WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB NMR Structure Validation Report ⓘ

Jun 6, 2023 – 04:12 AM EDT

|		
PDB ID	:	2MKJ
BMRB ID	:	19777
Title	:	Solution structure of tandem RRM domains of cytoplasmic polyadenylation element binding protein 4 (CPEB4) in free state
Authors	:	Afroz, T.; Skrisovska, L.; Belloc, E.; Boixet, J.G.; Mendez, R.; Allain, F.H.-T.
Deposited on	:	2014-02-07
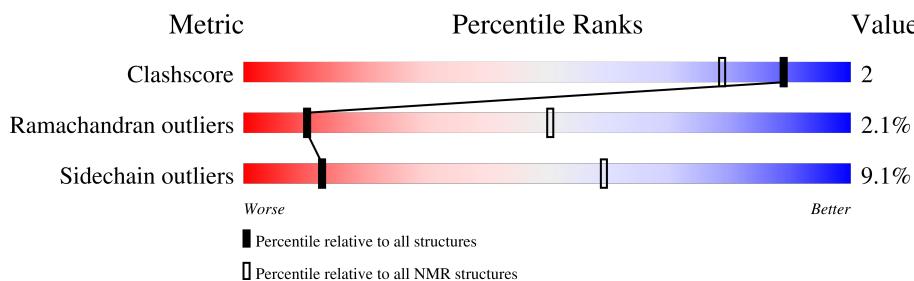
1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 68%.

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	Percentile Ranks	Value
Clashscore		2
Ramachandran outliers		2.1%
Sidechain outliers		9.1%

Worse — *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all NMR structures

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	203	81% 5% 13%

2 Ensemble composition and analysis ⓘ

This entry contains 20 models. Model 2 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:62-A:95, A:109-A:140, A:145-A:254 (176)	1.75	2

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

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

NmrClust was unable to cluster the ensemble.

Error message: Inconsistent models

3 Entry composition ⓘ

There is only 1 type of molecule in this entry. The entry contains 3182 atoms, of which 1582 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cytoplasmic polyadenylation element-binding protein 4.
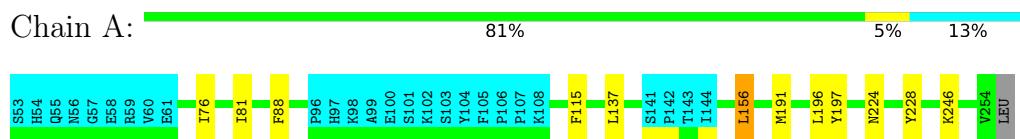
Mol	Chain	Residues	Atoms						Trace
1	A	202	Total	C	H	N	O	S	0
			3182	1023	1582	273	298	6	

4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: Cytoplasmic polyadenylation element-binding protein 4
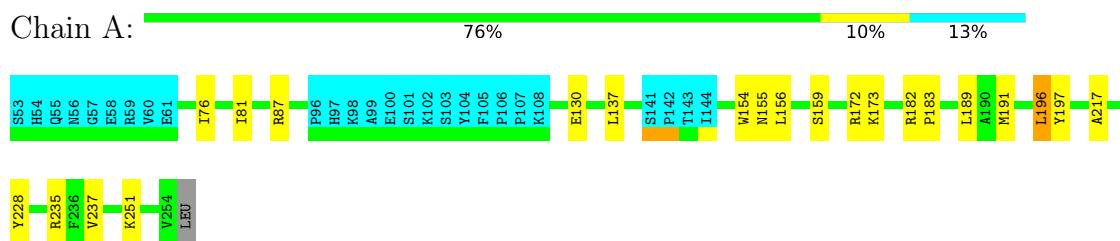
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.
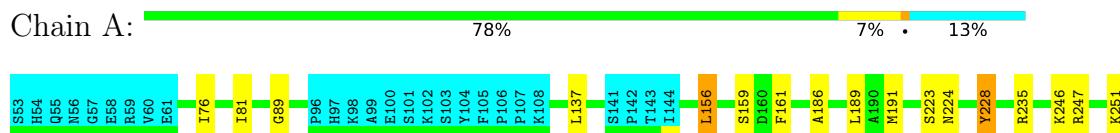
4.2.1 Score per residue for model 1

• Molecule 1: Cytoplasmic polyadenylation element-binding protein 4

4.2.2 Score per residue for model 2 (medoid)

• Molecule 1: Cytoplasmic polyadenylation element-binding protein 4

V254 LEU
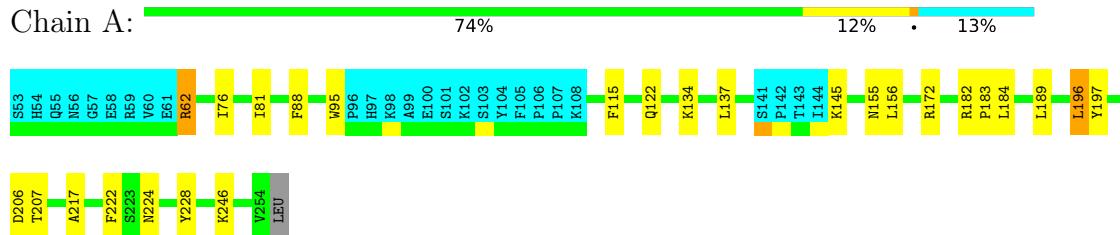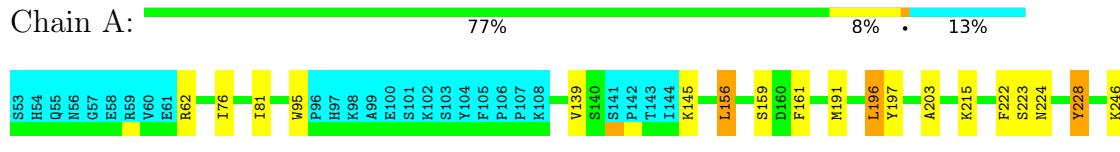
4.2.3 Score per residue for model 3

• Molecule 1: Cytoplasmic polyadenylation element-binding protein 4

Chain A: 74%   12%   •   13%

S53 H54 Q55 N56 G57 E58 R59 V60 E61 R62 I76 I81 F88 W95 P96 H97 K98 A99 E100 S101 K102 S103 Y104 F105 P106 P107 K108 F115 Q122 K134 L137 S141 P142 T143 I144 K145 N155 L156 R172 R182 P183 L184 L189 L196 Y197

D206 T207 A217 F222 S223 N224 Y228 K246 V254 LEU
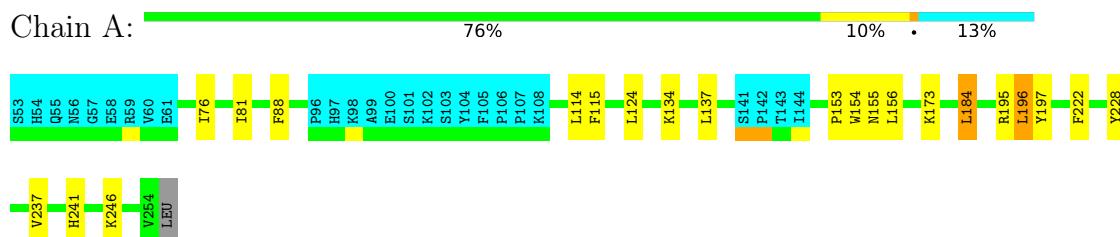
4.2.4 Score per residue for model 4

• Molecule 1: Cytoplasmic polyadenylation element-binding protein 4

Chain A: 77%   8%   •   13%

S53 H54 Q55 N56 G57 E58 R59 V60 E61 R62 I76 I81 W95 P96 H97 K98 A99 E100 S101 K102 S103 Y104 F105 P106 P107 K108 V139 S140 S141 P142 T143 I144 K145 L156 S159 D160 F161 M191 L196 Y197 A203 K215 F222 S223 N224 Y228 K246

V254 LEU
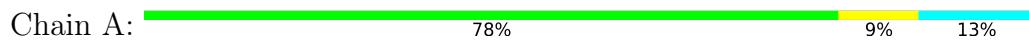
4.2.5 Score per residue for model 5

• Molecule 1: Cytoplasmic polyadenylation element-binding protein 4

Chain A: 76%   10%   •   13%

S53 H54 Q55 N56 G57 E58 R59 V60 E61 I76 I81 F88 P96 H97 K98 A99 E100 S101 K102 S103 Y104 F105 P106 P107 K108 L114 F115 L124 K134 L137 S141 P142 T143 I144 P153 W154 N155 L156 K173 L184 R195 L196 Y197 F222 Y228

V237 H241 K246 V254 LEU
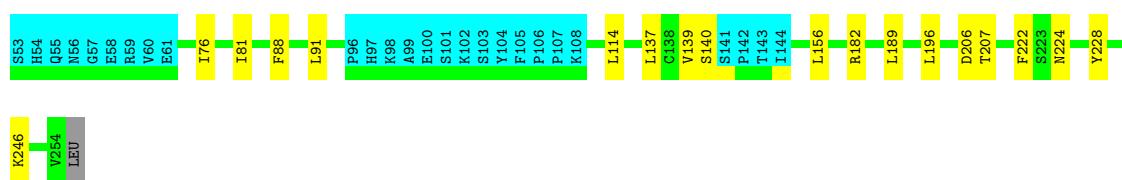
4.2.6 Score per residue for model 6

• Molecule 1: Cytoplasmic polyadenylation element-binding protein 4

Chain A: 78%   9%   13%

S53 H54 Q55 N56 G57 E58 R59 V60 E61 I76 I81 F88 L91 P96 H97 K98 A99 E100 S101 K102 S103 Y104 F105 P106 P107 K108 L114 L137 C138 V139 S140 S141 P142 T143 I144 L156 R182 L189 L196 D206 T207 F222 S223 N224 Y228

K246 V254 LEU
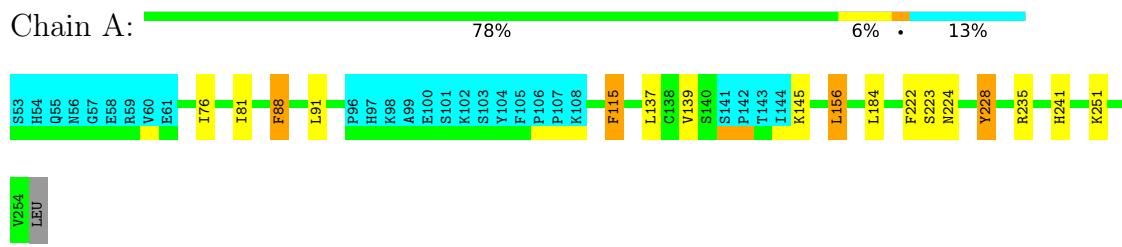
4.2.7 Score per residue for model 7

• Molecule 1: Cytoplasmic polyadenylation element-binding protein 4

Chain A: 80%   7%   13%

S53 H54 Q55 N56 G57 E58 R59 V60 E61 I76 I81 P96 H97 K98 A99 E100 S101 K102 S103 Y104 F105 P106 P107 K108 L114 F115 S141 P142 T143 I144 P153 L156 G165 R182 M191 L196 T207 Y228 L239 K246 V254 LEU
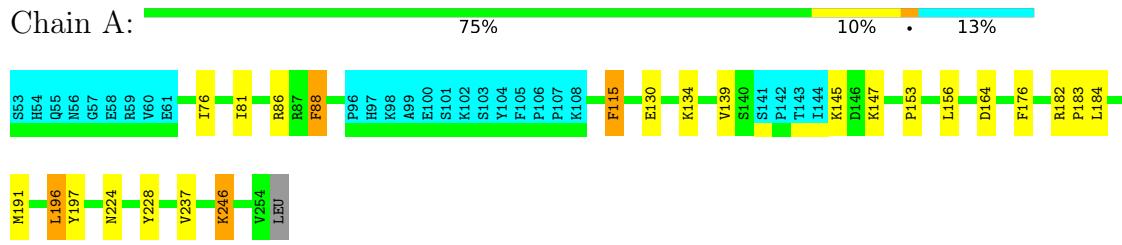
4.2.8 Score per residue for model 8

• Molecule 1: Cytoplasmic polyadenylation element-binding protein 4

Chain A: 78%   6% ·   13%

S53 H54 Q55 N56 G57 E58 R59 V60 E61 I76 I81 F88 L91 P96 H97 K98 A99 E100 S101 K102 S103 Y104 F105 P106 P107 K108 F115 L137 C138 V139 S140 S141 P142 T143 I144 K145 L156 L184 F222 S223 N224 Y228 R235 H241 K251

V254 LEU
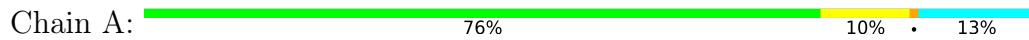
4.2.9 Score per residue for model 9

• Molecule 1: Cytoplasmic polyadenylation element-binding protein 4

Chain A: 75%   10% ·   13%

S53 H54 Q55 N56 G57 E58 R59 V60 E61 I76 I81 R86 R87 F88 P96 H97 K98 A99 E100 S101 K102 S103 Y104 F105 P106 P107 K108 F115 E130 K134 V139 S140 S141 P142 T143 I144 K145 D146 K147 P153 L156 D164 F176 R182 P183 L184

M191 L196 Y197 N224 Y228 V237 K246 V254 LEU

4.2.10 Score per residue for model 10

• Molecule 1: Cytoplasmic polyadenylation element-binding protein 4

Chain A: 76%   10% ·   13%

S53 H54 Q55 N56 G57 E58 R59 V60 E61 S64 F68 I76 I81 F88 P96 H97 K98 A99 E100 S101 K102 S103 Y104 F105 P106 P107 K108 L114 Q122 L137 S140 S141 P142 T143 I144 P153 L156 V180 P181 L189 A190 M191 L196 I205

D206 T207 N224 Y228 Q238 V254 LEU
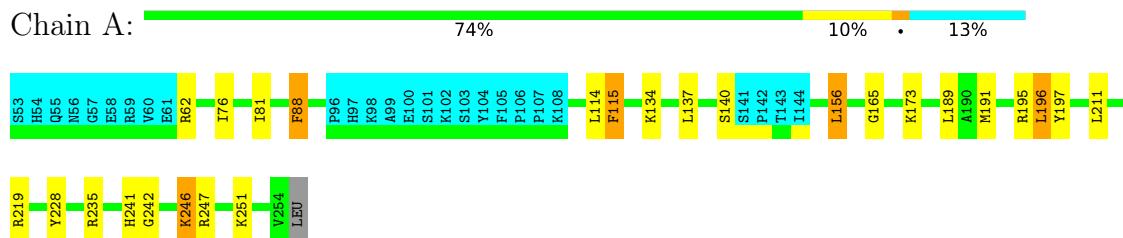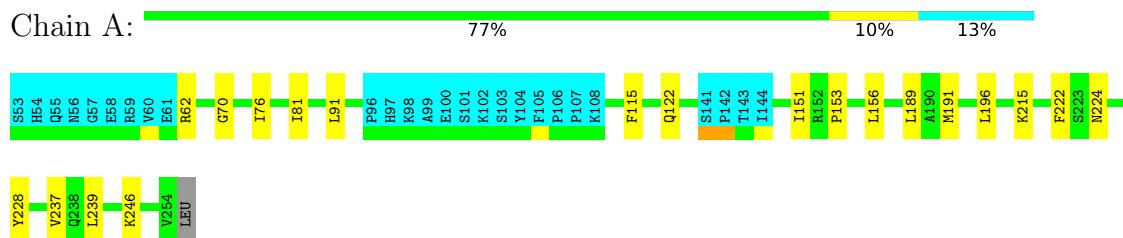
### 4.2.11 Score per residue for model 11

• Molecule 1: Cytoplasmic polyadenylation element-binding protein 4

Chain A: 74% 10% · 13%

S53 H54 Q55 N56 G57 E58 R59 V60 E61 R62 I76 I81 F88 P96 H97 K98 A99 E100 S101 K102 S103 Y104 F105 P106 P107 K108 L114 F115 K134 L137 S140 S141 P142 T143 I144 L156 G165 K173 L189 A190 M191 R195 L196 Y197 L211

R219 Y228 R235 H241 G242 K246 R247 K251 V254 LEU
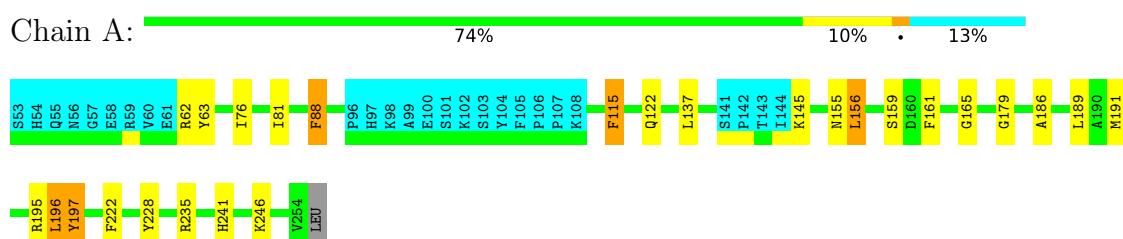
4.2.12 Score per residue for model 12

• Molecule 1: Cytoplasmic polyadenylation element-binding protein 4

Chain A: 77% 10% 13%

S53 H54 Q55 N56 G57 E58 R59 V60 E61 R62 G70 I76 I81 L91 P96 H97 K98 A99 E100 S101 K102 S103 Y104 F105 P106 P107 K108 F115 Q122 S141 P142 T143 I144 I151 R152 P153 L156 L189 A190 M191 L196 K215 F222 S223 N224

Y228 V237 Q238 L239 K246 V254 LEU
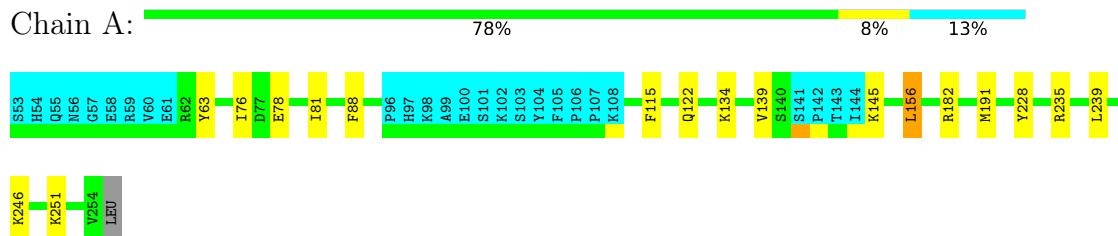
4.2.13 Score per residue for model 13

