Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2LPU
BMRB ID	:	18277
Title	:	Solution structures of KmAtg10
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Deposited on	:	2012-02-19

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 (1)) were used in the production of this report:

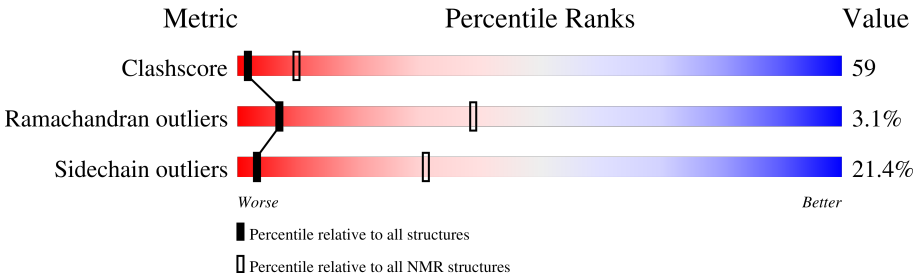
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
BMRB Restraints Analysis	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 93%.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	152	24% 57% 12% 5% •

2 Ensemble composition and analysis (i)

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: *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:1-A:101, A:108-A:147 (141)	0.63	2

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 6 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2447 atoms, of which 1221 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called KmAtg10.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	148	2447	786	1221	199	237	4	0

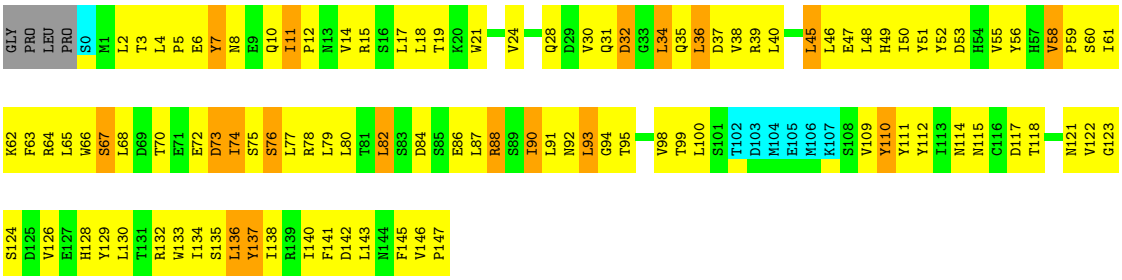
4 Residue-property plots (i)

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: KmAtg10

Chain A: 24% 57% 12% 5% •



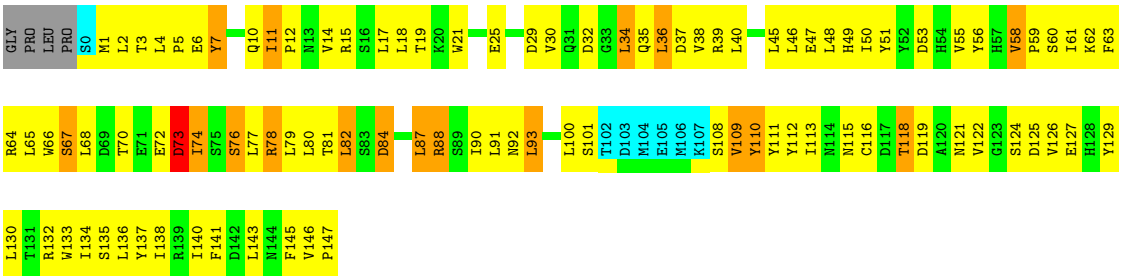
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: KmAtg10

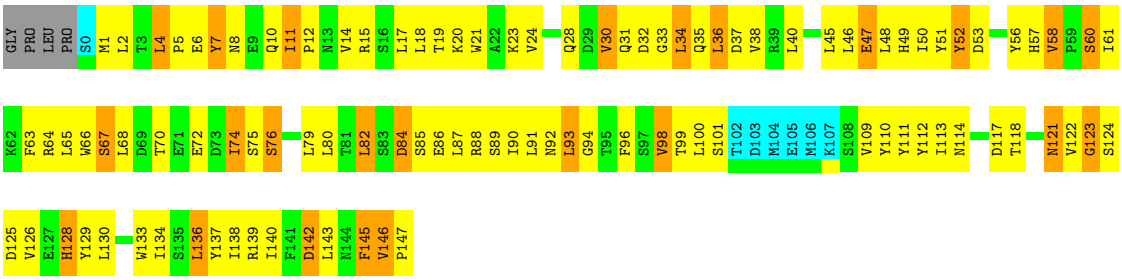
Chain A: 28% 53% 11% • 5% •



4.2.2 Score per residue for model 2 (medoid)

- Molecule 1: KmAtg10

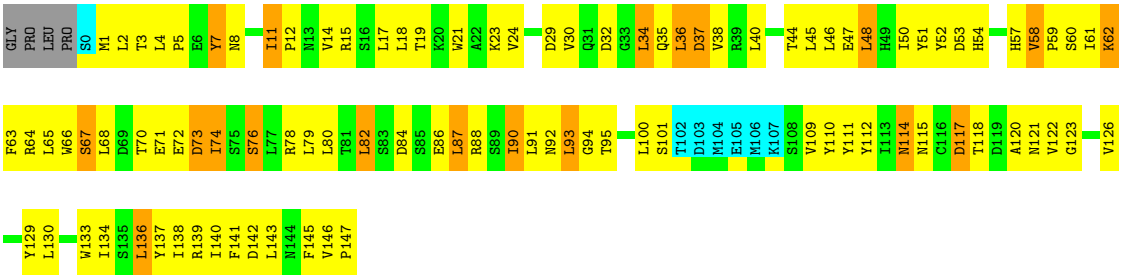
Chain A: 25% 52% 16% 5% •



4.2.3 Score per residue for model 3

- Molecule 1: KmAtg10

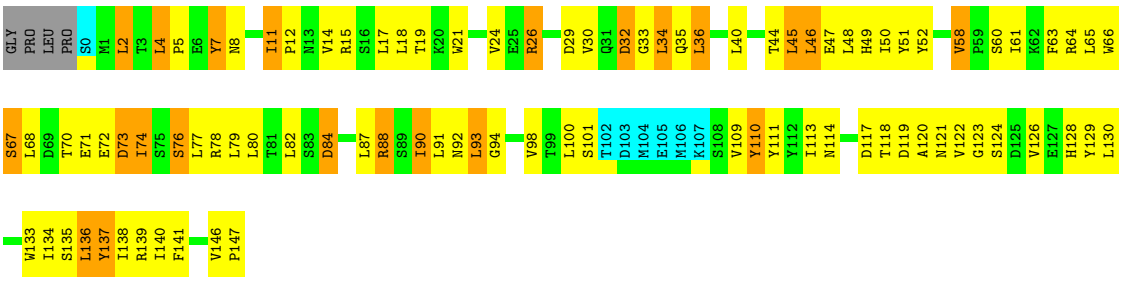
Chain A: 28% 52% 12% 5% •



4.2.4 Score per residue for model 4

- Molecule 1: KmAtg10

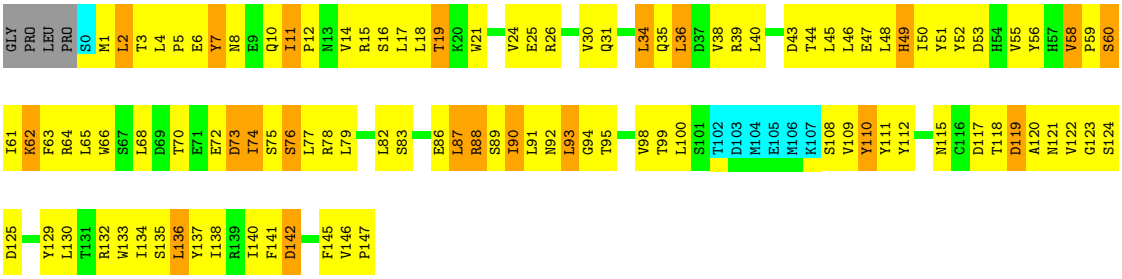
Chain A: 33% 45% 14% 5% •



4.2.5 Score per residue for model 5

- Molecule 1: KmAtg10

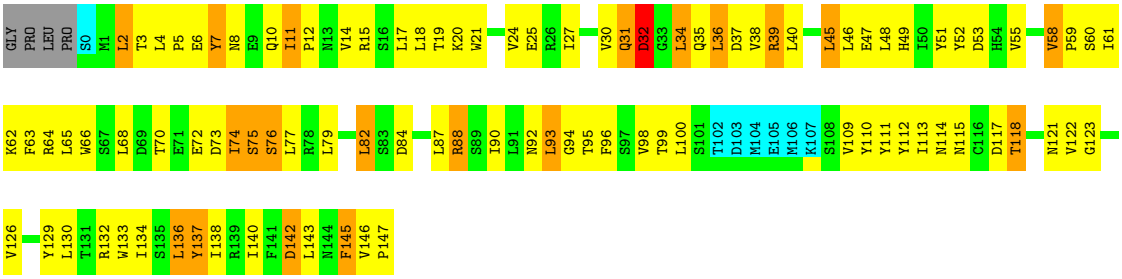
Chain A: 23% 56% 14% 5% •



4.2.6 Score per residue for model 6

- Molecule 1: KmAtg10

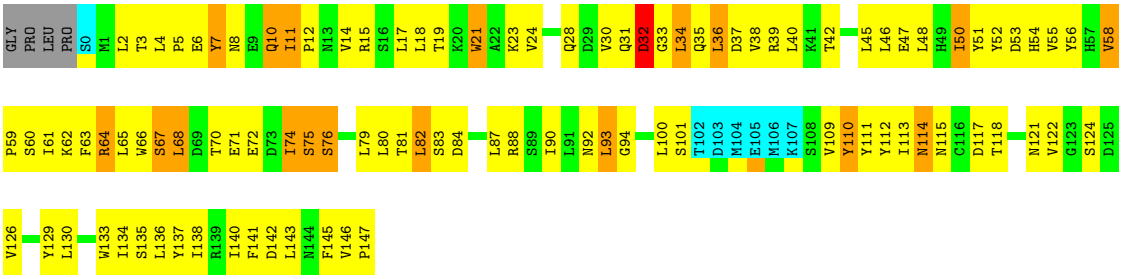
Chain A: 29% 50% 13% • 5% •



4.2.7 Score per residue for model 7

- Molecule 1: KmAtg10

Chain A: 26% 54% 12% • 5% •



4.2.8 Score per residue for model 8

- Molecule 1: KmAtg10

Chain A: 26% 53% 12% • 5% •

GLY PRO LEU PRO S0 M1 L2 T3 L4 P5 E6 Y7 N8 E9 Q10 I11 P12 N13 V14 R15 S16 L17 L18 T19 K20 W21 A22 K23 V24 Q28 D29 V30 Q31 D32 G33 L34 Q35 L36 D37 V38 R39 L40 T44 L45 L46 E47 L48 H49 I50 Y51 Y52 D53 H54 V55 Y56 H57 V58 P59

S60 I61 K62 F63 R64 L65 W66 S67 L68 D69 T70 E71 E72 D73 I74 S75 S76 L77 R78 L79 L80 T81 L82 S83 L87 R88 S89 I90 L91 N92 L93 G94 T95 V98 T99 L100 S101 T102 D103 M104 E105 M106 K107 S108 V109 Y110 Y111 Y112 D117 A120 N121 V122 G123 S124 D125 V126

E127 H128 Y129 L130 T131 R132 W133 I134 S135 L136 Y137 I138 R139 I140 F141 D142 L143 N144 F145 V146 P147

4.2.9 Score per residue for model 9

- Molecule 1: KmAtg10

Chain A: 30% 47% 15% • 5% •

GLY PRO LEU PRO S0 M1 L2 T3 L4 P5 E6 Y7 N8 E9 Q10 I11 P12 N13 V14 R15 S16 L17 L18 T19 K20 W21 A22 K23 V24 E25 Q31 D32 G33 L34 Q35 L36 D37 V38 R39 L40 D43 T44 L45 L46 E47 L48 H49 I50 Y51 Y52 D53 H54 V55 Y56 H57 V58 P59 S60

I61 K62 F63 R64 L65 W66 S67 L68 D69 T70 E71 E72 D73 I74 S75 S76 L77 R78 L79 L80 T81 L82 S83 D84 L87 R88 S89 I90 L91 N92 L93 G94 T95 F96 S97 V98 T99 L100 S101 T102 D103 M104 E105 M106 K107 S108 V109 Y110 Y111 N114 N115 C116 D117 A120 N121 V122 G123

V126 Y129 L130 W133 I134 S135 L136 Y137 I138 R139 I140 F141 V146 P147

4.2.10 Score per residue for model 10

- Molecule 1: KmAtg10

Chain A: 25% 55% 13% 5% •

GLY PRO LEU PRO S0 M1 L2 T3 L4 P5 E6 Y7 N8 E9 Q10 I11 P12 N13 V14 R15 S16 L17 L18 T19 K20 W21 A22 K23 V24 I27 Q28 D29 V30 Q31 D32 G33 L34 Q35 L36 D37 V38 R39 L40 D43 T44 L45 L46 E47 L48 H49 I50 Y51 V55 Y56 H57 V58 P59

S60 I61 K62 F63 R64 L65 W66 S67 L68 D69 T70 E71 E72 D73 I74 S75 S76 L77 R78 L79 L80 T81 L82 S83 D84 S85 E86 L87 R88 S89 I90 L91 N92 L93 V98 T99 L100 S101 T102 D103 M104 E105 M106 K107 S108 V109 Y110 Y111 Y112 I113 N114 N115 C116 D117 T118 N121 V122 G123

S124 D125 V126 Y129 L130 T131 R132 W133 I134 S135 L136 Y137 I138 R139 I140 F141 D142 L143 V146 P147

4.2.11 Score per residue for model 11

- Molecule 1: KmAtg10

Chain A: 35% 43% 14% • 5% •

GLY PRO LEU PRO S0 M1 L2 T3 L4 P5 E6 Y7 N8 E9 Q10 I11 P12 N13 V14 L17 L18 W21 V24 E25 R26 V30 L34 Q35 L36 D37 V38 R39 L40 T44 L45 L46 E47 L48 H49 I50 Y51 Y52 D53 H57 V58 P59 S60 I61 K62 F63 R64 L65 W66

S67 L68 D69 T70 E71 E72 D73 I74 S75 S76 L77 R78 L79 L80 T81 L82 S83 L87 R88 S89 I90 L91 N92 L93 G94 T95 L100 S101 T102 D103 M104 E105 M106 K107 S108 V109 Y110 Y111 N114 T118 D119 A120 N121 V122 G123 S124 D125 V126 Y129 L130 T131 R132 W133 I134 S135

L136 Y137 I138 R139 I140 F141 D142 V146 P147

4.2.12 Score per residue for model 12

- Molecule 1: KmAtg10

Chain A: 25% 54% 13% • 5% •

GLY PRO LEU PRO S0 M1 L2 T3 L4 P5 E6 Y7 N8 I11 P12 N13 V14 R15 S16 L17 L18 T19 K20 W21 R26 I27 Q28 D29 V30 Q31 D32 G33 L34 Q35 L36 D37 V38 R39 L40 K41 L45 L46 E47 L48 Y51 Y52 D53 H54 V55 Y56 H57 V58 P59 S60 I61 K62

F63 R64 L65 W66 S67 L68 D69 T70 E71 E72 D73 I74 S75 S76 L77 R78 L79 L80 T81 L82 S83 D84 S85 E86 L87 R88 S89 I90 L91 N92 L93 G94 T95 F96 S97 V98 T99 L100 S101 T102 D103 M104 E105 M106 K107 S108 V109 Y110 Y111 Y112 N115 C116 D117 T118 N121 V122 G123 S124

