2	A	29	THR	HG1	4.77	0.08 – 2.19	17.2
2	A	90	ASP	HB3	0.39	1.32 – 4.00	-8.5
2	A	20	GLN	HB3	-0.03	0.71 – 3.33	-7.8
2	A	199	ARG	HD3	1.22	1.81 – 4.39	-7.3
2	A	199	ARG	HG3	-0.25	0.15 – 2.94	-6.5

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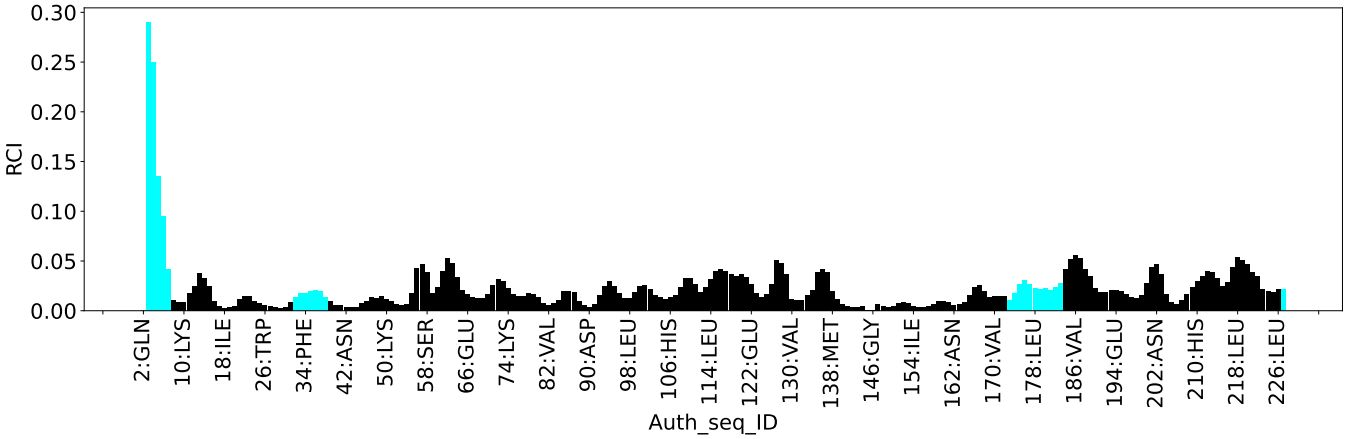
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
2	A	147	LYS	HD3	0.26	0.54 – 2.65	-6.3
2	A	90	ASP	HA	2.75	3.04 – 6.12	-5.9
2	A	32	GLY	HA3	1.86	2.08 – 5.71	-5.6

7.2.5 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	6749
Intra-residue (|i-j|=0)	1215
Sequential (|i-j|=1)	1557
Medium range (|i-j|>1 and |i-j|<5)	1216
Long range (|i-j|≥5)	2759
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	2
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	29.7
Number of long range restraints per residue[1]	12.2

[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)	21.9	0.2
0.2-0.5 (Medium)	3.2	0.47
>0.5 (Large)	None	None

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)

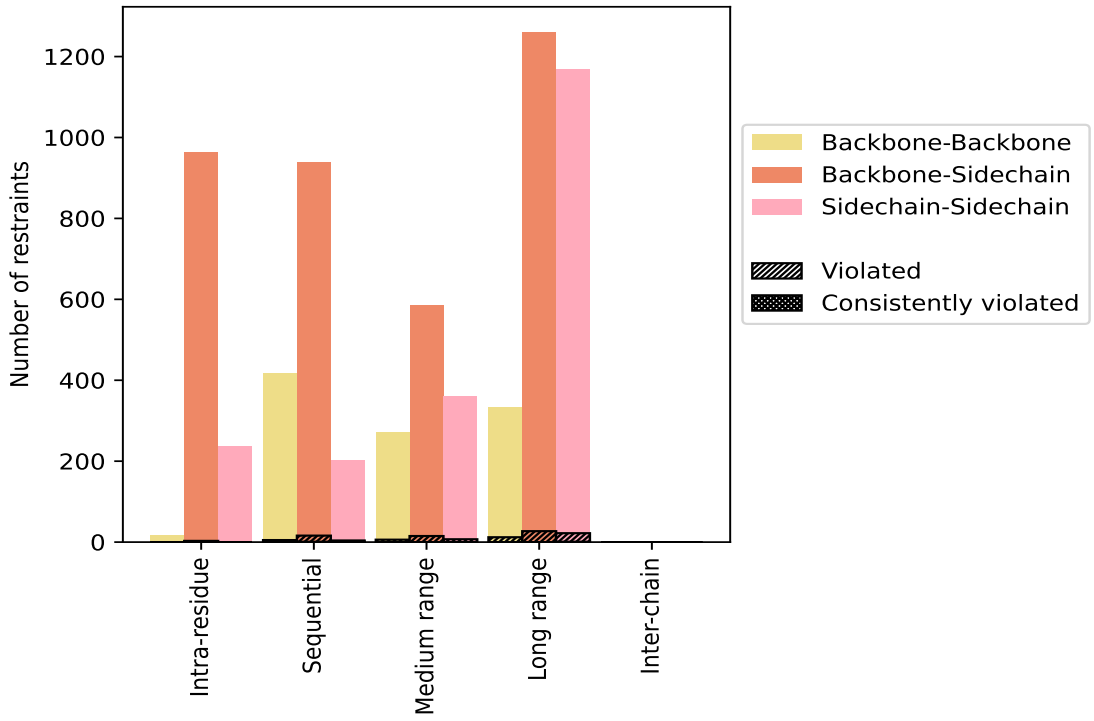
9.1 Summary of distance violations (i)

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)	1215	18.0	3	0.2	0.0	0	0.0	0.0
Backbone-Backbone	16	0.2	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	962	14.3	3	0.3	0.0	0	0.0	0.0
Sidechain-Sidechain	237	3.5	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	1557	23.1	25	1.6	0.4	2	0.1	0.0
Backbone-Backbone	417	6.2	5	1.2	0.1	0	0.0	0.0
Backbone-Sidechain	938	13.9	16	1.7	0.2	1	0.1	0.0
Sidechain-Sidechain	202	3.0	4	2.0	0.1	1	0.5	0.0
Medium range (|i-j|>1 & |i-j|<5)	1216	18.0	28	2.3	0.4	0	0.0	0.0
Backbone-Backbone	270	4.0	6	2.2	0.1	0	0.0	0.0
Backbone-Sidechain	585	8.7	15	2.6	0.2	0	0.0	0.0
Sidechain-Sidechain	361	5.3	7	1.9	0.1	0	0.0	0.0
Long range (|i-j|≥5)	2759	40.9	60	2.2	0.9	1	0.0	0.0
Backbone-Backbone	333	4.9	12	3.6	0.2	0	0.0	0.0
Backbone-Sidechain	1260	18.7	27	2.1	0.4	0	0.0	0.0
Sidechain-Sidechain	1166	17.3	21	1.8	0.3	1	0.1	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	2	0.0	1	50.0	0.0	0	0.0	0.0
Total	6749	100.0	117	1.7	1.7	3	0.0	0.0
Backbone-Backbone	1036	15.4	23	2.2	0.3	0	0.0	0.0
Backbone-Sidechain	3745	55.5	61	1.6	0.9	1	0.0	0.0
Sidechain-Sidechain	1968	29.2	33	1.7	0.5	2	0.1	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	2	4	8	0	14	0.15	0.22	0.03	0.14
2	0	6	5	8	0	19	0.15	0.22	0.03	0.14
3	1	4	5	10	0	20	0.15	0.21	0.03	0.15
4	1	4	5	11	0	21	0.15	0.21	0.03	0.14
5	0	4	5	13	0	22	0.15	0.23	0.04	0.14
6	2	7	4	12	0	25	0.16	0.25	0.04	0.16
7	1	4	7	13	0	25	0.15	0.23	0.04	0.13
8	1	4	5	8	0	18	0.15	0.22	0.03	0.15
9	0	4	4	16	0	24	0.16	0.34	0.06	0.15
10	1	6	6	10	0	23	0.17	0.36	0.06	0.15
11	2	5	8	15	0	30	0.14	0.21	0.03	0.14

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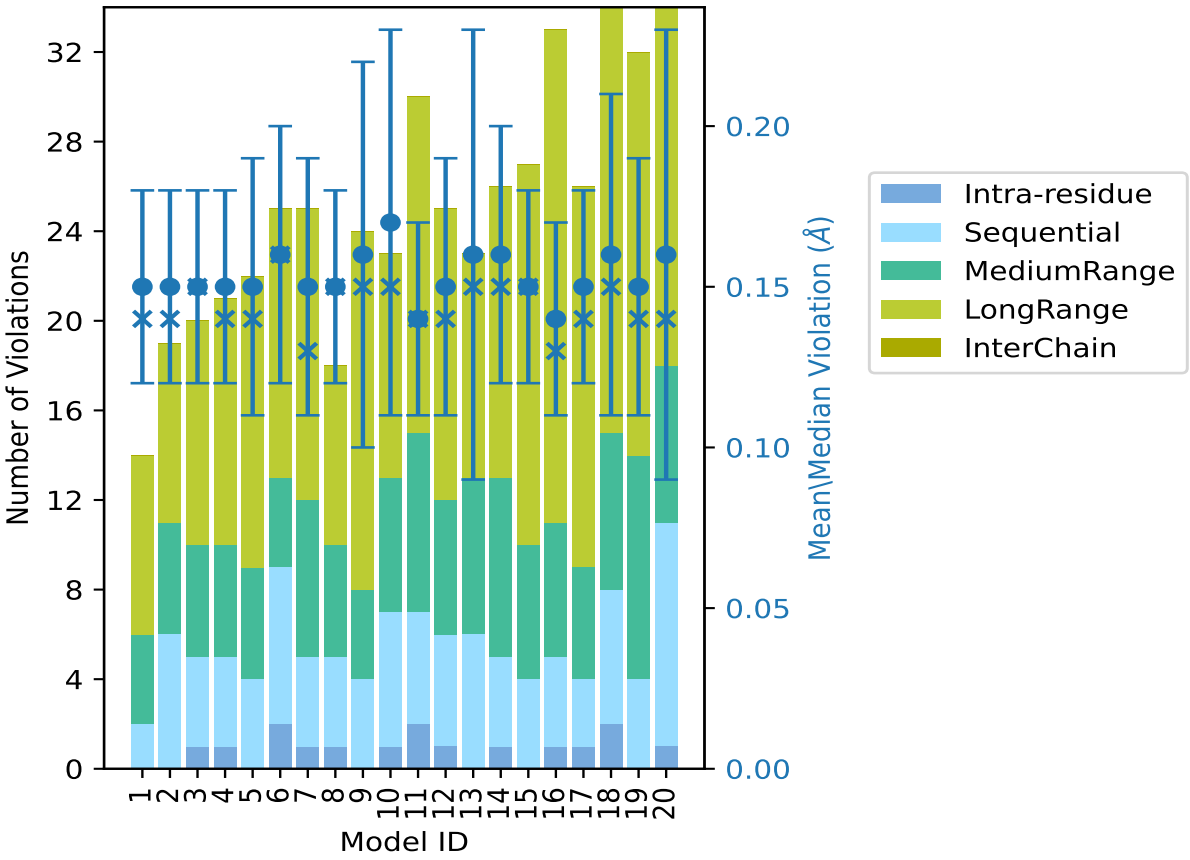
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	1	5	6	13	0	25	0.15	0.26	0.04	0.14
13	0	6	7	10	0	23	0.16	0.46	0.07	0.15
14	1	4	8	13	0	26	0.16	0.25	0.04	0.15
15	0	4	6	17	0	27	0.15	0.23	0.03	0.15
16	1	4	6	22	0	33	0.14	0.21	0.03	0.13
17	1	3	5	17	0	26	0.15	0.22	0.03	0.14
18	2	6	7	19	0	34	0.16	0.38	0.05	0.15
19	0	4	10	18	0	32	0.15	0.25	0.04	0.14
20	1	10	7	16	0	34	0.16	0.47	0.07	0.14

[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

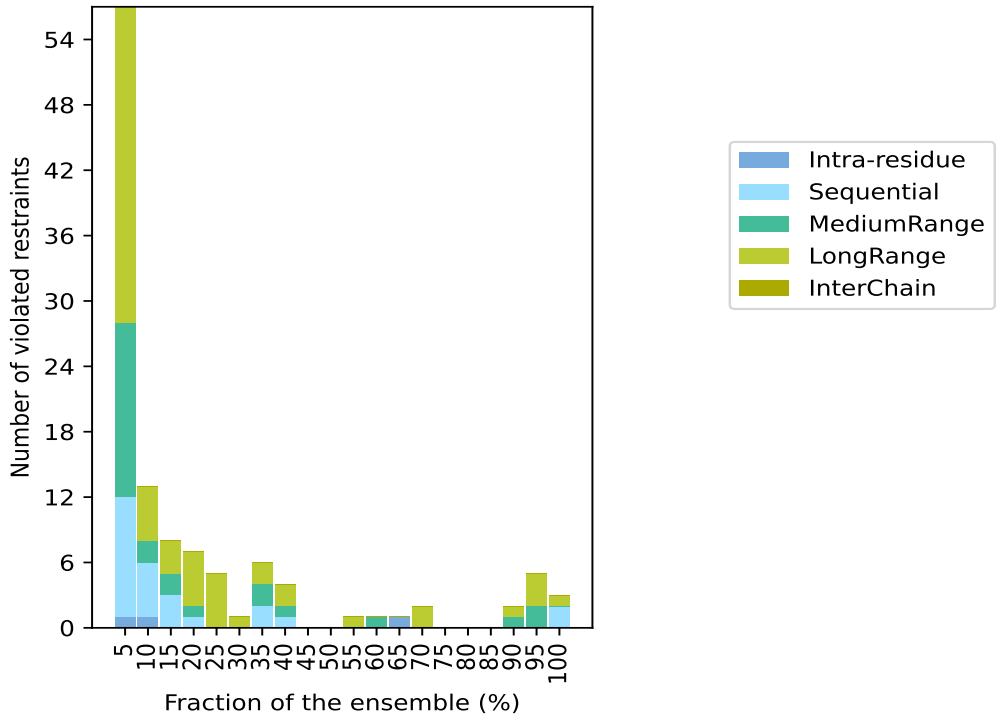
9.3 Distance violation statistics for the ensemble (i)

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, 6631(IR:1212, SQ:1532, MR:1188, LR:2699, 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]	%
1	11	16	29	0	57	1	5.0
1	5	2	5	0	13	2	10.0
0	3	2	3	0	8	3	15.0
0	1	1	5	0	7	4	20.0
0	0	0	5	0	5	5	25.0
0	0	0	1	0	1	6	30.0
0	2	2	2	0	6	7	35.0
0	1	1	2	0	4	8	40.0
0	0	0	0	0	0	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	1	0	1	11	55.0
0	0	1	0	0	1	12	60.0
1	0	0	0	0	1	13	65.0
0	0	0	2	0	2	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	1	1	0	2	18	90.0
0	0	2	3	0	5	19	95.0
0	2	0	1	0	3	20	100.0