• Molecule 1: Cytoplasmic polyadenylation element-binding protein 4

Chain A: 74% 10% · 13%

S53 H54 Q55 N56 G57 E58 R59 V60 E61 R62 Y63 I76 I81 F88 P96 H97 K98 A99 E100 S101 K102 S103 Y104 F105 P106 P107 K108 F115 Q122 L137 S141 P142 T143 I144 K145 N155 L156 S159 D160 F161 G165 G179 A186 L189 A190 M191

R195 L196 Y197 F222 Y228 R235 H241 K246 V254 LEU
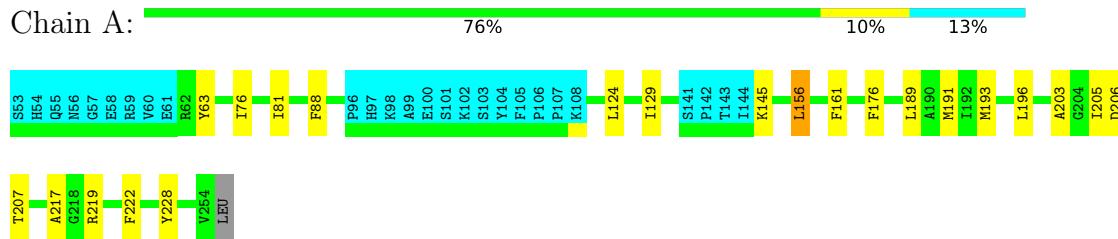
4.2.14 Score per residue for model 14

• Molecule 1: Cytoplasmic polyadenylation element-binding protein 4

Chain A: 78%   8%   13%

S53 H54 Q55 N56 G57 E58 R59 V60 E61 R62 Y63 I76 D77 E78 I81 F88 P96 H97 K98 A99 E100 S101 K102 S103 Y104 F105 P106 P107 K108 F115 Q122 K134 V139 S140 S141 P142 T143 I144 K145 L156 R182 M191 Y228 R235 L239

K246 K251 V254 LEU
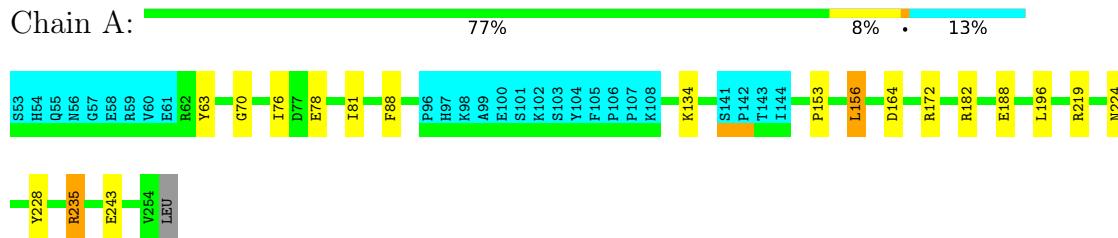
4.2.15 Score per residue for model 15

• Molecule 1: Cytoplasmic polyadenylation element-binding protein 4

Chain A: 76%   10%   13%

S53 H54 Q55 N56 G57 E58 R59 V60 E61 R62 Y63 I76 I81 F88 P96 H97 K98 A99 E100 S101 K102 S103 Y104 F105 P106 P107 K108 L124 I129 S141 P142 T143 I144 K145 L156 F161 F176 L189 A190 M191 I192 M193 L196 A203 G204 I205 D206

T207 A217 G218 R219 F222 Y228 V254 LEU
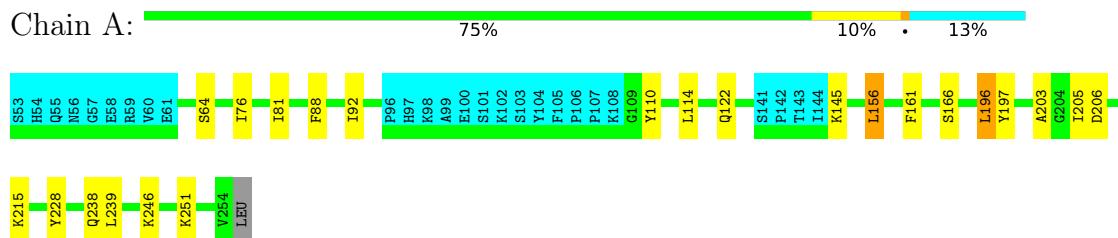
4.2.16 Score per residue for model 16

• Molecule 1: Cytoplasmic polyadenylation element-binding protein 4

Chain A: 77%   8%   •   13%

S53 H54 Q55 N56 G57 E58 R59 V60 E61 R62 Y63 G70 I76 D77 E78 I81 F88 P96 H97 K98 A99 E100 S101 K102 S103 Y104 F105 P106 P107 K108 K134 S141 P142 T143 I144 P153 L156 D164 R172 R182 E188 L196 R219 N224

Y228 R235 E243 V254 LEU
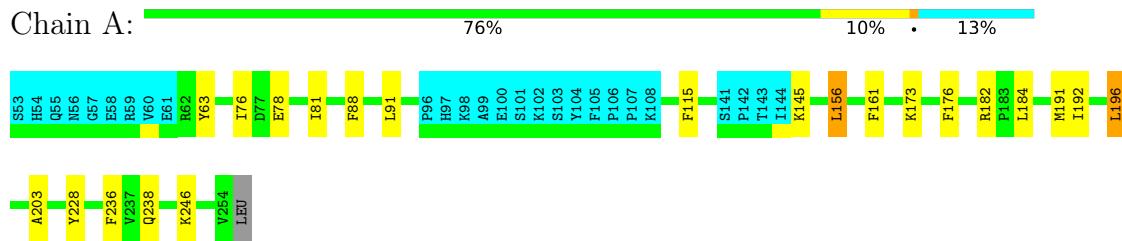
4.2.17 Score per residue for model 17

• Molecule 1: Cytoplasmic polyadenylation element-binding protein 4

Chain A: 75%   10%   •   13%

S53 H54 Q55 N56 G57 E58 R59 V60 E61 S64 I76 I81 F88 I92 P96 H97 K98 A99 E100 S101 K102 S103 Y104 F105 P106 P107 K108 G109 Y110 L114 Q122 S141 P142 T143 I144 K145 L156 F161 S166 L196 Y197 A203 G204 I205 D206

K215 Y228 Q238 L239 K246 K251 V254 LEU
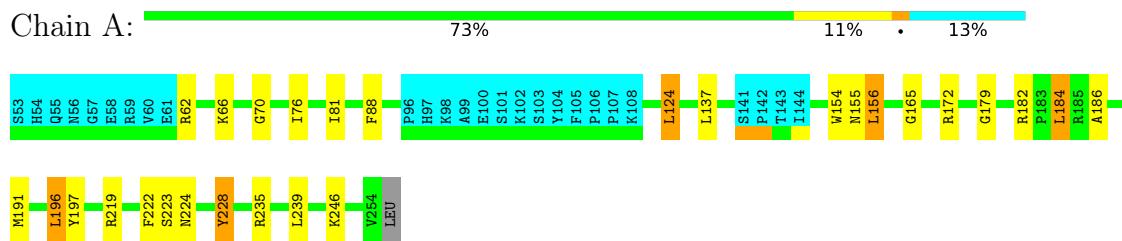
4.2.18 Score per residue for model 18

• Molecule 1: Cytoplasmic polyadenylation element-binding protein 4

Chain A:
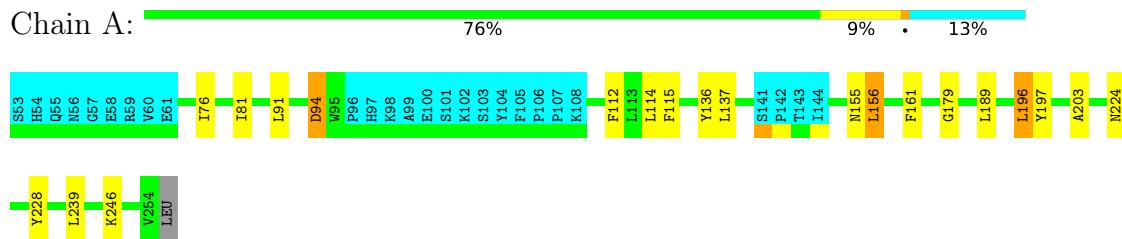
4.2.19 Score per residue for model 19

• Molecule 1: Cytoplasmic polyadenylation element-binding protein 4

Chain A:

4.2.20 Score per residue for model 20

• Molecule 1: Cytoplasmic polyadenylation element-binding protein 4

Chain A:

5 Refinement protocol and experimental data overview ⓘ

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

Of the 30 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
Amber	refinement	
CYANA	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	1
Total number of shifts	1720
Number of shifts mapped to atoms	1719
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	68%

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1392	1381	1381	5±3
All	All	27840	27620	27620	99

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models Worst	Total
1:A:156:LEU:HD13	1:A:156:LEU:H	0.77	1.39	10	12
1:A:196:LEU:CD1	1:A:197:TYR:H	0.63	2.07	11	2
1:A:156:LEU:H	1:A:156:LEU:CD1	0.62	2.08	20	6
1:A:156:LEU:HD13	1:A:156:LEU:N	0.57	2.14	16	3
1:A:189:LEU:HD23	1:A:189:LEU:C	0.52	2.24	3	5
1:A:88:PHE:CD1	1:A:115:PHE:CZ	0.52	2.98	11	4
1:A:88:PHE:CE1	1:A:115:PHE:CZ	0.50	3.00	5	3
1:A:161:PHE:CZ	1:A:203:ALA:HB3	0.50	2.40	18	3
1:A:196:LEU:HD12	1:A:197:TYR:H	0.49	1.65	11	5
1:A:154:TRP:CG	1:A:155:ASN:N	0.48	2.81	1	2
1:A:196:LEU:HD13	1:A:197:TYR:CD2	0.48	2.43	1	4
1:A:189:LEU:C	1:A:189:LEU:HD13	0.47	2.30	2	2
1:A:241:HIS:CG	1:A:242:GLY:N	0.47	2.83	11	1
1:A:94:ASP:CB	1:A:112:PHE:H	0.46	2.22	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:192:ILE:O	1:A:196:LEU:CD2	0.45	2.64	18	1
1:A:223:SER:HA	1:A:228:TYR:CD2	0.45	2.46	8	3
1:A:173:LYS:HA	1:A:173:LYS:HE2	0.45	1.87	18	2
1:A:88:PHE:CZ	1:A:124:LEU:HD12	0.45	2.47	5	1
1:A:182:ARG:N	1:A:183:PRO:CD	0.44	2.81	9	3
1:A:154:TRP:CD1	1:A:155:ASN:N	0.44	2.85	19	1
1:A:156:LEU:CD1	1:A:156:LEU:N	0.44	2.81	12	4
1:A:64:SER:HB2	1:A:156:LEU:HD12	0.43	1.90	17	2
1:A:63:TYR:CD1	1:A:63:TYR:N	0.43	2.85	15	2
1:A:223:SER:HA	1:A:228:TYR:CG	0.43	2.48	4	1
1:A:94:ASP:HA	1:A:112:PHE:O	0.43	2.13	20	1
1:A:161:PHE:CZ	1:A:203:ALA:CB	0.43	3.01	17	2
1:A:88:PHE:CE2	1:A:115:PHE:CE2	0.43	3.07	8	1
1:A:246:LYS:HE2	1:A:246:LYS:H	0.43	1.74	11	1
1:A:184:LEU:CD2	1:A:186:ALA:H	0.43	2.27	19	1
1:A:241:HIS:CG	1:A:242:GLY:H	0.42	2.32	11	1
1:A:68:PHE:CD1	1:A:68:PHE:C	0.42	2.92	10	1
1:A:180:VAL:N	1:A:181:PRO:CD	0.42	2.82	10	1
1:A:94:ASP:CB	1:A:112:PHE:N	0.42	2.82	20	1
1:A:196:LEU:CD2	1:A:196:LEU:N	0.41	2.84	18	1
1:A:189:LEU:C	1:A:189:LEU:HD23	0.41	2.36	11	1
1:A:238:GLN:C	1:A:239:LEU:HD22	0.41	2.36	17	1
1:A:161:PHE:CD1	1:A:186:ALA:CB	0.41	3.04	2	1
1:A:156:LEU:N	1:A:156:LEU:HD12	0.41	2.30	7	1
1:A:196:LEU:HD12	1:A:197:TYR:N	0.41	2.30	20	1
1:A:184:LEU:C	1:A:184:LEU:HD12	0.41	2.36	18	1
1:A:62:ARG:N	1:A:62:ARG:CD	0.41	2.84	3	1
1:A:88:PHE:CG	1:A:115:PHE:CZ	0.41	3.09	11	1
1:A:156:LEU:N	1:A:156:LEU:CD1	0.41	2.83	16	1
1:A:124:LEU:CD1	1:A:137:LEU:HD21	0.41	2.46	19	1
1:A:205:ILE:O	1:A:207:THR:N	0.40	2.54	10	1
1:A:189:LEU:HD13	1:A:189:LEU:C	0.40	2.36	20	1
1:A:161:PHE:CE2	1:A:186:ALA:HB3	0.40	2.52	13	1
1:A:92:ILE:HD12	1:A:92:ILE:N	0.40	2.31	17	1
1:A:129:ILE:HD12	1:A:129:ILE:N	0.40	2.31	15	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the backbone conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	175/203 (86%)	152±3 (87±2%)	19±4 (11±2%)	4±2 (2±1%)	10	50
All	All	3500/4060 (86%)	3042 (87%)	383 (11%)	75 (2%)	10	50

All 30 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	246	LYS	6
1	A	153	PRO	6
1	A	206	ASP	5
1	A	139	VAL	5
1	A	182	ARG	5
1	A	159	SER	4
1	A	165	GLY	4
1	A	217	ALA	3
1	A	222	PHE	3
1	A	70	GLY	3
1	A	179	GLY	3
1	A	78	GLU	3
1	A	247	ARG	2
1	A	237	VAL	2
1	A	140	SER	2
1	A	164	ASP	2
1	A	239	LEU	2
1	A	145	LYS	2
1	A	235	ARG	2
1	A	87	ARG	1
1	A	89	GLY	1
1	A	184	LEU	1
1	A	86	ARG	1
1	A	63	TYR	1
1	A	243	GLU	1
1	A	110	TYR	1
1	A	166	SER	1

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Mol	Chain	Res	Type	Models (Total)
1	A	236	PHE	1
1	A	219	ARG	1
1	A	94	ASP	1

6.3.2   Protein sidechains ⓘ

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	150/175 (86%)	136±2 (91±1%)	14±2 (9±1%)	13	59
All	All	3000/3500 (86%)	2726 (91%)	274 (9%)	13	59

All 49 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	76	ILE	20
1	A	81	ILE	20
1	A	228	TYR	20
1	A	156	LEU	17
1	A	196	LEU	17
1	A	191	MET	13
1	A	224	ASN	11
1	A	88	PHE	11
1	A	137	LEU	10
1	A	246	LYS	10
1	A	115	PHE	8
1	A	235	ARG	7
1	A	145	LYS	7
1	A	114	LEU	7
1	A	251	LYS	6
1	A	62	ARG	6
1	A	122	GLN	6
1	A	134	LYS	6
1	A	222	PHE	6
1	A	184	LEU	5
1	A	91	LEU	5
1	A	172	ARG	4

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Mol	Chain	Res	Type	Models (Total)
1	A	207	THR	4
1	A	155	ASN	3
1	A	215	LYS	3
1	A	195	ARG	3
1	A	241	HIS	3
1	A	239	LEU	3
1	A	176	PHE	3
1	A	219	ARG	3
1	A	130	GLU	2
1	A	173	LYS	2
1	A	237	VAL	2
1	A	95	TRP	2
1	A	238	GLN	2
1	A	63	TYR	2
1	A	124	LEU	2
1	A	205	ILE	2
1	A	182	ARG	1
1	A	147	LYS	1
1	A	68	PHE	1
1	A	211	LEU	1
1	A	151	ILE	1
1	A	197	TYR	1
1	A	189	LEU	1
1	A	193	MET	1
1	A	188	GLU	1
1	A	66	LYS	1
1	A	136	TYR	1

6.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

6.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers ⓘ

There are no such molecules in this entry.

6.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

7   Chemical shift validation ⓘ

The completeness of assignment taking into account all chemical shift lists is 68% for the well-defined parts and 62% for the entire structure.

7.1   Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *CPEB4RRM12_ assigned_ chemical_ shifts*

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	1720
Number of shifts mapped to atoms	1719
Number of unparsed shifts	0
Number of shifts with mapping errors	1
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	9

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- No matching atom found in the structure. All 1 occurrences are reported below.

List ID	Chain	Res	Type	Atom	Shift Data		
					Value	Uncertainty	Ambiguity
1	A	255	LEU	H	7.998	0.000	.