Y129 L130 W133 I134 S135 L136 Y137 I138 R139 I140 F141 D142 L143 N144 F145 V146 P147

4.2.13 Score per residue for model 13

- Molecule 1: KmAtg10

Chain A: 28% 53% 11% • 5% •

GLY PRO LEU PRO S0 M1 L2 T3 L4 P5 E6 Y7 N8 E9 Q10 I11 P12 N13 V14 R15 S16 L17 L18 T19 K20 W21 V24 E25 R26 I27 Q28 D29 V30 Q31 D32 G33 L34 Q35 L36 D37 V38 R39 L40 T44 L45 L46 E47 L48 H49 I50 Y51 Y52 D53 H54 V55 V58 P59

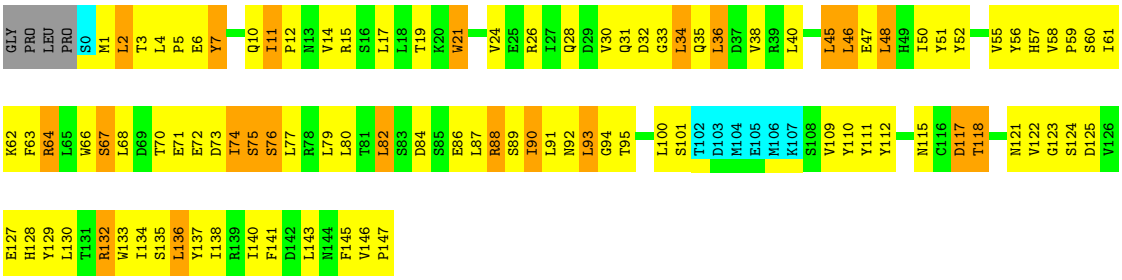
S60 I61 K62 F63 R64 L65 W66 S67 L68 D69 T70 E71 E72 D73 I74 S75 S76 L77 R78 L79 L80 T81 L82 S83 E86 L87 R88 S89 I90 L91 N92 L93 F96 S97 V98 T99 L100 S101 T102 D103 M104 E105 M106 K107 S108 V109 Y110 Y111 N114 N115 T118 D119 V122 G123 S124

D125 V126 E127 H128 Y129 L130 T131 R132 W133 I134 S135 L136 Y137 I138 R139 I140 F141 D142 L143 N144 F145 V146 P147

4.2.14 Score per residue for model 14

- Molecule 1: KmAtg10

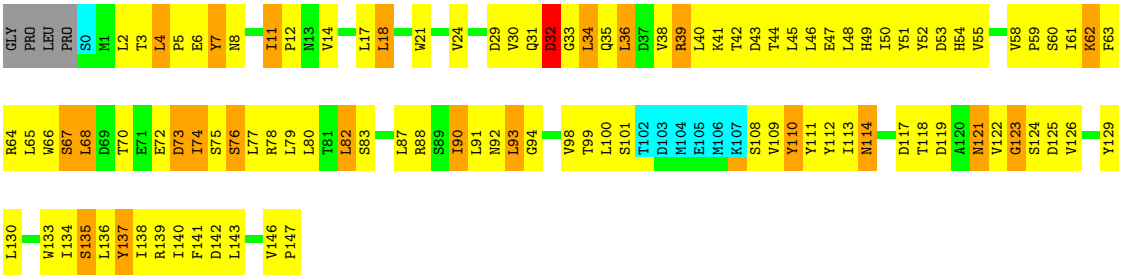
Chain A: 27% 51% 14% 5% •



4.2.15 Score per residue for model 15

- Molecule 1: KmAtg10

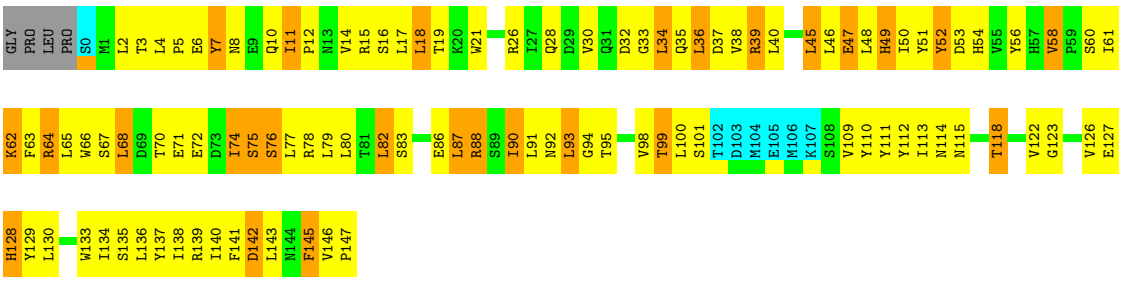
Chain A: 24% 54% 14% • 5% •



4.2.16 Score per residue for model 16

- Molecule 1: KmAtg10

Chain A: 24% 51% 18% 5% •



4.2.17 Score per residue for model 17

- Molecule 1: KmAtg10

Chain A: 30% 47% 16% 5% •

GLY PRO LEU PRO S0 M1 L2 T3 L4 P5 E6 Y7 N8 E9 Q10 I11 P12 N13 V14 R15 S16 L17 L18 T19 K20 W21 V24 E25 R26 T27 Q28 Q31 D32 G33 L34 Q35 L36 D37 V38 R39 L40 D43 T44 L45 L46 E47 L48 H49 I50 Y51 Y52 D53 H57 V58 P59 S60

I61 K62 F63 R64 L65 W66 S67 L68 D69 T70 E71 E72 D73 I74 S75 S76 L77 R78 L79 L80 T81 L82 S83 D84 S85 E86 L87 R88 S89 I90 L91 N92 L93 G94 T95 L100 S101 T102 D103 M104 E105 M106 K107 S108 V109 Y110 Y111 N114 N115 C116 D117 N121 V122 G123 S124 D125 V126

E127 H128 Y129 L130 T131 R132 W133 I134 S135 L136 Y137 I138 R139 I140 F141 D142 F145 V146 P147

4.2.18 Score per residue for model 18

- Molecule 1: KmAtg10

Chain A: 28% 50% 13% • 5% •

GLY PRO LEU PRO S0 M1 L2 T3 L4 P5 E6 Y7 N8 I11 P12 N13 V14 R15 S16 L17 L18 T19 K20 W21 V24 Q28 D29 V30 Q31 D32 G33 L34 Q35 L36 D37 V38 R39 L40 K41 T42 D43 T44 L45 L46 E47 L48 H49 I50 Y51 Y52 D53 H54 V55 Y56 H57 V58 P59

S60 I61 K62 F63 R64 L65 W66 S67 L68 D69 T70 E71 E72 D73 I74 S75 S76 L77 R78 L79 L80 T81 L82 S83 D84 L87 R88 S89 I90 L91 N92 L93 G94 T95 F96 S97 V98 T99 L100 S101 T102 D103 M104 E105 M106 K107 Y110 Y111 Y112 N115 T118 D119 A120 N121 V122

D125 Y129 L130 T131 R132 W133 I134 S135 L136 Y137 I138 R139 I140 F141 D142 V146 P147

4.2.19 Score per residue for model 19

- Molecule 1: KmAtg10

Chain A: 26% 54% 12% 5% •

GLY PRO LEU PRO S0 M1 L2 T3 L4 P5 E6 Y7 N8 E9 Q10 I11 P12 N13 V14 R15 S16 L17 L18 T19 K20 W21 A22 K23 V24 Q28 D29 V30 Q31 D32 G33 L34 Q35 L36 D37 V38 R39 L40 L45 L46 E47 L48 H49 I50 Y51 Y52 D53 H54 V55 V58 P59 S60 I61

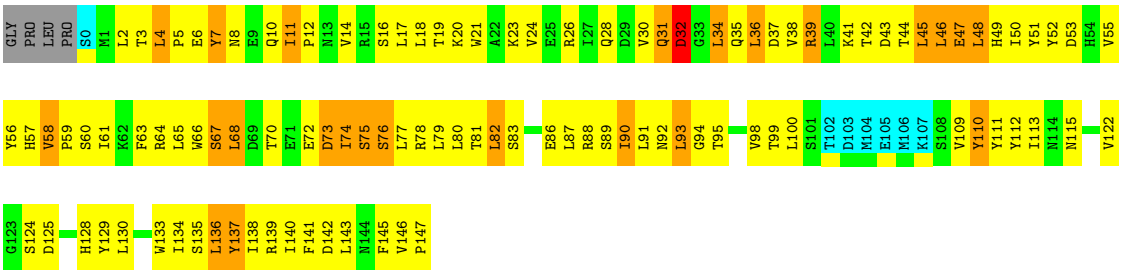
K62 F63 R64 L65 W66 S67 L68 D69 T70 E71 E72 D73 I74 S75 S76 L77 R78 L79 L80 T81 L82 E86 L87 R88 S89 I90 L91 N92 L93 G94 V98 T99 L100 S101 T102 D103 M104 E105 M106 K107 S108 V109 Y110 Y111 Y112 I113 N114 N115 T118 N121 V122 G123 S124 D125 V126 E127

H128 Y129 L130 T131 R132 W133 I134 S135 L136 Y137 I138 R139 I140 F141 D142 L143 N144 F145 V146 P147

4.2.20 Score per residue for model 20

- Molecule 1: KmAtg10

Chain A: 22% 55% 16% • 5% •



5 Refinement protocol and experimental data overview (i)

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: *target function.*

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

Software name	**Classification**	**Version**
Sparky	refinement	3.113
TALOS+	structure solution	1.01
CYANA	structure solution	2.1
CYANA	refinement	2.1

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1961
Number of shifts mapped to atoms	1961
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

6 Model quality (i)

6.1 Standard geometry (i)

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

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	1171	1167	1159	137±9
All	All	23420	23340	23180	2731

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 59.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:LEU:HD11	1:A:91:LEU:HD12	1.10	1.19	4	3
1:A:40:LEU:HD13	1:A:90:ILE:HD12	1.09	1.20	18	8
1:A:65:LEU:HD11	1:A:87:LEU:HD13	1.08	1.23	18	8
1:A:21:TRP:CH2	1:A:38:VAL:HG21	1.03	1.88	7	10
1:A:87:LEU:HD21	1:A:91:LEU:HD12	0.97	1.35	9	7
1:A:40:LEU:CD1	1:A:90:ILE:HD12	0.93	1.94	5	5
1:A:100:LEU:HD11	1:A:109:VAL:HG12	0.92	1.39	7	7
1:A:45:LEU:HD12	1:A:46:LEU:N	0.92	1.79	14	5
1:A:17:LEU:HD21	1:A:134:ILE:HG21	0.91	1.37	15	6
1:A:100:LEU:HD12	1:A:110:TYR:O	0.91	1.64	14	9
1:A:21:TRP:CZ3	1:A:138:ILE:HD11	0.90	2.02	8	11
1:A:21:TRP:CZ2	1:A:38:VAL:HG11	0.90	2.02	6	10
1:A:122:VAL:HG22	1:A:136:LEU:HD13	0.89	1.41	13	6
1:A:7:TYR:CD2	1:A:130:LEU:HD11	0.89	2.02	5	18