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

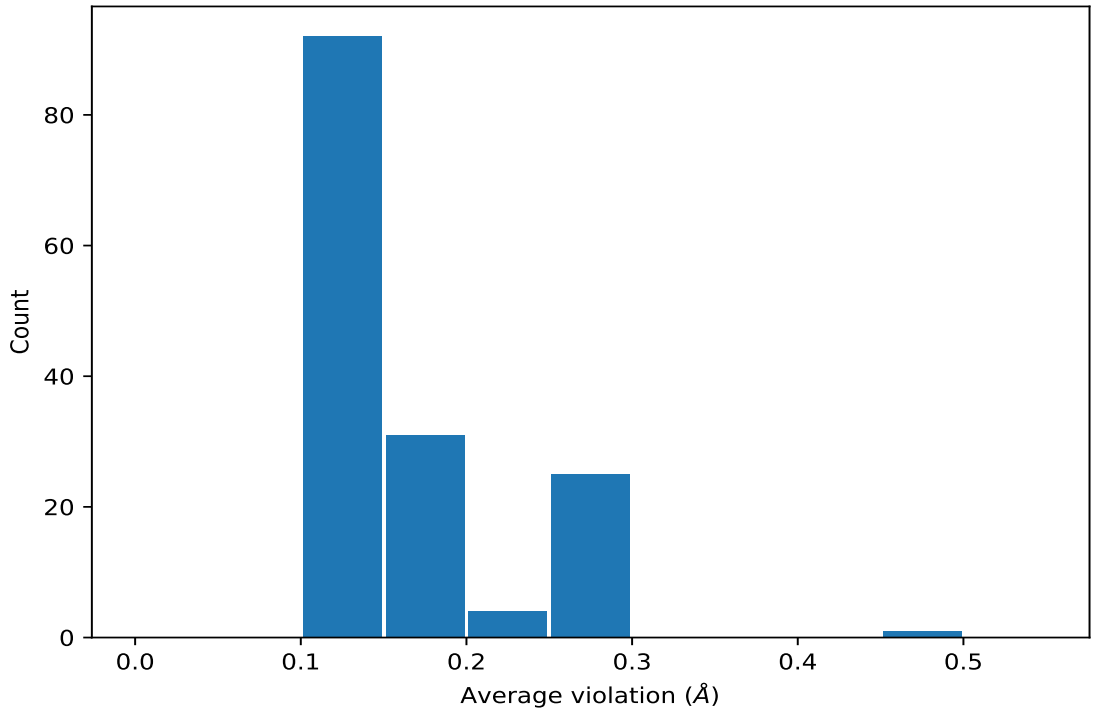
9.3.1 Bar graph : Distance violation statistics for the ensemble



9.4 Most violated distance restraints in the ensemble

9.4.1 Histogram : Distribution of mean distance violations

The following histogram shows the distribution of the average value of the violation. The average is calculated for each restraint that is violated in more than one model over all the violated models in the ensemble



9.4.2 Table: Most violated distance restraints

The following table provides the mean and the standard deviation of the 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)
(3,3)	1:A:210:HIS:NE2	2:A:302:ZN:ZN	20	0.22	0.01	0.22
(3,5)	2:A:301:ZN:ZN	2:A:302:ZN:ZN	20	0.21	0.01	0.21
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG21	20	0.14	0.01	0.14
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG22	20	0.14	0.01	0.14
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG23	20	0.14	0.01	0.14
(3,4)	1:A:90:ASP:OD2	2:A:302:ZN:ZN	19	0.21	0.01	0.2
(1,2775)	1:A:9:ILE:HB	1:A:19:SER:H	19	0.15	0.01	0.16
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD11	19	0.15	0.02	0.15
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD12	19	0.15	0.02	0.15
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD13	19	0.15	0.02	0.15
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD11	19	0.15	0.02	0.15
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD12	19	0.15	0.02	0.15
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD13	19	0.15	0.02	0.15
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD11	19	0.15	0.02	0.15
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD12	19	0.15	0.02	0.15
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD13	19	0.15	0.02	0.15

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2842)	1:A:20:GLN:HA	1:A:25:VAL:H	19	0.14	0.02	0.14
(1,4510)	1:A:193:ILE:HG12	1:A:195:ASN:H	19	0.14	0.02	0.13
(1,3163)	1:A:54:LEU:HA	1:A:56:ASP:H	18	0.15	0.02	0.15
(1,3413)	1:A:68:ILE:HD11	1:A:79:VAL:H	18	0.14	0.02	0.14
(1,3413)	1:A:68:ILE:HD12	1:A:79:VAL:H	18	0.14	0.02	0.14
(1,3413)	1:A:68:ILE:HD13	1:A:79:VAL:H	18	0.14	0.02	0.14
(1,4092)	1:A:87:ALA:H	1:A:153:ASN:H	14	0.14	0.02	0.13
(1,2685)	1:A:54:LEU:H	1:A:82:VAL:HB	14	0.13	0.02	0.13
(1,4699)	1:A:213:VAL:H	1:A:213:VAL:HB	13	0.12	0.01	0.12
(1,4675)	1:A:208:PRO:HD3	1:A:210:HIS:H	12	0.14	0.03	0.14
(1,2790)	1:A:7:THR:HA	1:A:20:GLN:H	11	0.14	0.01	0.13
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG11	8	0.15	0.0	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG12	8	0.15	0.0	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG13	8	0.15	0.0	0.15
(1,3058)	1:A:46:LEU:H	1:A:54:LEU:HB3	8	0.14	0.03	0.14
(1,2800)	1:A:8:VAL:HB	1:A:20:GLN:H	8	0.14	0.01	0.14
(1,2518)	1:A:195:ASN:HB3	1:A:198:LYS:HB2	8	0.13	0.01	0.12
(1,2518)	1:A:195:ASN:HB3	1:A:198:LYS:HB3	8	0.13	0.01	0.12
(1,6653)	1:A:214:GLY:HA3	1:A:215:ASP:HB2	7	0.19	0.01	0.19
(1,6653)	1:A:214:GLY:HA3	1:A:215:ASP:HB3	7	0.19	0.01	0.19
(1,6659)	1:A:215:ASP:HB2	1:A:216:LYS:HA	7	0.17	0.0	0.17
(1,6659)	1:A:215:ASP:HB3	1:A:216:LYS:HA	7	0.17	0.0	0.17
(1,3799)	1:A:113:GLU:HB2	1:A:116:LYS:H	7	0.15	0.04	0.16
(1,3799)	1:A:113:GLU:HB3	1:A:116:LYS:H	7	0.15	0.04	0.16
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD21	7	0.12	0.01	0.12
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD22	7	0.12	0.01	0.12
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD23	7	0.12	0.01	0.12
(1,2097)	1:A:58:SER:HB2	1:A:67:LEU:HG	7	0.12	0.01	0.12
(1,4040)	1:A:148:GLY:H	1:A:151:GLU:H	7	0.12	0.01	0.11
(3,2)	1:A:168:CYS:SG	2:A:302:ZN:ZN	6	0.19	0.03	0.2
(1,5457)	1:A:39:VAL:HG11	1:A:59:TRP:HE1	6	0.13	0.01	0.12
(1,5457)	1:A:39:VAL:HG12	1:A:59:TRP:HE1	6	0.13	0.01	0.12
(1,5457)	1:A:39:VAL:HG13	1:A:59:TRP:HE1	6	0.13	0.01	0.12
(1,5457)	1:A:39:VAL:HG21	1:A:59:TRP:HE1	6	0.13	0.01	0.12
(1,5457)	1:A:39:VAL:HG22	1:A:59:TRP:HE1	6	0.13	0.01	0.12
(1,5457)	1:A:39:VAL:HG23	1:A:59:TRP:HE1	6	0.13	0.01	0.12
(1,795)	1:A:57:SER:H	1:A:92:ILE:HG21	5	0.16	0.01	0.17
(1,795)	1:A:57:SER:H	1:A:92:ILE:HG22	5	0.16	0.01	0.17
(1,795)	1:A:57:SER:H	1:A:92:ILE:HG23	5	0.16	0.01	0.17
(1,4940)	1:A:115:ALA:H	1:A:120:TYR:HD1	5	0.14	0.01	0.14
(1,4940)	1:A:115:ALA:H	1:A:120:TYR:HD2	5	0.14	0.01	0.14
(1,3572)	1:A:95:ILE:H	1:A:120:TYR:HE1	5	0.14	0.02	0.14

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3572)	1:A:95:ILE:H	1:A:120:TYR:HE2	5	0.14	0.02	0.14
(1,3701)	1:A:83:ILE:HA	1:A:107:SER:H	5	0.13	0.03	0.12
(1,773)	1:A:84:ILE:HD11	1:A:92:ILE:HB	5	0.13	0.01	0.13
(1,773)	1:A:84:ILE:HD12	1:A:92:ILE:HB	5	0.13	0.01	0.13
(1,773)	1:A:84:ILE:HD13	1:A:92:ILE:HB	5	0.13	0.01	0.13
(1,370)	1:A:28:HIS:H	1:A:42:ASN:HA	4	0.13	0.02	0.13
(1,2130)	1:A:219:LEU:HD11	1:A:222:THR:HG1	4	0.13	0.02	0.13
(1,2130)	1:A:219:LEU:HD12	1:A:222:THR:HG1	4	0.13	0.02	0.13
(1,2130)	1:A:219:LEU:HD13	1:A:222:THR:HG1	4	0.13	0.02	0.13
(1,867)	1:A:57:SER:H	1:A:105:ALA:HB1	4	0.12	0.01	0.12
(1,867)	1:A:57:SER:H	1:A:105:ALA:HB2	4	0.12	0.01	0.12
(1,867)	1:A:57:SER:H	1:A:105:ALA:HB3	4	0.12	0.01	0.12
(1,2166)	1:A:83:ILE:HG21	1:A:107:SER:H	4	0.12	0.02	0.11
(1,2166)	1:A:83:ILE:HG22	1:A:107:SER:H	4	0.12	0.02	0.11
(1,2166)	1:A:83:ILE:HG23	1:A:107:SER:H	4	0.12	0.02	0.11
(1,2618)	1:A:57:SER:HA	1:A:91:ARG:HA	4	0.12	0.01	0.12
(1,5671)	1:A:54:LEU:HD11	1:A:55:VAL:H	4	0.12	0.01	0.12
(1,5671)	1:A:54:LEU:HD12	1:A:55:VAL:H	4	0.12	0.01	0.12
(1,5671)	1:A:54:LEU:HD13	1:A:55:VAL:H	4	0.12	0.01	0.12
(1,5671)	1:A:54:LEU:HD21	1:A:55:VAL:H	4	0.12	0.01	0.12
(1,5671)	1:A:54:LEU:HD22	1:A:55:VAL:H	4	0.12	0.01	0.12
(1,5671)	1:A:54:LEU:HD23	1:A:55:VAL:H	4	0.12	0.01	0.12
(1,1406)	1:A:84:ILE:HG21	1:A:91:ARG:HA	4	0.12	0.0	0.12
(1,1406)	1:A:84:ILE:HG22	1:A:91:ARG:HA	4	0.12	0.0	0.12
(1,1406)	1:A:84:ILE:HG23	1:A:91:ARG:HA	4	0.12	0.0	0.12
(1,2053)	1:A:45:VAL:HA	1:A:53:VAL:HG21	3	0.19	0.01	0.18
(1,2053)	1:A:45:VAL:HA	1:A:53:VAL:HG22	3	0.19	0.01	0.18
(1,2053)	1:A:45:VAL:HA	1:A:53:VAL:HG23	3	0.19	0.01	0.18
(1,5878)	1:A:90:ASP:HB2	1:A:91:ARG:HB2	3	0.17	0.01	0.17
(1,5878)	1:A:90:ASP:HB2	1:A:91:ARG:HB3	3	0.17	0.01	0.17
(1,5878)	1:A:90:ASP:HB3	1:A:91:ARG:HB2	3	0.17	0.01	0.17
(1,5878)	1:A:90:ASP:HB3	1:A:91:ARG:HB3	3	0.17	0.01	0.17
(1,1447)	1:A:190:SER:HB2	1:A:226:LEU:HB2	3	0.16	0.0	0.16
(1,1447)	1:A:190:SER:HB2	1:A:226:LEU:HB3	3	0.16	0.0	0.16
(1,1447)	1:A:190:SER:HB3	1:A:226:LEU:HB2	3	0.16	0.0	0.16
(1,1447)	1:A:190:SER:HB3	1:A:226:LEU:HB3	3	0.16	0.0	0.16
(1,4800)	1:A:224:ASP:H	1:A:226:LEU:HB2	3	0.16	0.0	0.16
(1,4800)	1:A:224:ASP:H	1:A:226:LEU:HB3	3	0.16	0.0	0.16
(1,2963)	1:A:32:GLY:HA2	1:A:33:SER:H	3	0.14	0.02	0.13
(1,3168)	1:A:56:ASP:H	1:A:57:SER:H	3	0.13	0.03	0.11
(1,3173)	1:A:58:SER:H	1:A:95:ILE:H	3	0.12	0.01	0.12
(1,4796)	1:A:222:THR:HG1	1:A:224:ASP:H	3	0.11	0.0	0.11