7.1.2   Chemical shift referencing ⓘ

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_\alpha$	137	2.96 ± 0.12	Should be applied
$^{13}C_\beta$	124	2.91 ± 0.06	Should be applied
$^{13}C'$	0	—	None (insufficient data)
^{15}N	170	-0.51 ± 0.30	None needed (imprecise)

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 68%, i.e. 1638 atoms were assigned a chemical shift out of a possible 2421. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	612/870 (70%)	320/354 (90%)	133/352 (38%)	159/164 (97%)
Sidechain	893/1358 (66%)	625/883 (71%)	260/420 (62%)	8/55 (15%)
Aromatic	133/193 (69%)	81/93 (87%)	50/97 (52%)	2/3 (67%)
Overall	1638/2421 (68%)	1026/1330 (77%)	443/869 (51%)	169/222 (76%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 62%, i.e. 1719 atoms were assigned a chemical shift out of a possible 2765. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	642/993 (65%)	335/403 (83%)	137/404 (34%)	170/186 (91%)
Sidechain	931/1546 (60%)	651/1003 (65%)	271/480 (56%)	9/63 (14%)
Aromatic	146/226 (65%)	89/110 (81%)	55/111 (50%)	2/5 (40%)
Overall	1719/2765 (62%)	1075/1516 (71%)	463/995 (47%)	181/254 (71%)

7.1.4 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.
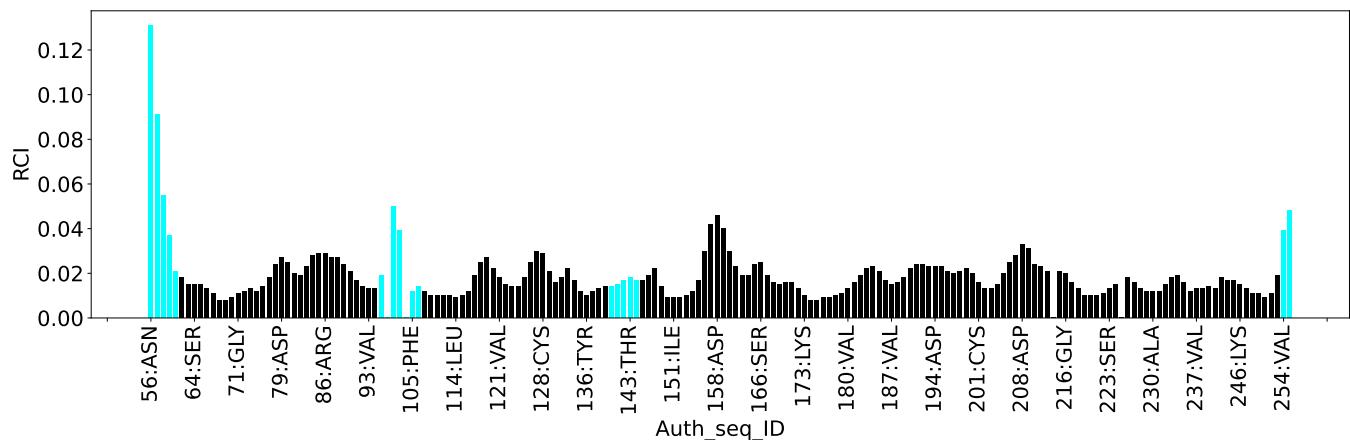
List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	76	ILE	CG1	11.00	$19.24 - 36.26$	-9.8
1	A	214	PRO	HD3	0.44	$1.76 - 5.48$	-8.5
1	A	214	PRO	HD2	0.91	$1.93 - 5.38$	-7.9
1	A	205	ILE	CG1	14.50	$19.24 - 36.26$	-7.8
1	A	214	PRO	HG3	-0.38	$0.33 - 3.48$	-7.3
1	A	175	ILE	CG1	17.13	$19.24 - 36.26$	-6.2
1	A	214	PRO	HG2	0.18	$0.41 - 3.45$	-5.8
1	A	134	LYS	CE	37.29	$37.57 - 46.21$	-5.3
1	A	95	TRP	CZ2	121.45	$107.20 - 121.33$	5.1

7.1.5 Random Coil Index (RCI) plots ⓘ

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	2493
Intra-residue ($|i-j|$=0)	496
Sequential ($|i-j|$=1)	718
Medium range ($|i-j|$>1 and $|i-j|$<5)	426
Long range ($|i-j|$≥5)	731
Inter-chain	0
Hydrogen bond restraints	122
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	12.3
Number of long range restraints per residue[1]	3.9

[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)	23.1	0.2
0.2-0.5 (Medium)	15.1	0.48
>0.5 (Large)	1.6	1.56

8.2.2 Average number of dihedral-angle violations per model ⓘ

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

9   Distance violation analysis (i)
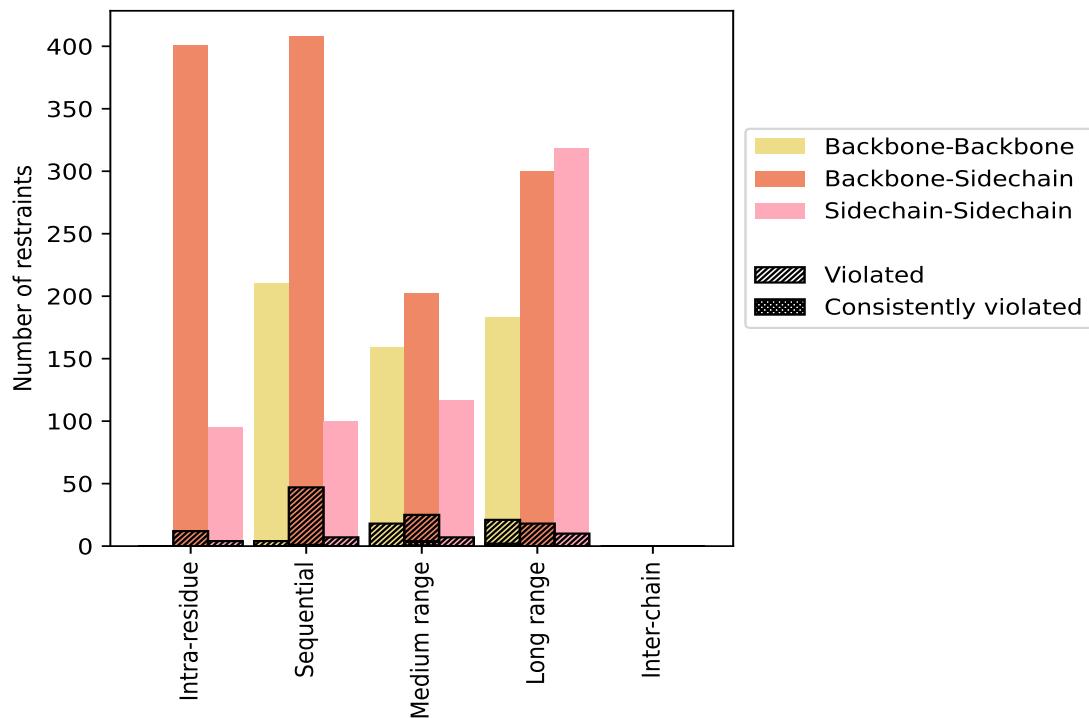
9.1   Summary of distance violations (i)

The following table shows the summary of distance violations in different restraint categories based on the sequence separation of the atoms involved. Each category is further sub-divided into three sub-categories based on the atoms involved. Violations less than 0.1 Å are not included in the statistics.

Restraints type	Count	$\%^1$	Violated[3]			Consistently Violated[4]		
			Count	$\%^2$	$\%^1$	Count	$\%^2$	$\%^1$
Intra-residue (|i-j|=0)	496	19.9	16	3.2	0.6	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	401	16.1	12	3.0	0.5	0	0.0	0.0
Sidechain-Sidechain	95	3.8	4	4.2	0.2	0	0.0	0.0
Sequential (|i-j|=1)	718	28.8	58	8.1	2.3	1	0.1	0.0
Backbone-Backbone	210	8.4	4	1.9	0.2	0	0.0	0.0
Backbone-Sidechain	408	16.4	47	11.5	1.9	1	0.2	0.0
Sidechain-Sidechain	100	4.0	7	7.0	0.3	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	426	17.1	43	10.1	1.7	4	0.9	0.2
Backbone-Backbone	107	4.3	11	10.3	0.4	0	0.0	0.0
Backbone-Sidechain	202	8.1	25	12.4	1.0	4	2.0	0.2
Sidechain-Sidechain	117	4.7	7	6.0	0.3	0	0.0	0.0
Long range (|i-j|≥5)	731	29.3	38	5.2	1.5	0	0.0	0.0
Backbone-Backbone	113	4.5	10	8.8	0.4	0	0.0	0.0
Backbone-Sidechain	300	12.0	18	6.0	0.7	0	0.0	0.0
Sidechain-Sidechain	318	12.8	10	3.1	0.4	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	122	4.9	18	14.8	0.7	2	1.6	0.1
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2493	100.0	173	6.9	6.9	7	0.3	0.3
Backbone-Backbone	552	22.1	43	7.8	1.7	2	0.4	0.1
Backbone-Sidechain	1311	52.6	102	7.8	4.1	5	0.4	0.2
Sidechain-Sidechain	630	25.3	28	4.4	1.1	0	0.0	0.0

[1] percentage calculated with respect to the total number of distance restraints, [2] percentage calculated with respect to the number of restraints in a particular restraint category, [3] violated in at least one model, [4] violated in all the models

9.1.1　Bar chart : Distribution of distance restraints and violations ⓘ

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

9.2　Distance violation statistics for each model ⓘ

The following table provides the distance violation statistics for each model in the ensemble. Violations less than 0.1 Å are not included in the statistics.

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	2	9	13	8	0	32	0.22	0.76	0.12	0.18
2	3	10	13	10	0	36	0.25	1.56	0.24	0.18
3	2	11	18	8	0	39	0.2	0.4	0.09	0.17
4	2	7	22	12	0	43	0.23	1.25	0.18	0.2
5	2	10	13	9	0	34	0.2	0.83	0.13	0.16
6	6	9	13	10	0	38	0.23	0.58	0.11	0.21
7	5	16	15	10	0	46	0.2	0.98	0.14	0.16
8	4	9	16	11	0	40	0.21	0.55	0.11	0.18
9	2	11	14	9	0	36	0.2	0.99	0.15	0.16
10	2	13	14	8	0	37	0.21	0.46	0.08	0.18
11	3	7	15	8	0	33	0.23	0.93	0.16	0.18
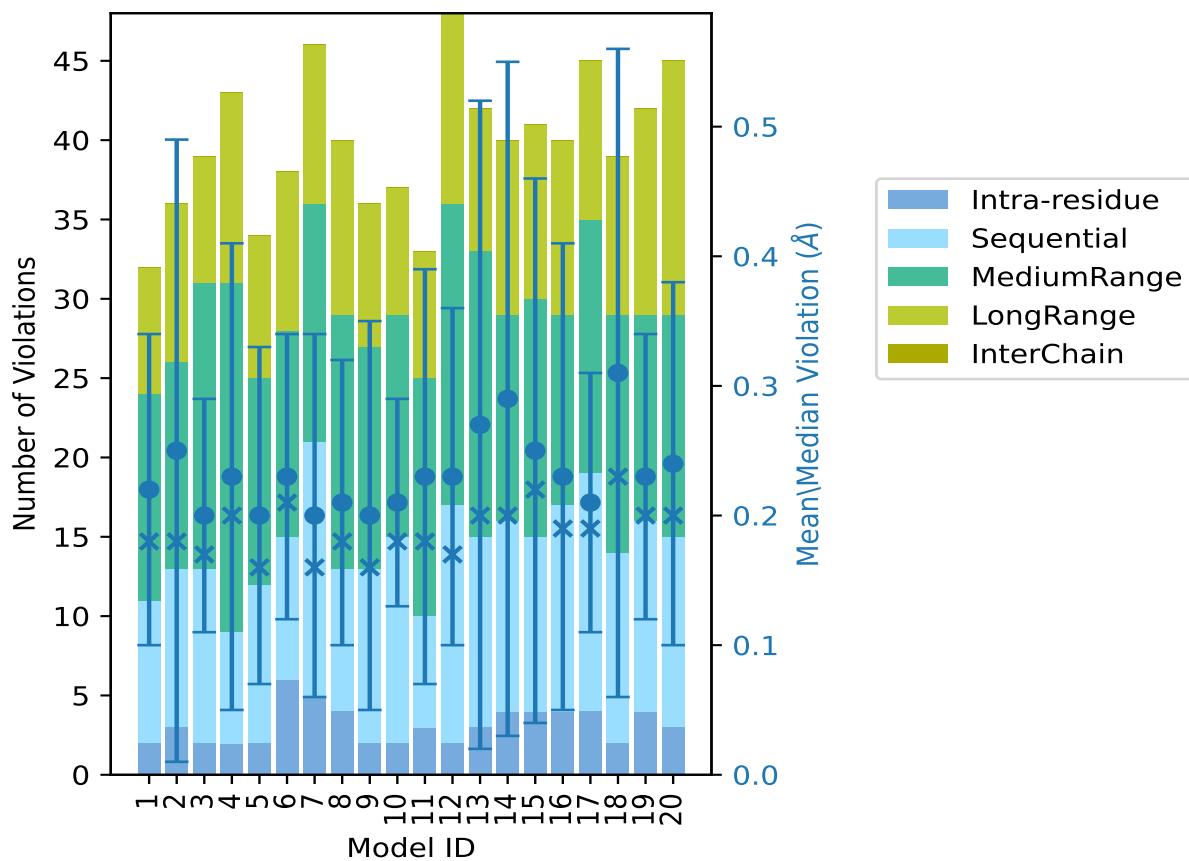
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Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	2	15	19	12	0	48	0.23	0.77	0.13	0.17
13	3	12	18	9	0	42	0.27	1.5	0.25	0.2
14	4	12	13	11	0	40	0.29	1.23	0.26	0.2
15	4	11	15	11	0	41	0.25	1.42	0.21	0.22
16	4	13	12	11	0	40	0.23	1.23	0.18	0.19
17	4	15	16	10	0	45	0.21	0.55	0.1	0.19
18	2	12	15	10	0	39	0.31	1.42	0.25	0.23
19	4	12	13	13	0	42	0.23	0.61	0.11	0.2
20	3	12	14	16	0	45	0.24	0.8	0.14	0.2

[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 ⓘ
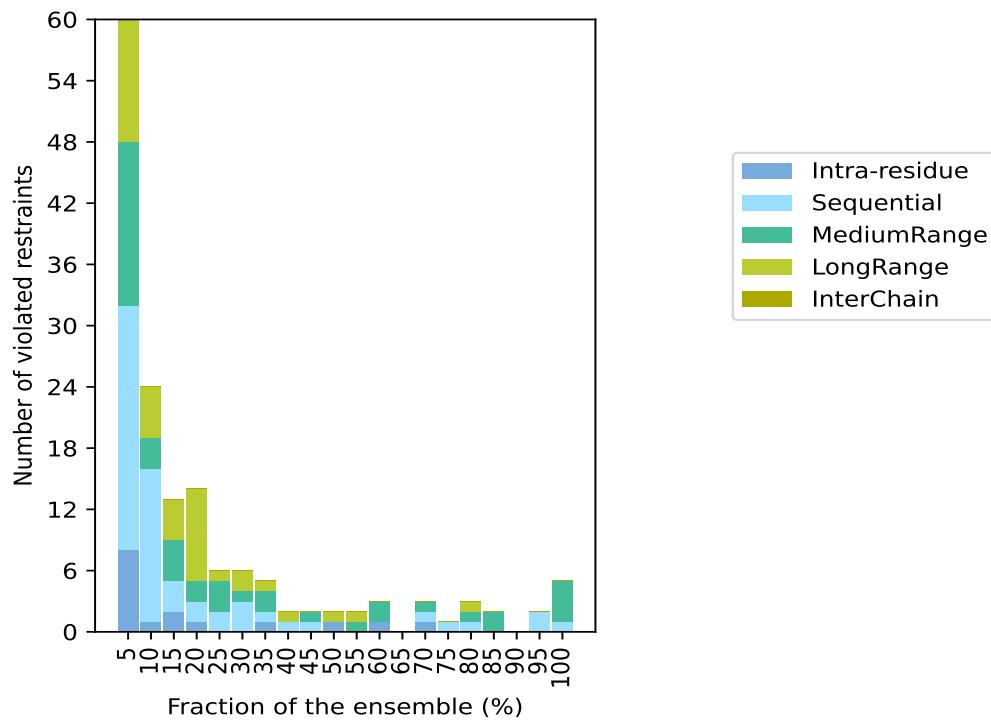
Violation analysis may find that some restraints are violated in few models and some are violated in most of models. The following table provides this information as number of violated restraints for a given fraction of the ensemble. In total, 2216(IR:480, SQ:660, MR:383, LR:693, IC:0) restraints are 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]	%
8	24	16	12	0	60	1	5.0
1	15	3	5	0	24	2	10.0
2	3	4	4	0	13	3	15.0
1	2	2	9	0	14	4	20.0
0	2	3	1	0	6	5	25.0
0	3	1	2	0	6	6	30.0
1	1	2	1	0	5	7	35.0
0	1	0	1	0	2	8	40.0
0	1	1	0	0	2	9	45.0
1	0	0	1	0	2	10	50.0
0	0	1	1	0	2	11	55.0
1	0	2	0	0	3	12	60.0
0	0	0	0	0	0	13	65.0
1	1	1	0	0	3	14	70.0
0	1	0	0	0	1	15	75.0
0	1	1	1	0	3	16	80.0
0	0	2	0	0	2	17	85.0
0	0	0	0	0	0	18	90.0
0	2	0	0	0	2	19	95.0
0	1	4	0	0	5	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
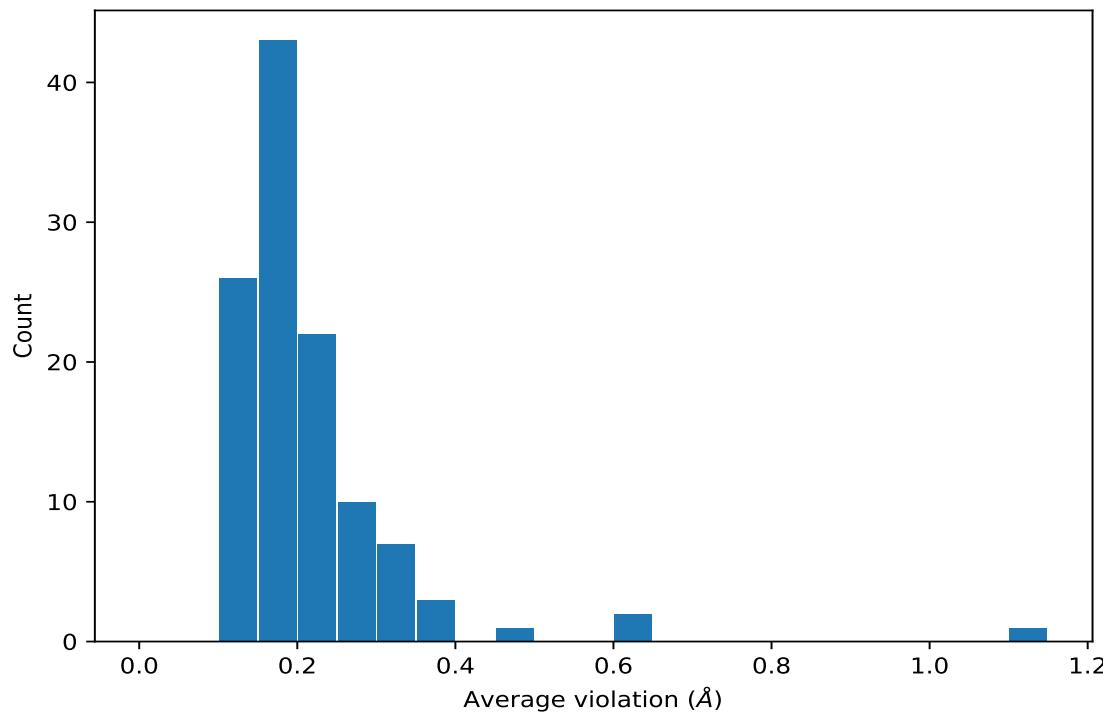
### 9.3.1 Bar graph : Distance violation statistics for the ensemble ⓘ