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:LEU:CD1	1:A:91:LEU:HD12	0.89	1.97	4	2
1:A:100:LEU:HD13	1:A:111:TYR:CD1	0.88	2.03	10	9
1:A:65:LEU:HD11	1:A:87:LEU:HD23	0.88	1.46	4	2
1:A:2:LEU:HD13	1:A:126:VAL:HG13	0.88	1.44	3	8
1:A:14:VAL:O	1:A:18:LEU:HD23	0.88	1.66	10	5
1:A:65:LEU:O	1:A:79:LEU:HD12	0.87	1.68	12	17
1:A:36:LEU:HD13	1:A:36:LEU:N	0.87	1.82	2	4
1:A:21:TRP:CZ3	1:A:38:VAL:HG21	0.87	2.04	6	7
1:A:40:LEU:HD13	1:A:90:ILE:CD1	0.86	2.00	5	5
1:A:100:LEU:HD12	1:A:111:TYR:CE1	0.86	2.06	5	8
1:A:17:LEU:HD13	1:A:147:PRO:CB	0.86	2.00	19	14
1:A:14:VAL:CG1	1:A:134:ILE:HD13	0.86	2.01	12	6
1:A:61:ILE:HD12	1:A:137:TYR:CD2	0.85	2.06	16	4
1:A:46:LEU:HD21	1:A:63:PHE:CD1	0.85	2.05	18	10
1:A:7:TYR:OH	1:A:11:ILE:HD11	0.85	1.71	4	12
1:A:122:VAL:CG2	1:A:136:LEU:HD22	0.85	2.01	18	3
1:A:17:LEU:HD12	1:A:18:LEU:N	0.85	1.87	8	9
1:A:100:LEU:HD22	1:A:111:TYR:CE1	0.85	2.06	20	7
1:A:28:GLN:O	1:A:34:LEU:HD23	0.84	1.73	8	8
1:A:4:LEU:HD23	1:A:54:HIS:CE1	0.83	2.08	15	1
1:A:122:VAL:HG23	1:A:136:LEU:HD22	0.83	1.50	18	2
1:A:15:ARG:O	1:A:19:THR:HG23	0.83	1.72	3	13
1:A:48:LEU:HD12	1:A:141:PHE:CE2	0.83	2.09	9	7
1:A:87:LEU:HD22	1:A:87:LEU:O	0.83	1.74	3	2
1:A:38:VAL:O	1:A:45:LEU:HD22	0.82	1.74	3	9
1:A:55:VAL:HG13	1:A:56:TYR:CD2	0.82	2.09	14	2
1:A:118:THR:HG22	1:A:129:TYR:OH	0.82	1.74	12	6
1:A:14:VAL:HG22	1:A:130:LEU:O	0.81	1.73	13	19
1:A:121:ASN:OD1	1:A:122:VAL:HG23	0.81	1.75	17	1
1:A:121:ASN:HB3	1:A:136:LEU:HD21	0.81	1.52	18	1
1:A:87:LEU:HD11	1:A:91:LEU:CD1	0.81	2.05	4	2
1:A:122:VAL:HG11	1:A:129:TYR:CE1	0.81	2.10	18	2
1:A:7:TYR:CZ	1:A:11:ILE:HD11	0.81	2.11	10	11
1:A:64:ARG:HB3	1:A:79:LEU:HD11	0.81	1.50	7	13
1:A:27:ILE:CD1	1:A:36:LEU:HD23	0.81	2.06	10	2
1:A:122:VAL:HG22	1:A:136:LEU:CD1	0.81	2.05	19	4
1:A:100:LEU:HD21	1:A:109:VAL:CG1	0.80	2.06	19	6
1:A:64:ARG:CB	1:A:79:LEU:HD11	0.80	2.06	13	7
1:A:38:VAL:HG12	1:A:40:LEU:CD2	0.80	2.05	10	1
1:A:21:TRP:CH2	1:A:38:VAL:HG11	0.79	2.12	13	5
1:A:61:ILE:HD12	1:A:137:TYR:CD1	0.79	2.13	5	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:LEU:HD13	1:A:46:LEU:O	0.79	1.77	16	11
1:A:67:SER:HB2	1:A:80:LEU:HD11	0.78	1.53	12	18
1:A:122:VAL:HG11	1:A:129:TYR:CD1	0.78	2.13	18	2
1:A:53:ASP:OD1	1:A:55:VAL:HG23	0.78	1.76	18	6
1:A:100:LEU:HD23	1:A:101:SER:N	0.78	1.94	11	7
1:A:18:LEU:HD12	1:A:36:LEU:HD22	0.78	1.53	10	2
1:A:17:LEU:HD13	1:A:147:PRO:HB3	0.78	1.55	11	11
1:A:66:TRP:CZ2	1:A:79:LEU:HD12	0.77	2.15	10	1
1:A:100:LEU:HD13	1:A:111:TYR:CE1	0.77	2.15	18	9
1:A:40:LEU:HD13	1:A:46:LEU:CB	0.77	2.09	9	6
1:A:48:LEU:HD11	1:A:141:PHE:CZ	0.76	2.16	14	5
1:A:44:THR:HG23	1:A:66:TRP:O	0.76	1.78	20	10
1:A:79:LEU:HD21	1:A:109:VAL:HB	0.76	1.56	3	8
1:A:14:VAL:HG13	1:A:134:ILE:HG12	0.76	1.56	8	7
1:A:130:LEU:O	1:A:134:ILE:HG22	0.76	1.81	1	11
1:A:4:LEU:HD23	1:A:52:TYR:CD2	0.76	2.15	9	1
1:A:134:ILE:HD12	1:A:137:TYR:CE2	0.76	2.16	20	9
1:A:117:ASP:HB3	1:A:120:ALA:HB3	0.75	1.58	8	3
1:A:122:VAL:HB	1:A:136:LEU:HD13	0.75	1.56	9	5
1:A:100:LEU:HD12	1:A:111:TYR:CE2	0.75	2.16	11	1
1:A:92:ASN:CG	1:A:143:LEU:HD12	0.75	2.02	12	13
1:A:21:TRP:CE3	1:A:138:ILE:HD11	0.75	2.16	8	1
1:A:45:LEU:HD11	1:A:47:GLU:HG3	0.75	1.58	4	4
1:A:92:ASN:O	1:A:140:ILE:HG23	0.74	1.82	14	11
1:A:37:ASP:OD1	1:A:45:LEU:HD21	0.74	1.83	1	4
1:A:65:LEU:CD1	1:A:87:LEU:HD13	0.74	2.10	18	2
1:A:36:LEU:N	1:A:36:LEU:HD12	0.74	1.98	10	15
1:A:63:PHE:CE2	1:A:113:ILE:HD11	0.74	2.18	7	1
1:A:2:LEU:HD21	1:A:7:TYR:HB2	0.74	1.59	7	15
1:A:45:LEU:HD22	1:A:46:LEU:N	0.74	1.98	8	6
1:A:136:LEU:C	1:A:136:LEU:HD12	0.73	2.04	6	1
1:A:45:LEU:HD13	1:A:46:LEU:N	0.73	1.98	3	9
1:A:100:LEU:HD21	1:A:109:VAL:HG11	0.73	1.57	19	1
1:A:65:LEU:HD11	1:A:87:LEU:CD2	0.73	2.14	4	1
1:A:16:SER:O	1:A:19:THR:HG23	0.73	1.84	20	5
1:A:33:GLY:O	1:A:34:LEU:HD12	0.73	1.84	16	2
1:A:63:PHE:CE2	1:A:91:LEU:HD11	0.72	2.19	5	6
1:A:100:LEU:HD12	1:A:111:TYR:CZ	0.72	2.19	19	5
1:A:66:TRP:CE2	1:A:79:LEU:HD12	0.72	2.20	10	1
1:A:18:LEU:HD23	1:A:36:LEU:HD21	0.72	1.62	12	7
1:A:17:LEU:HD13	1:A:147:PRO:HB2	0.71	1.61	20	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:39:ARG:CZ	1:A:68:LEU:HD13	0.71	2.16	9	3
1:A:45:LEU:HD12	1:A:45:LEU:C	0.71	2.06	14	5
1:A:53:ASP:OD2	1:A:55:VAL:HG23	0.71	1.86	13	4
1:A:2:LEU:CD1	1:A:126:VAL:HG13	0.71	2.14	3	8
1:A:37:ASP:CG	1:A:45:LEU:HD21	0.71	2.05	7	3
1:A:45:LEU:C	1:A:45:LEU:HD13	0.71	2.06	11	14
1:A:61:ILE:CD1	1:A:137:TYR:CD1	0.71	2.74	14	4
1:A:87:LEU:C	1:A:87:LEU:HD23	0.71	2.05	5	2
1:A:61:ILE:CD1	1:A:137:TYR:CD2	0.71	2.74	6	3
1:A:35:GLN:C	1:A:36:LEU:HD13	0.71	2.06	2	4
1:A:82:LEU:HD13	1:A:86:GLU:HB2	0.70	1.62	13	9
1:A:37:ASP:OD2	1:A:45:LEU:HD21	0.70	1.85	12	1
1:A:63:PHE:CZ	1:A:91:LEU:CD1	0.70	2.74	10	12
1:A:137:TYR:CD1	1:A:137:TYR:C	0.70	2.64	19	9
1:A:55:VAL:CG1	1:A:56:TYR:CD2	0.70	2.75	20	1
1:A:2:LEU:HD12	1:A:126:VAL:HG13	0.70	1.62	4	2
1:A:46:LEU:HD13	1:A:46:LEU:C	0.70	2.06	14	5
1:A:55:VAL:CG1	1:A:56:TYR:CE2	0.70	2.75	20	1
1:A:48:LEU:HD21	1:A:61:ILE:HG23	0.70	1.64	10	4
1:A:45:LEU:HD22	1:A:46:LEU:H	0.69	1.45	8	4
1:A:136:LEU:CD2	1:A:137:TYR:CD2	0.69	2.76	2	2
1:A:87:LEU:C	1:A:87:LEU:HD13	0.69	2.07	3	2
1:A:36:LEU:N	1:A:36:LEU:CD1	0.69	2.56	2	17
1:A:134:ILE:O	1:A:138:ILE:HG22	0.69	1.88	20	10
1:A:4:LEU:C	1:A:4:LEU:HD13	0.69	2.07	17	5
1:A:63:PHE:CE1	1:A:111:TYR:CG	0.69	2.81	1	2
1:A:14:VAL:HG13	1:A:134:ILE:HD13	0.68	1.65	4	6
1:A:4:LEU:HD11	1:A:32:ASP:OD1	0.68	1.88	19	1
1:A:46:LEU:C	1:A:46:LEU:HD22	0.68	2.08	20	1
1:A:40:LEU:HD13	1:A:46:LEU:HB2	0.68	1.64	9	2
1:A:100:LEU:HD11	1:A:109:VAL:CG1	0.68	2.18	17	6
1:A:122:VAL:HG21	1:A:132:ARG:O	0.68	1.89	5	1
1:A:51:TYR:CE1	1:A:60:SER:CB	0.67	2.76	18	3
1:A:4:LEU:HD21	1:A:32:ASP:OD1	0.67	1.89	19	2
1:A:61:ILE:HD11	1:A:137:TYR:HB2	0.67	1.65	15	1
1:A:48:LEU:C	1:A:48:LEU:HD13	0.67	2.10	1	5
1:A:92:ASN:ND2	1:A:143:LEU:HD12	0.67	2.05	7	5
1:A:48:LEU:CD1	1:A:141:PHE:CE2	0.67	2.78	20	5
1:A:2:LEU:HD11	1:A:7:TYR:CA	0.67	2.20	5	4
1:A:14:VAL:O	1:A:18:LEU:HD13	0.67	1.89	12	1
1:A:18:LEU:HD23	1:A:36:LEU:CD2	0.66	2.20	12	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:87:LEU:O	1:A:87:LEU:HD13	0.66	1.90	6	2
1:A:133:TRP:NE1	1:A:137:TYR:CE1	0.66	2.63	8	4
1:A:4:LEU:HD13	1:A:4:LEU:O	0.66	1.90	11	20
1:A:4:LEU:HD23	1:A:52:TYR:CD1	0.66	2.25	17	8
1:A:65:LEU:HD13	1:A:82:LEU:HD11	0.66	1.68	12	1
1:A:18:LEU:HD12	1:A:36:LEU:CD2	0.66	2.21	16	2
1:A:137:TYR:CD1	1:A:138:ILE:N	0.66	2.64	20	6
1:A:63:PHE:CE1	1:A:111:TYR:CB	0.66	2.79	1	5
1:A:2:LEU:HD21	1:A:7:TYR:CB	0.66	2.20	5	1
1:A:61:ILE:CD1	1:A:137:TYR:CG	0.65	2.79	1	11
1:A:51:TYR:CZ	1:A:60:SER:CB	0.65	2.79	18	16
1:A:133:TRP:NE1	1:A:137:TYR:CE2	0.65	2.64	2	6
1:A:100:LEU:HD21	1:A:109:VAL:HG13	0.65	1.69	16	3
1:A:90:ILE:HD13	1:A:90:ILE:N	0.65	2.05	13	3
1:A:37:ASP:OD1	1:A:45:LEU:HD11	0.65	1.92	7	2
1:A:46:LEU:HD21	1:A:63:PHE:CD2	0.65	2.26	16	5
1:A:2:LEU:HD11	1:A:7:TYR:HA	0.65	1.69	17	4
1:A:11:ILE:N	1:A:12:PRO:CD	0.65	2.60	14	20
1:A:65:LEU:CD1	1:A:82:LEU:HD11	0.65	2.22	12	1
1:A:66:TRP:CE3	1:A:77:LEU:CD1	0.64	2.80	16	16
1:A:4:LEU:N	1:A:5:PRO:CD	0.64	2.60	17	20
1:A:18:LEU:HD13	1:A:36:LEU:CD1	0.64	2.22	7	1
1:A:87:LEU:HD21	1:A:91:LEU:CD1	0.64	2.21	1	2
1:A:61:ILE:CD1	1:A:133:TRP:CZ2	0.64	2.80	17	6
1:A:4:LEU:HD13	1:A:4:LEU:C	0.64	2.13	14	12
1:A:40:LEU:HD13	1:A:46:LEU:HB3	0.64	1.69	6	8
1:A:64:ARG:NH2	1:A:66:TRP:CZ2	0.64	2.65	18	5
1:A:101:SER:O	1:A:109:VAL:HG13	0.64	1.92	14	1
1:A:132:ARG:NE	1:A:136:LEU:HD13	0.64	2.08	18	1
1:A:46:LEU:HD23	1:A:65:LEU:HD23	0.64	1.68	13	5
1:A:67:SER:CB	1:A:80:LEU:HD21	0.64	2.23	1	14
1:A:74:ILE:HD11	1:A:76:SER:HB2	0.64	1.70	3	20
1:A:93:LEU:CD2	1:A:93:LEU:N	0.64	2.60	17	20
1:A:18:LEU:HD21	1:A:36:LEU:CD2	0.64	2.23	2	1
1:A:66:TRP:CE3	1:A:77:LEU:HD13	0.64	2.28	16	11
1:A:21:TRP:CZ3	1:A:138:ILE:CD1	0.62	2.81	8	1
1:A:45:LEU:HD13	1:A:45:LEU:C	0.62	2.14	3	1
1:A:36:LEU:HD12	1:A:36:LEU:H	0.62	1.55	17	15
1:A:64:ARG:NH2	1:A:66:TRP:CH2	0.62	2.68	18	4
1:A:122:VAL:CG1	1:A:129:TYR:CZ	0.62	2.82	6	4
1:A:46:LEU:C	1:A:46:LEU:HD13	0.62	2.14	17	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:63:PHE:CZ	1:A:91:LEU:HD11	0.62	2.29	17	13
1:A:137:TYR:CG	1:A:138:ILE:N	0.62	2.67	17	9
1:A:100:LEU:CD1	1:A:109:VAL:HG12	0.62	2.24	6	6
1:A:45:LEU:HD21	1:A:47:GLU:OE2	0.62	1.95	14	1
1:A:64:ARG:O	1:A:66:TRP:CD1	0.62	2.53	16	13
1:A:2:LEU:CD1	1:A:126:VAL:HG23	0.62	2.25	11	3
1:A:38:VAL:HG12	1:A:40:LEU:HD12	0.61	1.72	19	5
1:A:66:TRP:CZ2	1:A:79:LEU:HD13	0.61	2.29	2	10
1:A:110:TYR:CD1	1:A:110:TYR:N	0.61	2.68	19	9
1:A:100:LEU:HD13	1:A:111:TYR:CG	0.61	2.29	8	2
1:A:55:VAL:HG23	1:A:56:TYR:CD2	0.61	2.30	5	2
1:A:7:TYR:CD1	1:A:130:LEU:HD11	0.61	2.31	8	1
1:A:2:LEU:HD13	1:A:126:VAL:HG23	0.61	1.71	11	2
1:A:100:LEU:HD21	1:A:109:VAL:HG21	0.61	1.70	1	1
1:A:122:VAL:HB	1:A:136:LEU:HD22	0.61	1.71	16	1
1:A:21:TRP:CZ3	1:A:38:VAL:CG2	0.61	2.83	11	7
1:A:124:SER:O	1:A:129:TYR:CD1	0.61	2.53	20	7
1:A:61:ILE:CD1	1:A:137:TYR:CB	0.61	2.79	7	6
1:A:87:LEU:CD1	1:A:111:TYR:CE1	0.61	2.83	5	2
1:A:63:PHE:HE2	1:A:113:ILE:HD11	0.61	1.55	7	1
1:A:65:LEU:HD11	1:A:87:LEU:CD1	0.61	2.15	18	6
1:A:7:TYR:CE1	1:A:8:ASN:OD1	0.61	2.54	6	3
1:A:27:ILE:HD11	1:A:36:LEU:HD23	0.61	1.72	10	1
1:A:122:VAL:CG2	1:A:136:LEU:HD13	0.61	2.26	20	3
1:A:100:LEU:HD22	1:A:111:TYR:HE1	0.60	1.52	13	3
1:A:109:VAL:O	1:A:110:TYR:CD1	0.60	2.55	16	2
1:A:7:TYR:CD1	1:A:8:ASN:OD1	0.60	2.55	6	2
1:A:51:TYR:CD1	1:A:51:TYR:O	0.60	2.55	18	4
1:A:15:ARG:HA	1:A:18:LEU:HD22	0.60	1.73	12	1
1:A:136:LEU:HD23	1:A:137:TYR:CD2	0.60	2.31	2	4
1:A:48:LEU:CD2	1:A:61:ILE:HG23	0.60	2.26	10	2
1:A:134:ILE:O	1:A:138:ILE:CG2	0.60	2.50	20	10
1:A:55:VAL:HG12	1:A:56:TYR:CD2	0.60	2.31	12	3
1:A:7:TYR:CD1	1:A:8:ASN:N	0.60	2.70	13	12
1:A:7:TYR:CE2	1:A:8:ASN:OD1	0.60	2.55	8	1
1:A:48:LEU:HD13	1:A:49:HIS:N	0.60	2.12	19	4
1:A:61:ILE:HD11	1:A:133:TRP:CZ2	0.60	2.32	17	6
1:A:52:TYR:C	1:A:52:TYR:CD1	0.60	2.75	11	4
1:A:48:LEU:CD1	1:A:141:PHE:CZ	0.59	2.85	14	6
1:A:62:LYS:CD	1:A:112:TYR:CZ	0.59	2.85	7	1
1:A:55:VAL:HG12	1:A:56:TYR:CD1	0.59	2.32	18	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:47:GLU:OE1	1:A:66:TRP:CD1	0.59	2.55	14	1
1:A:51:TYR:CE1	1:A:60:SER:OG	0.59	2.55	17	2
1:A:93:LEU:N	1:A:93:LEU:HD22	0.59	2.13	5	20
1:A:18:LEU:CD1	1:A:36:LEU:HD22	0.59	2.27	10	2
1:A:61:ILE:HD12	1:A:137:TYR:HD2	0.59	1.56	16	1
1:A:2:LEU:HB2	1:A:126:VAL:HG22	0.59	1.74	9	1
1:A:67:SER:CB	1:A:80:LEU:HD11	0.59	2.26	12	2
1:A:51:TYR:CE2	1:A:60:SER:OG	0.59	2.55	8	4
1:A:121:ASN:CB	1:A:136:LEU:HD21	0.59	2.26	18	1
1:A:51:TYR:CE2	1:A:53:ASP:OD2	0.59	2.56	17	1
1:A:66:TRP:CE3	1:A:79:LEU:N	0.59	2.71	16	6
1:A:14:VAL:HG11	1:A:134:ILE:HD13	0.59	1.74	16	2
1:A:48:LEU:HD13	1:A:48:LEU:C	0.59	2.18	19	1
1:A:56:TYR:O	1:A:58:VAL:HG22	0.59	1.97	2	2
1:A:89:SER:HB3	1:A:90:ILE:HD13	0.59	1.74	10	3
1:A:124:SER:O	1:A:129:TYR:CE1	0.58	2.56	19	5
1:A:7:TYR:C	1:A:7:TYR:CD1	0.58	2.76	5	1
1:A:100:LEU:HD21	1:A:109:VAL:HG12	0.58	1.75	15	1
1:A:61:ILE:HD11	1:A:137:TYR:CG	0.58	2.33	20	5
1:A:81:THR:CG2	1:A:109:VAL:HG21	0.58	2.29	10	1
1:A:100:LEU:C	1:A:100:LEU:HD23	0.58	2.19	1	2
1:A:14:VAL:HG23	1:A:130:LEU:HB3	0.58	1.76	4	8
1:A:57:HIS:O	1:A:58:VAL:HG13	0.58	1.98	8	3
1:A:4:LEU:HD23	1:A:52:TYR:CG	0.58	2.33	17	5
1:A:14:VAL:HG13	1:A:134:ILE:CD1	0.58	2.28	17	6
1:A:46:LEU:CD2	1:A:63:PHE:CD2	0.58	2.86	16	3
1:A:81:THR:HG21	1:A:109:VAL:HG21	0.58	1.74	10	1
1:A:122:VAL:CG1	1:A:129:TYR:CE1	0.58	2.86	18	4
1:A:48:LEU:HD23	1:A:141:PHE:CE2	0.58	2.34	12	3
1:A:18:LEU:HD21	1:A:134:ILE:CD1	0.57	2.28	18	1
1:A:117:ASP:HB2	1:A:120:ALA:HB3	0.57	1.75	5	1
1:A:38:VAL:HG12	1:A:40:LEU:CD1	0.57	2.29	19	4
1:A:14:VAL:HG13	1:A:134:ILE:HG21	0.57	1.76	10	1
1:A:145:PHE:C	1:A:145:PHE:CD1	0.57	2.76	13	6
1:A:61:ILE:CD1	1:A:133:TRP:CH2	0.57	2.87	6	1
1:A:39:ARG:NH1	1:A:68:LEU:HD13	0.57	2.15	7	1
1:A:55:VAL:HG13	1:A:56:TYR:CG	0.57	2.35	20	1
1:A:96:PHE:CD2	1:A:140:ILE:HD11	0.57	2.34	2	3