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,3433)	1:A:81:ASP:H	1:A:82:VAL:HB	2	0.46	0.0	0.46
(1,5795)	1:A:71:VAL:HG21	1:A:79:VAL:HG11	2	0.28	0.03	0.28
(1,5795)	1:A:71:VAL:HG21	1:A:79:VAL:HG12	2	0.28	0.03	0.28
(1,5795)	1:A:71:VAL:HG21	1:A:79:VAL:HG13	2	0.28	0.03	0.28
(1,5795)	1:A:71:VAL:HG21	1:A:79:VAL:HG21	2	0.28	0.03	0.28
(1,5795)	1:A:71:VAL:HG21	1:A:79:VAL:HG22	2	0.28	0.03	0.28
(1,5795)	1:A:71:VAL:HG21	1:A:79:VAL:HG23	2	0.28	0.03	0.28
(1,5795)	1:A:71:VAL:HG22	1:A:79:VAL:HG11	2	0.28	0.03	0.28
(1,5795)	1:A:71:VAL:HG22	1:A:79:VAL:HG12	2	0.28	0.03	0.28
(1,5795)	1:A:71:VAL:HG22	1:A:79:VAL:HG13	2	0.28	0.03	0.28
(1,5795)	1:A:71:VAL:HG22	1:A:79:VAL:HG21	2	0.28	0.03	0.28
(1,5795)	1:A:71:VAL:HG22	1:A:79:VAL:HG22	2	0.28	0.03	0.28
(1,5795)	1:A:71:VAL:HG22	1:A:79:VAL:HG23	2	0.28	0.03	0.28
(1,5795)	1:A:71:VAL:HG23	1:A:79:VAL:HG11	2	0.28	0.03	0.28
(1,5795)	1:A:71:VAL:HG23	1:A:79:VAL:HG12	2	0.28	0.03	0.28
(1,5795)	1:A:71:VAL:HG23	1:A:79:VAL:HG13	2	0.28	0.03	0.28
(1,5795)	1:A:71:VAL:HG23	1:A:79:VAL:HG21	2	0.28	0.03	0.28
(1,5795)	1:A:71:VAL:HG23	1:A:79:VAL:HG22	2	0.28	0.03	0.28
(1,5795)	1:A:71:VAL:HG23	1:A:79:VAL:HG23	2	0.28	0.03	0.28
(1,2104)	1:A:68:ILE:HB	1:A:79:VAL:HB	2	0.27	0.07	0.27
(1,5679)	1:A:55:VAL:HA	1:A:82:VAL:HG11	2	0.26	0.03	0.26
(1,5679)	1:A:55:VAL:HA	1:A:82:VAL:HG12	2	0.26	0.03	0.26
(1,5679)	1:A:55:VAL:HA	1:A:82:VAL:HG13	2	0.26	0.03	0.26
(1,5679)	1:A:55:VAL:HA	1:A:82:VAL:HG21	2	0.26	0.03	0.26
(1,5679)	1:A:55:VAL:HA	1:A:82:VAL:HG22	2	0.26	0.03	0.26
(1,5679)	1:A:55:VAL:HA	1:A:82:VAL:HG23	2	0.26	0.03	0.26
(1,1154)	1:A:172:SER:HA	1:A:173:THR:HB	2	0.22	0.03	0.22
(1,2836)	1:A:173:THR:H	1:A:173:THR:HG21	2	0.16	0.01	0.16
(1,2836)	1:A:173:THR:H	1:A:173:THR:HG22	2	0.16	0.01	0.16
(1,2836)	1:A:173:THR:H	1:A:173:THR:HG23	2	0.16	0.01	0.16
(1,686)	1:A:81:ASP:HA	1:A:82:VAL:HB	2	0.16	0.0	0.16
(1,5440)	1:A:35:ASN:HD21	1:A:39:VAL:HG11	2	0.16	0.04	0.16
(1,5440)	1:A:35:ASN:HD21	1:A:39:VAL:HG12	2	0.16	0.04	0.16
(1,5440)	1:A:35:ASN:HD21	1:A:39:VAL:HG13	2	0.16	0.04	0.16
(1,5440)	1:A:35:ASN:HD21	1:A:39:VAL:HG21	2	0.16	0.04	0.16
(1,5440)	1:A:35:ASN:HD21	1:A:39:VAL:HG22	2	0.16	0.04	0.16
(1,5440)	1:A:35:ASN:HD21	1:A:39:VAL:HG23	2	0.16	0.04	0.16
(1,2109)	1:A:67:LEU:H	1:A:68:ILE:HD11	2	0.12	0.01	0.12
(1,2109)	1:A:67:LEU:H	1:A:68:ILE:HD12	2	0.12	0.01	0.12
(1,2109)	1:A:67:LEU:H	1:A:68:ILE:HD13	2	0.12	0.01	0.12
(1,39)	1:A:34:PHE:HD1	1:A:39:VAL:HB	2	0.12	0.0	0.12
(1,39)	1:A:34:PHE:HD2	1:A:39:VAL:HB	2	0.12	0.0	0.12

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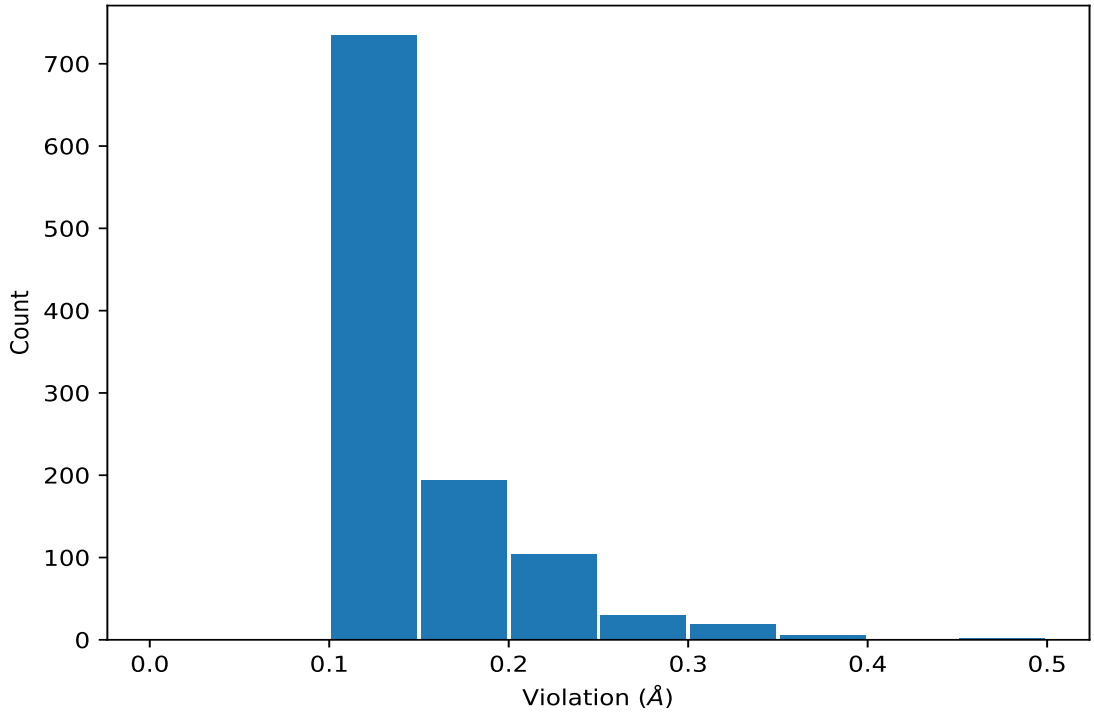
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,317)	1:A:186:VAL:HG21	1:A:187:ASN:HB2	2	0.12	0.0	0.12
(1,317)	1:A:186:VAL:HG21	1:A:187:ASN:HB3	2	0.12	0.0	0.12
(1,317)	1:A:186:VAL:HG22	1:A:187:ASN:HB2	2	0.12	0.0	0.12
(1,317)	1:A:186:VAL:HG22	1:A:187:ASN:HB3	2	0.12	0.0	0.12
(1,317)	1:A:186:VAL:HG23	1:A:187:ASN:HB2	2	0.12	0.0	0.12
(1,317)	1:A:186:VAL:HG23	1:A:187:ASN:HB3	2	0.12	0.0	0.12
(1,899)	1:A:109:ALA:HB1	1:A:113:GLU:H	2	0.12	0.0	0.12
(1,899)	1:A:109:ALA:HB2	1:A:113:GLU:H	2	0.12	0.0	0.12
(1,899)	1:A:109:ALA:HB3	1:A:113:GLU:H	2	0.12	0.0	0.12
(1,1463)	1:A:190:SER:HA	1:A:226:LEU:HB2	2	0.12	0.0	0.12
(1,1463)	1:A:190:SER:HA	1:A:226:LEU:HB3	2	0.12	0.0	0.12

[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 (i)

The following table lists the absolute value of the violation for each restraint in the ensemble sorted by its value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3433)	1:A:81:ASP:H	1:A:82:VAL:HB	20	0.47
(1,3433)	1:A:81:ASP:H	1:A:82:VAL:HB	13	0.46
(1,5895)	1:A:95:ILE:HG13	1:A:121:GLU:HB2	18	0.38
(1,5895)	1:A:95:ILE:HG13	1:A:121:GLU:HB3	18	0.38
(1,982)	1:A:150:THR:HG21	1:A:152:ASP:H	10	0.36
(1,982)	1:A:150:THR:HG22	1:A:152:ASP:H	10	0.36
(1,982)	1:A:150:THR:HG23	1:A:152:ASP:H	10	0.36
(1,2104)	1:A:68:ILE:HB	1:A:79:VAL:HB	9	0.34
(1,5795)	1:A:71:VAL:HG21	1:A:79:VAL:HG11	9	0.31
(1,5795)	1:A:71:VAL:HG21	1:A:79:VAL:HG12	9	0.31
(1,5795)	1:A:71:VAL:HG21	1:A:79:VAL:HG13	9	0.31
(1,5795)	1:A:71:VAL:HG21	1:A:79:VAL:HG21	9	0.31
(1,5795)	1:A:71:VAL:HG21	1:A:79:VAL:HG22	9	0.31
(1,5795)	1:A:71:VAL:HG21	1:A:79:VAL:HG23	9	0.31
(1,5795)	1:A:71:VAL:HG22	1:A:79:VAL:HG11	9	0.31
(1,5795)	1:A:71:VAL:HG22	1:A:79:VAL:HG12	9	0.31
(1,5795)	1:A:71:VAL:HG22	1:A:79:VAL:HG13	9	0.31
(1,5795)	1:A:71:VAL:HG22	1:A:79:VAL:HG21	9	0.31
(1,5795)	1:A:71:VAL:HG22	1:A:79:VAL:HG22	9	0.31
(1,5795)	1:A:71:VAL:HG22	1:A:79:VAL:HG23	9	0.31
(1,5795)	1:A:71:VAL:HG23	1:A:79:VAL:HG11	9	0.31
(1,5795)	1:A:71:VAL:HG23	1:A:79:VAL:HG12	9	0.31
(1,5795)	1:A:71:VAL:HG23	1:A:79:VAL:HG13	9	0.31
(1,5795)	1:A:71:VAL:HG23	1:A:79:VAL:HG21	9	0.31
(1,5795)	1:A:71:VAL:HG23	1:A:79:VAL:HG22	9	0.31
(1,5795)	1:A:71:VAL:HG23	1:A:79:VAL:HG23	9	0.31
(1,5679)	1:A:55:VAL:HA	1:A:82:VAL:HG11	20	0.29
(1,5679)	1:A:55:VAL:HA	1:A:82:VAL:HG12	20	0.29
(1,5679)	1:A:55:VAL:HA	1:A:82:VAL:HG13	20	0.29
(1,5679)	1:A:55:VAL:HA	1:A:82:VAL:HG21	20	0.29
(1,5679)	1:A:55:VAL:HA	1:A:82:VAL:HG22	20	0.29
(1,5679)	1:A:55:VAL:HA	1:A:82:VAL:HG23	20	0.29
(1,4075)	1:A:150:THR:HA	1:A:151:GLU:H	10	0.28
(1,770)	1:A:96:LYS:HA	1:A:121:GLU:HG3	18	0.27
(1,3206)	1:A:39:VAL:HB	1:A:59:TRP:HE1	12	0.26
(1,5795)	1:A:71:VAL:HG21	1:A:79:VAL:HG11	14	0.25
(1,5795)	1:A:71:VAL:HG21	1:A:79:VAL:HG12	14	0.25

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5795)	1:A:71:VAL:HG21	1:A:79:VAL:HG13	14	0.25
(1,5795)	1:A:71:VAL:HG21	1:A:79:VAL:HG21	14	0.25
(1,5795)	1:A:71:VAL:HG21	1:A:79:VAL:HG22	14	0.25
(1,5795)	1:A:71:VAL:HG21	1:A:79:VAL:HG23	14	0.25
(1,5795)	1:A:71:VAL:HG22	1:A:79:VAL:HG11	14	0.25
(1,5795)	1:A:71:VAL:HG22	1:A:79:VAL:HG12	14	0.25
(1,5795)	1:A:71:VAL:HG22	1:A:79:VAL:HG13	14	0.25
(1,5795)	1:A:71:VAL:HG22	1:A:79:VAL:HG21	14	0.25
(1,5795)	1:A:71:VAL:HG22	1:A:79:VAL:HG22	14	0.25
(1,5795)	1:A:71:VAL:HG22	1:A:79:VAL:HG23	14	0.25
(1,5795)	1:A:71:VAL:HG23	1:A:79:VAL:HG11	14	0.25
(1,5795)	1:A:71:VAL:HG23	1:A:79:VAL:HG12	14	0.25
(1,5795)	1:A:71:VAL:HG23	1:A:79:VAL:HG13	14	0.25
(1,5795)	1:A:71:VAL:HG23	1:A:79:VAL:HG21	14	0.25
(1,5795)	1:A:71:VAL:HG23	1:A:79:VAL:HG22	14	0.25
(1,5795)	1:A:71:VAL:HG23	1:A:79:VAL:HG23	14	0.25
(1,5439)	1:A:35:ASN:HB2	1:A:37:GLU:H	19	0.25
(1,5439)	1:A:35:ASN:HB3	1:A:37:GLU:H	19	0.25
(1,1154)	1:A:172:SER:HA	1:A:173:THR:HB	6	0.25
(1,1901)	1:A:8:VAL:HG21	1:A:19:SER:HA	10	0.24
(1,1901)	1:A:8:VAL:HG22	1:A:19:SER:HA	10	0.24
(1,1901)	1:A:8:VAL:HG23	1:A:19:SER:HA	10	0.24
(3,5)	2:A:301:ZN:ZN	2:A:302:ZN:ZN	9	0.23
(3,5)	2:A:301:ZN:ZN	2:A:302:ZN:ZN	15	0.23
(3,4)	1:A:90:ASP:OD2	2:A:302:ZN:ZN	6	0.23
(3,4)	1:A:90:ASP:OD2	2:A:302:ZN:ZN	7	0.23
(3,3)	1:A:210:HIS:NE2	2:A:302:ZN:ZN	5	0.23
(3,3)	1:A:210:HIS:NE2	2:A:302:ZN:ZN	6	0.23
(3,3)	1:A:210:HIS:NE2	2:A:302:ZN:ZN	7	0.23
(3,3)	1:A:210:HIS:NE2	2:A:302:ZN:ZN	15	0.23
(3,5)	2:A:301:ZN:ZN	2:A:302:ZN:ZN	2	0.22
(3,5)	2:A:301:ZN:ZN	2:A:302:ZN:ZN	5	0.22
(3,5)	2:A:301:ZN:ZN	2:A:302:ZN:ZN	8	0.22
(3,5)	2:A:301:ZN:ZN	2:A:302:ZN:ZN	17	0.22
(3,5)	2:A:301:ZN:ZN	2:A:302:ZN:ZN	18	0.22
(3,5)	2:A:301:ZN:ZN	2:A:302:ZN:ZN	19	0.22
(3,4)	1:A:90:ASP:OD2	2:A:302:ZN:ZN	12	0.22
(3,3)	1:A:210:HIS:NE2	2:A:302:ZN:ZN	1	0.22
(3,3)	1:A:210:HIS:NE2	2:A:302:ZN:ZN	2	0.22
(3,3)	1:A:210:HIS:NE2	2:A:302:ZN:ZN	8	0.22
(3,3)	1:A:210:HIS:NE2	2:A:302:ZN:ZN	9	0.22
(3,3)	1:A:210:HIS:NE2	2:A:302:ZN:ZN	12	0.22