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)
(1,1225)	1:A:211:LEU:H	1:A:215:LYS:HG2	20	0.63	0.33	0.76
(1,221)	1:A:194:ASP:HA	1:A:196:LEU:HG	20	0.37	0.36	0.26
(1,1180)	1:A:189:LEU:H	1:A:192:ILE:HG13	20	0.32	0.07	0.32
(1,215)	1:A:248:VAL:HA	1:A:249:GLU:HB3	20	0.3	0.04	0.3
(2,109)	1:A:213:TYR:H	1:A:208:ASP:O	20	0.21	0.03	0.2
(2,115)	1:A:154:TRP:H	1:A:64:SER:O	20	0.2	0.03	0.2
(1,2323)	1:A:210:GLU:HB2	1:A:212:LYS:H	20	0.18	0.03	0.19
(1,1668)	1:A:166:SER:HB3	1:A:167:GLN:HB3	19	0.29	0.1	0.31
(1,314)	1:A:193:MET:HG2	1:A:194:ASP:HB3	19	0.24	0.05	0.23
(2,116)	1:A:154:TRP:N	1:A:64:SER:O	18	0.15	0.03	0.15
(1,207)	1:A:159:SER:HA	1:A:161:PHE:H	17	0.21	0.08	0.17
(1,1764)	1:A:187:VAL:HA	1:A:191:MET:HB2	17	0.17	0.03	0.17
(1,1446)	1:A:71:GLY:H	1:A:85:PHE:HZ	16	0.25	0.13	0.19
(1,1665)	1:A:192:ILE:HG12	1:A:195:ARG:H	16	0.14	0.02	0.14
(1,1790)	1:A:226:GLN:HE22	1:A:227:SER:HA	16	0.14	0.06	0.12
(1,1560)	1:A:187:VAL:HA	1:A:188:GLU:HG3	15	0.32	0.08	0.35

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,527)	1:A:237:VAL:H	1:A:238:GLN:HB2	14	0.45	0.16	0.45
(1,484)	1:A:134:LYS:HB3	1:A:134:LYS:HD2	14	0.32	0.02	0.32
(1,1360)	1:A:231:ALA:HA	1:A:235:ARG:H	14	0.26	0.06	0.26
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD13	12	0.28	0.03	0.29
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD11	12	0.28	0.03	0.29
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD12	12	0.28	0.03	0.29
(1,1083)	1:A:159:SER:HB3	1:A:161:PHE:H	12	0.23	0.1	0.22
(1,1983)	1:A:85:PHE:HB2	1:A:88:PHE:HA	12	0.22	0.07	0.2
(1,119)	1:A:78:GLU:HG3	1:A:95:TRP:HZ2	11	0.19	0.06	0.2
(1,1373)	1:A:224:ASN:HD22	1:A:227:SER:H	11	0.17	0.05	0.18
(2,65)	1:A:196:LEU:H	1:A:192:ILE:O	11	0.16	0.03	0.16
(1,1417)	1:A:238:GLN:HB3	1:A:238:GLN:HE22	10	0.16	0.08	0.14
(1,127)	1:A:95:TRP:HZ3	1:A:113:LEU:HA	10	0.16	0.05	0.14
(1,120)	1:A:154:TRP:HH2	1:A:155:ASN:H	9	0.22	0.1	0.2
(1,934)	1:A:168:PRO:HA	1:A:170:ASP:H	9	0.2	0.08	0.19
(1,1533)	1:A:172:ARG:HA	1:A:173:LYS:HE2	8	0.2	0.07	0.2
(1,1705)	1:A:140:SER:HB2	1:A:146:ASP:HA	8	0.15	0.03	0.15
(2,73)	1:A:229:ILE:H	1:A:225:GLN:O	8	0.12	0.02	0.12
(1,511)	1:A:167:GLN:HB2	1:A:167:GLN:HE22	7	0.24	0.14	0.22
(1,1858)	1:A:196:LEU:HD11	1:A:197:TYR:H	7	0.19	0.08	0.16
(1,1858)	1:A:196:LEU:HD12	1:A:197:TYR:H	7	0.19	0.08	0.16
(1,1858)	1:A:196:LEU:HD13	1:A:197:TYR:H	7	0.19	0.08	0.16
(1,382)	1:A:180:VAL:HA	1:A:188:GLU:HG2	7	0.17	0.06	0.15
(1,172)	1:A:74:PRO:HA	1:A:76:ILE:H	7	0.15	0.02	0.16
(1,2246)	1:A:154:TRP:HE1	1:A:158:ASP:H	7	0.13	0.01	0.13
(1,492)	1:A:234:ALA:H	1:A:235:ARG:HB3	6	0.26	0.08	0.24
(1,287)	1:A:137:LEU:HB3	1:A:149:VAL:HB	6	0.22	0.08	0.24
(1,546)	1:A:134:LYS:HG2	1:A:151:ILE:H	6	0.2	0.08	0.16
(1,246)	1:A:184:LEU:HA	1:A:187:VAL:HB	6	0.19	0.05	0.18
(1,1415)	1:A:238:GLN:HE22	1:A:239:LEU:H	6	0.17	0.04	0.15
(1,2093)	1:A:136:TYR:HA	1:A:137:LEU:HB3	6	0.14	0.02	0.14
(1,305)	1:A:63:TYR:HB3	1:A:65:ARG:H	5	1.1	0.51	1.42
(1,2314)	1:A:208:ASP:HB2	1:A:212:LYS:H	5	0.25	0.05	0.27
(1,1551)	1:A:141:SER:H	1:A:144:ILE:HB	5	0.2	0.09	0.17
(1,1652)	1:A:245:ASP:HB2	1:A:246:LYS:HD3	5	0.19	0.03	0.19
(1,2171)	1:A:234:ALA:HA	1:A:235:ARG:HA	5	0.18	0.01	0.18
(1,253)	1:A:91:LEU:HA	1:A:114:LEU:H	5	0.17	0.03	0.17
(2,119)	1:A:159:SER:H	1:A:155:ASN:O	5	0.13	0.02	0.13
(2,61)	1:A:192:ILE:H	1:A:188:GLU:O	5	0.11	0.0	0.11
(1,262)	1:A:63:TYR:HA	1:A:155:ASN:H	4	0.61	0.29	0.56
(1,1062)	1:A:206:ASP:HB2	1:A:217:ALA:H	4	0.27	0.06	0.25
(1,365)	1:A:133:GLY:H	1:A:134:LYS:HE3	4	0.25	0.04	0.26

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Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,2107)	1:A:63:TYR:HA	1:A:155:ASN:HB3	4	0.24	0.11	0.21
(1,1013)	1:A:141:SER:H	1:A:145:LYS:H	4	0.2	0.09	0.18
(1,1521)	1:A:208:ASP:HB2	1:A:212:LYS:HA	4	0.19	0.03	0.2
(1,2136)	1:A:91:LEU:HA	1:A:117:ASP:H	4	0.19	0.05	0.16
(1,407)	1:A:130:GLU:H	1:A:130:GLU:HG3	4	0.18	0.01	0.18
(1,293)	1:A:206:ASP:H	1:A:218:GLY:HA2	4	0.18	0.03	0.17
(1,293)	1:A:206:ASP:H	1:A:218:GLY:HA3	4	0.18	0.03	0.17
(1,1438)	1:A:70:GLY:H	1:A:149:VAL:HA	4	0.17	0.04	0.18
(1,303)	1:A:235:ARG:HD3	1:A:236:PHE:H	4	0.17	0.03	0.18
(1,1086)	1:A:129:ILE:H	1:A:138:CYS:HA	4	0.16	0.05	0.16
(1,1617)	1:A:180:VAL:HB	1:A:188:GLU:HG2	4	0.16	0.04	0.16
(1,156)	1:A:174:THR:HB	1:A:253:TYR:HA	4	0.12	0.01	0.12
(1,2155)	1:A:238:GLN:HA	1:A:239:LEU:HB2	3	0.31	0.17	0.29
(1,1048)	1:A:134:LYS:H	1:A:134:LYS:HE3	3	0.21	0.04	0.22
(1,315)	1:A:184:LEU:HB2	1:A:187:VAL:HB	3	0.2	0.1	0.14
(1,1440)	1:A:70:GLY:H	1:A:85:PHE:HZ	3	0.19	0.03	0.18
(1,1642)	1:A:208:ASP:HB2	1:A:210:GLU:HB3	3	0.16	0.03	0.16
(1,1605)	1:A:131:GLU:HB2	1:A:134:LYS:HG3	3	0.16	0.03	0.17
(1,1655)	1:A:246:LYS:HB3	1:A:246:LYS:HD3	3	0.15	0.04	0.15
(1,1080)	1:A:129:ILE:H	1:A:138:CYS:HB2	3	0.14	0.02	0.13
(1,901)	1:A:237:VAL:HG21	1:A:238:GLN:H	3	0.13	0.01	0.13
(1,901)	1:A:237:VAL:HG22	1:A:238:GLN:H	3	0.13	0.01	0.13
(1,901)	1:A:237:VAL:HG23	1:A:238:GLN:H	3	0.13	0.01	0.13
(1,108)	1:A:235:ARG:HD2	1:A:236:PHE:HZ	3	0.13	0.01	0.13
(1,316)	1:A:63:TYR:HB3	1:A:155:ASN:HA	3	0.13	0.02	0.13
(1,494)	1:A:77:ASP:H	1:A:80:GLU:HB3	3	0.12	0.01	0.12
(1,1591)	1:A:163:MET:HB2	1:A:200:VAL:HB	3	0.12	0.01	0.12
(2,63)	1:A:194:ASP:H	1:A:190:ALA:O	3	0.12	0.01	0.11
(1,1720)	1:A:195:ARG:HA	1:A:196:LEU:HG	2	0.39	0.28	0.39
(1,310)	1:A:235:ARG:H	1:A:235:ARG:HD2	2	0.38	0.02	0.38
(1,1624)	1:A:168:PRO:HB3	1:A:169:LEU:H	2	0.3	0.02	0.3
(1,1583)	1:A:78:GLU:HG3	1:A:79:ASP:HA	2	0.3	0.08	0.3
(1,912)	1:A:65:ARG:H	1:A:114:LEU:HB2	2	0.24	0.1	0.24
(1,1565)	1:A:184:LEU:HB2	1:A:188:GLU:HG3	2	0.22	0.06	0.22
(1,1243)	1:A:226:GLN:HG2	1:A:229:ILE:H	2	0.22	0.02	0.22
(1,2015)	1:A:194:ASP:HA	1:A:198:GLY:H	2	0.22	0.1	0.22
(1,378)	1:A:63:TYR:HA	1:A:155:ASN:HB2	2	0.2	0.04	0.2
(1,444)	1:A:238:GLN:HG3	1:A:239:LEU:H	2	0.19	0.07	0.19
(1,612)	1:A:246:LYS:HG2	1:A:247:ARG:H	2	0.19	0.04	0.19
(1,612)	1:A:246:LYS:HG3	1:A:247:ARG:H	2	0.19	0.04	0.19
(1,409)	1:A:177:VAL:H	1:A:219:ARG:HB2	2	0.18	0.03	0.18
(2,28)	1:A:112:PHE:H	1:A:94:ASP:O	2	0.18	0.07	0.18

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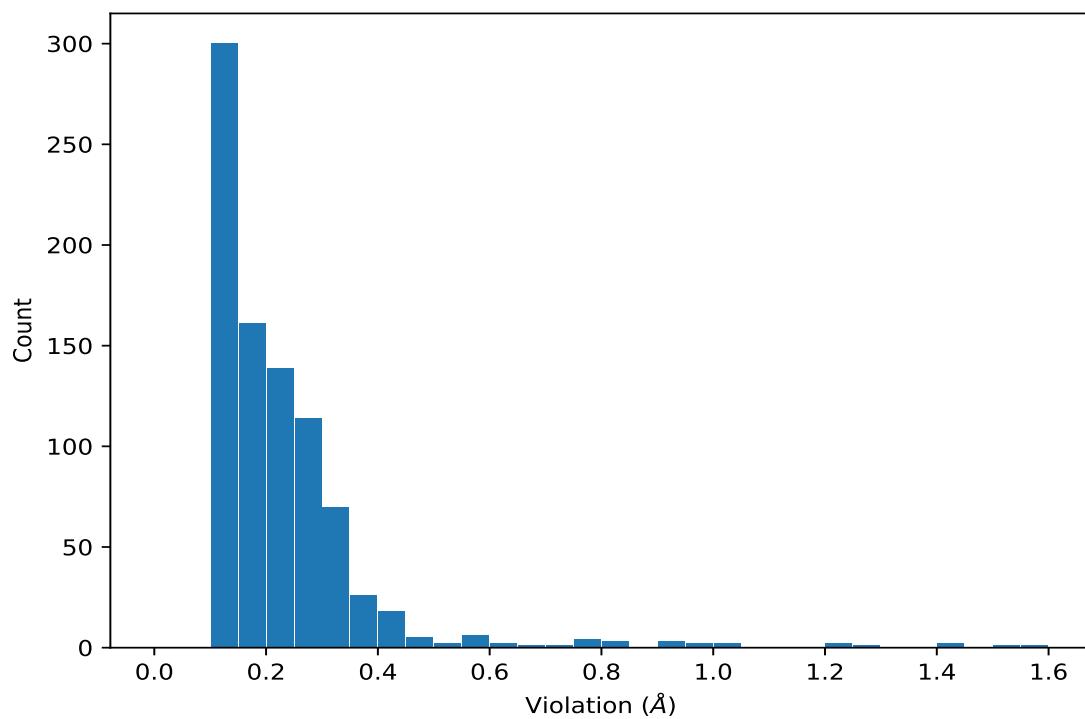
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1441)	1:A:225:GLN:HE22	1:A:226:GLN:H	2	0.18	0.0	0.18
(1,194)	1:A:244:ILE:HA	1:A:245:ASP:HB2	2	0.16	0.04	0.16
(1,312)	1:A:235:ARG:HD2	1:A:236:PHE:H	2	0.16	0.04	0.16
(1,1738)	1:A:223:SER:HB3	1:A:224:ASN:HA	2	0.16	0.05	0.16
(1,1368)	1:A:196:LEU:HG	1:A:197:TYR:H	2	0.15	0.03	0.15
(1,450)	1:A:238:GLN:HG2	1:A:239:LEU:H	2	0.15	0.0	0.15
(2,64)	1:A:195:ARG:H	1:A:191:MET:O	2	0.14	0.01	0.14
(1,443)	1:A:163:MET:HG3	1:A:164:ASP:H	2	0.14	0.01	0.14
(1,950)	1:A:143:THR:H	1:A:144:ILE:H	2	0.14	0.02	0.14
(1,1022)	1:A:208:ASP:H	1:A:215:LYS:HB2	2	0.14	0.01	0.14
(2,9)	1:A:123:ALA:H	1:A:119:SER:O	2	0.12	0.01	0.12
(1,183)	1:A:198:GLY:H	1:A:227:SER:HA	2	0.12	0.01	0.12
(1,1463)	1:A:142:PRO:HB3	1:A:143:THR:H	2	0.12	0.0	0.12
(1,1463)	1:A:142:PRO:HB2	1:A:143:THR:H	2	0.12	0.0	0.12
(1,1465)	1:A:199:GLY:H	1:A:200:VAL:H	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 ⓘ

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)
(1,221)	1:A:194:ASP:HA	1:A:196:LEU:HG	2	1.56
(1,305)	1:A:63:TYR:HB3	1:A:65:ARG:H	13	1.5
(1,305)	1:A:63:TYR:HB3	1:A:65:ARG:H	15	1.42
(1,305)	1:A:63:TYR:HB3	1:A:65:ARG:H	18	1.42
(1,508)	1:A:226:GLN:HG3	1:A:229:ILE:HG12	4	1.25
(1,221)	1:A:194:ASP:HA	1:A:196:LEU:HG	14	1.23
(1,1225)	1:A:211:LEU:H	1:A:215:LYS:HG2	16	1.23
(1,305)	1:A:63:TYR:HB3	1:A:65:ARG:H	14	1.04
(1,262)	1:A:63:TYR:HA	1:A:155:ASN:H	14	1.0
(1,1225)	1:A:211:LEU:H	1:A:215:LYS:HG2	9	0.99
(1,1225)	1:A:211:LEU:H	1:A:215:LYS:HG2	7	0.98
(1,1225)	1:A:211:LEU:H	1:A:215:LYS:HG2	11	0.93
(1,1225)	1:A:211:LEU:H	1:A:215:LYS:HG2	13	0.93
(1,1225)	1:A:211:LEU:H	1:A:215:LYS:HG2	14	0.91
(1,1225)	1:A:211:LEU:H	1:A:215:LYS:HG2	5	0.83
(1,1225)	1:A:211:LEU:H	1:A:215:LYS:HG2	18	0.81

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1225)	1:A:211:LEU:H	1:A:215:LYS:HG2	20	0.8
(1,262)	1:A:63:TYR:HA	1:A:155:ASN:H	18	0.78
(1,527)	1:A:237:VAL:H	1:A:238:GLN:HB2	13	0.77
(1,1225)	1:A:211:LEU:H	1:A:215:LYS:HG2	12	0.77
(1,1225)	1:A:211:LEU:H	1:A:215:LYS:HG2	1	0.76
(1,1494)	1:A:235:ARG:HA	1:A:235:ARG:HD2	20	0.71
(1,1720)	1:A:195:ARG:HA	1:A:196:LEU:HG	18	0.67
(1,527)	1:A:237:VAL:H	1:A:238:GLN:HB2	11	0.64
(1,2160)	1:A:175:ILE:H	1:A:219:ARG:HA	19	0.61
(1,527)	1:A:237:VAL:H	1:A:238:GLN:HB2	12	0.59
(1,527)	1:A:237:VAL:H	1:A:238:GLN:HB2	6	0.58
(1,1446)	1:A:71:GLY:H	1:A:85:PHE:HZ	16	0.58
(1,221)	1:A:194:ASP:HA	1:A:196:LEU:HG	18	0.57
(1,527)	1:A:237:VAL:H	1:A:238:GLN:HB2	8	0.55
(1,511)	1:A:167:GLN:HB2	1:A:167:GLN:HE22	17	0.55
(1,2155)	1:A:238:GLN:HA	1:A:239:LEU:HB2	12	0.52
(1,527)	1:A:237:VAL:H	1:A:238:GLN:HB2	9	0.51
(1,1225)	1:A:211:LEU:H	1:A:215:LYS:HG2	17	0.48
(1,1668)	1:A:166:SER:HB3	1:A:167:GLN:HB3	8	0.47
(1,1446)	1:A:71:GLY:H	1:A:85:PHE:HZ	19	0.47
(2,27)	1:A:94:ASP:H	1:A:112:PHE:O	20	0.46
(1,527)	1:A:237:VAL:H	1:A:238:GLN:HB2	10	0.46
(1,527)	1:A:237:VAL:H	1:A:238:GLN:HB2	18	0.44
(1,1560)	1:A:187:VAL:HA	1:A:188:GLU:HG3	2	0.44
(1,120)	1:A:154:TRP:HH2	1:A:155:ASN:H	19	0.44
(1,1668)	1:A:166:SER:HB3	1:A:167:GLN:HB3	20	0.43
(1,1668)	1:A:166:SER:HB3	1:A:167:GLN:HB3	5	0.42
(1,1560)	1:A:187:VAL:HA	1:A:188:GLU:HG3	6	0.42
(1,527)	1:A:237:VAL:H	1:A:238:GLN:HB2	15	0.41
(1,310)	1:A:235:ARG:H	1:A:235:ARG:HD2	19	0.41
(1,2107)	1:A:63:TYR:HA	1:A:155:ASN:HB3	15	0.41
(1,1180)	1:A:189:LEU:H	1:A:192:ILE:HG13	8	0.41
(1,1180)	1:A:189:LEU:H	1:A:192:ILE:HG13	12	0.41
(1,1083)	1:A:159:SER:HB3	1:A:161:PHE:H	18	0.41
(1,1668)	1:A:166:SER:HB3	1:A:167:GLN:HB3	14	0.4
(1,1417)	1:A:238:GLN:HB3	1:A:238:GLN:HE22	3	0.4
(1,1225)	1:A:211:LEU:H	1:A:215:LYS:HG2	8	0.4
(1,1180)	1:A:189:LEU:H	1:A:192:ILE:HG13	7	0.4
(1,1180)	1:A:189:LEU:H	1:A:192:ILE:HG13	13	0.4
(1,1180)	1:A:189:LEU:H	1:A:192:ILE:HG13	14	0.4
(1,492)	1:A:234:ALA:H	1:A:235:ARG:HB3	17	0.39
(1,1668)	1:A:166:SER:HB3	1:A:167:GLN:HB3	6	0.39