1:A:100:LEU:HD12	1:A:111:TYR:HE1	0.57	1.58	16	1
1:A:21:TRP:CE2	1:A:142:ASP:OD2	0.57	2.58	3	4
1:A:18:LEU:HD21	1:A:134:ILE:HD11	0.57	1.75	18	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:46:LEU:HD22	1:A:64:ARG:O	0.57	1.99	18	3
1:A:21:TRP:CE3	1:A:24:VAL:CG2	0.57	2.88	18	12
1:A:21:TRP:CE2	1:A:142:ASP:OD1	0.57	2.58	19	4
1:A:2:LEU:O	1:A:2:LEU:HD23	0.57	2.00	9	1
1:A:47:GLU:OE2	1:A:66:TRP:CD1	0.57	2.58	12	1
1:A:79:LEU:HD21	1:A:109:VAL:O	0.57	2.00	7	2
1:A:38:VAL:HG12	1:A:40:LEU:HD22	0.57	1.76	10	1
1:A:4:LEU:HD21	1:A:32:ASP:CG	0.57	2.20	19	1
1:A:15:ARG:HD2	1:A:34:LEU:HD21	0.57	1.76	7	2
1:A:52:TYR:CD1	1:A:52:TYR:C	0.57	2.78	2	4
1:A:7:TYR:HD1	1:A:130:LEU:HD11	0.57	1.58	8	1
1:A:2:LEU:HD12	1:A:6:GLU:HB3	0.56	1.75	20	6
1:A:21:TRP:CH2	1:A:38:VAL:CG1	0.56	2.87	13	1
1:A:61:ILE:HD13	1:A:137:TYR:CG	0.56	2.35	17	3
1:A:98:VAL:HG23	1:A:113:ILE:HG12	0.56	1.77	2	1
1:A:47:GLU:CG	1:A:49:HIS:NE2	0.56	2.68	16	7
1:A:23:LYS:HB2	1:A:38:VAL:HG13	0.56	1.78	2	5
1:A:136:LEU:HD12	1:A:137:TYR:N	0.56	2.15	6	1
1:A:40:LEU:HD12	1:A:46:LEU:HB2	0.56	1.78	14	3
1:A:56:TYR:CD2	1:A:116:CYS:O	0.56	2.59	9	2
1:A:14:VAL:HG12	1:A:18:LEU:HD23	0.56	1.78	15	1
1:A:55:VAL:CG2	1:A:56:TYR:CD2	0.55	2.89	5	1
1:A:63:PHE:CZ	1:A:111:TYR:CB	0.55	2.89	19	6
1:A:66:TRP:CZ2	1:A:79:LEU:CD1	0.55	2.89	10	1
1:A:40:LEU:CD1	1:A:65:LEU:CD2	0.55	2.84	13	2
1:A:31:GLN:O	1:A:31:GLN:CG	0.55	2.55	17	2
1:A:122:VAL:HG13	1:A:136:LEU:HD13	0.55	1.79	19	1
1:A:4:LEU:CD2	1:A:52:TYR:CG	0.55	2.90	17	3
1:A:30:VAL:HG22	1:A:34:LEU:N	0.55	2.16	14	7
1:A:53:ASP:CG	1:A:55:VAL:HG22	0.55	2.22	5	1
1:A:61:ILE:HD13	1:A:137:TYR:HB3	0.55	1.79	10	3
1:A:121:ASN:HB3	1:A:136:LEU:HD11	0.55	1.76	9	1
1:A:51:TYR:CZ	1:A:60:SER:OG	0.55	2.60	16	10
1:A:109:VAL:C	1:A:110:TYR:CG	0.55	2.80	16	2
1:A:133:TRP:CD1	1:A:137:TYR:CE2	0.54	2.94	1	6
1:A:58:VAL:HG11	1:A:118:THR:HG22	0.54	1.78	16	2
1:A:52:TYR:CD1	1:A:53:ASP:N	0.54	2.75	12	5
1:A:4:LEU:CD2	1:A:52:TYR:CD1	0.54	2.89	2	3
1:A:21:TRP:CE3	1:A:24:VAL:HG23	0.54	2.37	17	13
1:A:63:PHE:CE1	1:A:111:TYR:HB2	0.54	2.38	15	5
1:A:56:TYR:CG	1:A:116:CYS:O	0.54	2.61	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:51:TYR:CE2	1:A:60:SER:CB	0.53	2.92	19	3
1:A:21:TRP:CZ2	1:A:38:VAL:CG1	0.53	2.88	6	1
1:A:7:TYR:HD2	1:A:130:LEU:HD11	0.53	1.64	4	7
1:A:17:LEU:HD12	1:A:17:LEU:C	0.53	2.22	6	12
1:A:63:PHE:CZ	1:A:111:TYR:HB3	0.53	2.39	9	7
1:A:63:PHE:CE2	1:A:91:LEU:CD1	0.53	2.91	14	1
1:A:34:LEU:N	1:A:50:ILE:CG2	0.53	2.71	16	11
1:A:87:LEU:HD12	1:A:111:TYR:CE1	0.53	2.38	5	1
1:A:74:ILE:H	1:A:74:ILE:HD13	0.53	1.63	7	20
1:A:46:LEU:HG	1:A:65:LEU:HD23	0.53	1.80	4	2
1:A:61:ILE:HD11	1:A:133:TRP:CH2	0.53	2.38	6	1
1:A:2:LEU:HD23	1:A:59:PRO:HD3	0.53	1.81	13	3
1:A:129:TYR:O	1:A:133:TRP:CB	0.53	2.57	18	17
1:A:2:LEU:HD11	1:A:7:TYR:CB	0.53	2.34	5	2
1:A:38:VAL:CG1	1:A:40:LEU:CD2	0.53	2.83	10	1
1:A:4:LEU:HD22	1:A:52:TYR:CG	0.53	2.39	4	3
1:A:134:ILE:O	1:A:138:ILE:N	0.53	2.42	10	8
1:A:51:TYR:CD1	1:A:51:TYR:N	0.53	2.77	10	2
1:A:100:LEU:CD1	1:A:111:TYR:CE1	0.53	2.90	16	4
1:A:133:TRP:CD1	1:A:137:TYR:CE1	0.53	2.97	13	2
1:A:36:LEU:H	1:A:36:LEU:HD22	0.52	1.64	14	2
1:A:122:VAL:HG22	1:A:136:LEU:CD2	0.52	2.34	19	2
1:A:51:TYR:CE2	1:A:60:SER:HB2	0.52	2.39	19	6
1:A:136:LEU:C	1:A:136:LEU:CD1	0.52	2.77	6	1
1:A:14:VAL:HG13	1:A:134:ILE:CG1	0.52	2.30	8	7
1:A:39:ARG:CD	1:A:41:LYS:O	0.52	2.57	20	4
1:A:122:VAL:HG13	1:A:123:GLY:N	0.52	2.20	12	9
1:A:87:LEU:HD11	1:A:91:LEU:HG	0.52	1.80	15	1
1:A:58:VAL:HG11	1:A:118:THR:CG2	0.52	2.34	6	2
1:A:80:LEU:O	1:A:81:THR:HG23	0.52	2.04	20	3
1:A:14:VAL:HG21	1:A:130:LEU:HD12	0.52	1.82	2	4
1:A:7:TYR:HA	1:A:130:LEU:HD21	0.52	1.81	19	10
1:A:62:LYS:NZ	1:A:110:TYR:CD2	0.52	2.71	7	2
1:A:141:PHE:N	1:A:141:PHE:CD1	0.52	2.77	15	4
1:A:122:VAL:HG13	1:A:129:TYR:CE1	0.52	2.40	9	4
1:A:48:LEU:HD21	1:A:61:ILE:CG2	0.52	2.33	10	2
1:A:81:THR:CG2	1:A:109:VAL:CG2	0.51	2.88	10	1
1:A:16:SER:O	1:A:19:THR:CG2	0.51	2.58	12	2
1:A:11:ILE:N	1:A:12:PRO:HD2	0.51	2.20	8	20
1:A:87:LEU:HD13	1:A:87:LEU:C	0.51	2.25	6	1
1:A:18:LEU:HD13	1:A:36:LEU:HD13	0.51	1.82	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:64:ARG:NH2	1:A:79:LEU:HD13	0.51	2.20	10	1
1:A:4:LEU:C	1:A:4:LEU:CD1	0.51	2.79	3	20
1:A:4:LEU:N	1:A:5:PRO:HD2	0.51	2.21	9	20
1:A:86:GLU:O	1:A:89:SER:CB	0.51	2.58	10	6
1:A:48:LEU:CD2	1:A:137:TYR:OH	0.51	2.59	20	4
1:A:62:LYS:HD2	1:A:112:TYR:CE2	0.51	2.41	15	2
1:A:36:LEU:HD13	1:A:48:LEU:HD12	0.51	1.82	10	2
1:A:100:LEU:CD2	1:A:109:VAL:CG1	0.51	2.85	19	1
1:A:61:ILE:HG21	1:A:113:ILE:HD12	0.51	1.82	1	3
1:A:23:LYS:NZ	1:A:40:LEU:HD22	0.51	2.21	10	1
1:A:63:PHE:CE1	1:A:111:TYR:CD2	0.51	2.99	2	3
1:A:40:LEU:HD22	1:A:90:ILE:HB	0.51	1.82	4	4
1:A:98:VAL:CG1	1:A:99:THR:N	0.51	2.74	6	4
1:A:100:LEU:HD23	1:A:100:LEU:C	0.51	2.26	16	3
1:A:139:ARG:NH2	1:A:146:VAL:HG11	0.51	2.20	2	1
1:A:98:VAL:HG23	1:A:113:ILE:HA	0.51	1.81	4	1
1:A:18:LEU:HD21	1:A:36:LEU:HD21	0.51	1.83	2	1
1:A:88:ARG:O	1:A:88:ARG:CD	0.51	2.59	10	5
1:A:55:VAL:HG13	1:A:56:TYR:CD1	0.51	2.41	20	1
1:A:58:VAL:HB	1:A:118:THR:HG21	0.51	1.82	3	2
1:A:101:SER:O	1:A:110:TYR:CD1	0.51	2.64	7	1
1:A:72:GLU:O	1:A:73:ASP:CB	0.50	2.60	15	12
1:A:82:LEU:HD21	1:A:87:LEU:HB2	0.50	1.84	11	4
1:A:48:LEU:C	1:A:48:LEU:CD1	0.50	2.80	1	5
1:A:67:SER:HB2	1:A:80:LEU:HD21	0.50	1.82	14	9
1:A:45:LEU:C	1:A:45:LEU:CD1	0.50	2.80	14	10
1:A:15:ARG:O	1:A:19:THR:CG2	0.50	2.59	5	2
1:A:87:LEU:HD23	1:A:88:ARG:N	0.50	2.21	8	4
1:A:51:TYR:CD1	1:A:51:TYR:C	0.50	2.85	11	4
1:A:100:LEU:CD1	1:A:111:TYR:CE2	0.50	2.93	11	1
1:A:63:PHE:CZ	1:A:91:LEU:HD12	0.50	2.41	13	1
1:A:29:ASP:HA	1:A:34:LEU:HD23	0.50	1.83	1	4
1:A:82:LEU:N	1:A:82:LEU:CD2	0.50	2.75	15	8
1:A:135:SER:O	1:A:139:ARG:CD	0.50	2.60	17	6
1:A:14:VAL:CG2	1:A:130:LEU:O	0.50	2.60	8	7
1:A:66:TRP:CZ3	1:A:79:LEU:HB2	0.50	2.42	17	10
1:A:51:TYR:CE2	1:A:60:SER:HB3	0.50	2.42	4	4
1:A:87:LEU:HD13	1:A:111:TYR:CE1	0.50	2.42	8	1
1:A:53:ASP:CG	1:A:55:VAL:HG12	0.50	2.27	20	1
1:A:27:ILE:HD13	1:A:36:LEU:HD23	0.50	1.84	12	3
1:A:46:LEU:CD2	1:A:63:PHE:CD1	0.50	2.95	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:17:LEU:HD21	1:A:134:ILE:CG2	0.50	2.37	8	2
1:A:25:GLU:CD	1:A:39:ARG:CG	0.50	2.80	9	1
1:A:61:ILE:HG13	1:A:133:TRP:CZ2	0.50	2.42	13	2
1:A:122:VAL:HG13	1:A:129:TYR:CZ	0.50	2.41	6	1
1:A:3:THR:O	1:A:52:TYR:CE2	0.50	2.65	15	2
1:A:21:TRP:CH2	1:A:38:VAL:CG2	0.50	2.87	19	3
1:A:115:ASN:CB	1:A:137:TYR:OH	0.50	2.60	16	1
1:A:51:TYR:CZ	1:A:60:SER:HB2	0.50	2.42	19	10
1:A:63:PHE:CE2	1:A:141:PHE:CE1	0.50	3.00	10	2
1:A:100:LEU:CD1	1:A:110:TYR:O	0.50	2.60	20	2
1:A:109:VAL:CG2	1:A:110:TYR:N	0.49	2.75	1	1
1:A:51:TYR:CE1	1:A:60:SER:HB3	0.49	2.42	14	3
1:A:72:GLU:HB2	1:A:74:ILE:HG23	0.49	1.84	19	8
1:A:47:GLU:O	1:A:63:PHE:CB	0.49	2.60	7	2
1:A:48:LEU:HD11	1:A:141:PHE:CE2	0.49	2.41	13	1
1:A:63:PHE:CE1	1:A:111:TYR:HB3	0.49	2.43	19	2
1:A:113:ILE:HD11	1:A:141:PHE:CZ	0.49	2.43	16	2
1:A:132:ARG:O	1:A:136:LEU:N	0.49	2.45	13	3
1:A:20:LYS:HB2	1:A:145:PHE:CE1	0.49	2.42	19	5
1:A:52:TYR:CD2	1:A:54:HIS:CE1	0.49	3.01	3	1
1:A:122:VAL:CG1	1:A:123:GLY:N	0.49	2.75	11	9
1:A:98:VAL:HG22	1:A:99:THR:N	0.49	2.22	16	8
1:A:61:ILE:HG13	1:A:133:TRP:CH2	0.49	2.43	13	3
1:A:130:LEU:O	1:A:134:ILE:CG2	0.49	2.61	7	6
1:A:118:THR:CG2	1:A:129:TYR:OH	0.49	2.60	14	4
1:A:46:LEU:C	1:A:46:LEU:CD1	0.49	2.81	14	4
1:A:46:LEU:HD21	1:A:63:PHE:HB2	0.49	1.84	12	2
1:A:31:GLN:O	1:A:32:ASP:CB	0.49	2.59	6	12
1:A:45:LEU:CD1	1:A:66:TRP:CD1	0.49	2.96	15	1
1:A:48:LEU:HD12	1:A:141:PHE:CE1	0.49	2.43	13	2
1:A:114:ASN:HD22	1:A:114:ASN:N	0.49	2.04	7	2
1:A:64:ARG:HB2	1:A:79:LEU:HD11	0.49	1.85	10	2
1:A:53:ASP:OD2	1:A:55:VAL:CG2	0.49	2.60	13	1
1:A:134:ILE:HG23	1:A:135:SER:N	0.49	2.23	14	7
1:A:79:LEU:HD21	1:A:109:VAL:CB	0.49	2.36	3	1
1:A:18:LEU:CD1	1:A:36:LEU:HD11	0.49	2.38	7	1
1:A:135:SER:O	1:A:138:ILE:HG22	0.49	2.08	7	1
1:A:51:TYR:O	1:A:60:SER:CB	0.49	2.61	18	2
1:A:145:PHE:CZ	1:A:147:PRO:HG3	0.48	2.43	2	5
1:A:135:SER:OG	1:A:147:PRO:CG	0.48	2.60	15	4
1:A:118:THR:CG2	1:A:119:ASP:N	0.48	2.76	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:TYR:O	1:A:131:THR:N	0.48	2.46	13	1
1:A:18:LEU:HD11	1:A:21:TRP:CE3	0.48	2.43	1	2
1:A:58:VAL:CG1	1:A:118:THR:HG21	0.48	2.38	6	2
1:A:62:LYS:HD3	1:A:112:TYR:CZ	0.48	2.43	7	4
1:A:51:TYR:O	1:A:51:TYR:CG	0.48	2.66	9	4
1:A:51:TYR:CZ	1:A:60:SER:HB3	0.48	2.42	12	11
1:A:81:THR:HG21	1:A:109:VAL:CG2	0.48	2.38	10	1
1:A:48:LEU:HD21	1:A:137:TYR:OH	0.48	2.09	11	2
1:A:48:LEU:CD1	1:A:141:PHE:CE1	0.48	2.96	14	1
1:A:92:ASN:OD1	1:A:143:LEU:HD12	0.48	2.09	19	4
1:A:7:TYR:CE2	1:A:130:LEU:HD11	0.48	2.43	5	3
1:A:134:ILE:O	1:A:138:ILE:CB	0.48	2.61	20	7
1:A:87:LEU:O	1:A:87:LEU:CD2	0.48	2.62	16	2
1:A:110:TYR:N	1:A:110:TYR:CD1	0.48	2.81	1	1
1:A:46:LEU:O	1:A:46:LEU:CD1	0.48	2.60	5	6
1:A:87:LEU:CD1	1:A:111:TYR:CD1	0.48	2.97	5	2
1:A:55:VAL:HG11	1:A:56:TYR:CE2	0.48	2.44	20	1
1:A:74:ILE:O	1:A:75:SER:CB	0.48	2.62	12	11
1:A:136:LEU:HD23	1:A:137:TYR:N	0.48	2.24	11	2
1:A:58:VAL:CG1	1:A:118:THR:CG2	0.48	2.92	6	1
1:A:121:ASN:N	1:A:121:ASN:HD22	0.48	2.06	9	1
1:A:132:ARG:CD	1:A:136:LEU:HD13	0.48	2.38	18	1
1:A:62:LYS:HD3	1:A:112:TYR:CE1	0.48	2.44	8	5
1:A:18:LEU:CD2	1:A:36:LEU:HD21	0.48	2.39	2	1
1:A:138:ILE:HG12	1:A:145:PHE:CE2	0.48	2.44	8	3
1:A:62:LYS:HD2	1:A:112:TYR:CZ	0.48	2.43	7	1
1:A:124:SER:O	1:A:125:ASP:C	0.48	2.52	20	1
1:A:7:TYR:CD1	1:A:7:TYR:C	0.47	2.87	11	12
1:A:67:SER:HB3	1:A:80:LEU:HD21	0.47	1.85	10	5
1:A:133:TRP:CD1	1:A:136:LEU:HD22	0.47	2.44	12	2
1:A:135:SER:HA	1:A:138:ILE:HG22	0.47	1.85	19	6
1:A:66:TRP:CH2	1:A:79:LEU:HB2	0.47	2.44	16	1
1:A:35:GLN:C	1:A:35:GLN:NE2	0.47	2.68	5	16
1:A:48:LEU:HD22	1:A:137:TYR:OH	0.47	2.09	4	1
1:A:46:LEU:HD11	1:A:141:PHE:CE2	0.47	2.45	12	1
1:A:129:TYR:O	1:A:133:TRP:N	0.47	2.47	9	17
1:A:90:ILE:N	1:A:90:ILE:CD1	0.47	2.72	13	2
1:A:59:PRO:HB2	1:A:133:TRP:CZ2	0.47	2.45	6	2
1:A:14:VAL:O	1:A:18:LEU:CD2	0.47	2.63	15	1
1:A:122:VAL:HG23	1:A:136:LEU:CD2	0.47	2.33	18	1
1:A:51:TYR:CG	1:A:51:TYR:O	0.47	2.67	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:61:ILE:HD13	1:A:137:TYR:CD1	0.47	2.45	1	2
1:A:110:TYR:HB2	1:A:112:TYR:CE2	0.47	2.45	8	5
1:A:118:THR:O	1:A:122:VAL:N	0.47	2.48	19	5
1:A:92:ASN:N	1:A:140:ILE:O	0.47	2.47	11	8
1:A:21:TRP:HB2	1:A:145:PHE:CE2	0.47	2.44	8	1
1:A:15:ARG:CB	1:A:34:LEU:CD2	0.47	2.93	16	1
1:A:3:THR:OG1	1:A:6:GLU:CG	0.47	2.63	6	10
1:A:40:LEU:HD12	1:A:90:ILE:HB	0.47	1.86	10	1
1:A:40:LEU:CD2	1:A:90:ILE:HD12	0.47	2.40	15	2
1:A:11:ILE:HD11	1:A:33:GLY:HA2	0.47	1.87	14	1
1:A:87:LEU:HD22	1:A:111:TYR:CZ	0.47	2.44	18	1
1:A:51:TYR:O	1:A:51:TYR:CD1	0.47	2.67	20	1
1:A:67:SER:N	1:A:78:ARG:O	0.47	2.48	4	6
1:A:21:TRP:CD2	1:A:24:VAL:HG23	0.47	2.45	2	5
1:A:93:LEU:O	1:A:95:THR:N	0.47	2.48	8	11
1:A:21:TRP:NE1	1:A:142:ASP:OD1	0.47	2.48	5	2
1:A:44:THR:CG2	1:A:66:TRP:O	0.47	2.63	18	3
1:A:63:PHE:CE2	1:A:141:PHE:CZ	0.47	3.03	10	1
1:A:134:ILE:CD1	1:A:137:TYR:CE2	0.47	2.96	20	4
1:A:91:LEU:HD23	1:A:91:LEU:N	0.47	2.25	13	1
1:A:18:LEU:CD1	1:A:36:LEU:CD2	0.47	2.93	16	1
1:A:132:ARG:O	1:A:132:ARG:CD	0.47	2.63	17	1
1:A:124:SER:O	1:A:126:VAL:N	0.46	2.48	11	2
1:A:96:PHE:CE2	1:A:140:ILE:HD11	0.46	2.45	13	2
1:A:7:TYR:CZ	1:A:11:ILE:CD1	0.46	2.96	4	3
1:A:98:VAL:CG2	1:A:99:THR:N	0.46	2.78	18	4
1:A:124:SER:O	1:A:126:VAL:HG23	0.46	2.10	1	1
1:A:51:TYR:CE1	1:A:60:SER:HB2	0.46	2.46	18	2
1:A:96:PHE:HZ	1:A:136:LEU:HD13	0.46	1.71	6	1
1:A:62:LYS:HB2	1:A:112:TYR:CD2	0.46	2.46	16	1
1:A:18:LEU:CD2	1:A:36:LEU:CD2	0.46	2.92	2	1
1:A:62:LYS:HD3	1:A:112:TYR:CE2	0.46	2.46	3	3
1:A:21:TRP:HE1	1:A:23:LYS:NZ	0.46	2.09	20	1
1:A:46:LEU:C	1:A:46:LEU:CD2	0.46	2.82	20	1
1:A:92:ASN:CG	1:A:143:LEU:CD1	0.46	2.83	2	3
1:A:138:ILE:HG12	1:A:145:PHE:CE1	0.46	2.46	14	2
1:A:7:TYR:CD2	1:A:59:PRO:HB3	0.46	2.45	6	1
1:A:118:THR:O	1:A:121:ASN:N	0.46	2.49	19	5
1:A:65:LEU:O	1:A:79:LEU:CD1	0.46	2.64	3	5
1:A:142:ASP:OD2	1:A:142:ASP:N	0.46	2.48	5	1