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,3)	1:A:210:HIS:NE2	2:A:302:ZN:ZN	17	0.22
(3,3)	1:A:210:HIS:NE2	2:A:302:ZN:ZN	18	0.22
(3,3)	1:A:210:HIS:NE2	2:A:302:ZN:ZN	19	0.22
(3,3)	1:A:210:HIS:NE2	2:A:302:ZN:ZN	20	0.22
(1,5679)	1:A:55:VAL:HA	1:A:82:VAL:HG11	13	0.22
(1,5679)	1:A:55:VAL:HA	1:A:82:VAL:HG12	13	0.22
(1,5679)	1:A:55:VAL:HA	1:A:82:VAL:HG13	13	0.22
(1,5679)	1:A:55:VAL:HA	1:A:82:VAL:HG21	13	0.22
(1,5679)	1:A:55:VAL:HA	1:A:82:VAL:HG22	13	0.22
(1,5679)	1:A:55:VAL:HA	1:A:82:VAL:HG23	13	0.22
(1,5411)	1:A:32:GLY:HA2	1:A:33:SER:H	19	0.22
(1,5411)	1:A:32:GLY:HA3	1:A:33:SER:H	19	0.22
(3,5)	2:A:301:ZN:ZN	2:A:302:ZN:ZN	1	0.21
(3,5)	2:A:301:ZN:ZN	2:A:302:ZN:ZN	4	0.21
(3,5)	2:A:301:ZN:ZN	2:A:302:ZN:ZN	6	0.21
(3,5)	2:A:301:ZN:ZN	2:A:302:ZN:ZN	7	0.21
(3,5)	2:A:301:ZN:ZN	2:A:302:ZN:ZN	11	0.21
(3,5)	2:A:301:ZN:ZN	2:A:302:ZN:ZN	12	0.21
(3,5)	2:A:301:ZN:ZN	2:A:302:ZN:ZN	14	0.21
(3,5)	2:A:301:ZN:ZN	2:A:302:ZN:ZN	20	0.21
(3,4)	1:A:90:ASP:OD2	2:A:302:ZN:ZN	2	0.21
(3,4)	1:A:90:ASP:OD2	2:A:302:ZN:ZN	3	0.21
(3,4)	1:A:90:ASP:OD2	2:A:302:ZN:ZN	5	0.21
(3,4)	1:A:90:ASP:OD2	2:A:302:ZN:ZN	11	0.21
(3,4)	1:A:90:ASP:OD2	2:A:302:ZN:ZN	19	0.21
(3,4)	1:A:90:ASP:OD2	2:A:302:ZN:ZN	20	0.21
(3,3)	1:A:210:HIS:NE2	2:A:302:ZN:ZN	3	0.21
(3,3)	1:A:210:HIS:NE2	2:A:302:ZN:ZN	4	0.21
(3,3)	1:A:210:HIS:NE2	2:A:302:ZN:ZN	11	0.21
(3,3)	1:A:210:HIS:NE2	2:A:302:ZN:ZN	14	0.21
(3,3)	1:A:210:HIS:NE2	2:A:302:ZN:ZN	16	0.21
(3,2)	1:A:168:CYS:SG	2:A:302:ZN:ZN	6	0.21
(3,2)	1:A:168:CYS:SG	2:A:302:ZN:ZN	7	0.21
(1,6653)	1:A:214:GLY:HA3	1:A:215:ASP:HB2	4	0.21
(1,6653)	1:A:214:GLY:HA3	1:A:215:ASP:HB3	4	0.21
(1,3163)	1:A:54:LEU:HA	1:A:56:ASP:H	13	0.21
(1,2053)	1:A:45:VAL:HA	1:A:53:VAL:HG21	6	0.21
(1,2053)	1:A:45:VAL:HA	1:A:53:VAL:HG22	6	0.21
(1,2053)	1:A:45:VAL:HA	1:A:53:VAL:HG23	6	0.21
(3,5)	2:A:301:ZN:ZN	2:A:302:ZN:ZN	3	0.2
(3,5)	2:A:301:ZN:ZN	2:A:302:ZN:ZN	13	0.2
(3,5)	2:A:301:ZN:ZN	2:A:302:ZN:ZN	16	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(3,4)	1:A:90:ASP:OD2	2:A:302:ZN:ZN	1	0.2
(3,4)	1:A:90:ASP:OD2	2:A:302:ZN:ZN	4	0.2
(3,4)	1:A:90:ASP:OD2	2:A:302:ZN:ZN	9	0.2
(3,4)	1:A:90:ASP:OD2	2:A:302:ZN:ZN	10	0.2
(3,4)	1:A:90:ASP:OD2	2:A:302:ZN:ZN	13	0.2
(3,4)	1:A:90:ASP:OD2	2:A:302:ZN:ZN	14	0.2
(3,4)	1:A:90:ASP:OD2	2:A:302:ZN:ZN	15	0.2
(3,4)	1:A:90:ASP:OD2	2:A:302:ZN:ZN	16	0.2
(3,4)	1:A:90:ASP:OD2	2:A:302:ZN:ZN	17	0.2
(3,4)	1:A:90:ASP:OD2	2:A:302:ZN:ZN	18	0.2
(3,3)	1:A:210:HIS:NE2	2:A:302:ZN:ZN	10	0.2
(3,3)	1:A:210:HIS:NE2	2:A:302:ZN:ZN	13	0.2
(3,2)	1:A:168:CYS:SG	2:A:302:ZN:ZN	3	0.2
(3,2)	1:A:168:CYS:SG	2:A:302:ZN:ZN	10	0.2
(1,6653)	1:A:214:GLY:HA3	1:A:215:ASP:HB2	12	0.2
(1,6653)	1:A:214:GLY:HA3	1:A:215:ASP:HB3	12	0.2
(1,6653)	1:A:214:GLY:HA3	1:A:215:ASP:HB2	18	0.2
(1,6653)	1:A:214:GLY:HA3	1:A:215:ASP:HB3	18	0.2
(1,5440)	1:A:35:ASN:HD21	1:A:39:VAL:HG11	14	0.2
(1,5440)	1:A:35:ASN:HD21	1:A:39:VAL:HG12	14	0.2
(1,5440)	1:A:35:ASN:HD21	1:A:39:VAL:HG13	14	0.2
(1,5440)	1:A:35:ASN:HD21	1:A:39:VAL:HG21	14	0.2
(1,5440)	1:A:35:ASN:HD21	1:A:39:VAL:HG22	14	0.2
(1,5440)	1:A:35:ASN:HD21	1:A:39:VAL:HG23	14	0.2
(1,4675)	1:A:208:PRO:HD3	1:A:210:HIS:H	12	0.2
(1,3867)	1:A:95:ILE:HG13	1:A:121:GLU:H	18	0.2
(1,3799)	1:A:113:GLU:HB2	1:A:116:LYS:H	8	0.2
(1,3799)	1:A:113:GLU:HB3	1:A:116:LYS:H	8	0.2
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD11	19	0.2
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD12	19	0.2
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD13	19	0.2
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD11	19	0.2
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD12	19	0.2
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD13	19	0.2
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD11	19	0.2
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD12	19	0.2
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD13	19	0.2
(1,3058)	1:A:46:LEU:H	1:A:54:LEU:HB3	18	0.2
(1,2104)	1:A:68:ILE:HB	1:A:79:VAL:HB	14	0.2
(1,6653)	1:A:214:GLY:HA3	1:A:215:ASP:HB2	6	0.19
(1,6653)	1:A:214:GLY:HA3	1:A:215:ASP:HB3	6	0.19
(1,5809)	1:A:78:ARG:HA	1:A:79:VAL:HG11	14	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5809)	1:A:78:ARG:HA	1:A:79:VAL:HG12	14	0.19
(1,5809)	1:A:78:ARG:HA	1:A:79:VAL:HG13	14	0.19
(1,5809)	1:A:78:ARG:HA	1:A:79:VAL:HG21	14	0.19
(1,5809)	1:A:78:ARG:HA	1:A:79:VAL:HG22	14	0.19
(1,5809)	1:A:78:ARG:HA	1:A:79:VAL:HG23	14	0.19
(1,4675)	1:A:208:PRO:HD3	1:A:210:HIS:H	10	0.19
(1,4510)	1:A:193:ILE:HG12	1:A:195:ASN:H	11	0.19
(1,3799)	1:A:113:GLU:HB2	1:A:116:LYS:H	18	0.19
(1,3799)	1:A:113:GLU:HB3	1:A:116:LYS:H	18	0.19
(1,3701)	1:A:83:ILE:HA	1:A:107:SER:H	15	0.19
(1,1161)	1:A:171:LYS:H	1:A:175:ALA:HB1	11	0.19
(1,1161)	1:A:171:LYS:H	1:A:175:ALA:HB2	11	0.19
(1,1161)	1:A:171:LYS:H	1:A:175:ALA:HB3	11	0.19
(1,1154)	1:A:172:SER:HA	1:A:173:THR:HB	11	0.19
(3,2)	1:A:168:CYS:SG	2:A:302:ZN:ZN	16	0.18
(1,795)	1:A:57:SER:H	1:A:92:ILE:HG21	16	0.18
(1,795)	1:A:57:SER:H	1:A:92:ILE:HG22	16	0.18
(1,795)	1:A:57:SER:H	1:A:92:ILE:HG23	16	0.18
(1,6653)	1:A:214:GLY:HA3	1:A:215:ASP:HB2	2	0.18
(1,6653)	1:A:214:GLY:HA3	1:A:215:ASP:HB3	2	0.18
(1,6653)	1:A:214:GLY:HA3	1:A:215:ASP:HB2	13	0.18
(1,6653)	1:A:214:GLY:HA3	1:A:215:ASP:HB3	13	0.18
(1,5878)	1:A:90:ASP:HB2	1:A:91:ARG:HB2	6	0.18
(1,5878)	1:A:90:ASP:HB2	1:A:91:ARG:HB3	6	0.18
(1,5878)	1:A:90:ASP:HB3	1:A:91:ARG:HB2	6	0.18
(1,5878)	1:A:90:ASP:HB3	1:A:91:ARG:HB3	6	0.18
(1,4092)	1:A:87:ALA:H	1:A:153:ASN:H	13	0.18
(1,3799)	1:A:113:GLU:HB2	1:A:116:LYS:H	3	0.18
(1,3799)	1:A:113:GLU:HB3	1:A:116:LYS:H	3	0.18
(1,3413)	1:A:68:ILE:HD11	1:A:79:VAL:H	14	0.18
(1,3413)	1:A:68:ILE:HD12	1:A:79:VAL:H	14	0.18
(1,3413)	1:A:68:ILE:HD13	1:A:79:VAL:H	14	0.18
(1,3413)	1:A:68:ILE:HD11	1:A:79:VAL:H	16	0.18
(1,3413)	1:A:68:ILE:HD12	1:A:79:VAL:H	16	0.18
(1,3413)	1:A:68:ILE:HD13	1:A:79:VAL:H	16	0.18
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD11	20	0.18
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD12	20	0.18
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD13	20	0.18
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD11	20	0.18
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD12	20	0.18
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD13	20	0.18
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD11	20	0.18