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1560)	1:A:187:VAL:HA	1:A:188:GLU:HG3	17	0.39
(1,1359)	1:A:235:ARG:H	1:A:235:ARG:HD3	6	0.39
(1,1180)	1:A:189:LEU:H	1:A:192:ILE:HG13	2	0.39
(1,1180)	1:A:189:LEU:H	1:A:192:ILE:HG13	6	0.39
(1,527)	1:A:237:VAL:H	1:A:238:GLN:HB2	3	0.38
(1,221)	1:A:194:ASP:HA	1:A:196:LEU:HG	8	0.38
(1,215)	1:A:248:VAL:HA	1:A:249:GLU:HB3	3	0.38
(1,207)	1:A:159:SER:HA	1:A:161:PHE:H	20	0.38
(1,1560)	1:A:187:VAL:HA	1:A:188:GLU:HG3	4	0.38
(1,1560)	1:A:187:VAL:HA	1:A:188:GLU:HG3	13	0.38
(1,1083)	1:A:159:SER:HB3	1:A:161:PHE:H	16	0.38
(1,934)	1:A:168:PRO:HA	1:A:170:ASP:H	4	0.37
(1,546)	1:A:134:LYS:HG2	1:A:151:ILE:H	20	0.37
(1,1668)	1:A:166:SER:HB3	1:A:167:GLN:HB3	19	0.37
(1,1583)	1:A:78:GLU:HG3	1:A:79:ASP:HA	18	0.37
(1,1560)	1:A:187:VAL:HA	1:A:188:GLU:HG3	10	0.37
(1,1446)	1:A:71:GLY:H	1:A:85:PHE:HZ	2	0.37
(1,1180)	1:A:189:LEU:H	1:A:192:ILE:HG13	15	0.37
(1,1078)	1:A:113:LEU:H	1:A:114:LEU:HB3	20	0.37
(1,484)	1:A:134:LYS:HB3	1:A:134:LYS:HD2	2	0.36
(1,310)	1:A:235:ARG:H	1:A:235:ARG:HD2	6	0.36
(1,1560)	1:A:187:VAL:HA	1:A:188:GLU:HG3	3	0.36
(1,1551)	1:A:141:SER:H	1:A:144:ILE:HB	13	0.36
(1,1062)	1:A:206:ASP:HB2	1:A:217:ALA:H	10	0.36
(1,215)	1:A:248:VAL:HA	1:A:249:GLU:HB3	19	0.35
(1,1560)	1:A:187:VAL:HA	1:A:188:GLU:HG3	12	0.35
(1,1360)	1:A:231:ALA:HA	1:A:235:ARG:H	14	0.35
(1,1225)	1:A:211:LEU:H	1:A:215:LYS:HG2	4	0.35
(1,912)	1:A:65:ARG:H	1:A:114:LEU:HB2	20	0.34
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD13	4	0.34
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD11	4	0.34
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD12	4	0.34
(1,484)	1:A:134:LYS:HB3	1:A:134:LYS:HD2	7	0.34
(1,315)	1:A:184:LEU:HB2	1:A:187:VAL:HB	1	0.34
(1,287)	1:A:137:LEU:HB3	1:A:149:VAL:HB	12	0.34
(1,262)	1:A:63:TYR:HA	1:A:155:ASN:H	15	0.34
(1,215)	1:A:248:VAL:HA	1:A:249:GLU:HB3	13	0.34
(1,215)	1:A:248:VAL:HA	1:A:249:GLU:HB3	20	0.34
(1,1668)	1:A:166:SER:HB3	1:A:167:GLN:HB3	15	0.34
(1,1668)	1:A:166:SER:HB3	1:A:167:GLN:HB3	18	0.34
(1,1560)	1:A:187:VAL:HA	1:A:188:GLU:HG3	15	0.34
(1,1360)	1:A:231:ALA:HA	1:A:235:ARG:H	11	0.34

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1225)	1:A:211:LEU:H	1:A:215:LYS:HG2	19	0.34
(1,1018)	1:A:140:SER:HA	1:A:146:ASP:H	17	0.34
(1,484)	1:A:134:LYS:HB3	1:A:134:LYS:HD2	15	0.33
(1,484)	1:A:134:LYS:HB3	1:A:134:LYS:HD2	18	0.33
(1,484)	1:A:134:LYS:HB3	1:A:134:LYS:HD2	19	0.33
(1,262)	1:A:63:TYR:HA	1:A:155:ASN:H	13	0.33
(1,215)	1:A:248:VAL:HA	1:A:249:GLU:HB3	4	0.33
(1,215)	1:A:248:VAL:HA	1:A:249:GLU:HB3	5	0.33
(1,215)	1:A:248:VAL:HA	1:A:249:GLU:HB3	6	0.33
(1,215)	1:A:248:VAL:HA	1:A:249:GLU:HB3	16	0.33
(1,207)	1:A:159:SER:HA	1:A:161:PHE:H	2	0.33
(1,1983)	1:A:85:PHE:HB2	1:A:88:PHE:HA	6	0.33
(1,1858)	1:A:196:LEU:HD11	1:A:197:TYR:H	11	0.33
(1,1858)	1:A:196:LEU:HD12	1:A:197:TYR:H	11	0.33
(1,1858)	1:A:196:LEU:HD13	1:A:197:TYR:H	11	0.33
(1,1668)	1:A:166:SER:HB3	1:A:167:GLN:HB3	10	0.33
(1,1360)	1:A:231:ALA:HA	1:A:235:ARG:H	1	0.33
(1,1180)	1:A:189:LEU:H	1:A:192:ILE:HG13	10	0.33
(1,1180)	1:A:189:LEU:H	1:A:192:ILE:HG13	11	0.33
(1,1013)	1:A:141:SER:H	1:A:145:LYS:H	3	0.33
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD13	8	0.32
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD11	8	0.32
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD12	8	0.32
(1,492)	1:A:234:ALA:H	1:A:235:ARG:HB3	7	0.32
(1,484)	1:A:134:LYS:HB3	1:A:134:LYS:HD2	1	0.32
(1,484)	1:A:134:LYS:HB3	1:A:134:LYS:HD2	4	0.32
(1,484)	1:A:134:LYS:HB3	1:A:134:LYS:HD2	8	0.32
(1,484)	1:A:134:LYS:HB3	1:A:134:LYS:HD2	10	0.32
(1,484)	1:A:134:LYS:HB3	1:A:134:LYS:HD2	12	0.32
(1,484)	1:A:134:LYS:HB3	1:A:134:LYS:HD2	17	0.32
(1,314)	1:A:193:MET:HG2	1:A:194:ASP:HB3	15	0.32
(1,207)	1:A:159:SER:HA	1:A:161:PHE:H	16	0.32
(1,2015)	1:A:194:ASP:HA	1:A:198:GLY:H	12	0.32
(1,1983)	1:A:85:PHE:HB2	1:A:88:PHE:HA	13	0.32
(1,1624)	1:A:168:PRO:HB3	1:A:169:LEU:H	15	0.32
(1,1533)	1:A:172:ARG:HA	1:A:173:LYS:HE2	14	0.32
(1,120)	1:A:154:TRP:HH2	1:A:155:ASN:H	14	0.32
(1,1180)	1:A:189:LEU:H	1:A:192:ILE:HG13	1	0.32
(1,1083)	1:A:159:SER:HB3	1:A:161:PHE:H	12	0.32
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD13	10	0.31
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD11	10	0.31
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD12	10	0.31

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,382)	1:A:180:VAL:HA	1:A:188:GLU:HG2	3	0.31
(1,314)	1:A:193:MET:HG2	1:A:194:ASP:HB3	18	0.31
(1,221)	1:A:194:ASP:HA	1:A:196:LEU:HG	1	0.31
(1,215)	1:A:248:VAL:HA	1:A:249:GLU:HB3	12	0.31
(1,215)	1:A:248:VAL:HA	1:A:249:GLU:HB3	18	0.31
(1,1668)	1:A:166:SER:HB3	1:A:167:GLN:HB3	13	0.31
(1,1636)	1:A:246:LYS:HG2	1:A:247:ARG:HB3	7	0.31
(1,1636)	1:A:246:LYS:HG3	1:A:247:ARG:HB3	7	0.31
(1,1225)	1:A:211:LEU:H	1:A:215:LYS:HG2	2	0.31
(1,1083)	1:A:159:SER:HB3	1:A:161:PHE:H	13	0.31
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD13	18	0.3
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD11	18	0.3
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD12	18	0.3
(1,527)	1:A:237:VAL:H	1:A:238:GLN:HB2	19	0.3
(1,484)	1:A:134:LYS:HB3	1:A:134:LYS:HD2	6	0.3
(1,484)	1:A:134:LYS:HB3	1:A:134:LYS:HD2	13	0.3
(1,365)	1:A:133:GLY:H	1:A:134:LYS:HE3	20	0.3
(1,221)	1:A:194:ASP:HA	1:A:196:LEU:HG	3	0.3
(1,215)	1:A:248:VAL:HA	1:A:249:GLU:HB3	8	0.3
(1,207)	1:A:159:SER:HA	1:A:161:PHE:H	4	0.3
(1,1858)	1:A:196:LEU:HD11	1:A:197:TYR:H	13	0.3
(1,1858)	1:A:196:LEU:HD12	1:A:197:TYR:H	13	0.3
(1,1858)	1:A:196:LEU:HD13	1:A:197:TYR:H	13	0.3
(1,1790)	1:A:226:GLN:HE22	1:A:227:SER:HA	12	0.3
(1,1560)	1:A:187:VAL:HA	1:A:188:GLU:HG3	18	0.3
(1,1360)	1:A:231:ALA:HA	1:A:235:ARG:H	15	0.3
(2,109)	1:A:213:TYR:H	1:A:208:ASP:O	18	0.29
(1,963)	1:A:234:ALA:H	1:A:236:PHE:H	18	0.29
(1,934)	1:A:168:PRO:HA	1:A:170:ASP:H	16	0.29
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD13	11	0.29
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD11	11	0.29
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD12	11	0.29
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD13	14	0.29
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD11	14	0.29
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD12	14	0.29
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD13	19	0.29
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD11	19	0.29
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD12	19	0.29
(1,484)	1:A:134:LYS:HB3	1:A:134:LYS:HD2	14	0.29
(1,314)	1:A:193:MET:HG2	1:A:194:ASP:HB3	7	0.29
(1,314)	1:A:193:MET:HG2	1:A:194:ASP:HB3	14	0.29
(1,2314)	1:A:208:ASP:HB2	1:A:212:LYS:H	6	0.29

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,221)	1:A:194:ASP:HA	1:A:196:LEU:HG	5	0.29
(1,221)	1:A:194:ASP:HA	1:A:196:LEU:HG	7	0.29
(1,2155)	1:A:238:GLN:HA	1:A:239:LEU:HB2	20	0.29
(1,1983)	1:A:85:PHE:HB2	1:A:88:PHE:HA	18	0.29
(1,1790)	1:A:226:GLN:HE22	1:A:227:SER:HA	4	0.29
(1,1464)	1:A:199:GLY:H	1:A:200:VAL:HB	12	0.29
(1,1360)	1:A:231:ALA:HA	1:A:235:ARG:H	12	0.29
(1,1180)	1:A:189:LEU:H	1:A:192:ILE:HG13	3	0.29
(1,1180)	1:A:189:LEU:H	1:A:192:ILE:HG13	20	0.29
(1,287)	1:A:137:LEU:HB3	1:A:149:VAL:HB	4	0.28
(1,2314)	1:A:208:ASP:HB2	1:A:212:LYS:H	3	0.28
(1,215)	1:A:248:VAL:HA	1:A:249:GLU:HB3	1	0.28
(1,215)	1:A:248:VAL:HA	1:A:249:GLU:HB3	9	0.28
(1,215)	1:A:248:VAL:HA	1:A:249:GLU:HB3	17	0.28
(1,1668)	1:A:166:SER:HB3	1:A:167:GLN:HB3	17	0.28
(1,1624)	1:A:168:PRO:HB3	1:A:169:LEU:H	18	0.28
(1,1565)	1:A:184:LEU:HB2	1:A:188:GLU:HG3	8	0.28
(1,1560)	1:A:187:VAL:HA	1:A:188:GLU:HG3	1	0.28
(1,1462)	1:A:141:SER:H	1:A:143:THR:H	7	0.28
(1,1446)	1:A:71:GLY:H	1:A:85:PHE:HZ	9	0.28
(1,1446)	1:A:71:GLY:H	1:A:85:PHE:HZ	17	0.28
(1,1360)	1:A:231:ALA:HA	1:A:235:ARG:H	2	0.28
(1,1143)	1:A:227:SER:H	1:A:229:ILE:HG12	4	0.28
(2,115)	1:A:154:TRP:H	1:A:64:SER:O	8	0.27
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD13	17	0.27
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD11	17	0.27
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD12	17	0.27
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD13	20	0.27
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD11	20	0.27
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD12	20	0.27
(1,527)	1:A:237:VAL:H	1:A:238:GLN:HB2	2	0.27
(1,511)	1:A:167:GLN:HB2	1:A:167:GLN:HE22	6	0.27
(1,365)	1:A:133:GLY:H	1:A:134:LYS:HE3	11	0.27
(1,314)	1:A:193:MET:HG2	1:A:194:ASP:HB3	17	0.27
(1,2314)	1:A:208:ASP:HB2	1:A:212:LYS:H	10	0.27
(1,215)	1:A:248:VAL:HA	1:A:249:GLU:HB3	10	0.27
(1,2136)	1:A:91:LEU:HA	1:A:117:ASP:H	17	0.27
(1,1983)	1:A:85:PHE:HB2	1:A:88:PHE:HA	10	0.27
(1,1560)	1:A:187:VAL:HA	1:A:188:GLU:HG3	14	0.27
(1,1373)	1:A:224:ASN:HD22	1:A:227:SER:H	12	0.27
(1,1360)	1:A:231:ALA:HA	1:A:235:ARG:H	3	0.27
(1,127)	1:A:95:TRP:HZ3	1:A:113:LEU:HA	11	0.27

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,119)	1:A:78:GLU:HG3	1:A:95:TRP:HZ2	16	0.27
(1,1180)	1:A:189:LEU:H	1:A:192:ILE:HG13	17	0.27
(1,1180)	1:A:189:LEU:H	1:A:192:ILE:HG13	19	0.27
(2,115)	1:A:154:TRP:H	1:A:64:SER:O	16	0.26
(2,109)	1:A:213:TYR:H	1:A:208:ASP:O	3	0.26
(1,511)	1:A:167:GLN:HB2	1:A:167:GLN:HE22	16	0.26
(1,492)	1:A:234:ALA:H	1:A:235:ARG:HB3	6	0.26
(1,444)	1:A:238:GLN:HG3	1:A:239:LEU:H	13	0.26
(1,314)	1:A:193:MET:HG2	1:A:194:ASP:HB3	4	0.26
(1,314)	1:A:193:MET:HG2	1:A:194:ASP:HB3	6	0.26
(1,314)	1:A:193:MET:HG2	1:A:194:ASP:HB3	19	0.26
(1,287)	1:A:137:LEU:HB3	1:A:149:VAL:HB	14	0.26
(1,246)	1:A:184:LEU:HA	1:A:187:VAL:HB	3	0.26
(1,221)	1:A:194:ASP:HA	1:A:196:LEU:HG	12	0.26
(1,221)	1:A:194:ASP:HA	1:A:196:LEU:HG	16	0.26
(1,2107)	1:A:63:TYR:HA	1:A:155:ASN:HB3	14	0.26
(1,1983)	1:A:85:PHE:HB2	1:A:88:PHE:HA	12	0.26
(1,1668)	1:A:166:SER:HB3	1:A:167:GLN:HB3	7	0.26
(1,1662)	1:A:251:LYS:HA	1:A:251:LYS:HD2	14	0.26
(1,1227)	1:A:219:ARG:HB3	1:A:220:VAL:H	19	0.26
(1,1225)	1:A:211:LEU:H	1:A:215:LYS:HG2	10	0.26
(1,119)	1:A:78:GLU:HG3	1:A:95:TRP:HZ2	15	0.26
(1,1180)	1:A:189:LEU:H	1:A:192:ILE:HG13	9	0.26
(1,1062)	1:A:206:ASP:HB2	1:A:217:ALA:H	6	0.26
(2,28)	1:A:112:PHE:H	1:A:94:ASP:O	20	0.25
(1,378)	1:A:63:TYR:HA	1:A:155:ASN:HB2	19	0.25
(1,2314)	1:A:208:ASP:HB2	1:A:212:LYS:H	15	0.25
(1,221)	1:A:194:ASP:HA	1:A:196:LEU:HG	15	0.25
(1,215)	1:A:248:VAL:HA	1:A:249:GLU:HB3	11	0.25
(1,215)	1:A:248:VAL:HA	1:A:249:GLU:HB3	15	0.25
(1,207)	1:A:159:SER:HA	1:A:161:PHE:H	6	0.25
(1,1668)	1:A:166:SER:HB3	1:A:167:GLN:HB3	4	0.25
(1,1533)	1:A:172:ARG:HA	1:A:173:LYS:HE2	19	0.25
(1,1446)	1:A:71:GLY:H	1:A:85:PHE:HZ	13	0.25
(1,1415)	1:A:238:GLN:HE22	1:A:239:LEU:H	17	0.25
(1,1360)	1:A:231:ALA:HA	1:A:235:ARG:H	4	0.25
(1,120)	1:A:154:TRP:HH2	1:A:155:ASN:H	10	0.25
(1,1180)	1:A:189:LEU:H	1:A:192:ILE:HG13	4	0.25
(1,1083)	1:A:159:SER:HB3	1:A:161:PHE:H	6	0.25
(1,1048)	1:A:134:LYS:H	1:A:134:LYS:HE3	16	0.25
(2,84)	1:A:220:VAL:H	1:A:175:ILE:O	19	0.24
(2,109)	1:A:213:TYR:H	1:A:208:ASP:O	4	0.24