1:A:77:LEU:HD12	1:A:77:LEU:C	0.46	2.31	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:TYR:HB2	1:A:112:TYR:CE1	0.46	2.46	15	2
1:A:17:LEU:HD13	1:A:147:PRO:CG	0.46	2.40	19	2
1:A:30:VAL:CG2	1:A:33:GLY:C	0.46	2.84	15	6
1:A:53:ASP:OD1	1:A:55:VAL:HG22	0.46	2.10	5	1
1:A:53:ASP:OD1	1:A:55:VAL:CG2	0.46	2.64	7	3
1:A:100:LEU:HD12	1:A:110:TYR:C	0.46	2.30	14	2
1:A:84:ASP:O	1:A:87:LEU:N	0.46	2.49	10	3
1:A:61:ILE:HG13	1:A:137:TYR:CD1	0.46	2.46	2	1
1:A:66:TRP:CE2	1:A:79:LEU:HD13	0.46	2.45	2	4
1:A:61:ILE:HD11	1:A:137:TYR:CD2	0.46	2.46	20	1
1:A:47:GLU:OE1	1:A:49:HIS:NE2	0.46	2.49	2	2
1:A:21:TRP:NE1	1:A:23:LYS:CG	0.46	2.78	3	1
1:A:2:LEU:HD22	1:A:129:TYR:CD2	0.46	2.46	14	2
1:A:142:ASP:OD1	1:A:145:PHE:N	0.46	2.49	17	2
1:A:61:ILE:HD13	1:A:137:TYR:HB2	0.46	1.87	9	2
1:A:100:LEU:CD1	1:A:111:TYR:CZ	0.46	2.99	15	2
1:A:37:ASP:OD1	1:A:45:LEU:CD2	0.46	2.64	16	1
1:A:132:ARG:NE	1:A:136:LEU:CD1	0.46	2.78	18	1
1:A:33:GLY:CA	1:A:50:ILE:O	0.45	2.63	10	6
1:A:117:ASP:O	1:A:121:ASN:N	0.45	2.49	6	5
1:A:133:TRP:O	1:A:136:LEU:CB	0.45	2.65	7	1
1:A:137:TYR:O	1:A:140:ILE:N	0.45	2.48	17	4
1:A:21:TRP:CD1	1:A:23:LYS:HG3	0.45	2.46	20	1
1:A:115:ASN:O	1:A:115:ASN:ND2	0.45	2.50	7	6
1:A:122:VAL:O	1:A:124:SER:N	0.45	2.49	17	3
1:A:60:SER:OG	1:A:61:ILE:N	0.45	2.49	3	1
1:A:4:LEU:CD2	1:A:52:TYR:CB	0.45	2.94	6	1
1:A:100:LEU:HD22	1:A:111:TYR:CZ	0.45	2.45	8	1
1:A:117:ASP:O	1:A:120:ALA:N	0.45	2.50	9	1
1:A:11:ILE:HG23	1:A:34:LEU:CD1	0.45	2.42	10	1
1:A:47:GLU:OE2	1:A:49:HIS:CE1	0.45	2.70	11	1
1:A:21:TRP:CH2	1:A:138:ILE:HD11	0.45	2.45	15	3
1:A:129:TYR:O	1:A:132:ARG:N	0.45	2.48	13	1
1:A:25:GLU:OE2	1:A:39:ARG:NH2	0.45	2.50	5	2
1:A:59:PRO:O	1:A:115:ASN:ND2	0.45	2.50	3	9
1:A:62:LYS:HB2	1:A:112:TYR:CD1	0.45	2.46	5	1
1:A:18:LEU:CD1	1:A:36:LEU:CD1	0.45	2.93	7	1
1:A:10:GLN:NE2	1:A:130:LEU:HD23	0.45	2.26	9	1
1:A:24:VAL:HG22	1:A:38:VAL:HG22	0.45	1.88	14	1
1:A:39:ARG:NE	1:A:41:LYS:C	0.45	2.70	15	2
1:A:43:ASP:O	1:A:68:LEU:N	0.45	2.49	20	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:30:VAL:HG23	1:A:33:GLY:C	0.45	2.31	4	7
1:A:117:ASP:O	1:A:121:ASN:ND2	0.45	2.50	2	10
1:A:15:ARG:HB3	1:A:34:LEU:HD13	0.45	1.87	7	1
1:A:87:LEU:HD22	1:A:111:TYR:CE1	0.45	2.46	20	1
1:A:65:LEU:CD1	1:A:87:LEU:HD23	0.45	2.30	4	1
1:A:88:ARG:NE	1:A:91:LEU:O	0.45	2.50	8	1
1:A:40:LEU:CD1	1:A:46:LEU:CB	0.45	2.92	17	2
1:A:52:TYR:CE1	1:A:53:ASP:C	0.45	2.89	16	2
1:A:129:TYR:C	1:A:131:THR:N	0.45	2.67	13	1
1:A:3:THR:C	1:A:52:TYR:CE2	0.45	2.90	14	1
1:A:137:TYR:O	1:A:140:ILE:CG1	0.45	2.64	15	1
1:A:84:ASP:O	1:A:86:GLU:N	0.45	2.49	10	4
1:A:115:ASN:ND2	1:A:115:ASN:O	0.45	2.50	3	2
1:A:113:ILE:CG2	1:A:137:TYR:CE1	0.45	3.00	6	1
1:A:138:ILE:HG21	1:A:147:PRO:CD	0.45	2.42	7	1
1:A:7:TYR:CE2	1:A:59:PRO:HB3	0.45	2.46	6	1
1:A:61:ILE:HD12	1:A:137:TYR:CG	0.45	2.47	16	3
1:A:4:LEU:HA	1:A:52:TYR:CE1	0.45	2.47	3	1
1:A:28:GLN:CG	1:A:29:ASP:N	0.45	2.79	10	2
1:A:45:LEU:HD12	1:A:66:TRP:CD1	0.45	2.47	10	1
1:A:59:PRO:HB2	1:A:133:TRP:CH2	0.45	2.46	10	1
1:A:122:VAL:O	1:A:123:GLY:C	0.45	2.55	17	6
1:A:113:ILE:HG21	1:A:137:TYR:CD2	0.45	2.46	7	1
1:A:134:ILE:O	1:A:138:ILE:HB	0.45	2.12	20	4
1:A:84:ASP:O	1:A:88:ARG:N	0.45	2.50	4	4
1:A:38:VAL:O	1:A:45:LEU:CD2	0.45	2.63	20	2
1:A:99:THR:N	1:A:112:TYR:O	0.44	2.50	8	3
1:A:4:LEU:HD23	1:A:52:TYR:CB	0.44	2.41	5	2
1:A:47:GLU:CD	1:A:49:HIS:NE2	0.44	2.70	11	2
1:A:39:ARG:NE	1:A:41:LYS:O	0.44	2.49	15	2
1:A:2:LEU:HD11	1:A:7:TYR:HB2	0.44	1.89	5	1
1:A:51:TYR:O	1:A:60:SER:N	0.44	2.50	16	2
1:A:29:ASP:OD2	1:A:30:VAL:N	0.44	2.50	15	2
1:A:40:LEU:HD12	1:A:65:LEU:CD2	0.44	2.41	13	1
1:A:133:TRP:CZ3	1:A:137:TYR:CE2	0.44	3.04	20	1
1:A:66:TRP:CH2	1:A:79:LEU:HD13	0.44	2.47	4	1
1:A:52:TYR:OH	1:A:57:HIS:ND1	0.44	2.50	14	3
1:A:46:LEU:HD23	1:A:65:LEU:CD2	0.44	2.41	13	1
1:A:55:VAL:HG13	1:A:56:TYR:CE2	0.44	2.46	14	1
1:A:82:LEU:HD22	1:A:86:GLU:HB3	0.44	1.89	14	1
1:A:14:VAL:HG12	1:A:18:LEU:CD2	0.44	2.43	15	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:53:ASP:OD1	1:A:56:TYR:CD2	0.44	2.70	2	1
1:A:30:VAL:HG22	1:A:33:GLY:C	0.44	2.32	7	1
1:A:62:LYS:CD	1:A:112:TYR:CE2	0.44	3.01	15	1
1:A:10:GLN:NE2	1:A:127:GLU:O	0.44	2.51	8	4
1:A:45:LEU:O	1:A:66:TRP:N	0.44	2.50	1	1
1:A:64:ARG:HD3	1:A:110:TYR:CD2	0.44	2.48	5	2
1:A:128:HIS:CB	1:A:131:THR:OG1	0.44	2.65	19	1
1:A:17:LEU:HD11	1:A:134:ILE:HG12	0.44	1.88	20	1
1:A:45:LEU:HB2	1:A:68:LEU:HD11	0.44	1.89	20	1
1:A:63:PHE:CD1	1:A:63:PHE:C	0.44	2.91	1	1
1:A:53:ASP:O	1:A:57:HIS:N	0.44	2.50	3	1
1:A:100:LEU:HD13	1:A:111:TYR:CD2	0.44	2.47	8	1
1:A:142:ASP:CG	1:A:145:PHE:CB	0.44	2.86	5	1
1:A:61:ILE:HD13	1:A:137:TYR:CD2	0.44	2.44	6	1
1:A:122:VAL:HG22	1:A:136:LEU:HD22	0.44	1.81	18	2
1:A:25:GLU:CD	1:A:39:ARG:NH2	0.44	2.71	6	1
1:A:56:TYR:CE1	1:A:116:CYS:HB2	0.44	2.47	9	1
1:A:47:GLU:OE1	1:A:66:TRP:NE1	0.44	2.51	10	1
1:A:142:ASP:OD2	1:A:145:PHE:N	0.44	2.50	20	1
1:A:30:VAL:HG22	1:A:34:LEU:CA	0.44	2.43	14	3
1:A:45:LEU:HD12	1:A:46:LEU:H	0.44	1.63	6	3
1:A:96:PHE:CZ	1:A:136:LEU:HD13	0.44	2.47	6	1
1:A:82:LEU:H	1:A:82:LEU:HD23	0.44	1.72	18	2
1:A:134:ILE:CG2	1:A:135:SER:N	0.43	2.81	5	4
1:A:87:LEU:O	1:A:87:LEU:HD22	0.43	2.12	6	2
1:A:59:PRO:HG2	1:A:133:TRP:CD2	0.43	2.48	7	1
1:A:4:LEU:CD1	1:A:8:ASN:ND2	0.43	2.81	11	1
1:A:135:SER:O	1:A:139:ARG:NE	0.43	2.51	17	1
1:A:61:ILE:CD1	1:A:137:TYR:HB2	0.43	2.44	11	3
1:A:47:GLU:OE2	1:A:49:HIS:NE2	0.43	2.51	11	1
1:A:2:LEU:HD22	1:A:129:TYR:HD2	0.43	1.73	14	2
1:A:28:GLN:NE2	1:A:35:GLN:OE1	0.43	2.51	20	4
1:A:15:ARG:HB3	1:A:34:LEU:CD2	0.43	2.43	16	2
1:A:40:LEU:HD23	1:A:90:ILE:HD12	0.43	1.90	15	1
1:A:59:PRO:HG2	1:A:133:TRP:CE2	0.43	2.48	6	3
1:A:82:LEU:HD22	1:A:86:GLU:CB	0.43	2.43	14	1
1:A:32:ASP:OD2	1:A:32:ASP:N	0.43	2.50	4	1
1:A:56:TYR:CB	1:A:58:VAL:CG2	0.43	2.96	5	1
1:A:39:ARG:NH2	1:A:42:THR:O	0.43	2.51	7	1
1:A:122:VAL:HG11	1:A:129:TYR:CZ	0.43	2.48	11	1
1:A:119:ASP:OD2	1:A:119:ASP:N	0.43	2.51	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:113:ILE:HG21	1:A:137:TYR:CE1	0.43	2.47	6	1
1:A:4:LEU:HD11	1:A:8:ASN:ND2	0.43	2.28	11	1
1:A:100:LEU:C	1:A:100:LEU:CD2	0.43	2.87	16	2
1:A:21:TRP:HB3	1:A:24:VAL:HG23	0.43	1.90	6	2
1:A:117:ASP:OD1	1:A:117:ASP:N	0.43	2.52	14	1
1:A:84:ASP:C	1:A:86:GLU:N	0.43	2.70	10	4
1:A:55:VAL:HG23	1:A:56:TYR:CG	0.43	2.48	5	1
1:A:63:PHE:O	1:A:111:TYR:N	0.43	2.52	5	1
1:A:10:GLN:NE2	1:A:126:VAL:O	0.43	2.52	7	1
1:A:23:LYS:CB	1:A:38:VAL:HG13	0.43	2.43	7	1
1:A:142:ASP:OD2	1:A:145:PHE:CB	0.43	2.67	7	1
1:A:64:ARG:CD	1:A:109:VAL:O	0.43	2.66	2	1
1:A:128:HIS:CD2	1:A:128:HIS:N	0.43	2.86	2	2
1:A:122:VAL:CG2	1:A:136:LEU:CD2	0.43	2.93	7	1
1:A:20:LYS:O	1:A:22:ALA:N	0.43	2.52	8	1
1:A:99:THR:O	1:A:112:TYR:N	0.43	2.51	8	1
1:A:33:GLY:O	1:A:34:LEU:CD1	0.43	2.63	16	1
1:A:136:LEU:C	1:A:136:LEU:HD23	0.43	2.34	1	1
1:A:67:SER:CB	1:A:80:LEU:CD2	0.43	2.97	14	1
1:A:7:TYR:CA	1:A:130:LEU:HD21	0.42	2.43	11	2
1:A:47:GLU:OE2	1:A:66:TRP:NE1	0.42	2.51	4	2
1:A:137:TYR:C	1:A:139:ARG:N	0.42	2.71	17	4
1:A:60:SER:C	1:A:61:ILE:CG1	0.42	2.87	18	1
1:A:56:TYR:HB2	1:A:58:VAL:CG2	0.42	2.44	5	1
1:A:66:TRP:CZ3	1:A:79:LEU:CB	0.42	3.02	16	1
1:A:117:ASP:OD2	1:A:121:ASN:ND2	0.42	2.53	5	1
1:A:10:GLN:CB	1:A:130:LEU:HB2	0.42	2.45	8	6
1:A:4:LEU:HD21	1:A:32:ASP:OD2	0.42	2.14	10	2
1:A:66:TRP:CE3	1:A:79:LEU:CA	0.42	3.02	16	1
1:A:139:ARG:CZ	1:A:139:ARG:HB2	0.42	2.43	3	1
1:A:109:VAL:C	1:A:110:TYR:CD1	0.42	2.93	5	1
1:A:97:SER:O	1:A:98:VAL:HG23	0.42	2.15	12	1
1:A:129:TYR:O	1:A:130:LEU:C	0.42	2.57	13	1
1:A:63:PHE:CD1	1:A:111:TYR:HB2	0.42	2.50	1	1
1:A:98:VAL:HG22	1:A:99:THR:H	0.42	1.73	19	2
1:A:123:GLY:O	1:A:124:SER:C	0.42	2.58	10	5
1:A:132:ARG:O	1:A:133:TRP:C	0.42	2.58	13	1
1:A:3:THR:HG23	1:A:6:GLU:OE1	0.42	2.13	20	1
1:A:61:ILE:CD1	1:A:137:TYR:HB3	0.42	2.44	16	4
1:A:21:TRP:CE2	1:A:23:LYS:HB2	0.42	2.49	3	1
1:A:118:THR:HG22	1:A:129:TYR:CZ	0.42	2.50	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:16:SER:O	1:A:19:THR:OG1	0.42	2.36	5	2
1:A:4:LEU:CD2	1:A:52:TYR:CD2	0.42	2.98	9	1
1:A:135:SER:OG	1:A:147:PRO:CD	0.42	2.67	15	1
1:A:61:ILE:HD12	1:A:137:TYR:HB3	0.42	1.91	16	1
1:A:82:LEU:N	1:A:82:LEU:HD23	0.42	2.30	18	1
1:A:84:ASP:N	1:A:84:ASP:OD1	0.42	2.52	4	1
1:A:48:LEU:CD2	1:A:61:ILE:CG2	0.42	2.98	10	1
1:A:124:SER:OG	1:A:125:ASP:N	0.42	2.52	2	2
1:A:109:VAL:HG22	1:A:110:TYR:N	0.42	2.30	4	1
1:A:138:ILE:O	1:A:142:ASP:OD2	0.42	2.38	5	1
1:A:87:LEU:HG	1:A:111:TYR:CE1	0.42	2.50	19	1
1:A:35:GLN:CD	1:A:35:GLN:C	0.42	2.79	10	1
1:A:36:LEU:CD1	1:A:48:LEU:HD12	0.42	2.44	16	2
1:A:66:TRP:CZ3	1:A:79:LEU:N	0.42	2.88	16	1
1:A:46:LEU:HD22	1:A:47:GLU:N	0.42	2.30	20	1
1:A:17:LEU:HD12	1:A:18:LEU:HD23	0.41	1.92	5	1
1:A:18:LEU:O	1:A:21:TRP:N	0.41	2.53	8	1
1:A:87:LEU:HD23	1:A:87:LEU:C	0.41	2.36	8	1
1:A:35:GLN:C	1:A:35:GLN:CD	0.41	2.79	16	5
1:A:4:LEU:CD2	1:A:52:TYR:HB3	0.41	2.45	6	1
1:A:139:ARG:NH2	1:A:146:VAL:CG1	0.41	2.83	2	1
1:A:26:ARG:NH1	1:A:35:GLN:OE1	0.41	2.54	4	1
1:A:67:SER:HB3	1:A:80:LEU:CD2	0.41	2.46	10	2
1:A:61:ILE:HD11	1:A:137:TYR:CB	0.41	2.42	15	1
1:A:113:ILE:HD11	1:A:141:PHE:CE1	0.41	2.50	16	1
1:A:46:LEU:HD11	1:A:63:PHE:HB2	0.41	1.93	1	2
1:A:18:LEU:CD2	1:A:36:LEU:HD22	0.41	2.46	1	1
1:A:87:LEU:C	1:A:87:LEU:CD1	0.41	2.88	1	2
1:A:35:GLN:CD	1:A:35:GLN:O	0.41	2.59	2	2
1:A:63:PHE:CE1	1:A:91:LEU:HD11	0.41	2.50	10	1
1:A:48:LEU:C	1:A:49:HIS:CD2	0.41	2.94	11	1
1:A:88:ARG:C	1:A:90:ILE:N	0.41	2.73	12	1
1:A:88:ARG:O	1:A:91:LEU:O	0.41	2.39	5	4
1:A:21:TRP:CZ2	1:A:142:ASP:OD2	0.41	2.74	6	1
1:A:35:GLN:O	1:A:35:GLN:NE2	0.41	2.54	19	2
1:A:40:LEU:CD1	1:A:46:LEU:HB3	0.41	2.43	9	1
1:A:128:HIS:O	1:A:131:THR:OG1	0.41	2.38	13	1
1:A:122:VAL:C	1:A:124:SER:N	0.41	2.73	15	2
1:A:36:LEU:CD2	1:A:48:LEU:HD12	0.41	2.45	19	1
1:A:47:GLU:HG3	1:A:49:HIS:NE2	0.41	2.31	1	1
1:A:114:ASN:N	1:A:114:ASN:HD22	0.41	2.14	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:115:ASN:O	1:A:115:ASN:CG	0.41	2.59	12	3
1:A:122:VAL:HG12	1:A:124:SER:H	0.41	1.76	10	1
1:A:137:TYR:CD1	1:A:141:PHE:CE1	0.41	3.09	12	1
1:A:87:LEU:CD2	1:A:91:LEU:HG	0.41	2.46	16	1
1:A:115:ASN:O	1:A:118:THR:CB	0.41	2.69	18	1
1:A:142:ASP:O	1:A:142:ASP:OD2	0.41	2.39	19	1
1:A:21:TRP:CZ2	1:A:38:VAL:HG21	0.41	2.45	7	1
1:A:61:ILE:HD12	1:A:137:TYR:CB	0.41	2.46	16	1
1:A:37:ASP:OD1	1:A:47:GLU:OE2	0.40	2.40	1	1
1:A:7:TYR:HA	1:A:130:LEU:CD2	0.40	2.46	11	1
1:A:101:SER:HB3	1:A:110:TYR:CE1	0.40	2.51	11	1
1:A:100:LEU:HB2	1:A:111:TYR:CD1	0.40	2.51	12	1
1:A:40:LEU:CD1	1:A:46:LEU:HB2	0.40	2.47	14	1
1:A:47:GLU:CB	1:A:49:HIS:NE2	0.40	2.84	16	1
1:A:132:ARG:O	1:A:136:LEU:CB	0.40	2.69	1	1
1:A:52:TYR:OH	1:A:57:HIS:CG	0.40	2.74	14	1
1:A:2:LEU:HB2	1:A:126:VAL:HG13	0.40	1.93	17	1
1:A:64:ARG:HD2	1:A:110:TYR:CD2	0.40	2.51	18	1
1:A:30:VAL:CG2	1:A:34:LEU:N	0.40	2.84	20	1
1:A:80:LEU:O	1:A:81:THR:CG2	0.40	2.69	20	1
1:A:84:ASP:O	1:A:85:SER:C	0.40	2.60	2	2
1:A:65:LEU:HD12	1:A:111:TYR:OH	0.40	2.15	3	1
1:A:141:PHE:CD1	1:A:141:PHE:N	0.40	2.90	9	1
1:A:142:ASP:O	1:A:142:ASP:OD1	0.40	2.39	3	1
1:A:37:ASP:CG	1:A:47:GLU:OE1	0.40	2.60	8	1
1:A:3:THR:CB	1:A:5:PRO:HD2	0.40	2.47	9	1
1:A:17:LEU:HD12	1:A:18:LEU:HD22	0.40	1.93	10	1
1:A:98:VAL:HG22	1:A:113:ILE:HA	0.40	1.93	10	1
1:A:113:ILE:CD1	1:A:141:PHE:CE1	0.40	3.04	16	1
1:A:35:GLN:NE2	1:A:37:ASP:OD2	0.40	2.55	18	1
1:A:55:VAL:CG1	1:A:56:TYR:CZ	0.40	3.04	20	1
1:A:59:PRO:O	1:A:115:ASN:CG	0.40	2.60	20	1
1:A:56:TYR:CZ	1:A:116:CYS:HB2	0.40	2.51	1	1
1:A:113:ILE:O	1:A:114:ASN:C	0.40	2.59	2	1
1:A:2:LEU:HB2	1:A:126:VAL:CG2	0.40	2.45	9	1
1:A:40:LEU:HD23	1:A:46:LEU:CB	0.40	2.46	10	1
1:A:96:PHE:CG	1:A:140:ILE:HD11	0.40	2.52	12	1
1:A:39:ARG:CD	1:A:44:THR:O	0.40	2.70	13	1
1:A:46:LEU:HD21	1:A:63:PHE:CG	0.40	2.52	16	1
1:A:82:LEU:HD12	1:A:86:GLU:HB3	0.40	1.92	20	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	140/152 (92%)	121±2 (86±2%)	15±3 (10±2%)	4±1 (3±1%)	7 39
All	All	2800/3040 (92%)	2421 (86%)	293 (10%)	86 (3%)	7 39