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD12	20	0.18
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD13	20	0.18
(1,3168)	1:A:56:ASP:H	1:A:57:SER:H	20	0.18
(1,3058)	1:A:46:LEU:H	1:A:54:LEU:HB3	5	0.18
(1,2757)	1:A:8:VAL:HA	1:A:18:ILE:H	10	0.18
(1,2053)	1:A:45:VAL:HA	1:A:53:VAL:HG21	5	0.18
(1,2053)	1:A:45:VAL:HA	1:A:53:VAL:HG22	5	0.18
(1,2053)	1:A:45:VAL:HA	1:A:53:VAL:HG23	5	0.18
(1,2053)	1:A:45:VAL:HA	1:A:53:VAL:HG21	18	0.18
(1,2053)	1:A:45:VAL:HA	1:A:53:VAL:HG22	18	0.18
(1,2053)	1:A:45:VAL:HA	1:A:53:VAL:HG23	18	0.18
(3,5)	2:A:301:ZN:ZN	2:A:302:ZN:ZN	10	0.17
(1,795)	1:A:57:SER:H	1:A:92:ILE:HG21	17	0.17
(1,795)	1:A:57:SER:H	1:A:92:ILE:HG22	17	0.17
(1,795)	1:A:57:SER:H	1:A:92:ILE:HG23	17	0.17
(1,795)	1:A:57:SER:H	1:A:92:ILE:HG21	19	0.17
(1,795)	1:A:57:SER:H	1:A:92:ILE:HG22	19	0.17
(1,795)	1:A:57:SER:H	1:A:92:ILE:HG23	19	0.17
(1,6659)	1:A:215:ASP:HB2	1:A:216:LYS:HA	2	0.17
(1,6659)	1:A:215:ASP:HB3	1:A:216:LYS:HA	2	0.17
(1,6659)	1:A:215:ASP:HB2	1:A:216:LYS:HA	4	0.17
(1,6659)	1:A:215:ASP:HB3	1:A:216:LYS:HA	4	0.17
(1,6659)	1:A:215:ASP:HB2	1:A:216:LYS:HA	12	0.17
(1,6659)	1:A:215:ASP:HB3	1:A:216:LYS:HA	12	0.17
(1,6659)	1:A:215:ASP:HB2	1:A:216:LYS:HA	18	0.17
(1,6659)	1:A:215:ASP:HB3	1:A:216:LYS:HA	18	0.17
(1,6653)	1:A:214:GLY:HA3	1:A:215:ASP:HB2	10	0.17
(1,6653)	1:A:214:GLY:HA3	1:A:215:ASP:HB3	10	0.17
(1,5878)	1:A:90:ASP:HB2	1:A:91:ARG:HB2	5	0.17
(1,5878)	1:A:90:ASP:HB2	1:A:91:ARG:HB3	5	0.17
(1,5878)	1:A:90:ASP:HB3	1:A:91:ARG:HB2	5	0.17
(1,5878)	1:A:90:ASP:HB3	1:A:91:ARG:HB3	5	0.17
(1,4510)	1:A:193:ILE:HG12	1:A:195:ASN:H	15	0.17
(1,4092)	1:A:87:ALA:H	1:A:153:ASN:H	5	0.17
(1,3572)	1:A:95:ILE:H	1:A:120:TYR:HE1	16	0.17
(1,3572)	1:A:95:ILE:H	1:A:120:TYR:HE2	16	0.17
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD11	2	0.17
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD12	2	0.17
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD13	2	0.17
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD11	2	0.17
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD12	2	0.17
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD13	2	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD11	2	0.17
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD12	2	0.17
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD13	2	0.17
(1,3163)	1:A:54:LEU:HA	1:A:56:ASP:H	1	0.17
(1,3163)	1:A:54:LEU:HA	1:A:56:ASP:H	4	0.17
(1,3163)	1:A:54:LEU:HA	1:A:56:ASP:H	17	0.17
(1,2836)	1:A:173:THR:H	1:A:173:THR:HG21	6	0.17
(1,2836)	1:A:173:THR:H	1:A:173:THR:HG22	6	0.17
(1,2836)	1:A:173:THR:H	1:A:173:THR:HG23	6	0.17
(1,2775)	1:A:9:ILE:HB	1:A:19:SER:H	8	0.17
(1,2775)	1:A:9:ILE:HB	1:A:19:SER:H	20	0.17
(1,2685)	1:A:54:LEU:H	1:A:82:VAL:HB	18	0.17
(1,1986)	1:A:34:PHE:HB2	1:A:39:VAL:HG11	20	0.17
(1,1986)	1:A:34:PHE:HB2	1:A:39:VAL:HG12	20	0.17
(1,1986)	1:A:34:PHE:HB2	1:A:39:VAL:HG13	20	0.17
(1,686)	1:A:81:ASP:HA	1:A:82:VAL:HB	13	0.16
(1,686)	1:A:81:ASP:HA	1:A:82:VAL:HB	20	0.16
(1,6659)	1:A:215:ASP:HB2	1:A:216:LYS:HA	6	0.16
(1,6659)	1:A:215:ASP:HB3	1:A:216:LYS:HA	6	0.16
(1,6659)	1:A:215:ASP:HB2	1:A:216:LYS:HA	10	0.16
(1,6659)	1:A:215:ASP:HB3	1:A:216:LYS:HA	10	0.16
(1,6659)	1:A:215:ASP:HB2	1:A:216:LYS:HA	13	0.16
(1,6659)	1:A:215:ASP:HB3	1:A:216:LYS:HA	13	0.16
(1,4940)	1:A:115:ALA:H	1:A:120:TYR:HD1	16	0.16
(1,4940)	1:A:115:ALA:H	1:A:120:TYR:HD2	16	0.16
(1,4800)	1:A:224:ASP:H	1:A:226:LEU:HB2	7	0.16
(1,4800)	1:A:224:ASP:H	1:A:226:LEU:HB3	7	0.16
(1,4800)	1:A:224:ASP:H	1:A:226:LEU:HB2	19	0.16
(1,4800)	1:A:224:ASP:H	1:A:226:LEU:HB3	19	0.16
(1,4510)	1:A:193:ILE:HG12	1:A:195:ASN:H	9	0.16
(1,4510)	1:A:193:ILE:HG12	1:A:195:ASN:H	17	0.16
(1,4092)	1:A:87:ALA:H	1:A:153:ASN:H	6	0.16
(1,3799)	1:A:113:GLU:HB2	1:A:116:LYS:H	15	0.16
(1,3799)	1:A:113:GLU:HB3	1:A:116:LYS:H	15	0.16
(1,3572)	1:A:95:ILE:H	1:A:120:TYR:HE1	15	0.16
(1,3572)	1:A:95:ILE:H	1:A:120:TYR:HE2	15	0.16
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD11	4	0.16
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD12	4	0.16
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD13	4	0.16
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD11	4	0.16
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD12	4	0.16
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD13	4	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD11	4	0.16
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD12	4	0.16
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD13	4	0.16
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD11	5	0.16
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD12	5	0.16
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD13	5	0.16
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD11	5	0.16
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD12	5	0.16
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD13	5	0.16
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD11	5	0.16
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD12	5	0.16
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD13	5	0.16
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD11	6	0.16
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD12	6	0.16
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD13	6	0.16
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD11	6	0.16
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD12	6	0.16
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD13	6	0.16
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD11	6	0.16
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD12	6	0.16
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD13	6	0.16
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD11	11	0.16
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD12	11	0.16
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD13	11	0.16
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD11	11	0.16
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD12	11	0.16
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD13	11	0.16
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD11	11	0.16
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD12	11	0.16
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD13	11	0.16
(1,3163)	1:A:54:LEU:HA	1:A:56:ASP:H	7	0.16
(1,3163)	1:A:54:LEU:HA	1:A:56:ASP:H	12	0.16
(1,3058)	1:A:46:LEU:H	1:A:54:LEU:HB3	6	0.16
(1,2963)	1:A:32:GLY:HA2	1:A:33:SER:H	20	0.16
(1,2842)	1:A:20:GLN:HA	1:A:25:VAL:H	2	0.16
(1,2842)	1:A:20:GLN:HA	1:A:25:VAL:H	8	0.16
(1,2842)	1:A:20:GLN:HA	1:A:25:VAL:H	9	0.16
(1,2842)	1:A:20:GLN:HA	1:A:25:VAL:H	15	0.16
(1,2842)	1:A:20:GLN:HA	1:A:25:VAL:H	17	0.16
(1,2836)	1:A:173:THR:H	1:A:173:THR:HG21	11	0.16
(1,2836)	1:A:173:THR:H	1:A:173:THR:HG22	11	0.16
(1,2836)	1:A:173:THR:H	1:A:173:THR:HG23	11	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2790)	1:A:7:THR:HA	1:A:20:GLN:H	14	0.16
(1,2775)	1:A:9:ILE:HB	1:A:19:SER:H	2	0.16
(1,2775)	1:A:9:ILE:HB	1:A:19:SER:H	6	0.16
(1,2775)	1:A:9:ILE:HB	1:A:19:SER:H	9	0.16
(1,2775)	1:A:9:ILE:HB	1:A:19:SER:H	11	0.16
(1,2775)	1:A:9:ILE:HB	1:A:19:SER:H	13	0.16
(1,2775)	1:A:9:ILE:HB	1:A:19:SER:H	15	0.16
(1,2775)	1:A:9:ILE:HB	1:A:19:SER:H	17	0.16
(1,2775)	1:A:9:ILE:HB	1:A:19:SER:H	19	0.16
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG21	17	0.16
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG22	17	0.16
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG23	17	0.16
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG21	19	0.16
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG22	19	0.16
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG23	19	0.16
(1,1447)	1:A:190:SER:HB2	1:A:226:LEU:HB2	9	0.16
(1,1447)	1:A:190:SER:HB2	1:A:226:LEU:HB3	9	0.16
(1,1447)	1:A:190:SER:HB3	1:A:226:LEU:HB2	9	0.16
(1,1447)	1:A:190:SER:HB3	1:A:226:LEU:HB3	9	0.16
(1,1447)	1:A:190:SER:HB2	1:A:226:LEU:HB2	17	0.16
(1,1447)	1:A:190:SER:HB2	1:A:226:LEU:HB3	17	0.16
(1,1447)	1:A:190:SER:HB3	1:A:226:LEU:HB2	17	0.16
(1,1447)	1:A:190:SER:HB3	1:A:226:LEU:HB3	17	0.16
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG11	2	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG12	2	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG13	2	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG11	6	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG12	6	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG13	6	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG11	8	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG12	8	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG13	8	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG11	9	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG12	9	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG13	9	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG11	15	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG12	15	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG13	15	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG11	17	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG12	17	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG13	17	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG11	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG12	18	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG13	18	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG11	20	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG12	20	0.15
(2,4)	1:A:7:THR:HA	1:A:8:VAL:HG13	20	0.15
(1,795)	1:A:57:SER:H	1:A:92:ILE:HG21	15	0.15
(1,795)	1:A:57:SER:H	1:A:92:ILE:HG22	15	0.15
(1,795)	1:A:57:SER:H	1:A:92:ILE:HG23	15	0.15
(1,773)	1:A:84:ILE:HD11	1:A:92:ILE:HB	15	0.15
(1,773)	1:A:84:ILE:HD12	1:A:92:ILE:HB	15	0.15
(1,773)	1:A:84:ILE:HD13	1:A:92:ILE:HB	15	0.15
(1,5878)	1:A:90:ASP:HB2	1:A:91:ARG:HB2	7	0.15
(1,5878)	1:A:90:ASP:HB2	1:A:91:ARG:HB3	7	0.15
(1,5878)	1:A:90:ASP:HB3	1:A:91:ARG:HB2	7	0.15
(1,5878)	1:A:90:ASP:HB3	1:A:91:ARG:HB3	7	0.15
(1,5830)	1:A:82:VAL:HG11	1:A:83:ILE:H	20	0.15
(1,5830)	1:A:82:VAL:HG12	1:A:83:ILE:H	20	0.15
(1,5830)	1:A:82:VAL:HG13	1:A:83:ILE:H	20	0.15
(1,5830)	1:A:82:VAL:HG21	1:A:83:ILE:H	20	0.15
(1,5830)	1:A:82:VAL:HG22	1:A:83:ILE:H	20	0.15
(1,5830)	1:A:82:VAL:HG23	1:A:83:ILE:H	20	0.15
(1,5011)	1:A:34:PHE:HD1	1:A:37:GLU:HB2	14	0.15
(1,5011)	1:A:34:PHE:HD2	1:A:37:GLU:HB2	14	0.15
(1,4940)	1:A:115:ALA:H	1:A:120:TYR:HD1	17	0.15
(1,4940)	1:A:115:ALA:H	1:A:120:TYR:HD2	17	0.15
(1,4800)	1:A:224:ASP:H	1:A:226:LEU:HB2	5	0.15
(1,4800)	1:A:224:ASP:H	1:A:226:LEU:HB3	5	0.15
(1,4510)	1:A:193:ILE:HG12	1:A:195:ASN:H	3	0.15
(1,4510)	1:A:193:ILE:HG12	1:A:195:ASN:H	8	0.15
(1,4510)	1:A:193:ILE:HG12	1:A:195:ASN:H	12	0.15
(1,4510)	1:A:193:ILE:HG12	1:A:195:ASN:H	19	0.15
(1,4092)	1:A:87:ALA:H	1:A:153:ASN:H	16	0.15
(1,4040)	1:A:148:GLY:H	1:A:151:GLU:H	11	0.15
(1,370)	1:A:28:HIS:H	1:A:42:ASN:HA	7	0.15
(1,370)	1:A:28:HIS:H	1:A:42:ASN:HA	9	0.15
(1,3413)	1:A:68:ILE:HD11	1:A:79:VAL:H	8	0.15
(1,3413)	1:A:68:ILE:HD12	1:A:79:VAL:H	8	0.15
(1,3413)	1:A:68:ILE:HD13	1:A:79:VAL:H	8	0.15
(1,3413)	1:A:68:ILE:HD11	1:A:79:VAL:H	9	0.15
(1,3413)	1:A:68:ILE:HD12	1:A:79:VAL:H	9	0.15
(1,3413)	1:A:68:ILE:HD13	1:A:79:VAL:H	9	0.15
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD11	3	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD12	3	0.15
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD13	3	0.15
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD11	3	0.15
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD12	3	0.15
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD13	3	0.15
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD11	3	0.15
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD12	3	0.15
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD13	3	0.15