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,934)	1:A:168:PRO:HA	1:A:170:ASP:H	6	0.24
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD13	2	0.24
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD11	2	0.24
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD12	2	0.24
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD13	13	0.24
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD11	13	0.24
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD12	13	0.24
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD13	15	0.24
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD11	15	0.24
(1,621)	1:A:156:LEU:H	1:A:156:LEU:HD12	15	0.24
(1,546)	1:A:134:LYS:HG2	1:A:151:ILE:H	7	0.24
(1,527)	1:A:237:VAL:H	1:A:238:GLN:HB2	16	0.24
(1,365)	1:A:133:GLY:H	1:A:134:LYS:HE3	3	0.24
(1,314)	1:A:193:MET:HG2	1:A:194:ASP:HB3	2	0.24
(1,246)	1:A:184:LEU:HA	1:A:187:VAL:HB	9	0.24
(1,2323)	1:A:210:GLU:HB2	1:A:212:LYS:H	11	0.24
(1,221)	1:A:194:ASP:HA	1:A:196:LEU:HG	6	0.24
(1,215)	1:A:248:VAL:HA	1:A:249:GLU:HB3	2	0.24
(1,215)	1:A:248:VAL:HA	1:A:249:GLU:HB3	7	0.24
(1,1560)	1:A:187:VAL:HA	1:A:188:GLU:HG3	19	0.24
(1,1446)	1:A:71:GLY:H	1:A:85:PHE:HZ	15	0.24
(1,1243)	1:A:226:GLN:HG2	1:A:229:ILE:H	12	0.24
(1,119)	1:A:78:GLU:HG3	1:A:95:TRP:HZ2	20	0.24
(1,1062)	1:A:206:ASP:HB2	1:A:217:ALA:H	18	0.24
(1,1013)	1:A:141:SER:H	1:A:145:LYS:H	4	0.24
(2,65)	1:A:196:LEU:H	1:A:192:ILE:O	18	0.23
(2,115)	1:A:154:TRP:H	1:A:64:SER:O	17	0.23
(1,612)	1:A:246:LYS:HG2	1:A:247:ARG:H	7	0.23
(1,612)	1:A:246:LYS:HG3	1:A:247:ARG:H	7	0.23
(1,314)	1:A:193:MET:HG2	1:A:194:ASP:HB3	1	0.23
(1,314)	1:A:193:MET:HG2	1:A:194:ASP:HB3	16	0.23
(1,314)	1:A:193:MET:HG2	1:A:194:ASP:HB3	20	0.23
(1,215)	1:A:248:VAL:HA	1:A:249:GLU:HB3	14	0.23
(1,207)	1:A:159:SER:HA	1:A:161:PHE:H	14	0.23
(1,1764)	1:A:187:VAL:HA	1:A:191:MET:HB2	4	0.23
(1,1652)	1:A:245:ASP:HB2	1:A:246:LYS:HD3	1	0.23
(1,1617)	1:A:180:VAL:HB	1:A:188:GLU:HG2	5	0.23
(1,1533)	1:A:172:ARG:HA	1:A:173:LYS:HE2	13	0.23
(1,1521)	1:A:208:ASP:HB2	1:A:212:LYS:HA	8	0.23
(1,1510)	1:A:246:LYS:H	1:A:246:LYS:HE3	11	0.23
(1,1510)	1:A:246:LYS:H	1:A:246:LYS:HE2	11	0.23
(1,1440)	1:A:70:GLY:H	1:A:85:PHE:HZ	16	0.23

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1438)	1:A:70:GLY:H	1:A:149:VAL:HA	10	0.23
(1,1373)	1:A:224:ASN:HD22	1:A:227:SER:H	15	0.23
(1,1360)	1:A:231:ALA:HA	1:A:235:ARG:H	5	0.23
(1,1180)	1:A:189:LEU:H	1:A:192:ILE:HG13	5	0.23
(1,1180)	1:A:189:LEU:H	1:A:192:ILE:HG13	16	0.23
(1,1180)	1:A:189:LEU:H	1:A:192:ILE:HG13	18	0.23
(1,1083)	1:A:159:SER:HB3	1:A:161:PHE:H	2	0.23
(2,116)	1:A:154:TRP:N	1:A:64:SER:O	8	0.22
(2,115)	1:A:154:TRP:H	1:A:64:SER:O	9	0.22
(2,109)	1:A:213:TYR:H	1:A:208:ASP:O	8	0.22
(2,109)	1:A:213:TYR:H	1:A:208:ASP:O	15	0.22
(2,109)	1:A:213:TYR:H	1:A:208:ASP:O	20	0.22
(1,511)	1:A:167:GLN:HB2	1:A:167:GLN:HE22	5	0.22
(1,492)	1:A:234:ALA:H	1:A:235:ARG:HB3	9	0.22
(1,314)	1:A:193:MET:HG2	1:A:194:ASP:HB3	10	0.22
(1,293)	1:A:206:ASP:H	1:A:218:GLY:HA2	20	0.22
(1,293)	1:A:206:ASP:H	1:A:218:GLY:HA3	20	0.22
(1,2323)	1:A:210:GLU:HB2	1:A:212:LYS:H	12	0.22
(1,2323)	1:A:210:GLU:HB2	1:A:212:LYS:H	13	0.22
(1,221)	1:A:194:ASP:HA	1:A:196:LEU:HG	19	0.22
(1,1764)	1:A:187:VAL:HA	1:A:191:MET:HB2	16	0.22
(1,1668)	1:A:166:SER:HB3	1:A:167:GLN:HB3	16	0.22
(1,1652)	1:A:245:ASP:HB2	1:A:246:LYS:HD3	16	0.22
(1,1583)	1:A:78:GLU:HG3	1:A:79:ASP:HA	17	0.22
(1,1551)	1:A:141:SER:H	1:A:144:ILE:HB	12	0.22
(1,1225)	1:A:211:LEU:H	1:A:215:LYS:HG2	15	0.22
(1,120)	1:A:154:TRP:HH2	1:A:155:ASN:H	15	0.22
(1,119)	1:A:78:GLU:HG3	1:A:95:TRP:HZ2	3	0.22
(1,1086)	1:A:129:ILE:H	1:A:138:CYS:HA	20	0.22
(1,1048)	1:A:134:LYS:H	1:A:134:LYS:HE3	11	0.22
(2,42)	1:A:112:PHE:N	1:A:94:ASP:O	20	0.21
(2,115)	1:A:154:TRP:H	1:A:64:SER:O	2	0.21
(2,115)	1:A:154:TRP:H	1:A:64:SER:O	11	0.21
(2,109)	1:A:213:TYR:H	1:A:208:ASP:O	5	0.21
(2,109)	1:A:213:TYR:H	1:A:208:ASP:O	6	0.21
(2,109)	1:A:213:TYR:H	1:A:208:ASP:O	10	0.21
(2,109)	1:A:213:TYR:H	1:A:208:ASP:O	14	0.21
(1,409)	1:A:177:VAL:H	1:A:219:ARG:HB2	8	0.21
(1,382)	1:A:180:VAL:HA	1:A:188:GLU:HG2	6	0.21
(1,314)	1:A:193:MET:HG2	1:A:194:ASP:HB3	3	0.21
(1,287)	1:A:137:LEU:HB3	1:A:149:VAL:HB	18	0.21
(1,253)	1:A:91:LEU:HA	1:A:114:LEU:H	4	0.21

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2323)	1:A:210:GLU:HB2	1:A:212:LYS:H	4	0.21
(1,2323)	1:A:210:GLU:HB2	1:A:212:LYS:H	17	0.21
(1,221)	1:A:194:ASP:HA	1:A:196:LEU:HG	13	0.21
(1,2186)	1:A:113:LEU:HA	1:A:114:LEU:HB3	20	0.21
(1,1983)	1:A:85:PHE:HB2	1:A:88:PHE:HA	1	0.21
(1,194)	1:A:244:ILE:HA	1:A:245:ASP:HB2	13	0.21
(1,1764)	1:A:187:VAL:HA	1:A:191:MET:HB2	6	0.21
(1,1764)	1:A:187:VAL:HA	1:A:191:MET:HB2	7	0.21
(1,1521)	1:A:208:ASP:HB2	1:A:212:LYS:HA	19	0.21
(1,1360)	1:A:231:ALA:HA	1:A:235:ARG:H	13	0.21
(1,1360)	1:A:231:ALA:HA	1:A:235:ARG:H	18	0.21
(1,127)	1:A:95:TRP:HZ3	1:A:113:LEU:HA	19	0.21
(1,119)	1:A:78:GLU:HG3	1:A:95:TRP:HZ2	1	0.21
(1,1062)	1:A:206:ASP:HB2	1:A:217:ALA:H	7	0.21
(2,115)	1:A:154:TRP:H	1:A:64:SER:O	3	0.2
(2,115)	1:A:154:TRP:H	1:A:64:SER:O	6	0.2
(2,115)	1:A:154:TRP:H	1:A:64:SER:O	10	0.2
(2,115)	1:A:154:TRP:H	1:A:64:SER:O	19	0.2
(2,109)	1:A:213:TYR:H	1:A:208:ASP:O	1	0.2
(2,109)	1:A:213:TYR:H	1:A:208:ASP:O	2	0.2
(2,109)	1:A:213:TYR:H	1:A:208:ASP:O	11	0.2
(2,109)	1:A:213:TYR:H	1:A:208:ASP:O	13	0.2
(2,109)	1:A:213:TYR:H	1:A:208:ASP:O	17	0.2
(2,109)	1:A:213:TYR:H	1:A:208:ASP:O	19	0.2
(1,934)	1:A:168:PRO:HA	1:A:170:ASP:H	2	0.2
(1,495)	1:A:79:ASP:HB3	1:A:80:GLU:HB3	16	0.2
(1,492)	1:A:234:ALA:H	1:A:235:ARG:HB3	10	0.2
(1,407)	1:A:130:GLU:H	1:A:130:GLU:HG3	20	0.2
(1,314)	1:A:193:MET:HG2	1:A:194:ASP:HB3	9	0.2
(1,314)	1:A:193:MET:HG2	1:A:194:ASP:HB3	13	0.2
(1,312)	1:A:235:ARG:HD2	1:A:236:PHE:H	20	0.2
(1,303)	1:A:235:ARG:HD3	1:A:236:PHE:H	9	0.2
(1,303)	1:A:235:ARG:HD3	1:A:236:PHE:H	17	0.2
(1,2323)	1:A:210:GLU:HB2	1:A:212:LYS:H	7	0.2
(1,2323)	1:A:210:GLU:HB2	1:A:212:LYS:H	14	0.2
(1,221)	1:A:194:ASP:HA	1:A:196:LEU:HG	4	0.2
(1,2171)	1:A:234:ALA:HA	1:A:235:ARG:HA	17	0.2
(1,1983)	1:A:85:PHE:HB2	1:A:88:PHE:HA	11	0.2
(1,1764)	1:A:187:VAL:HA	1:A:191:MET:HB2	14	0.2
(1,1738)	1:A:223:SER:HB3	1:A:224:ASN:HA	14	0.2
(1,1705)	1:A:140:SER:HB2	1:A:146:ASP:HA	2	0.2
(1,1705)	1:A:140:SER:HB2	1:A:146:ASP:HA	20	0.2

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1655)	1:A:246:LYS:HB3	1:A:246:LYS:HD3	7	0.2
(1,1642)	1:A:208:ASP:HB2	1:A:210:GLU:HB3	4	0.2
(1,1533)	1:A:172:ARG:HA	1:A:173:LYS:HE2	17	0.2
(1,1415)	1:A:238:GLN:HE22	1:A:239:LEU:H	5	0.2
(1,1360)	1:A:231:ALA:HA	1:A:235:ARG:H	9	0.2
(1,1360)	1:A:231:ALA:HA	1:A:235:ARG:H	20	0.2
(1,1243)	1:A:226:GLN:HG2	1:A:229:ILE:H	4	0.2
(1,120)	1:A:154:TRP:HH2	1:A:155:ASN:H	8	0.2
(1,119)	1:A:78:GLU:HG3	1:A:95:TRP:HZ2	5	0.2
(1,1086)	1:A:129:ILE:H	1:A:138:CYS:HA	18	0.2
(1,1083)	1:A:159:SER:HB3	1:A:161:PHE:H	1	0.2
(2,115)	1:A:154:TRP:H	1:A:64:SER:O	4	0.19
(2,115)	1:A:154:TRP:H	1:A:64:SER:O	5	0.19
(2,115)	1:A:154:TRP:H	1:A:64:SER:O	7	0.19
(2,115)	1:A:154:TRP:H	1:A:64:SER:O	12	0.19
(2,115)	1:A:154:TRP:H	1:A:64:SER:O	13	0.19
(2,109)	1:A:213:TYR:H	1:A:208:ASP:O	16	0.19
(1,934)	1:A:168:PRO:HA	1:A:170:ASP:H	14	0.19
(1,527)	1:A:237:VAL:H	1:A:238:GLN:HB2	5	0.19
(1,407)	1:A:130:GLU:H	1:A:130:GLU:HG3	8	0.19
(1,365)	1:A:133:GLY:H	1:A:134:LYS:HE3	16	0.19
(1,253)	1:A:91:LEU:HA	1:A:114:LEU:H	10	0.19
(1,246)	1:A:184:LEU:HA	1:A:187:VAL:HB	17	0.19
(1,2323)	1:A:210:GLU:HB2	1:A:212:LYS:H	1	0.19
(1,2323)	1:A:210:GLU:HB2	1:A:212:LYS:H	5	0.19
(1,2323)	1:A:210:GLU:HB2	1:A:212:LYS:H	9	0.19
(1,2323)	1:A:210:GLU:HB2	1:A:212:LYS:H	20	0.19
(1,221)	1:A:194:ASP:HA	1:A:196:LEU:HG	17	0.19
(1,207)	1:A:159:SER:HA	1:A:161:PHE:H	18	0.19
(1,1764)	1:A:187:VAL:HA	1:A:191:MET:HB2	13	0.19
(1,1741)	1:A:156:LEU:H	1:A:156:LEU:HD21	16	0.19
(1,1741)	1:A:156:LEU:H	1:A:156:LEU:HD22	16	0.19
(1,1741)	1:A:156:LEU:H	1:A:156:LEU:HD23	16	0.19
(1,1668)	1:A:166:SER:HB3	1:A:167:GLN:HB3	3	0.19
(1,1652)	1:A:245:ASP:HB2	1:A:246:LYS:HD3	7	0.19
(1,1533)	1:A:172:ARG:HA	1:A:173:LYS:HE2	12	0.19
(1,1521)	1:A:208:ASP:HB2	1:A:212:LYS:HA	2	0.19
(1,1446)	1:A:71:GLY:H	1:A:85:PHE:HZ	1	0.19
(1,1446)	1:A:71:GLY:H	1:A:85:PHE:HZ	5	0.19
(1,1446)	1:A:71:GLY:H	1:A:85:PHE:HZ	6	0.19
(1,1446)	1:A:71:GLY:H	1:A:85:PHE:HZ	8	0.19
(1,1446)	1:A:71:GLY:H	1:A:85:PHE:HZ	11	0.19

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1438)	1:A:70:GLY:H	1:A:149:VAL:HA	13	0.19
(1,120)	1:A:154:TRP:HH2	1:A:155:ASN:H	7	0.19
(2,65)	1:A:196:LEU:H	1:A:192:ILE:O	4	0.18
(2,65)	1:A:196:LEU:H	1:A:192:ILE:O	10	0.18
(2,116)	1:A:154:TRP:N	1:A:64:SER:O	3	0.18
(2,116)	1:A:154:TRP:N	1:A:64:SER:O	4	0.18
(2,115)	1:A:154:TRP:H	1:A:64:SER:O	1	0.18
(2,109)	1:A:213:TYR:H	1:A:208:ASP:O	9	0.18
(1,546)	1:A:134:LYS:HG2	1:A:151:ILE:H	1	0.18
(1,493)	1:A:167:GLN:HB3	1:A:201:CYS:HB3	2	0.18
(1,382)	1:A:180:VAL:HA	1:A:188:GLU:HG2	12	0.18
(1,342)	1:A:208:ASP:HB3	1:A:215:LYS:HG2	19	0.18
(1,314)	1:A:193:MET:HG2	1:A:194:ASP:HB3	12	0.18
(1,2323)	1:A:210:GLU:HB2	1:A:212:LYS:H	16	0.18
(1,221)	1:A:194:ASP:HA	1:A:196:LEU:HG	11	0.18
(1,2171)	1:A:234:ALA:HA	1:A:235:ARG:HA	6	0.18
(1,2171)	1:A:234:ALA:HA	1:A:235:ARG:HA	16	0.18
(1,207)	1:A:159:SER:HA	1:A:161:PHE:H	17	0.18
(1,2028)	1:A:189:LEU:HA	1:A:193:MET:HG3	8	0.18
(1,1983)	1:A:85:PHE:HB2	1:A:88:PHE:HA	8	0.18
(1,1983)	1:A:85:PHE:HB2	1:A:88:PHE:HA	14	0.18
(1,1858)	1:A:196:LEU:HD11	1:A:197:TYR:H	20	0.18
(1,1858)	1:A:196:LEU:HD12	1:A:197:TYR:H	20	0.18
(1,1858)	1:A:196:LEU:HD13	1:A:197:TYR:H	20	0.18
(1,1764)	1:A:187:VAL:HA	1:A:191:MET:HB2	5	0.18
(1,1652)	1:A:245:ASP:HB2	1:A:246:LYS:HD3	15	0.18
(1,1605)	1:A:131:GLU:HB2	1:A:134:LYS:HG3	9	0.18
(1,1570)	1:A:245:ASP:HA	1:A:246:LYS:HB3	15	0.18
(1,1441)	1:A:225:GLN:HE22	1:A:226:GLN:H	3	0.18
(1,1440)	1:A:70:GLY:H	1:A:85:PHE:HZ	20	0.18
(1,1417)	1:A:238:GLN:HB3	1:A:238:GLN:HE22	17	0.18
(1,1373)	1:A:224:ASN:HD22	1:A:227:SER:H	1	0.18
(1,1373)	1:A:224:ASN:HD22	1:A:227:SER:H	2	0.18
(1,1373)	1:A:224:ASN:HD22	1:A:227:SER:H	4	0.18
(1,1373)	1:A:224:ASN:HD22	1:A:227:SER:H	20	0.18
(1,1368)	1:A:196:LEU:HG	1:A:197:TYR:H	2	0.18
(1,127)	1:A:95:TRP:HZ3	1:A:113:LEU:HA	8	0.18
(1,1268)	1:A:234:ALA:HA	1:A:236:PHE:H	18	0.18
(1,1083)	1:A:159:SER:HB3	1:A:161:PHE:H	20	0.18
(2,65)	1:A:196:LEU:H	1:A:192:ILE:O	20	0.17
(2,116)	1:A:154:TRP:N	1:A:64:SER:O	6	0.17
(2,116)	1:A:154:TRP:N	1:A:64:SER:O	9	0.17