All 14 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	94	GLY	17
1	A	32	ASP	14
1	A	73	ASP	12
1	A	83	SER	10
1	A	75	SER	8
1	A	31	GLN	6
1	A	2	LEU	5
1	A	123	GLY	3
1	A	85	SER	3
1	A	125	ASP	2
1	A	21	TRP	2
1	A	124	SER	2
1	A	96	PHE	1
1	A	130	LEU	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	136/146 (93%)	107±3 (79±2%)	29±3 (21±2%)	3 31
All	All	2720/2920 (93%)	2139 (79%)	581 (21%)	3 31

All 76 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	7	TYR	20
1	A	11	ILE	20
1	A	34	LEU	20
1	A	36	LEU	20
1	A	58	VAL	20
1	A	68	LEU	20
1	A	70	THR	20
1	A	74	ILE	20
1	A	76	SER	20
1	A	82	LEU	20
1	A	93	LEU	20
1	A	146	VAL	20
1	A	90	ILE	19
1	A	88	ARG	18
1	A	67	SER	16
1	A	110	TYR	12
1	A	32	ASP	12
1	A	136	LEU	12
1	A	114	ASN	11
1	A	45	LEU	11
1	A	137	TYR	10
1	A	4	LEU	9
1	A	26	ARG	9
1	A	39	ARG	9
1	A	73	ASP	8
1	A	10	GLN	8
1	A	128	HIS	8
1	A	62	LYS	8
1	A	49	HIS	8
1	A	1	MET	7
1	A	84	ASP	7
1	A	118	THR	7
1	A	142	ASP	7
1	A	37	ASP	6
1	A	121	ASN	6
1	A	145	PHE	6
1	A	132	ARG	6
1	A	78	ARG	5
1	A	87	LEU	5
1	A	71	GLU	5
1	A	64	ARG	5