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD11	9	0.15
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD12	9	0.15
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD13	9	0.15
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD11	9	0.15
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD12	9	0.15
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD13	9	0.15
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD11	9	0.15
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD12	9	0.15
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD13	9	0.15
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD11	13	0.15
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD12	13	0.15
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD13	13	0.15
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD11	13	0.15
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD12	13	0.15
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD13	13	0.15
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD11	13	0.15
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD12	13	0.15
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD13	13	0.15
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD11	15	0.15
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD12	15	0.15
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD13	15	0.15
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD11	15	0.15
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD12	15	0.15
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD13	15	0.15
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD11	15	0.15
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD12	15	0.15
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD13	15	0.15
(1,3163)	1:A:54:LEU:HA	1:A:56:ASP:H	3	0.15
(1,3163)	1:A:54:LEU:HA	1:A:56:ASP:H	9	0.15
(1,3163)	1:A:54:LEU:HA	1:A:56:ASP:H	10	0.15
(1,3163)	1:A:54:LEU:HA	1:A:56:ASP:H	14	0.15
(1,3163)	1:A:54:LEU:HA	1:A:56:ASP:H	15	0.15
(1,3163)	1:A:54:LEU:HA	1:A:56:ASP:H	18	0.15
(1,3163)	1:A:54:LEU:HA	1:A:56:ASP:H	19	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2982)	1:A:34:PHE:H	1:A:37:GLU:H	19	0.15
(1,2842)	1:A:20:GLN:HA	1:A:25:VAL:H	14	0.15
(1,2842)	1:A:20:GLN:HA	1:A:25:VAL:H	18	0.15
(1,2842)	1:A:20:GLN:HA	1:A:25:VAL:H	20	0.15
(1,2800)	1:A:8:VAL:HB	1:A:20:GLN:H	8	0.15
(1,2790)	1:A:7:THR:HA	1:A:20:GLN:H	1	0.15
(1,2790)	1:A:7:THR:HA	1:A:20:GLN:H	3	0.15
(1,2790)	1:A:7:THR:HA	1:A:20:GLN:H	4	0.15
(1,2775)	1:A:9:ILE:HB	1:A:19:SER:H	1	0.15
(1,2775)	1:A:9:ILE:HB	1:A:19:SER:H	3	0.15
(1,2775)	1:A:9:ILE:HB	1:A:19:SER:H	5	0.15
(1,2775)	1:A:9:ILE:HB	1:A:19:SER:H	7	0.15
(1,2775)	1:A:9:ILE:HB	1:A:19:SER:H	14	0.15
(1,2775)	1:A:9:ILE:HB	1:A:19:SER:H	18	0.15
(1,2685)	1:A:54:LEU:H	1:A:82:VAL:HB	10	0.15
(1,2166)	1:A:83:ILE:HG21	1:A:107:SER:H	15	0.15
(1,2166)	1:A:83:ILE:HG22	1:A:107:SER:H	15	0.15
(1,2166)	1:A:83:ILE:HG23	1:A:107:SER:H	15	0.15
(1,2130)	1:A:219:LEU:HD11	1:A:222:THR:HG1	20	0.15
(1,2130)	1:A:219:LEU:HD12	1:A:222:THR:HG1	20	0.15
(1,2130)	1:A:219:LEU:HD13	1:A:222:THR:HG1	20	0.15
(1,1938)	1:A:18:ILE:HA	1:A:19:SER:HA	10	0.15
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG21	3	0.15
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG22	3	0.15
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG23	3	0.15
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG21	6	0.15
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG22	6	0.15
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG23	6	0.15
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG21	15	0.15
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG22	15	0.15
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG23	15	0.15
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG21	18	0.15
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG22	18	0.15
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG23	18	0.15
(1,1447)	1:A:190:SER:HB2	1:A:226:LEU:HB2	4	0.15
(1,1447)	1:A:190:SER:HB2	1:A:226:LEU:HB3	4	0.15
(1,1447)	1:A:190:SER:HB3	1:A:226:LEU:HB2	4	0.15
(1,1447)	1:A:190:SER:HB3	1:A:226:LEU:HB3	4	0.15
(1,1160)	1:A:175:ALA:HB1	1:A:221:HIS:HD2	11	0.15
(1,1160)	1:A:175:ALA:HB2	1:A:221:HIS:HD2	11	0.15
(1,1160)	1:A:175:ALA:HB3	1:A:221:HIS:HD2	11	0.15
(2,2)	1:A:218:LEU:HD11	1:A:221:HIS:HB2	11	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,2)	1:A:218:LEU:HD12	1:A:221:HIS:HB2	11	0.14
(2,2)	1:A:218:LEU:HD13	1:A:221:HIS:HB2	11	0.14
(1,795)	1:A:57:SER:H	1:A:92:ILE:HG21	20	0.14
(1,795)	1:A:57:SER:H	1:A:92:ILE:HG22	20	0.14
(1,795)	1:A:57:SER:H	1:A:92:ILE:HG23	20	0.14
(1,5457)	1:A:39:VAL:HG11	1:A:59:TRP:HE1	16	0.14
(1,5457)	1:A:39:VAL:HG12	1:A:59:TRP:HE1	16	0.14
(1,5457)	1:A:39:VAL:HG13	1:A:59:TRP:HE1	16	0.14
(1,5457)	1:A:39:VAL:HG21	1:A:59:TRP:HE1	16	0.14
(1,5457)	1:A:39:VAL:HG22	1:A:59:TRP:HE1	16	0.14
(1,5457)	1:A:39:VAL:HG23	1:A:59:TRP:HE1	16	0.14
(1,5447)	1:A:37:GLU:HB2	1:A:39:VAL:HG11	12	0.14
(1,5447)	1:A:37:GLU:HB2	1:A:39:VAL:HG12	12	0.14
(1,5447)	1:A:37:GLU:HB2	1:A:39:VAL:HG13	12	0.14
(1,5447)	1:A:37:GLU:HB2	1:A:39:VAL:HG21	12	0.14
(1,5447)	1:A:37:GLU:HB2	1:A:39:VAL:HG22	12	0.14
(1,5447)	1:A:37:GLU:HB2	1:A:39:VAL:HG23	12	0.14
(1,4940)	1:A:115:ALA:H	1:A:120:TYR:HD1	15	0.14
(1,4940)	1:A:115:ALA:H	1:A:120:TYR:HD2	15	0.14
(1,4940)	1:A:115:ALA:H	1:A:120:TYR:HD1	19	0.14
(1,4940)	1:A:115:ALA:H	1:A:120:TYR:HD2	19	0.14
(1,4699)	1:A:213:VAL:H	1:A:213:VAL:HB	11	0.14
(1,4675)	1:A:208:PRO:HD3	1:A:210:HIS:H	7	0.14
(1,4675)	1:A:208:PRO:HD3	1:A:210:HIS:H	9	0.14
(1,4675)	1:A:208:PRO:HD3	1:A:210:HIS:H	16	0.14
(1,4675)	1:A:208:PRO:HD3	1:A:210:HIS:H	18	0.14
(1,4510)	1:A:193:ILE:HG12	1:A:195:ASN:H	2	0.14
(1,4092)	1:A:87:ALA:H	1:A:153:ASN:H	14	0.14
(1,4092)	1:A:87:ALA:H	1:A:153:ASN:H	18	0.14
(1,3701)	1:A:83:ILE:HA	1:A:107:SER:H	17	0.14
(1,3572)	1:A:95:ILE:H	1:A:120:TYR:HE1	19	0.14
(1,3572)	1:A:95:ILE:H	1:A:120:TYR:HE2	19	0.14
(1,3413)	1:A:68:ILE:HD11	1:A:79:VAL:H	2	0.14
(1,3413)	1:A:68:ILE:HD12	1:A:79:VAL:H	2	0.14
(1,3413)	1:A:68:ILE:HD13	1:A:79:VAL:H	2	0.14
(1,3413)	1:A:68:ILE:HD11	1:A:79:VAL:H	6	0.14
(1,3413)	1:A:68:ILE:HD12	1:A:79:VAL:H	6	0.14
(1,3413)	1:A:68:ILE:HD13	1:A:79:VAL:H	6	0.14
(1,3413)	1:A:68:ILE:HD11	1:A:79:VAL:H	11	0.14
(1,3413)	1:A:68:ILE:HD12	1:A:79:VAL:H	11	0.14
(1,3413)	1:A:68:ILE:HD13	1:A:79:VAL:H	11	0.14
(1,3413)	1:A:68:ILE:HD11	1:A:79:VAL:H	12	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3413)	1:A:68:ILE:HD12	1:A:79:VAL:H	12	0.14
(1,3413)	1:A:68:ILE:HD13	1:A:79:VAL:H	12	0.14
(1,3413)	1:A:68:ILE:HD11	1:A:79:VAL:H	19	0.14
(1,3413)	1:A:68:ILE:HD12	1:A:79:VAL:H	19	0.14
(1,3413)	1:A:68:ILE:HD13	1:A:79:VAL:H	19	0.14
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD11	1	0.14
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD12	1	0.14
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD13	1	0.14
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD11	1	0.14
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD12	1	0.14
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD13	1	0.14
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD11	1	0.14
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD12	1	0.14
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD13	1	0.14
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD11	7	0.14
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD12	7	0.14
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD13	7	0.14
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD11	7	0.14
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD12	7	0.14
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD13	7	0.14
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD11	7	0.14
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD12	7	0.14
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD13	7	0.14
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD11	8	0.14
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD12	8	0.14
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD13	8	0.14
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD11	8	0.14
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD12	8	0.14
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD13	8	0.14
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD11	8	0.14
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD12	8	0.14
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD13	8	0.14
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD11	10	0.14
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD12	10	0.14
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD13	10	0.14
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD11	10	0.14
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD12	10	0.14
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD13	10	0.14
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD11	10	0.14
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD12	10	0.14
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD13	10	0.14
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD11	14	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD12	14	0.14
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD13	14	0.14
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD11	14	0.14
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD12	14	0.14
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD13	14	0.14
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD11	14	0.14
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD12	14	0.14
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD13	14	0.14
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD11	16	0.14
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD12	16	0.14
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD13	16	0.14
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD11	16	0.14
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD12	16	0.14
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD13	16	0.14
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD11	16	0.14
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD12	16	0.14
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD13	16	0.14
(1,3163)	1:A:54:LEU:HA	1:A:56:ASP:H	8	0.14
(1,3163)	1:A:54:LEU:HA	1:A:56:ASP:H	11	0.14
(1,3163)	1:A:54:LEU:HA	1:A:56:ASP:H	20	0.14
(1,3058)	1:A:46:LEU:H	1:A:54:LEU:HB3	13	0.14
(1,3058)	1:A:46:LEU:H	1:A:54:LEU:HB3	20	0.14
(1,2991)	1:A:34:PHE:HD1	1:A:39:VAL:H	18	0.14
(1,2991)	1:A:34:PHE:HD2	1:A:39:VAL:H	18	0.14
(1,2842)	1:A:20:GLN:HA	1:A:25:VAL:H	1	0.14
(1,2842)	1:A:20:GLN:HA	1:A:25:VAL:H	3	0.14
(1,2842)	1:A:20:GLN:HA	1:A:25:VAL:H	4	0.14
(1,2842)	1:A:20:GLN:HA	1:A:25:VAL:H	6	0.14
(1,2800)	1:A:8:VAL:HB	1:A:20:GLN:H	6	0.14
(1,2800)	1:A:8:VAL:HB	1:A:20:GLN:H	9	0.14
(1,2800)	1:A:8:VAL:HB	1:A:20:GLN:H	18	0.14
(1,2800)	1:A:8:VAL:HB	1:A:20:GLN:H	20	0.14
(1,2790)	1:A:7:THR:HA	1:A:20:GLN:H	5	0.14
(1,2775)	1:A:9:ILE:HB	1:A:19:SER:H	4	0.14
(1,2775)	1:A:9:ILE:HB	1:A:19:SER:H	12	0.14
(1,2775)	1:A:9:ILE:HB	1:A:19:SER:H	16	0.14
(1,2685)	1:A:54:LEU:H	1:A:82:VAL:HB	6	0.14
(1,2518)	1:A:195:ASN:HB3	1:A:198:LYS:HB2	1	0.14
(1,2518)	1:A:195:ASN:HB3	1:A:198:LYS:HB3	1	0.14
(1,2518)	1:A:195:ASN:HB3	1:A:198:LYS:HB2	14	0.14
(1,2518)	1:A:195:ASN:HB3	1:A:198:LYS:HB3	14	0.14
(1,2394)	1:A:114:LEU:HB2	1:A:150:THR:HB	15	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2130)	1:A:219:LEU:HD11	1:A:222:THR:HG1	15	0.14
(1,2130)	1:A:219:LEU:HD12	1:A:222:THR:HG1	15	0.14
(1,2130)	1:A:219:LEU:HD13	1:A:222:THR:HG1	15	0.14
(1,2097)	1:A:58:SER:HB2	1:A:67:LEU:HG	16	0.14
(1,2097)	1:A:58:SER:HB2	1:A:67:LEU:HG	19	0.14
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG21	2	0.14
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG22	2	0.14