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(2,116)	1:A:154:TRP:N	1:A:64:SER:O	11	0.17
(2,115)	1:A:154:TRP:H	1:A:64:SER:O	15	0.17
(2,115)	1:A:154:TRP:H	1:A:64:SER:O	18	0.17
(2,109)	1:A:213:TYR:H	1:A:208:ASP:O	12	0.17
(1,511)	1:A:167:GLN:HB2	1:A:167:GLN:HE22	1	0.17
(1,407)	1:A:130:GLU:H	1:A:130:GLU:HG3	14	0.17
(1,407)	1:A:130:GLU:H	1:A:130:GLU:HG3	19	0.17
(1,293)	1:A:206:ASP:H	1:A:218:GLY:HA2	8	0.17
(1,293)	1:A:206:ASP:H	1:A:218:GLY:HA3	8	0.17
(1,293)	1:A:206:ASP:H	1:A:218:GLY:HA2	14	0.17
(1,293)	1:A:206:ASP:H	1:A:218:GLY:HA3	14	0.17
(1,253)	1:A:91:LEU:HA	1:A:114:LEU:H	16	0.17
(1,253)	1:A:91:LEU:HA	1:A:114:LEU:H	19	0.17
(1,246)	1:A:184:LEU:HA	1:A:187:VAL:HB	13	0.17
(1,2323)	1:A:210:GLU:HB2	1:A:212:LYS:H	2	0.17
(1,221)	1:A:194:ASP:HA	1:A:196:LEU:HG	10	0.17
(1,2171)	1:A:234:ALA:HA	1:A:235:ARG:HA	19	0.17
(1,2136)	1:A:91:LEU:HA	1:A:117:ASP:H	1	0.17
(1,207)	1:A:159:SER:HA	1:A:161:PHE:H	10	0.17
(1,207)	1:A:159:SER:HA	1:A:161:PHE:H	11	0.17
(1,1764)	1:A:187:VAL:HA	1:A:191:MET:HB2	2	0.17
(1,1764)	1:A:187:VAL:HA	1:A:191:MET:HB2	12	0.17
(1,1764)	1:A:187:VAL:HA	1:A:191:MET:HB2	19	0.17
(1,172)	1:A:74:PRO:HA	1:A:76:ILE:H	10	0.17
(1,1665)	1:A:192:ILE:HG12	1:A:195:ARG:H	7	0.17
(1,1665)	1:A:192:ILE:HG12	1:A:195:ARG:H	9	0.17
(1,1665)	1:A:192:ILE:HG12	1:A:195:ARG:H	14	0.17
(1,1665)	1:A:192:ILE:HG12	1:A:195:ARG:H	17	0.17
(1,1617)	1:A:180:VAL:HB	1:A:188:GLU:HG2	7	0.17
(1,1605)	1:A:131:GLU:HB2	1:A:134:LYS:HG3	5	0.17
(1,1560)	1:A:187:VAL:HA	1:A:188:GLU:HG3	9	0.17
(1,1551)	1:A:141:SER:H	1:A:144:ILE:HB	14	0.17
(1,1441)	1:A:225:GLN:HE22	1:A:226:GLN:H	18	0.17
(1,1256)	1:A:117:ASP:H	1:A:120:SER:HB3	3	0.17
(2,73)	1:A:229:ILE:H	1:A:225:GLN:O	12	0.16
(2,65)	1:A:196:LEU:H	1:A:192:ILE:O	1	0.16
(2,65)	1:A:196:LEU:H	1:A:192:ILE:O	3	0.16
(2,65)	1:A:196:LEU:H	1:A:192:ILE:O	15	0.16
(2,116)	1:A:154:TRP:N	1:A:64:SER:O	12	0.16
(2,116)	1:A:154:TRP:N	1:A:64:SER:O	17	0.16
(2,109)	1:A:213:TYR:H	1:A:208:ASP:O	7	0.16
(1,378)	1:A:63:TYR:HA	1:A:155:ASN:HB2	12	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,350)	1:A:249:GLU:H	1:A:249:GLU:HG3	12	0.16
(1,303)	1:A:235:ARG:HD3	1:A:236:PHE:H	10	0.16
(1,2323)	1:A:210:GLU:HB2	1:A:212:LYS:H	3	0.16
(1,2323)	1:A:210:GLU:HB2	1:A:212:LYS:H	18	0.16
(1,2323)	1:A:210:GLU:HB2	1:A:212:LYS:H	19	0.16
(1,221)	1:A:194:ASP:HA	1:A:196:LEU:HG	20	0.16
(1,2171)	1:A:234:ALA:HA	1:A:235:ARG:HA	7	0.16
(1,2136)	1:A:91:LEU:HA	1:A:117:ASP:H	16	0.16
(1,2107)	1:A:63:TYR:HA	1:A:155:ASN:HB3	2	0.16
(1,2093)	1:A:136:TYR:HA	1:A:137:LEU:HB3	12	0.16
(1,207)	1:A:159:SER:HA	1:A:161:PHE:H	7	0.16
(1,207)	1:A:159:SER:HA	1:A:161:PHE:H	19	0.16
(1,1858)	1:A:196:LEU:HD11	1:A:197:TYR:H	17	0.16
(1,1858)	1:A:196:LEU:HD12	1:A:197:TYR:H	17	0.16
(1,1858)	1:A:196:LEU:HD13	1:A:197:TYR:H	17	0.16
(1,1824)	1:A:239:LEU:HD11	1:A:240:GLN:H	7	0.16
(1,1824)	1:A:239:LEU:HD12	1:A:240:GLN:H	7	0.16
(1,1824)	1:A:239:LEU:HD13	1:A:240:GLN:H	7	0.16
(1,1764)	1:A:187:VAL:HA	1:A:191:MET:HB2	10	0.16
(1,1764)	1:A:187:VAL:HA	1:A:191:MET:HB2	18	0.16
(1,172)	1:A:74:PRO:HA	1:A:76:ILE:H	8	0.16
(1,172)	1:A:74:PRO:HA	1:A:76:ILE:H	11	0.16
(1,172)	1:A:74:PRO:HA	1:A:76:ILE:H	13	0.16
(1,1705)	1:A:140:SER:HB2	1:A:146:ASP:HA	9	0.16
(1,1665)	1:A:192:ILE:HG12	1:A:195:ARG:H	10	0.16
(1,1665)	1:A:192:ILE:HG12	1:A:195:ARG:H	12	0.16
(1,1642)	1:A:208:ASP:HB2	1:A:210:GLU:HB3	2	0.16
(1,1588)	1:A:78:GLU:HG2	1:A:80:GLU:H	17	0.16
(1,1565)	1:A:184:LEU:HB2	1:A:188:GLU:HG3	11	0.16
(1,1557)	1:A:80:GLU:HG3	1:A:81:ILE:HB	16	0.16
(1,1527)	1:A:240:GLN:HG3	1:A:245:ASP:HB3	5	0.16
(1,1438)	1:A:70:GLY:H	1:A:149:VAL:HA	18	0.16
(1,1417)	1:A:238:GLN:HB3	1:A:238:GLN:HE22	9	0.16
(1,1415)	1:A:238:GLN:HE22	1:A:239:LEU:H	1	0.16
(1,1356)	1:A:232:ILE:HA	1:A:235:ARG:H	13	0.16
(1,127)	1:A:95:TRP:HZ3	1:A:113:LEU:HA	14	0.16
(1,1183)	1:A:207:THR:HB	1:A:215:LYS:H	15	0.16
(1,1080)	1:A:129:ILE:H	1:A:138:CYS:HB2	8	0.16
(1,1048)	1:A:134:LYS:H	1:A:134:LYS:HE3	3	0.16
(1,1014)	1:A:141:SER:H	1:A:145:LYS:HA	17	0.16
(1,1011)	1:A:239:LEU:HD11	1:A:240:GLN:H	7	0.16
(1,1011)	1:A:239:LEU:HD12	1:A:240:GLN:H	7	0.16

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1011)	1:A:239:LEU:HD13	1:A:240:GLN:H	7	0.16
(1,1011)	1:A:239:LEU:HD21	1:A:240:GLN:H	7	0.16
(1,1011)	1:A:239:LEU:HD22	1:A:240:GLN:H	7	0.16
(1,1011)	1:A:239:LEU:HD23	1:A:240:GLN:H	7	0.16
(2,96)	1:A:220:VAL:N	1:A:175:ILE:O	19	0.15
(2,73)	1:A:229:ILE:H	1:A:225:GLN:O	4	0.15
(2,65)	1:A:196:LEU:H	1:A:192:ILE:O	9	0.15
(2,64)	1:A:195:ARG:H	1:A:191:MET:O	5	0.15
(2,119)	1:A:159:SER:H	1:A:155:ASN:O	16	0.15
(2,119)	1:A:159:SER:H	1:A:155:ASN:O	18	0.15
(2,116)	1:A:154:TRP:N	1:A:64:SER:O	1	0.15
(2,116)	1:A:154:TRP:N	1:A:64:SER:O	2	0.15
(2,116)	1:A:154:TRP:N	1:A:64:SER:O	10	0.15
(2,116)	1:A:154:TRP:N	1:A:64:SER:O	18	0.15
(2,115)	1:A:154:TRP:H	1:A:64:SER:O	20	0.15
(1,950)	1:A:143:THR:H	1:A:144:ILE:H	9	0.15
(1,912)	1:A:65:ARG:H	1:A:114:LEU:HB2	9	0.15
(1,901)	1:A:237:VAL:HG21	1:A:238:GLN:H	5	0.15
(1,901)	1:A:237:VAL:HG22	1:A:238:GLN:H	5	0.15
(1,901)	1:A:237:VAL:HG23	1:A:238:GLN:H	5	0.15
(1,612)	1:A:246:LYS:HG2	1:A:247:ARG:H	15	0.15
(1,612)	1:A:246:LYS:HG3	1:A:247:ARG:H	15	0.15
(1,546)	1:A:134:LYS:HG2	1:A:151:ILE:H	4	0.15
(1,450)	1:A:238:GLN:HG2	1:A:239:LEU:H	3	0.15
(1,409)	1:A:177:VAL:H	1:A:219:ARG:HB2	20	0.15
(1,382)	1:A:180:VAL:HA	1:A:188:GLU:HG2	2	0.15
(1,367)	1:A:128:CYS:HA	1:A:129:ILE:HB	18	0.15
(1,316)	1:A:63:TYR:HB3	1:A:155:ASN:HA	17	0.15
(1,314)	1:A:193:MET:HG2	1:A:194:ASP:HB3	5	0.15
(1,314)	1:A:193:MET:HG2	1:A:194:ASP:HB3	11	0.15
(1,293)	1:A:206:ASP:H	1:A:218:GLY:HA2	13	0.15
(1,293)	1:A:206:ASP:H	1:A:218:GLY:HA3	13	0.15
(1,246)	1:A:184:LEU:HA	1:A:187:VAL:HB	11	0.15
(1,2323)	1:A:210:GLU:HB2	1:A:212:LYS:H	6	0.15
(1,2323)	1:A:210:GLU:HB2	1:A:212:LYS:H	8	0.15
(1,2323)	1:A:210:GLU:HB2	1:A:212:LYS:H	10	0.15
(1,2246)	1:A:154:TRP:HE1	1:A:158:ASP:H	17	0.15
(1,221)	1:A:194:ASP:HA	1:A:196:LEU:HG	9	0.15
(1,2202)	1:A:144:ILE:HD11	1:A:145:LYS:H	10	0.15
(1,2202)	1:A:144:ILE:HD12	1:A:145:LYS:H	10	0.15
(1,2202)	1:A:144:ILE:HD13	1:A:145:LYS:H	10	0.15
(1,2093)	1:A:136:TYR:HA	1:A:137:LEU:HB3	18	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2093)	1:A:136:TYR:HA	1:A:137:LEU:HB3	19	0.15
(1,207)	1:A:159:SER:HA	1:A:161:PHE:H	8	0.15
(1,1764)	1:A:187:VAL:HA	1:A:191:MET:HB2	9	0.15
(1,1764)	1:A:187:VAL:HA	1:A:191:MET:HB2	11	0.15
(1,1764)	1:A:187:VAL:HA	1:A:191:MET:HB2	15	0.15
(1,1749)	1:A:184:LEU:HD22	1:A:188:GLU:H	7	0.15
(1,1749)	1:A:184:LEU:HD23	1:A:188:GLU:H	7	0.15
(1,1749)	1:A:184:LEU:HD21	1:A:188:GLU:H	7	0.15
(1,1705)	1:A:140:SER:HB2	1:A:146:ASP:HA	11	0.15
(1,1705)	1:A:140:SER:HB2	1:A:146:ASP:HA	12	0.15
(1,1668)	1:A:166:SER:HB3	1:A:167:GLN:HB3	2	0.15
(1,1655)	1:A:246:LYS:HB3	1:A:246:LYS:HD3	15	0.15
(1,1652)	1:A:245:ASP:HB2	1:A:246:LYS:HD3	10	0.15
(1,1651)	1:A:167:GLN:HB3	1:A:201:CYS:HB2	16	0.15
(1,1533)	1:A:172:ARG:HA	1:A:173:LYS:HE2	20	0.15
(1,1521)	1:A:208:ASP:HB2	1:A:212:LYS:HA	4	0.15
(1,1446)	1:A:71:GLY:H	1:A:85:PHE:HZ	10	0.15
(1,1440)	1:A:70:GLY:H	1:A:85:PHE:HZ	4	0.15
(1,127)	1:A:95:TRP:HZ3	1:A:113:LEU:HA	5	0.15
(1,1225)	1:A:211:LEU:H	1:A:215:LYS:HG2	3	0.15
(1,119)	1:A:78:GLU:HG3	1:A:95:TRP:HZ2	6	0.15
(1,1049)	1:A:131:GLU:HB2	1:A:134:LYS:H	20	0.15
(2,63)	1:A:194:ASP:H	1:A:190:ALA:O	13	0.14
(2,116)	1:A:154:TRP:N	1:A:64:SER:O	13	0.14
(2,116)	1:A:154:TRP:N	1:A:64:SER:O	16	0.14
(2,115)	1:A:154:TRP:H	1:A:64:SER:O	14	0.14
(1,934)	1:A:168:PRO:HA	1:A:170:ASP:H	7	0.14
(1,934)	1:A:168:PRO:HA	1:A:170:ASP:H	17	0.14
(1,552)	1:A:134:LYS:HG2	1:A:136:TYR:HB2	12	0.14
(1,546)	1:A:134:LYS:HG2	1:A:151:ILE:H	6	0.14
(1,494)	1:A:77:ASP:H	1:A:80:GLU:HB3	16	0.14
(1,492)	1:A:234:ALA:H	1:A:235:ARG:HB3	18	0.14
(1,450)	1:A:238:GLN:HG2	1:A:239:LEU:H	12	0.14
(1,443)	1:A:163:MET:HG3	1:A:164:ASP:H	14	0.14
(1,315)	1:A:184:LEU:HB2	1:A:187:VAL:HB	15	0.14
(1,2323)	1:A:210:GLU:HB2	1:A:212:LYS:H	15	0.14
(1,2314)	1:A:208:ASP:HB2	1:A:212:LYS:H	16	0.14
(1,2246)	1:A:154:TRP:HE1	1:A:158:ASP:H	15	0.14
(1,2136)	1:A:91:LEU:HA	1:A:117:ASP:H	12	0.14
(1,207)	1:A:159:SER:HA	1:A:161:PHE:H	13	0.14
(1,1983)	1:A:85:PHE:HB2	1:A:88:PHE:HA	17	0.14
(1,1858)	1:A:196:LEU:HD11	1:A:197:TYR:H	3	0.14