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Mol	Chain	Res	Type	Models (Total)
1	A	18	LEU	5
1	A	47	GLU	4
1	A	52	TYR	4
1	A	60	SER	4
1	A	48	LEU	4
1	A	117	ASP	4
1	A	46	LEU	4
1	A	2	LEU	4
1	A	43	ASP	4
1	A	119	ASP	4
1	A	125	ASP	4
1	A	54	HIS	4
1	A	31	GLN	3
1	A	42	THR	3
1	A	108	SER	2
1	A	30	VAL	2
1	A	50	ILE	2
1	A	29	ASP	2
1	A	8	ASN	2
1	A	109	VAL	1
1	A	98	VAL	1
1	A	3	THR	1
1	A	19	THR	1
1	A	124	SER	1
1	A	28	GLN	1
1	A	97	SER	1
1	A	126	VAL	1
1	A	79	LEU	1
1	A	131	THR	1
1	A	21	TRP	1
1	A	135	SER	1
1	A	99	THR	1
1	A	53	ASP	1
1	A	75	SER	1
1	A	129	TYR	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 93% for the well-defined parts and 93% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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

Total number of shifts	1961
Number of shifts mapped to atoms	1961
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	8

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	148	-0.29 ± 0.11	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	145	-0.12 ± 0.12	None needed (< 0.5 ppm)
$^{13}C'$	140	0.15 ± 0.09	None needed (< 0.5 ppm)
^{15}N	141	0.04 ± 0.46	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 93%, i.e. 1884 atoms were assigned a chemical shift out of a possible 2029. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	686/700 (98%)	278/281 (99%)	274/282 (97%)	134/137 (98%)
Sidechain	1060/1144 (93%)	709/747 (95%)	333/358 (93%)	18/39 (46%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	138/185 (75%)	82/90 (91%)	53/88 (60%)	3/7 (43%)
Overall	1884/2029 (93%)	1069/1118 (96%)	660/728 (91%)	155/183 (85%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 93%, i.e. 1961 atoms were assigned a chemical shift out of a possible 2117. 0 out of 34 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	721/735 (98%)	292/295 (99%)	288/296 (97%)	141/144 (98%)
Sidechain	1102/1197 (92%)	737/781 (94%)	347/376 (92%)	18/40 (45%)
Aromatic	138/185 (75%)	82/90 (91%)	53/88 (60%)	3/7 (43%)
Overall	1961/2117 (93%)	1111/1166 (95%)	688/760 (91%)	162/191 (85%)

7.1.4 Statistically unusual chemical shifts (i)

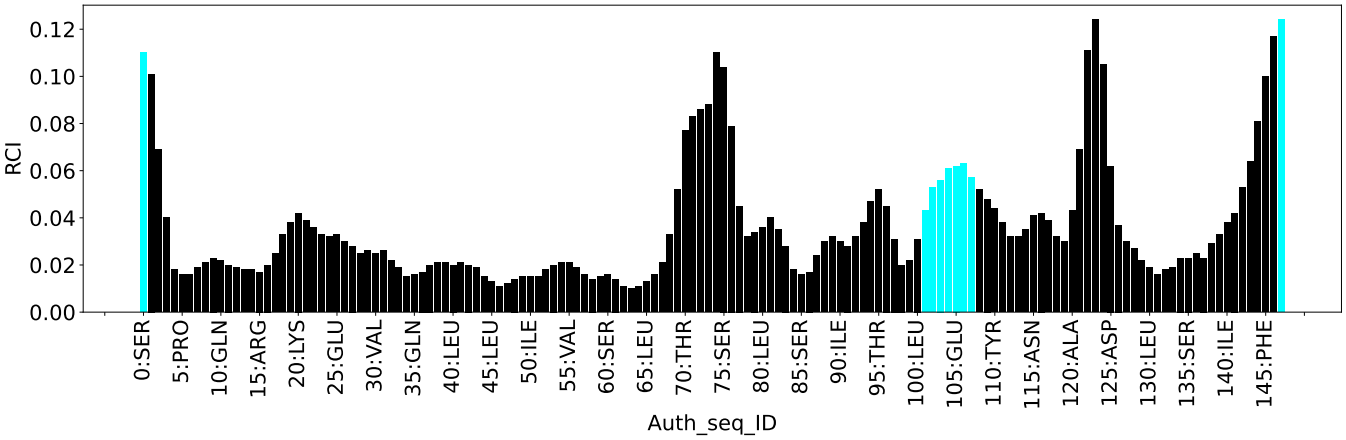
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	62	LYS	HE2	1.23	1.95 – 3.88	-8.7
1	A	23	LYS	HB2	-0.19	0.58 – 2.97	-8.2
1	A	60	SER	HB2	2.06	2.61 – 5.13	-7.2
1	A	62	LYS	HD2	0.26	0.58 – 2.64	-6.5
1	A	62	LYS	HE3	1.69	1.92 – 3.89	-6.2
1	A	59	PRO	HB3	-0.05	0.25 – 3.76	-5.8
1	A	111	TYR	HB2	0.90	1.09 – 4.72	-5.5
1	A	52	TYR	HB2	1.02	1.09 – 4.72	-5.2

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:


RCI
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0:SER
5:PRO
10:GLN
15:ARG
20:LYS
25:GLU
30:VAL
35:GLN
40:LEU
45:LEU
50:ILE
55:VAL
60:SER
65:LEU
70:THR
75:SER
80:LEU
85:SER
90:ILE
95:THR
100:LEU
105:GLU
110:TYR
115:ASN
120:ALA
125:ASP
130:LEU
135:SER
140:ILE
145:PHE
Auth_seq_ID

8 NMR restraints analysis (i)

8.1 Conformationally restricting restraints (i)

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	2901
Intra-residue (|i-j|=0)	763
Sequential (|i-j|=1)	780
Medium range (|i-j|>1 and |i-j|<5)	485
Long range (|i-j|≥5)	873
Inter-chain	0
Hydrogen bond restraints	0
Disulfide bond restraints	0
Total dihedral-angle restraints	0
Number of unmapped restraints	0
Number of restraints per residue	19.1
Number of long range restraints per residue[1]	5.7

[1]Long range hydrogen bonds and disulfide bonds are counted as long range restraints while calculating the number of long range restraints per residue

8.2 Residual restraint violations (i)

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 (i)

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)	1.4	0.19
0.2-0.5 (Medium)	0.1	0.29
>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)

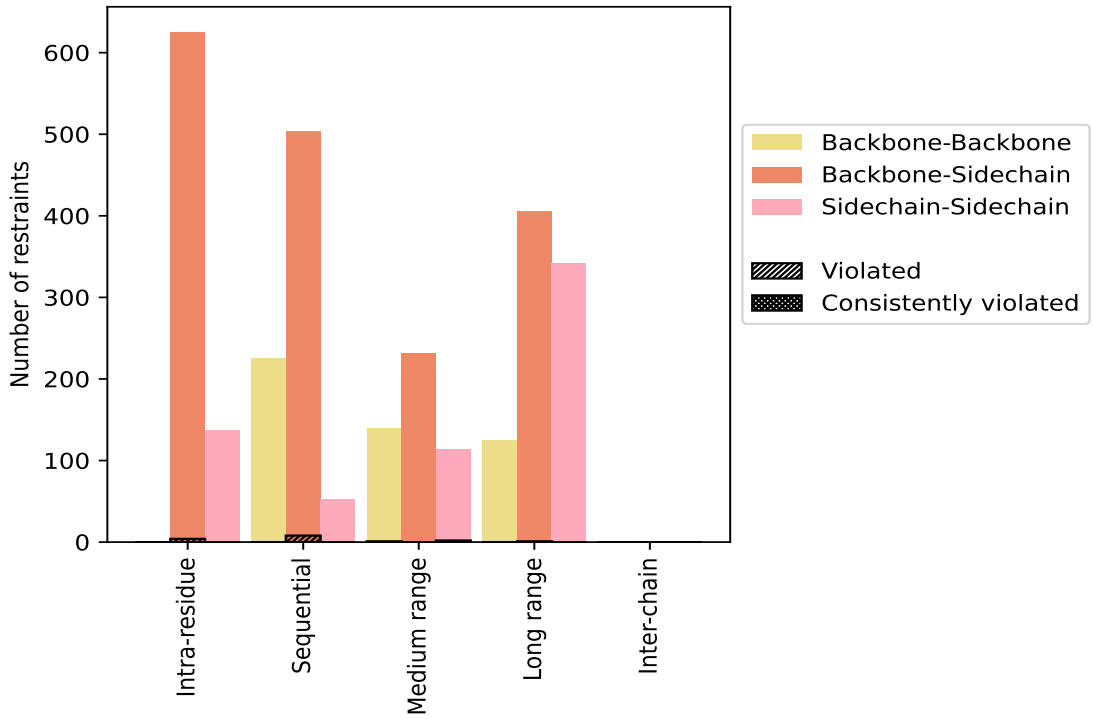
9.1 Summary of distance violations (i)

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)	763	26.3	4	0.5	0.1	0	0.0	0.0
Backbone-Backbone	1	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	625	21.5	4	0.6	0.1	0	0.0	0.0
Sidechain-Sidechain	137	4.7	0	0.0	0.0	0	0.0	0.0
Sequential (|i-j|=1)	780	26.9	8	1.0	0.3	0	0.0	0.0
Backbone-Backbone	225	7.8	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	503	17.3	8	1.6	0.3	0	0.0	0.0
Sidechain-Sidechain	52	1.8	0	0.0	0.0	0	0.0	0.0
Medium range (|i-j|>1 & |i-j|<5)	485	16.7	3	0.6	0.1	0	0.0	0.0
Backbone-Backbone	140	4.8	1	0.7	0.0	0	0.0	0.0
Backbone-Sidechain	231	8.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	114	3.9	2	1.8	0.1	0	0.0	0.0
Long range (|i-j|≥5)	873	30.1	1	0.1	0.0	0	0.0	0.0
Backbone-Backbone	125	4.3	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	406	14.0	1	0.2	0.0	0	0.0	0.0
Sidechain-Sidechain	342	11.8	0	0.0	0.0	0	0.0	0.0
Inter-chain	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Backbone	0	0.0	0	0.0	0.0	0	0.0	0.0
Backbone-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Sidechain-Sidechain	0	0.0	0	0.0	0.0	0	0.0	0.0
Hydrogen bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Disulfide bond	0	0.0	0	0.0	0.0	0	0.0	0.0
Total	2901	100.0	16	0.6	0.6	0	0.0	0.0
Backbone-Backbone	491	16.9	1	0.2	0.0	0	0.0	0.0
Backbone-Sidechain	1765	60.8	13	0.7	0.4	0	0.0	0.0
Sidechain-Sidechain	645	22.2	2	0.3	0.1	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 (i)



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 (i)

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

Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
1	0	0	0	0	0	0	0.0	0.0	0.0	0.0
2	2	0	1	0	0	3	0.13	0.15	0.02	0.12
3	1	0	0	0	0	1	0.19	0.19	0.0	0.19
4	0	1	0	0	0	1	0.13	0.13	0.0	0.13
5	0	1	0	0	0	1	0.14	0.14	0.0	0.14
6	0	0	0	0	0	0	0.0	0.0	0.0	0.0
7	1	0	0	1	0	2	0.14	0.15	0.01	0.14
8	0	2	0	0	0	2	0.14	0.14	0.0	0.14
9	0	1	0	0	0	1	0.13	0.13	0.0	0.13
10	1	0	1	0	0	2	0.18	0.22	0.04	0.18
11	0	1	0	0	0	1	0.12	0.12	0.0	0.12