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG23	2	0.14
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG21	8	0.14
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG22	8	0.14
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG23	8	0.14
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG21	11	0.14
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG22	11	0.14
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG23	11	0.14
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG21	12	0.14
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG22	12	0.14
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG23	12	0.14
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG21	14	0.14
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG22	14	0.14
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG23	14	0.14
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG21	20	0.14
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG22	20	0.14
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG23	20	0.14
(3,2)	1:A:168:CYS:SG	2:A:302:ZN:ZN	15	0.13
(2,9)	1:A:67:LEU:HD21	1:A:71:VAL:H	15	0.13
(2,9)	1:A:67:LEU:HD22	1:A:71:VAL:H	15	0.13
(2,9)	1:A:67:LEU:HD23	1:A:71:VAL:H	15	0.13
(1,867)	1:A:57:SER:H	1:A:105:ALA:HB1	15	0.13
(1,867)	1:A:57:SER:H	1:A:105:ALA:HB2	15	0.13
(1,867)	1:A:57:SER:H	1:A:105:ALA:HB3	15	0.13
(1,867)	1:A:57:SER:H	1:A:105:ALA:HB1	17	0.13
(1,867)	1:A:57:SER:H	1:A:105:ALA:HB2	17	0.13
(1,867)	1:A:57:SER:H	1:A:105:ALA:HB3	17	0.13
(1,773)	1:A:84:ILE:HD11	1:A:92:ILE:HB	16	0.13
(1,773)	1:A:84:ILE:HD12	1:A:92:ILE:HB	16	0.13
(1,773)	1:A:84:ILE:HD13	1:A:92:ILE:HB	16	0.13
(1,773)	1:A:84:ILE:HD11	1:A:92:ILE:HB	17	0.13
(1,773)	1:A:84:ILE:HD12	1:A:92:ILE:HB	17	0.13
(1,773)	1:A:84:ILE:HD13	1:A:92:ILE:HB	17	0.13
(1,773)	1:A:84:ILE:HD11	1:A:92:ILE:HB	19	0.13
(1,773)	1:A:84:ILE:HD12	1:A:92:ILE:HB	19	0.13
(1,773)	1:A:84:ILE:HD13	1:A:92:ILE:HB	19	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6437)	1:A:178:LEU:H	1:A:226:LEU:HD11	11	0.13
(1,6437)	1:A:178:LEU:H	1:A:226:LEU:HD12	11	0.13
(1,6437)	1:A:178:LEU:H	1:A:226:LEU:HD13	11	0.13
(1,6437)	1:A:178:LEU:H	1:A:226:LEU:HD21	11	0.13
(1,6437)	1:A:178:LEU:H	1:A:226:LEU:HD22	11	0.13
(1,6437)	1:A:178:LEU:H	1:A:226:LEU:HD23	11	0.13
(1,5671)	1:A:54:LEU:HD11	1:A:55:VAL:H	3	0.13
(1,5671)	1:A:54:LEU:HD12	1:A:55:VAL:H	3	0.13
(1,5671)	1:A:54:LEU:HD13	1:A:55:VAL:H	3	0.13
(1,5671)	1:A:54:LEU:HD21	1:A:55:VAL:H	3	0.13
(1,5671)	1:A:54:LEU:HD22	1:A:55:VAL:H	3	0.13
(1,5671)	1:A:54:LEU:HD23	1:A:55:VAL:H	3	0.13
(1,5457)	1:A:39:VAL:HG11	1:A:59:TRP:HE1	3	0.13
(1,5457)	1:A:39:VAL:HG12	1:A:59:TRP:HE1	3	0.13
(1,5457)	1:A:39:VAL:HG13	1:A:59:TRP:HE1	3	0.13
(1,5457)	1:A:39:VAL:HG21	1:A:59:TRP:HE1	3	0.13
(1,5457)	1:A:39:VAL:HG22	1:A:59:TRP:HE1	3	0.13
(1,5457)	1:A:39:VAL:HG23	1:A:59:TRP:HE1	3	0.13
(1,5457)	1:A:39:VAL:HG11	1:A:59:TRP:HE1	6	0.13
(1,5457)	1:A:39:VAL:HG12	1:A:59:TRP:HE1	6	0.13
(1,5457)	1:A:39:VAL:HG13	1:A:59:TRP:HE1	6	0.13
(1,5457)	1:A:39:VAL:HG21	1:A:59:TRP:HE1	6	0.13
(1,5457)	1:A:39:VAL:HG22	1:A:59:TRP:HE1	6	0.13
(1,5457)	1:A:39:VAL:HG23	1:A:59:TRP:HE1	6	0.13
(1,4940)	1:A:115:ALA:H	1:A:120:TYR:HD1	20	0.13
(1,4940)	1:A:115:ALA:H	1:A:120:TYR:HD2	20	0.13
(1,4675)	1:A:208:PRO:HD3	1:A:210:HIS:H	4	0.13
(1,4675)	1:A:208:PRO:HD3	1:A:210:HIS:H	8	0.13
(1,4675)	1:A:208:PRO:HD3	1:A:210:HIS:H	14	0.13
(1,4675)	1:A:208:PRO:HD3	1:A:210:HIS:H	20	0.13
(1,4510)	1:A:193:ILE:HG12	1:A:195:ASN:H	7	0.13
(1,4510)	1:A:193:ILE:HG12	1:A:195:ASN:H	10	0.13
(1,4510)	1:A:193:ILE:HG12	1:A:195:ASN:H	20	0.13
(1,4092)	1:A:87:ALA:H	1:A:153:ASN:H	4	0.13
(1,4092)	1:A:87:ALA:H	1:A:153:ASN:H	7	0.13
(1,4092)	1:A:87:ALA:H	1:A:153:ASN:H	20	0.13
(1,3777)	1:A:108:THR:HA	1:A:112:ALA:H	3	0.13
(1,3572)	1:A:95:ILE:H	1:A:120:TYR:HE1	17	0.13
(1,3572)	1:A:95:ILE:H	1:A:120:TYR:HE2	17	0.13
(1,3413)	1:A:68:ILE:HD11	1:A:79:VAL:H	3	0.13
(1,3413)	1:A:68:ILE:HD12	1:A:79:VAL:H	3	0.13
(1,3413)	1:A:68:ILE:HD13	1:A:79:VAL:H	3	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3413)	1:A:68:ILE:HD11	1:A:79:VAL:H	17	0.13
(1,3413)	1:A:68:ILE:HD12	1:A:79:VAL:H	17	0.13
(1,3413)	1:A:68:ILE:HD13	1:A:79:VAL:H	17	0.13
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD11	17	0.13
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD12	17	0.13
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD13	17	0.13
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD11	17	0.13
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD12	17	0.13
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD13	17	0.13
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD11	17	0.13
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD12	17	0.13
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD13	17	0.13
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD11	18	0.13
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD12	18	0.13
(1,329)	1:A:222:THR:HG21	1:A:226:LEU:HD13	18	0.13
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD11	18	0.13
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD12	18	0.13
(1,329)	1:A:222:THR:HG22	1:A:226:LEU:HD13	18	0.13
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD11	18	0.13
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD12	18	0.13
(1,329)	1:A:222:THR:HG23	1:A:226:LEU:HD13	18	0.13
(1,3196)	1:A:30:GLU:HA	1:A:59:TRP:HE1	12	0.13
(1,3173)	1:A:58:SER:H	1:A:95:ILE:H	16	0.13
(1,3170)	1:A:57:SER:H	1:A:84:ILE:HA	20	0.13
(1,3163)	1:A:54:LEU:HA	1:A:56:ASP:H	2	0.13
(1,2984)	1:A:33:SER:HA	1:A:37:GLU:H	19	0.13
(1,2963)	1:A:32:GLY:HA2	1:A:33:SER:H	7	0.13
(1,2842)	1:A:20:GLN:HA	1:A:25:VAL:H	7	0.13
(1,2842)	1:A:20:GLN:HA	1:A:25:VAL:H	16	0.13
(1,2842)	1:A:20:GLN:HA	1:A:25:VAL:H	19	0.13
(1,2800)	1:A:8:VAL:HB	1:A:20:GLN:H	2	0.13
(1,2800)	1:A:8:VAL:HB	1:A:20:GLN:H	15	0.13
(1,2800)	1:A:8:VAL:HB	1:A:20:GLN:H	17	0.13
(1,2790)	1:A:7:THR:HA	1:A:20:GLN:H	7	0.13
(1,2790)	1:A:7:THR:HA	1:A:20:GLN:H	11	0.13
(1,2790)	1:A:7:THR:HA	1:A:20:GLN:H	13	0.13
(1,2790)	1:A:7:THR:HA	1:A:20:GLN:H	16	0.13
(1,2790)	1:A:7:THR:HA	1:A:20:GLN:H	19	0.13
(1,2685)	1:A:54:LEU:H	1:A:82:VAL:HB	4	0.13
(1,2685)	1:A:54:LEU:H	1:A:82:VAL:HB	5	0.13
(1,2685)	1:A:54:LEU:H	1:A:82:VAL:HB	9	0.13
(1,2685)	1:A:54:LEU:H	1:A:82:VAL:HB	11	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2685)	1:A:54:LEU:H	1:A:82:VAL:HB	14	0.13
(1,2618)	1:A:57:SER:HA	1:A:91:ARG:HA	18	0.13
(1,2518)	1:A:195:ASN:HB3	1:A:198:LYS:HB2	5	0.13
(1,2518)	1:A:195:ASN:HB3	1:A:198:LYS:HB3	5	0.13
(1,2518)	1:A:195:ASN:HB3	1:A:198:LYS:HB2	16	0.13
(1,2518)	1:A:195:ASN:HB3	1:A:198:LYS:HB3	16	0.13
(1,2504)	1:A:192:SER:HB3	1:A:195:ASN:H	10	0.13
(1,2109)	1:A:67:LEU:H	1:A:68:ILE:HD11	14	0.13
(1,2109)	1:A:67:LEU:H	1:A:68:ILE:HD12	14	0.13
(1,2109)	1:A:67:LEU:H	1:A:68:ILE:HD13	14	0.13
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG21	1	0.13
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG22	1	0.13
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG23	1	0.13
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG21	7	0.13
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG22	7	0.13
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG23	7	0.13
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG21	9	0.13
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG22	9	0.13
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG23	9	0.13
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG21	10	0.13
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG22	10	0.13
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG23	10	0.13
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG21	13	0.13
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG22	13	0.13
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG23	13	0.13
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD21	9	0.13
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD22	9	0.13
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD23	9	0.13
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD21	11	0.13
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD22	11	0.13
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD23	11	0.13
(2,6)	1:A:32:GLY:H	1:A:40:PRO:HB2	9	0.12
(1,899)	1:A:109:ALA:HB1	1:A:113:GLU:H	18	0.12
(1,899)	1:A:109:ALA:HB2	1:A:113:GLU:H	18	0.12
(1,899)	1:A:109:ALA:HB3	1:A:113:GLU:H	18	0.12
(1,867)	1:A:57:SER:H	1:A:105:ALA:HB1	19	0.12
(1,867)	1:A:57:SER:H	1:A:105:ALA:HB2	19	0.12
(1,867)	1:A:57:SER:H	1:A:105:ALA:HB3	19	0.12
(1,773)	1:A:84:ILE:HD11	1:A:92:ILE:HB	20	0.12
(1,773)	1:A:84:ILE:HD12	1:A:92:ILE:HB	20	0.12
(1,773)	1:A:84:ILE:HD13	1:A:92:ILE:HB	20	0.12
(1,6722)	1:A:227:LYS:H	1:A:227:LYS:HG2	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6722)	1:A:227:LYS:H	1:A:227:LYS:HG3	18	0.12
(1,666)	1:A:68:ILE:HG21	1:A:78:ARG:HB2	9	0.12
(1,666)	1:A:68:ILE:HG21	1:A:78:ARG:HB3	9	0.12
(1,666)	1:A:68:ILE:HG22	1:A:78:ARG:HB2	9	0.12
(1,666)	1:A:68:ILE:HG22	1:A:78:ARG:HB3	9	0.12
(1,666)	1:A:68:ILE:HG23	1:A:78:ARG:HB2	9	0.12
(1,666)	1:A:68:ILE:HG23	1:A:78:ARG:HB3	9	0.12
(1,6397)	1:A:172:SER:HB2	1:A:173:THR:HG21	11	0.12
(1,6397)	1:A:172:SER:HB2	1:A:173:THR:HG22	11	0.12
(1,6397)	1:A:172:SER:HB2	1:A:173:THR:HG23	11	0.12
(1,6397)	1:A:172:SER:HB3	1:A:173:THR:HG21	11	0.12
(1,6397)	1:A:172:SER:HB3	1:A:173:THR:HG22	11	0.12
(1,6397)	1:A:172:SER:HB3	1:A:173:THR:HG23	11	0.12
(1,5703)	1:A:57:SER:HB2	1:A:64:THR:HB	16	0.12
(1,5703)	1:A:57:SER:HB3	1:A:64:THR:HB	16	0.12
(1,5671)	1:A:54:LEU:HD11	1:A:55:VAL:H	12	0.12
(1,5671)	1:A:54:LEU:HD12	1:A:55:VAL:H	12	0.12
(1,5671)	1:A:54:LEU:HD13	1:A:55:VAL:H	12	0.12
(1,5671)	1:A:54:LEU:HD21	1:A:55:VAL:H	12	0.12
(1,5671)	1:A:54:LEU:HD22	1:A:55:VAL:H	12	0.12
(1,5671)	1:A:54:LEU:HD23	1:A:55:VAL:H	12	0.12
(1,5671)	1:A:54:LEU:HD11	1:A:55:VAL:H	20	0.12
(1,5671)	1:A:54:LEU:HD12	1:A:55:VAL:H	20	0.12
(1,5671)	1:A:54:LEU:HD13	1:A:55:VAL:H	20	0.12
(1,5671)	1:A:54:LEU:HD21	1:A:55:VAL:H	20	0.12
(1,5671)	1:A:54:LEU:HD22	1:A:55:VAL:H	20	0.12
(1,5671)	1:A:54:LEU:HD23	1:A:55:VAL:H	20	0.12
(1,5457)	1:A:39:VAL:HG11	1:A:59:TRP:HE1	5	0.12
(1,5457)	1:A:39:VAL:HG12	1:A:59:TRP:HE1	5	0.12
(1,5457)	1:A:39:VAL:HG13	1:A:59:TRP:HE1	5	0.12
(1,5457)	1:A:39:VAL:HG21	1:A:59:TRP:HE1	5	0.12
(1,5457)	1:A:39:VAL:HG22	1:A:59:TRP:HE1	5	0.12
(1,5457)	1:A:39:VAL:HG23	1:A:59:TRP:HE1	5	0.12
(1,5457)	1:A:39:VAL:HG11	1:A:59:TRP:HE1	7	0.12
(1,5457)	1:A:39:VAL:HG12	1:A:59:TRP:HE1	7	0.12
(1,5457)	1:A:39:VAL:HG13	1:A:59:TRP:HE1	7	0.12
(1,5457)	1:A:39:VAL:HG21	1:A:59:TRP:HE1	7	0.12
(1,5457)	1:A:39:VAL:HG22	1:A:59:TRP:HE1	7	0.12
(1,5457)	1:A:39:VAL:HG23	1:A:59:TRP:HE1	7	0.12
(1,5457)	1:A:39:VAL:HG11	1:A:59:TRP:HE1	18	0.12
(1,5457)	1:A:39:VAL:HG12	1:A:59:TRP:HE1	18	0.12
(1,5457)	1:A:39:VAL:HG13	1:A:59:TRP:HE1	18	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,5457)	1:A:39:VAL:HG21	1:A:59:TRP:HE1	18	0.12
(1,5457)	1:A:39:VAL:HG22	1:A:59:TRP:HE1	18	0.12
(1,5457)	1:A:39:VAL:HG23	1:A:59:TRP:HE1	18	0.12
(1,5440)	1:A:35:ASN:HD21	1:A:39:VAL:HG11	17	0.12
(1,5440)	1:A:35:ASN:HD21	1:A:39:VAL:HG12	17	0.12
(1,5440)	1:A:35:ASN:HD21	1:A:39:VAL:HG13	17	0.12
(1,5440)	1:A:35:ASN:HD21	1:A:39:VAL:HG21	17	0.12
(1,5440)	1:A:35:ASN:HD21	1:A:39:VAL:HG22	17	0.12
(1,5440)	1:A:35:ASN:HD21	1:A:39:VAL:HG23	17	0.12
(1,4954)	1:A:81:ASP:HB2	1:A:106:HIS:HD2	18	0.12
(1,4954)	1:A:81:ASP:HB3	1:A:106:HIS:HD2	18	0.12
(1,4699)	1:A:213:VAL:H	1:A:213:VAL:HB	3	0.12
(1,4699)	1:A:213:VAL:H	1:A:213:VAL:HB	4	0.12
(1,4699)	1:A:213:VAL:H	1:A:213:VAL:HB	6	0.12
(1,4699)	1:A:213:VAL:H	1:A:213:VAL:HB	7	0.12
(1,4699)	1:A:213:VAL:H	1:A:213:VAL:HB	8	0.12
(1,4699)	1:A:213:VAL:H	1:A:213:VAL:HB	10	0.12
(1,4699)	1:A:213:VAL:H	1:A:213:VAL:HB	12	0.12
(1,4699)	1:A:213:VAL:H	1:A:213:VAL:HB	14	0.12
(1,4699)	1:A:213:VAL:H	1:A:213:VAL:HB	16	0.12
(1,4699)	1:A:213:VAL:H	1:A:213:VAL:HB	17	0.12