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1858)	1:A:196:LEU:HD12	1:A:197:TYR:H	3	0.14
(1,1858)	1:A:196:LEU:HD13	1:A:197:TYR:H	3	0.14
(1,1764)	1:A:187:VAL:HA	1:A:191:MET:HB2	8	0.14
(1,172)	1:A:74:PRO:HA	1:A:76:ILE:H	4	0.14
(1,1718)	1:A:195:ARG:H	1:A:196:LEU:HG	2	0.14
(1,1668)	1:A:166:SER:HB3	1:A:167:GLN:HB3	1	0.14
(1,1668)	1:A:166:SER:HB3	1:A:167:GLN:HB3	11	0.14
(1,1668)	1:A:166:SER:HB3	1:A:167:GLN:HB3	12	0.14
(1,1665)	1:A:192:ILE:HG12	1:A:195:ARG:H	1	0.14
(1,1665)	1:A:192:ILE:HG12	1:A:195:ARG:H	13	0.14
(1,1665)	1:A:192:ILE:HG12	1:A:195:ARG:H	20	0.14
(1,1617)	1:A:180:VAL:HB	1:A:188:GLU:HG2	18	0.14
(1,1560)	1:A:187:VAL:HA	1:A:188:GLU:HG3	16	0.14
(1,156)	1:A:174:THR:HB	1:A:253:TYR:HA	14	0.14
(1,1417)	1:A:238:GLN:HB3	1:A:238:GLN:HE22	5	0.14
(1,1417)	1:A:238:GLN:HB3	1:A:238:GLN:HE22	13	0.14
(1,1373)	1:A:224:ASN:HD22	1:A:227:SER:H	9	0.14
(1,1360)	1:A:231:ALA:HA	1:A:235:ARG:H	10	0.14
(1,1225)	1:A:211:LEU:H	1:A:215:LYS:HG2	6	0.14
(1,120)	1:A:154:TRP:HH2	1:A:155:ASN:H	12	0.14
(1,119)	1:A:78:GLU:HG3	1:A:95:TRP:HZ2	19	0.14
(1,1083)	1:A:159:SER:HB3	1:A:161:PHE:H	8	0.14
(1,1083)	1:A:159:SER:HB3	1:A:161:PHE:H	9	0.14
(1,108)	1:A:235:ARG:HD2	1:A:236:PHE:HZ	1	0.14
(1,1022)	1:A:208:ASP:H	1:A:215:LYS:HB2	3	0.14
(2,9)	1:A:123:ALA:H	1:A:119:SER:O	7	0.13
(2,73)	1:A:229:ILE:H	1:A:225:GLN:O	15	0.13
(2,65)	1:A:196:LEU:H	1:A:192:ILE:O	17	0.13
(2,64)	1:A:195:ARG:H	1:A:191:MET:O	12	0.13
(2,56)	1:A:203:ALA:H	1:A:161:PHE:O	15	0.13
(2,48)	1:A:129:ILE:H	1:A:136:TYR:O	13	0.13
(2,119)	1:A:159:SER:H	1:A:155:ASN:O	20	0.13
(2,116)	1:A:154:TRP:N	1:A:64:SER:O	5	0.13
(2,116)	1:A:154:TRP:N	1:A:64:SER:O	15	0.13
(1,934)	1:A:168:PRO:HA	1:A:170:ASP:H	3	0.13
(1,934)	1:A:168:PRO:HA	1:A:170:ASP:H	19	0.13
(1,901)	1:A:237:VAL:HG21	1:A:238:GLN:H	9	0.13
(1,901)	1:A:237:VAL:HG22	1:A:238:GLN:H	9	0.13
(1,901)	1:A:237:VAL:HG23	1:A:238:GLN:H	9	0.13
(1,695)	1:A:237:VAL:HG11	1:A:238:GLN:H	7	0.13
(1,695)	1:A:237:VAL:HG12	1:A:238:GLN:H	7	0.13
(1,695)	1:A:237:VAL:HG13	1:A:238:GLN:H	7	0.13

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,611)	1:A:81:ILE:HG12	1:A:82:THR:HA	14	0.13
(1,546)	1:A:134:LYS:HG2	1:A:151:ILE:H	14	0.13
(1,511)	1:A:167:GLN:HB2	1:A:167:GLN:HE22	9	0.13
(1,443)	1:A:163:MET:HG3	1:A:164:ASP:H	8	0.13
(1,382)	1:A:180:VAL:HA	1:A:188:GLU:HG2	10	0.13
(1,316)	1:A:63:TYR:HB3	1:A:155:ASN:HA	12	0.13
(1,305)	1:A:63:TYR:HB3	1:A:65:ARG:H	6	0.13
(1,2246)	1:A:154:TRP:HE1	1:A:158:ASP:H	6	0.13
(1,2246)	1:A:154:TRP:HE1	1:A:158:ASP:H	11	0.13
(1,2093)	1:A:136:TYR:HA	1:A:137:LEU:HB3	4	0.13
(1,207)	1:A:159:SER:HA	1:A:161:PHE:H	12	0.13
(1,1983)	1:A:85:PHE:HB2	1:A:88:PHE:HA	7	0.13
(1,1858)	1:A:196:LEU:HD11	1:A:197:TYR:H	9	0.13
(1,1858)	1:A:196:LEU:HD12	1:A:197:TYR:H	9	0.13
(1,1858)	1:A:196:LEU:HD13	1:A:197:TYR:H	9	0.13
(1,183)	1:A:198:GLY:H	1:A:227:SER:HA	4	0.13
(1,1790)	1:A:226:GLN:HE22	1:A:227:SER:HA	17	0.13
(1,1765)	1:A:187:VAL:HA	1:A:188:GLU:HG2	16	0.13
(1,172)	1:A:74:PRO:HA	1:A:76:ILE:H	12	0.13
(1,1705)	1:A:140:SER:HB2	1:A:146:ASP:HA	14	0.13
(1,1665)	1:A:192:ILE:HG12	1:A:195:ARG:H	4	0.13
(1,1665)	1:A:192:ILE:HG12	1:A:195:ARG:H	5	0.13
(1,1591)	1:A:163:MET:HB2	1:A:200:VAL:HB	3	0.13
(1,156)	1:A:174:THR:HB	1:A:253:TYR:HA	8	0.13
(1,1446)	1:A:71:GLY:H	1:A:85:PHE:HZ	7	0.13
(1,1417)	1:A:238:GLN:HB3	1:A:238:GLN:HE22	2	0.13
(1,1417)	1:A:238:GLN:HB3	1:A:238:GLN:HE22	6	0.13
(1,1417)	1:A:238:GLN:HB3	1:A:238:GLN:HE22	7	0.13
(1,1417)	1:A:238:GLN:HB3	1:A:238:GLN:HE22	16	0.13
(1,1415)	1:A:238:GLN:HE22	1:A:239:LEU:H	8	0.13
(1,1415)	1:A:238:GLN:HE22	1:A:239:LEU:H	11	0.13
(1,1415)	1:A:238:GLN:HE22	1:A:239:LEU:H	12	0.13
(1,1373)	1:A:224:ASN:HD22	1:A:227:SER:H	7	0.13
(1,127)	1:A:95:TRP:HZ3	1:A:113:LEU:HA	1	0.13
(1,127)	1:A:95:TRP:HZ3	1:A:113:LEU:HA	7	0.13
(1,119)	1:A:78:GLU:HG3	1:A:95:TRP:HZ2	2	0.13
(1,1080)	1:A:129:ILE:H	1:A:138:CYS:HB2	11	0.13
(1,108)	1:A:235:ARG:HD2	1:A:236:PHE:HZ	8	0.13
(1,1022)	1:A:208:ASP:H	1:A:215:LYS:HB2	17	0.13
(2,9)	1:A:123:ALA:H	1:A:119:SER:O	1	0.12
(2,73)	1:A:229:ILE:H	1:A:225:GLN:O	1	0.12
(2,65)	1:A:196:LEU:H	1:A:192:ILE:O	19	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,950)	1:A:143:THR:H	1:A:144:ILE:H	4	0.12
(1,901)	1:A:237:VAL:HG21	1:A:238:GLN:H	1	0.12
(1,901)	1:A:237:VAL:HG22	1:A:238:GLN:H	1	0.12
(1,901)	1:A:237:VAL:HG23	1:A:238:GLN:H	1	0.12
(1,494)	1:A:77:ASP:H	1:A:80:GLU:HB3	17	0.12
(1,444)	1:A:238:GLN:HG3	1:A:239:LEU:H	8	0.12
(1,406)	1:A:131:GLU:HG3	1:A:134:LYS:HE3	8	0.12
(1,382)	1:A:180:VAL:HA	1:A:188:GLU:HG2	4	0.12
(1,315)	1:A:184:LEU:HB2	1:A:187:VAL:HB	7	0.12
(1,312)	1:A:235:ARG:HD2	1:A:236:PHE:H	12	0.12
(1,303)	1:A:235:ARG:HD3	1:A:236:PHE:H	6	0.12
(1,287)	1:A:137:LEU:HB3	1:A:149:VAL:HB	7	0.12
(1,253)	1:A:91:LEU:HA	1:A:114:LEU:H	15	0.12
(1,246)	1:A:184:LEU:HA	1:A:187:VAL:HB	12	0.12
(1,2246)	1:A:154:TRP:HE1	1:A:158:ASP:H	8	0.12
(1,2107)	1:A:63:TYR:HA	1:A:155:ASN:HB3	8	0.12
(1,207)	1:A:159:SER:HA	1:A:161:PHE:H	3	0.12
(1,207)	1:A:159:SER:HA	1:A:161:PHE:H	9	0.12
(1,2015)	1:A:194:ASP:HA	1:A:198:GLY:H	11	0.12
(1,1983)	1:A:85:PHE:HB2	1:A:88:PHE:HA	3	0.12
(1,194)	1:A:244:ILE:HA	1:A:245:ASP:HB2	7	0.12
(1,1858)	1:A:196:LEU:HD11	1:A:197:TYR:H	7	0.12
(1,1858)	1:A:196:LEU:HD12	1:A:197:TYR:H	7	0.12
(1,1858)	1:A:196:LEU:HD13	1:A:197:TYR:H	7	0.12
(1,1790)	1:A:226:GLN:HE22	1:A:227:SER:HA	1	0.12
(1,1790)	1:A:226:GLN:HE22	1:A:227:SER:HA	2	0.12
(1,1790)	1:A:226:GLN:HE22	1:A:227:SER:HA	5	0.12
(1,1790)	1:A:226:GLN:HE22	1:A:227:SER:HA	10	0.12
(1,1790)	1:A:226:GLN:HE22	1:A:227:SER:HA	15	0.12
(1,1790)	1:A:226:GLN:HE22	1:A:227:SER:HA	16	0.12
(1,1705)	1:A:140:SER:HB2	1:A:146:ASP:HA	19	0.12
(1,1691)	1:A:247:ARG:HG2	1:A:248:VAL:H	16	0.12
(1,1665)	1:A:192:ILE:HG12	1:A:195:ARG:H	11	0.12
(1,1665)	1:A:192:ILE:HG12	1:A:195:ARG:H	15	0.12
(1,1665)	1:A:192:ILE:HG12	1:A:195:ARG:H	19	0.12
(1,1642)	1:A:208:ASP:HB2	1:A:210:GLU:HB3	8	0.12
(1,1617)	1:A:180:VAL:HB	1:A:188:GLU:HG2	13	0.12
(1,1605)	1:A:131:GLU:HB2	1:A:134:LYS:HG3	20	0.12
(1,1591)	1:A:163:MET:HB2	1:A:200:VAL:HB	6	0.12
(1,1586)	1:A:78:GLU:HG3	1:A:80:GLU:H	4	0.12
(1,1554)	1:A:85:PHE:HA	1:A:88:PHE:HB2	5	0.12
(1,1551)	1:A:141:SER:H	1:A:144:ILE:HB	5	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,1533)	1:A:172:ARG:HA	1:A:173:LYS:HE2	7	0.12
(1,1465)	1:A:199:GLY:H	1:A:200:VAL:H	17	0.12
(1,1463)	1:A:142:PRO:HB3	1:A:143:THR:H	5	0.12
(1,1463)	1:A:142:PRO:HB2	1:A:143:THR:H	5	0.12
(1,1446)	1:A:71:GLY:H	1:A:85:PHE:HZ	12	0.12
(1,1425)	1:A:88:PHE:HD1	1:A:89:GLY:H	13	0.12
(1,1425)	1:A:88:PHE:HD2	1:A:89:GLY:H	13	0.12
(1,1375)	1:A:224:ASN:HA	1:A:224:ASN:HD22	7	0.12
(1,1373)	1:A:224:ASN:HD22	1:A:227:SER:H	3	0.12
(1,1373)	1:A:224:ASN:HD22	1:A:227:SER:H	16	0.12
(1,1368)	1:A:196:LEU:HG	1:A:197:TYR:H	14	0.12
(1,1316)	1:A:163:MET:H	1:A:164:ASP:H	10	0.12
(1,1278)	1:A:122:GLN:HE22	1:A:123:ALA:HA	5	0.12
(1,1112)	1:A:134:LYS:HD3	1:A:135:LEU:H	5	0.12
(1,1086)	1:A:129:ILE:H	1:A:138:CYS:HA	5	0.12
(1,1086)	1:A:129:ILE:H	1:A:138:CYS:HA	9	0.12
(1,1083)	1:A:159:SER:HB3	1:A:161:PHE:H	3	0.12
(1,1080)	1:A:129:ILE:H	1:A:138:CYS:HB2	12	0.12
(1,108)	1:A:235:ARG:HD2	1:A:236:PHE:HZ	2	0.12
(1,1013)	1:A:141:SER:H	1:A:145:LYS:H	10	0.12
(1,1012)	1:A:141:SER:H	1:A:146:ASP:H	17	0.12
(2,73)	1:A:229:ILE:H	1:A:225:GLN:O	3	0.11
(2,73)	1:A:229:ILE:H	1:A:225:GLN:O	7	0.11
(2,73)	1:A:229:ILE:H	1:A:225:GLN:O	8	0.11
(2,73)	1:A:229:ILE:H	1:A:225:GLN:O	17	0.11
(2,65)	1:A:196:LEU:H	1:A:192:ILE:O	6	0.11
(2,63)	1:A:194:ASP:H	1:A:190:ALA:O	11	0.11
(2,63)	1:A:194:ASP:H	1:A:190:ALA:O	18	0.11
(2,61)	1:A:192:ILE:H	1:A:188:GLU:O	9	0.11
(2,61)	1:A:192:ILE:H	1:A:188:GLU:O	10	0.11
(2,61)	1:A:192:ILE:H	1:A:188:GLU:O	14	0.11
(2,61)	1:A:192:ILE:H	1:A:188:GLU:O	17	0.11
(2,61)	1:A:192:ILE:H	1:A:188:GLU:O	19	0.11
(2,28)	1:A:112:PHE:H	1:A:94:ASP:O	4	0.11
(2,22)	1:A:152:ARG:H	1:A:68:PHE:O	17	0.11
(2,119)	1:A:159:SER:H	1:A:155:ASN:O	4	0.11
(2,119)	1:A:159:SER:H	1:A:155:ASN:O	13	0.11
(2,116)	1:A:154:TRP:N	1:A:64:SER:O	14	0.11
(2,116)	1:A:154:TRP:N	1:A:64:SER:O	20	0.11
(1,548)	1:A:244:ILE:H	1:A:244:ILE:HG13	7	0.11
(1,538)	1:A:247:ARG:HG3	1:A:248:VAL:H	12	0.11
(1,511)	1:A:167:GLN:HB2	1:A:167:GLN:HE22	8	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,494)	1:A:77:ASP:H	1:A:80:GLU:HB3	20	0.11
(1,431)	1:A:240:GLN:HG2	1:A:245:ASP:HB3	12	0.11
(1,382)	1:A:180:VAL:HA	1:A:188:GLU:HG2	7	0.11
(1,316)	1:A:63:TYR:HB3	1:A:155:ASN:HA	20	0.11
(1,287)	1:A:137:LEU:HB3	1:A:149:VAL:HB	9	0.11
(1,2301)	1:A:205:ILE:H	1:A:154:TRP:HZ2	4	0.11
(1,2246)	1:A:154:TRP:HE1	1:A:158:ASP:H	13	0.11
(1,2246)	1:A:154:TRP:HE1	1:A:158:ASP:H	19	0.11
(1,2155)	1:A:238:GLN:HA	1:A:239:LEU:HB2	2	0.11
(1,2093)	1:A:136:TYR:HA	1:A:137:LEU:HB3	14	0.11
(1,2093)	1:A:136:TYR:HA	1:A:137:LEU:HB3	17	0.11
(1,183)	1:A:198:GLY:H	1:A:227:SER:HA	19	0.11
(1,182)	1:A:197:TYR:HB2	1:A:227:SER:HA	18	0.11
(1,1790)	1:A:226:GLN:HE22	1:A:227:SER:HA	3	0.11
(1,1790)	1:A:226:GLN:HE22	1:A:227:SER:HA	7	0.11
(1,1790)	1:A:226:GLN:HE22	1:A:227:SER:HA	8	0.11
(1,1790)	1:A:226:GLN:HE22	1:A:227:SER:HA	9	0.11
(1,1790)	1:A:226:GLN:HE22	1:A:227:SER:HA	13	0.11
(1,1790)	1:A:226:GLN:HE22	1:A:227:SER:HA	19	0.11
(1,1790)	1:A:226:GLN:HE22	1:A:227:SER:HA	20	0.11
(1,1764)	1:A:187:VAL:HA	1:A:191:MET:HB2	3	0.11
(1,1738)	1:A:223:SER:HB3	1:A:224:ASN:HA	17	0.11
(1,1720)	1:A:195:ARG:HA	1:A:196:LEU:HG	14	0.11
(1,172)	1:A:74:PRO:HA	1:A:76:ILE:H	15	0.11
(1,1709)	1:A:140:SER:HB3	1:A:141:SER:H	10	0.11
(1,1705)	1:A:140:SER:HB2	1:A:146:ASP:HA	7	0.11
(1,1665)	1:A:192:ILE:HG12	1:A:195:ARG:H	2	0.11
(1,1665)	1:A:192:ILE:HG12	1:A:195:ARG:H	3	0.11
(1,1655)	1:A:246:LYS:HB3	1:A:246:LYS:HD3	6	0.11
(1,1591)	1:A:163:MET:HB2	1:A:200:VAL:HB	16	0.11
(1,156)	1:A:174:THR:HB	1:A:253:TYR:HA	3	0.11
(1,156)	1:A:174:THR:HB	1:A:253:TYR:HA	6	0.11
(1,1551)	1:A:141:SER:H	1:A:144:ILE:HB	4	0.11
(1,1533)	1:A:172:ARG:HA	1:A:173:LYS:HE2	3	0.11
(1,1520)	1:A:208:ASP:HB2	1:A:215:LYS:HB2	16	0.11
(1,1465)	1:A:199:GLY:H	1:A:200:VAL:H	20	0.11
(1,1463)	1:A:142:PRO:HB3	1:A:143:THR:H	19	0.11
(1,1463)	1:A:142:PRO:HB2	1:A:143:THR:H	19	0.11
(1,1446)	1:A:71:GLY:H	1:A:85:PHE:HZ	20	0.11
(1,1438)	1:A:70:GLY:H	1:A:149:VAL:HA	9	0.11
(1,1417)	1:A:238:GLN:HB3	1:A:238:GLN:HE22	15	0.11
(1,1373)	1:A:224:ASN:HD22	1:A:227:SER:H	19	0.11

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,127)	1:A:95:TRP:HZ3	1:A:113:LEU:HA	2	0.11
(1,127)	1:A:95:TRP:HZ3	1:A:113:LEU:HA	4	0.11
(1,127)	1:A:95:TRP:HZ3	1:A:113:LEU:HA	15	0.11
(1,120)	1:A:154:TRP:HH2	1:A:155:ASN:H	6	0.11
(1,120)	1:A:154:TRP:HH2	1:A:155:ASN:H	9	0.11
(1,119)	1:A:78:GLU:HG3	1:A:95:TRP:HZ2	8	0.11
(1,119)	1:A:78:GLU:HG3	1:A:95:TRP:HZ2	11	0.11
(1,1083)	1:A:159:SER:HB3	1:A:161:PHE:H	5	0.11
(1,1034)	1:A:78:GLU:HG3	1:A:79:ASP:H	13	0.11
(1,1013)	1:A:141:SER:H	1:A:145:LYS:H	5	0.11

10 Dihedral-angle violation analysis ⓘ

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