(1,4699)	1:A:213:VAL:H	1:A:213:VAL:HB	18	0.12
(1,4699)	1:A:213:VAL:H	1:A:213:VAL:HB	20	0.12
(1,4675)	1:A:208:PRO:HD3	1:A:210:HIS:H	2	0.12
(1,4566)	1:A:222:THR:HB	1:A:226:LEU:H	12	0.12
(1,4510)	1:A:193:ILE:HG12	1:A:195:ASN:H	1	0.12
(1,4510)	1:A:193:ILE:HG12	1:A:195:ASN:H	14	0.12
(1,4092)	1:A:87:ALA:H	1:A:153:ASN:H	1	0.12
(1,4092)	1:A:87:ALA:H	1:A:153:ASN:H	9	0.12
(1,4092)	1:A:87:ALA:H	1:A:153:ASN:H	11	0.12
(1,4092)	1:A:87:ALA:H	1:A:153:ASN:H	12	0.12
(1,4092)	1:A:87:ALA:H	1:A:153:ASN:H	17	0.12
(1,4040)	1:A:148:GLY:H	1:A:151:GLU:H	7	0.12
(1,39)	1:A:34:PHE:HD1	1:A:39:VAL:HB	10	0.12
(1,39)	1:A:34:PHE:HD2	1:A:39:VAL:HB	10	0.12
(1,3701)	1:A:83:ILE:HA	1:A:107:SER:H	19	0.12
(1,3413)	1:A:68:ILE:HD11	1:A:79:VAL:H	4	0.12
(1,3413)	1:A:68:ILE:HD12	1:A:79:VAL:H	4	0.12
(1,3413)	1:A:68:ILE:HD13	1:A:79:VAL:H	4	0.12
(1,3413)	1:A:68:ILE:HD11	1:A:79:VAL:H	5	0.12
(1,3413)	1:A:68:ILE:HD12	1:A:79:VAL:H	5	0.12
(1,3413)	1:A:68:ILE:HD13	1:A:79:VAL:H	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,3413)	1:A:68:ILE:HD11	1:A:79:VAL:H	7	0.12
(1,3413)	1:A:68:ILE:HD12	1:A:79:VAL:H	7	0.12
(1,3413)	1:A:68:ILE:HD13	1:A:79:VAL:H	7	0.12
(1,3413)	1:A:68:ILE:HD11	1:A:79:VAL:H	10	0.12
(1,3413)	1:A:68:ILE:HD12	1:A:79:VAL:H	10	0.12
(1,3413)	1:A:68:ILE:HD13	1:A:79:VAL:H	10	0.12
(1,3413)	1:A:68:ILE:HD11	1:A:79:VAL:H	13	0.12
(1,3413)	1:A:68:ILE:HD12	1:A:79:VAL:H	13	0.12
(1,3413)	1:A:68:ILE:HD13	1:A:79:VAL:H	13	0.12
(1,3173)	1:A:58:SER:H	1:A:95:ILE:H	15	0.12
(1,317)	1:A:186:VAL:HG21	1:A:187:ASN:HB2	18	0.12
(1,317)	1:A:186:VAL:HG21	1:A:187:ASN:HB3	18	0.12
(1,317)	1:A:186:VAL:HG22	1:A:187:ASN:HB2	18	0.12
(1,317)	1:A:186:VAL:HG22	1:A:187:ASN:HB3	18	0.12
(1,317)	1:A:186:VAL:HG23	1:A:187:ASN:HB2	18	0.12
(1,317)	1:A:186:VAL:HG23	1:A:187:ASN:HB3	18	0.12
(1,3163)	1:A:54:LEU:HA	1:A:56:ASP:H	16	0.12
(1,3100)	1:A:48:THR:H	1:A:51:GLY:HA2	20	0.12
(1,2963)	1:A:32:GLY:HA2	1:A:33:SER:H	9	0.12
(1,2875)	1:A:22:ASN:H	1:A:26:TRP:HE1	5	0.12
(1,2842)	1:A:20:GLN:HA	1:A:25:VAL:H	5	0.12
(1,2842)	1:A:20:GLN:HA	1:A:25:VAL:H	11	0.12
(1,2842)	1:A:20:GLN:HA	1:A:25:VAL:H	12	0.12
(1,2790)	1:A:7:THR:HA	1:A:20:GLN:H	12	0.12
(1,2685)	1:A:54:LEU:H	1:A:82:VAL:HB	3	0.12
(1,2685)	1:A:54:LEU:H	1:A:82:VAL:HB	8	0.12
(1,2685)	1:A:54:LEU:H	1:A:82:VAL:HB	12	0.12
(1,2618)	1:A:57:SER:HA	1:A:91:ARG:HA	8	0.12
(1,2618)	1:A:57:SER:HA	1:A:91:ARG:HA	12	0.12
(1,2518)	1:A:195:ASN:HB3	1:A:198:LYS:HB2	4	0.12
(1,2518)	1:A:195:ASN:HB3	1:A:198:LYS:HB3	4	0.12
(1,2518)	1:A:195:ASN:HB3	1:A:198:LYS:HB2	13	0.12
(1,2518)	1:A:195:ASN:HB3	1:A:198:LYS:HB3	13	0.12
(1,2518)	1:A:195:ASN:HB3	1:A:198:LYS:HB2	18	0.12
(1,2518)	1:A:195:ASN:HB3	1:A:198:LYS:HB3	18	0.12
(1,2130)	1:A:219:LEU:HD11	1:A:222:THR:HG1	2	0.12
(1,2130)	1:A:219:LEU:HD12	1:A:222:THR:HG1	2	0.12
(1,2130)	1:A:219:LEU:HD13	1:A:222:THR:HG1	2	0.12
(1,2109)	1:A:67:LEU:H	1:A:68:ILE:HD11	16	0.12
(1,2109)	1:A:67:LEU:H	1:A:68:ILE:HD12	16	0.12
(1,2109)	1:A:67:LEU:H	1:A:68:ILE:HD13	16	0.12
(1,2097)	1:A:58:SER:HB2	1:A:67:LEU:HG	7	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2097)	1:A:58:SER:HB2	1:A:67:LEU:HG	14	0.12
(1,1981)	1:A:33:SER:HB3	1:A:38:ALA:HB1	18	0.12
(1,1981)	1:A:33:SER:HB3	1:A:38:ALA:HB2	18	0.12
(1,1981)	1:A:33:SER:HB3	1:A:38:ALA:HB3	18	0.12
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG21	4	0.12
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG22	4	0.12
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG23	4	0.12
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG21	5	0.12
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG22	5	0.12
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG23	5	0.12
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG21	16	0.12
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG22	16	0.12
(1,150)	1:A:14:GLY:H	1:A:15:THR:HG23	16	0.12
(1,1463)	1:A:190:SER:HA	1:A:226:LEU:HB2	7	0.12
(1,1463)	1:A:190:SER:HA	1:A:226:LEU:HB3	7	0.12
(1,1406)	1:A:84:ILE:HG21	1:A:91:ARG:HA	16	0.12
(1,1406)	1:A:84:ILE:HG22	1:A:91:ARG:HA	16	0.12
(1,1406)	1:A:84:ILE:HG23	1:A:91:ARG:HA	16	0.12
(1,1406)	1:A:84:ILE:HG21	1:A:91:ARG:HA	19	0.12
(1,1406)	1:A:84:ILE:HG22	1:A:91:ARG:HA	19	0.12
(1,1406)	1:A:84:ILE:HG23	1:A:91:ARG:HA	19	0.12
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD21	4	0.12
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD22	4	0.12
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD23	4	0.12
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD21	5	0.12
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD22	5	0.12
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD23	5	0.12
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD21	12	0.12
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD22	12	0.12
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD23	12	0.12
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD21	16	0.12
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD22	16	0.12
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD23	16	0.12
(2,7)	1:A:218:LEU:H	1:A:219:LEU:HG	11	0.11
(1,899)	1:A:109:ALA:HB1	1:A:113:GLU:H	13	0.11
(1,899)	1:A:109:ALA:HB2	1:A:113:GLU:H	13	0.11
(1,899)	1:A:109:ALA:HB3	1:A:113:GLU:H	13	0.11
(1,867)	1:A:57:SER:H	1:A:105:ALA:HB1	20	0.11
(1,867)	1:A:57:SER:H	1:A:105:ALA:HB2	20	0.11
(1,867)	1:A:57:SER:H	1:A:105:ALA:HB3	20	0.11
(1,6691)	1:A:222:THR:HA	1:A:223:LEU:HD11	19	0.11
(1,6691)	1:A:222:THR:HA	1:A:223:LEU:HD12	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,6691)	1:A:222:THR:HA	1:A:223:LEU:HD13	19	0.11
(1,6691)	1:A:222:THR:HA	1:A:223:LEU:HD21	19	0.11
(1,6691)	1:A:222:THR:HA	1:A:223:LEU:HD22	19	0.11
(1,6691)	1:A:222:THR:HA	1:A:223:LEU:HD23	19	0.11
(1,6408)	1:A:173:THR:HB	1:A:218:LEU:HD11	11	0.11
(1,6408)	1:A:173:THR:HB	1:A:218:LEU:HD12	11	0.11
(1,6408)	1:A:173:THR:HB	1:A:218:LEU:HD13	11	0.11
(1,6408)	1:A:173:THR:HB	1:A:218:LEU:HD21	11	0.11
(1,6408)	1:A:173:THR:HB	1:A:218:LEU:HD22	11	0.11
(1,6408)	1:A:173:THR:HB	1:A:218:LEU:HD23	11	0.11
(1,6388)	1:A:171:LYS:HB2	1:A:175:ALA:H	11	0.11
(1,6388)	1:A:171:LYS:HB3	1:A:175:ALA:H	11	0.11
(1,5893)	1:A:95:ILE:HG12	1:A:121:GLU:HB2	18	0.11
(1,5893)	1:A:95:ILE:HG12	1:A:121:GLU:HB3	18	0.11
(1,5671)	1:A:54:LEU:HD11	1:A:55:VAL:H	5	0.11
(1,5671)	1:A:54:LEU:HD12	1:A:55:VAL:H	5	0.11
(1,5671)	1:A:54:LEU:HD13	1:A:55:VAL:H	5	0.11
(1,5671)	1:A:54:LEU:HD21	1:A:55:VAL:H	5	0.11
(1,5671)	1:A:54:LEU:HD22	1:A:55:VAL:H	5	0.11
(1,5671)	1:A:54:LEU:HD23	1:A:55:VAL:H	5	0.11
(1,5217)	1:A:8:VAL:HG11	1:A:17:SER:HA	10	0.11
(1,5217)	1:A:8:VAL:HG12	1:A:17:SER:HA	10	0.11
(1,5217)	1:A:8:VAL:HG13	1:A:17:SER:HA	10	0.11
(1,5217)	1:A:8:VAL:HG21	1:A:17:SER:HA	10	0.11
(1,5217)	1:A:8:VAL:HG22	1:A:17:SER:HA	10	0.11
(1,5217)	1:A:8:VAL:HG23	1:A:17:SER:HA	10	0.11
(1,4796)	1:A:222:THR:HG1	1:A:224:ASP:H	7	0.11
(1,4796)	1:A:222:THR:HG1	1:A:224:ASP:H	11	0.11
(1,4796)	1:A:222:THR:HG1	1:A:224:ASP:H	19	0.11
(1,4675)	1:A:208:PRO:HD3	1:A:210:HIS:H	6	0.11
(1,4510)	1:A:193:ILE:HG12	1:A:195:ASN:H	4	0.11
(1,4510)	1:A:193:ILE:HG12	1:A:195:ASN:H	5	0.11
(1,4510)	1:A:193:ILE:HG12	1:A:195:ASN:H	6	0.11
(1,4510)	1:A:193:ILE:HG12	1:A:195:ASN:H	13	0.11
(1,4510)	1:A:193:ILE:HG12	1:A:195:ASN:H	16	0.11
(1,4319)	1:A:177:ASP:HB2	1:A:178:LEU:H	3	0.11
(1,4265)	1:A:170:VAL:H	1:A:222:THR:HG1	11	0.11
(1,4040)	1:A:148:GLY:H	1:A:151:GLU:H	14	0.11
(1,4040)	1:A:148:GLY:H	1:A:151:GLU:H	16	0.11
(1,4040)	1:A:148:GLY:H	1:A:151:GLU:H	17	0.11
(1,4040)	1:A:148:GLY:H	1:A:151:GLU:H	18	0.11
(1,4040)	1:A:148:GLY:H	1:A:151:GLU:H	20	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,39)	1:A:34:PHE:HD1	1:A:39:VAL:HB	11	0.11
(1,39)	1:A:34:PHE:HD2	1:A:39:VAL:HB	11	0.11
(1,3799)	1:A:113:GLU:HB2	1:A:116:LYS:H	12	0.11
(1,3799)	1:A:113:GLU:HB3	1:A:116:LYS:H	12	0.11
(1,3799)	1:A:113:GLU:HB2	1:A:116:LYS:H	13	0.11
(1,3799)	1:A:113:GLU:HB3	1:A:116:LYS:H	13	0.11
(1,3799)	1:A:113:GLU:HB2	1:A:116:LYS:H	19	0.11
(1,3799)	1:A:113:GLU:HB3	1:A:116:LYS:H	19	0.11
(1,3749)	1:A:110:LEU:HB2	1:A:111:THR:H	20	0.11
(1,3701)	1:A:83:ILE:HA	1:A:107:SER:H	16	0.11
(1,3701)	1:A:83:ILE:HA	1:A:107:SER:H	20	0.11
(1,370)	1:A:28:HIS:H	1:A:42:ASN:HA	14	0.11
(1,370)	1:A:28:HIS:H	1:A:42:ASN:HA	16	0.11
(1,3572)	1:A:95:ILE:H	1:A:120:TYR:HE1	20	0.11
(1,3572)	1:A:95:ILE:H	1:A:120:TYR:HE2	20	0.11
(1,3413)	1:A:68:ILE:HD11	1:A:79:VAL:H	1	0.11
(1,3413)	1:A:68:ILE:HD12	1:A:79:VAL:H	1	0.11
(1,3413)	1:A:68:ILE:HD13	1:A:79:VAL:H	1	0.11
(1,3413)	1:A:68:ILE:HD11	1:A:79:VAL:H	18	0.11
(1,3413)	1:A:68:ILE:HD12	1:A:79:VAL:H	18	0.11
(1,3413)	1:A:68:ILE:HD13	1:A:79:VAL:H	18	0.11
(1,3173)	1:A:58:SER:H	1:A:95:ILE:H	19	0.11
(1,317)	1:A:186:VAL:HG21	1:A:187:ASN:HB2	2	0.11
(1,317)	1:A:186:VAL:HG21	1:A:187:ASN:HB3	2	0.11
(1,317)	1:A:186:VAL:HG22	1:A:187:ASN:HB2	2	0.11
(1,317)	1:A:186:VAL:HG22	1:A:187:ASN:HB3	2	0.11
(1,317)	1:A:186:VAL:HG23	1:A:187:ASN:HB2	2	0.11
(1,317)	1:A:186:VAL:HG23	1:A:187:ASN:HB3	2	0.11
(1,3168)	1:A:56:ASP:H	1:A:57:SER:H	15	0.11
(1,3168)	1:A:56:ASP:H	1:A:57:SER:H	16	0.11
(1,3158)	1:A:56:ASP:H	1:A:82:VAL:HB	15	0.11
(1,3130)	1:A:52:LEU:H	1:A:81:ASP:H	13	0.11
(1,3058)	1:A:46:LEU:H	1:A:54:LEU:HB3	2	0.11
(1,3058)	1:A:46:LEU:H	1:A:54:LEU:HB3	9	0.11
(1,3058)	1:A:46:LEU:H	1:A:54:LEU:HB3	14	0.11
(1,2842)	1:A:20:GLN:HA	1:A:25:VAL:H	13	0.11
(1,2685)	1:A:54:LEU:H	1:A:82:VAL:HB	1	0.11
(1,2685)	1:A:54:LEU:H	1:A:82:VAL:HB	2	0.11
(1,2685)	1:A:54:LEU:H	1:A:82:VAL:HB	7	0.11
(1,2623)	1:A:135:PHE:HA	1:A:138:MET:HG2	13	0.11
(1,2623)	1:A:135:PHE:HA	1:A:138:MET:HG3	13	0.11
(1,2618)	1:A:57:SER:HA	1:A:91:ARG:HA	3	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2591)	1:A:196:VAL:HA	1:A:219:LEU:HD11	19	0.11
(1,2591)	1:A:196:VAL:HA	1:A:219:LEU:HD12	19	0.11
(1,2591)	1:A:196:VAL:HA	1:A:219:LEU:HD13	19	0.11
(1,2583)	1:A:172:SER:HA	1:A:218:LEU:HA	11	0.11
(1,2518)	1:A:195:ASN:HB3	1:A:198:LYS:HB2	6	0.11
(1,2518)	1:A:195:ASN:HB3	1:A:198:LYS:HB3	6	0.11
(1,2256)	1:A:87:ALA:HB1	1:A:151:GLU:H	10	0.11
(1,2256)	1:A:87:ALA:HB2	1:A:151:GLU:H	10	0.11
(1,2256)	1:A:87:ALA:HB3	1:A:151:GLU:H	10	0.11
(1,2249)	1:A:110:LEU:HG	1:A:111:THR:HA	8	0.11
(1,2190)	1:A:89:ALA:HB1	1:A:120:TYR:HD1	16	0.11
(1,2190)	1:A:89:ALA:HB1	1:A:120:TYR:HD2	16	0.11
(1,2190)	1:A:89:ALA:HB2	1:A:120:TYR:HD1	16	0.11
(1,2190)	1:A:89:ALA:HB2	1:A:120:TYR:HD2	16	0.11
(1,2190)	1:A:89:ALA:HB3	1:A:120:TYR:HD1	16	0.11
(1,2190)	1:A:89:ALA:HB3	1:A:120:TYR:HD2	16	0.11
(1,2168)	1:A:84:ILE:HA	1:A:91:ARG:HA	19	0.11
(1,2166)	1:A:83:ILE:HG21	1:A:107:SER:H	16	0.11
(1,2166)	1:A:83:ILE:HG22	1:A:107:SER:H	16	0.11
(1,2166)	1:A:83:ILE:HG23	1:A:107:SER:H	16	0.11
(1,2166)	1:A:83:ILE:HG21	1:A:107:SER:H	17	0.11
(1,2166)	1:A:83:ILE:HG22	1:A:107:SER:H	17	0.11
(1,2166)	1:A:83:ILE:HG23	1:A:107:SER:H	17	0.11
(1,2166)	1:A:83:ILE:HG21	1:A:107:SER:H	19	0.11
(1,2166)	1:A:83:ILE:HG22	1:A:107:SER:H	19	0.11
(1,2166)	1:A:83:ILE:HG23	1:A:107:SER:H	19	0.11
(1,2130)	1:A:219:LEU:HD11	1:A:222:THR:HG1	19	0.11
(1,2130)	1:A:219:LEU:HD12	1:A:222:THR:HG1	19	0.11
(1,2130)	1:A:219:LEU:HD13	1:A:222:THR:HG1	19	0.11
(1,2097)	1:A:58:SER:HB2	1:A:67:LEU:HG	4	0.11
(1,2097)	1:A:58:SER:HB2	1:A:67:LEU:HG	12	0.11
(1,2097)	1:A:58:SER:HB2	1:A:67:LEU:HG	17	0.11
(1,1463)	1:A:190:SER:HA	1:A:226:LEU:HB2	5	0.11
(1,1463)	1:A:190:SER:HA	1:A:226:LEU:HB3	5	0.11
(1,1406)	1:A:84:ILE:HG21	1:A:91:ARG:HA	15	0.11
(1,1406)	1:A:84:ILE:HG22	1:A:91:ARG:HA	15	0.11
(1,1406)	1:A:84:ILE:HG23	1:A:91:ARG:HA	15	0.11
(1,1406)	1:A:84:ILE:HG21	1:A:91:ARG:HA	17	0.11
(1,1406)	1:A:84:ILE:HG22	1:A:91:ARG:HA	17	0.11
(1,1406)	1:A:84:ILE:HG23	1:A:91:ARG:HA	17	0.11
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD21	8	0.11
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD22	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1209)	1:A:196:VAL:HA	1:A:219:LEU:HD23	8	0.11

10 Dihedral-angle violation analysis (i)

No dihedral-angle restraints found