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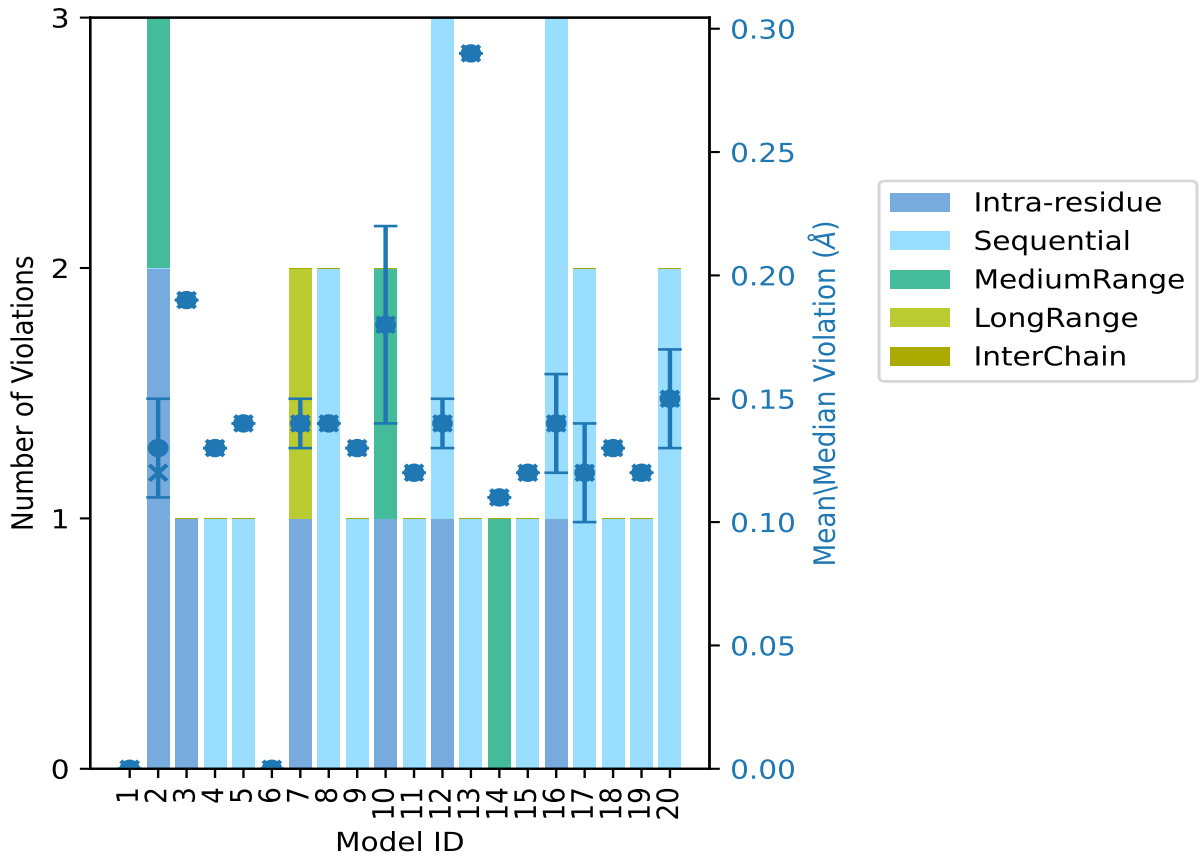
Model ID	Number of violations						Mean (Å)	Max (Å)	SD[6] (Å)	Median (Å)
	IR[1]	SQ[2]	MR[3]	LR[4]	IC[5]	Total				
12	1	2	0	0	0	3	0.14	0.15	0.01	0.14
13	0	1	0	0	0	1	0.29	0.29	0.0	0.29
14	0	0	1	0	0	1	0.11	0.11	0.0	0.11
15	0	1	0	0	0	1	0.12	0.12	0.0	0.12
16	1	2	0	0	0	3	0.14	0.16	0.02	0.14
17	0	2	0	0	0	2	0.12	0.14	0.02	0.12
18	0	1	0	0	0	1	0.13	0.13	0.0	0.13
19	0	1	0	0	0	1	0.12	0.12	0.0	0.12
20	0	2	0	0	0	2	0.15	0.16	0.02	0.15

[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 (i)



The mean(dot),median(x) and the standard deviation are shown in blue with respect to the y axis on the right

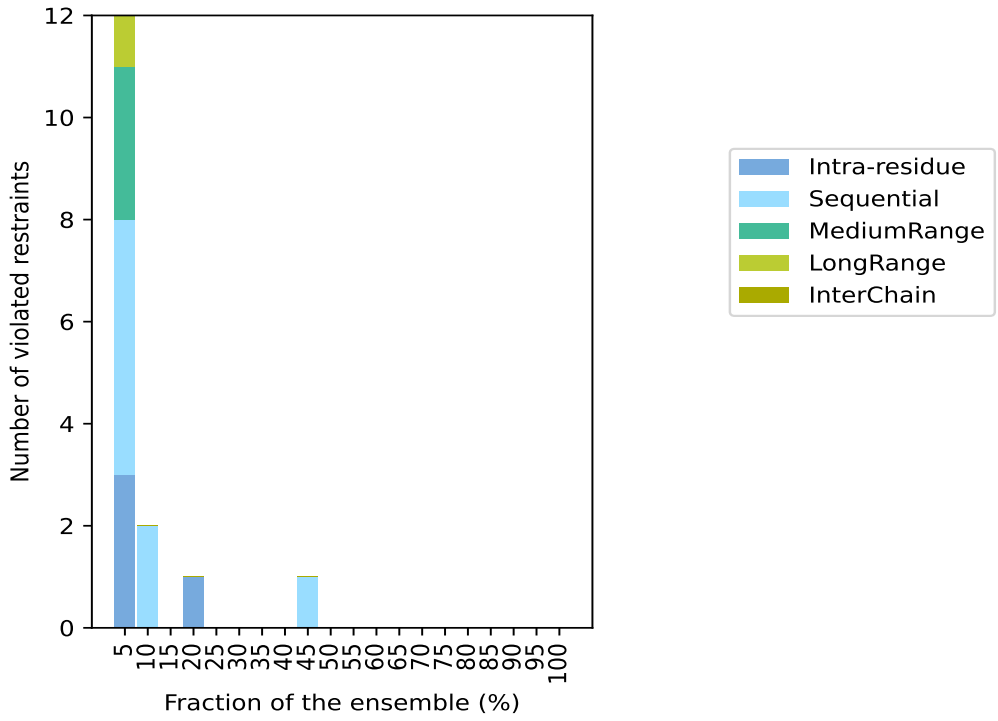
9.3 Distance violation statistics for the ensemble (i)

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, 2885(IR:759, SQ:772, MR:482, LR:872, 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]	%
3	5	3	1	0	12	1	5.0
0	2	0	0	0	2	2	10.0
0	0	0	0	0	0	3	15.0
1	0	0	0	0	1	4	20.0
0	0	0	0	0	0	5	25.0
0	0	0	0	0	0	6	30.0
0	0	0	0	0	0	7	35.0
0	0	0	0	0	0	8	40.0
0	1	0	0	0	1	9	45.0
0	0	0	0	0	0	10	50.0
0	0	0	0	0	0	11	55.0
0	0	0	0	0	0	12	60.0
0	0	0	0	0	0	13	65.0
0	0	0	0	0	0	14	70.0
0	0	0	0	0	0	15	75.0
0	0	0	0	0	0	16	80.0
0	0	0	0	0	0	17	85.0
0	0	0	0	0	0	18	90.0
0	0	0	0	0	0	19	95.0
0	0	0	0	0	0	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

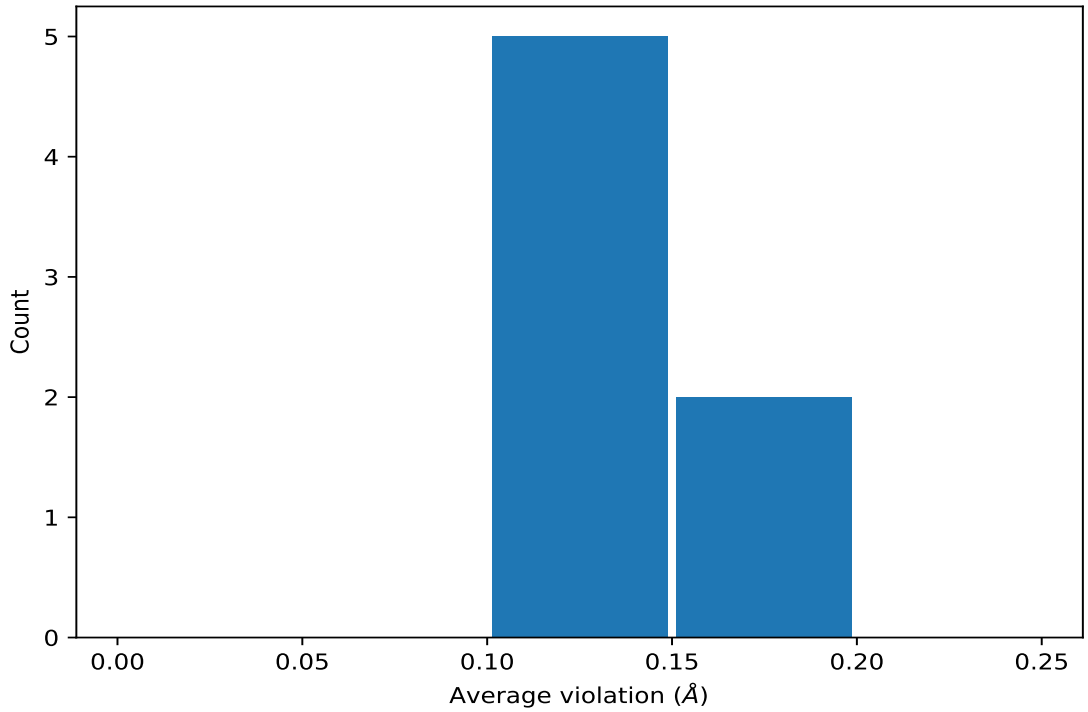
9.3.1 Bar graph : Distance violation statistics for the ensemble (i)



9.4 Most violated distance restraints in the ensemble (i)

9.4.1 Histogram : Distribution of mean distance violations (i)

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



9.4.2 Table: Most violated distance restraints (i)

The following table provides the mean and the standard deviation of the violation for each restraint sorted by number of violated models and the mean value. The Key (restraint list ID, restraint ID) is the unique identifier for a given restraint. Rows with same key represent combinatorial or ambiguous restraints and are counted as a single restraint.

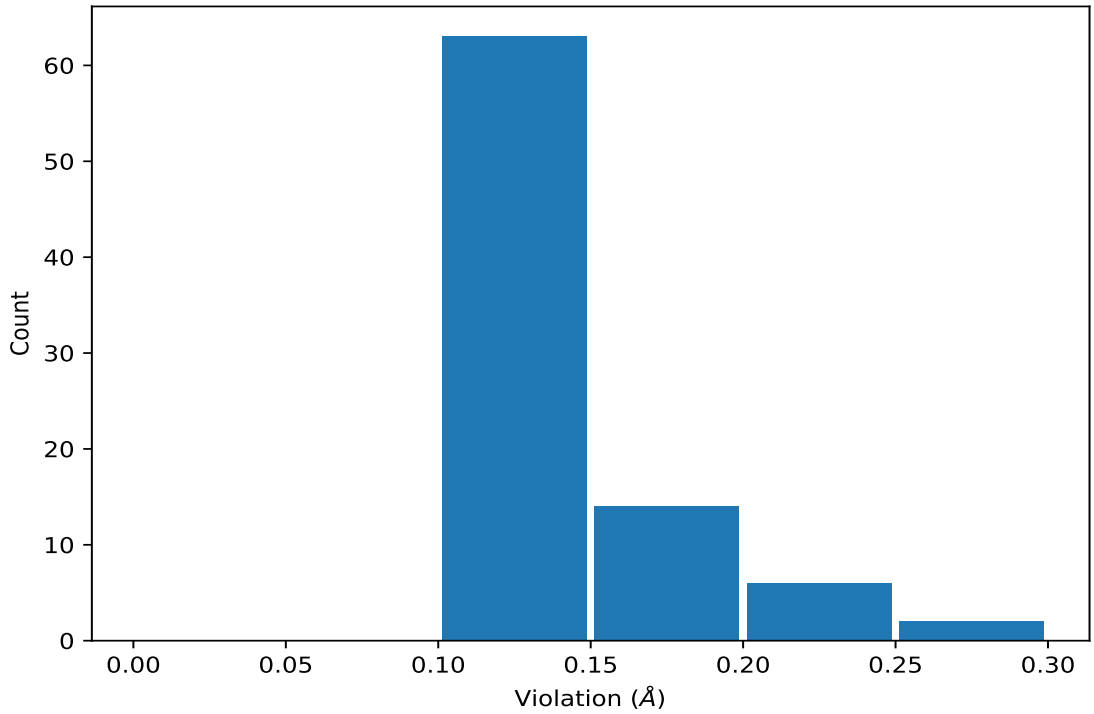
Key	Atom-1	Atom-2	Models[1]	Mean (Å)	SD[1] (Å)	Median (Å)
(1,1814)	1:A:92:ASN:HA	1:A:93:LEU:HG	9	0.13	0.01	0.13
(1,2651)	1:A:73:ASP:H	1:A:73:ASP:HB2	4	0.14	0.01	0.14
(1,2651)	1:A:73:ASP:H	1:A:73:ASP:HB3	4	0.14	0.01	0.14
(1,2399)	1:A:37:ASP:HB2	1:A:38:VAL:H	2	0.16	0.01	0.16
(1,2399)	1:A:37:ASP:HB3	1:A:38:VAL:H	2	0.16	0.01	0.16
(1,142)	1:A:144:ASN:H	1:A:145:PHE:HD1	2	0.13	0.01	0.13
(1,142)	1:A:144:ASN:H	1:A:145:PHE:HD2	2	0.13	0.01	0.13

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

9.5 All violated distance restraints (i)

9.5.1 Histogram : Distribution of distance violations (i)

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



9.5.2 Table : All distance violations (i)

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

Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2782)	1:A:106:MET:HB2	1:A:107:LYS:H	13	0.29
(1,2782)	1:A:106:MET:HB3	1:A:107:LYS:H	13	0.29
(1,2411)	1:A:38:VAL:HG11	1:A:40:LEU:HG	10	0.22
(1,2411)	1:A:38:VAL:HG12	1:A:40:LEU:HG	10	0.22
(1,2411)	1:A:38:VAL:HG13	1:A:40:LEU:HG	10	0.22
(1,2411)	1:A:38:VAL:HG21	1:A:40:LEU:HG	10	0.22
(1,2411)	1:A:38:VAL:HG22	1:A:40:LEU:HG	10	0.22
(1,2411)	1:A:38:VAL:HG23	1:A:40:LEU:HG	10	0.22
(1,1408)	1:A:3:THR:H	1:A:3:THR:HG21	3	0.19
(1,1408)	1:A:3:THR:H	1:A:3:THR:HG22	3	0.19
(1,1408)	1:A:3:THR:H	1:A:3:THR:HG23	3	0.19
(1,2831)	1:A:125:ASP:HB2	1:A:126:VAL:H	20	0.16
(1,2831)	1:A:125:ASP:HB3	1:A:126:VAL:H	20	0.16
(1,2399)	1:A:37:ASP:HB2	1:A:38:VAL:H	16	0.16
(1,2399)	1:A:37:ASP:HB3	1:A:38:VAL:H	16	0.16
(1,2651)	1:A:73:ASP:H	1:A:73:ASP:HB2	2	0.15

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2651)	1:A:73:ASP:H	1:A:73:ASP:HB3	2	0.15
(1,2399)	1:A:37:ASP:HB2	1:A:38:VAL:H	12	0.15
(1,2399)	1:A:37:ASP:HB3	1:A:38:VAL:H	12	0.15
(1,1198)	1:A:61:ILE:HA	1:A:113:ILE:HD11	7	0.15
(1,1198)	1:A:61:ILE:HA	1:A:113:ILE:HD12	7	0.15
(1,1198)	1:A:61:ILE:HA	1:A:113:ILE:HD13	7	0.15
(1,703)	1:A:31:GLN:HG2	1:A:32:ASP:H	5	0.14
(1,2651)	1:A:73:ASP:H	1:A:73:ASP:HB2	16	0.14
(1,2651)	1:A:73:ASP:H	1:A:73:ASP:HB3	16	0.14
(1,1959)	1:A:40:LEU:HA	1:A:40:LEU:HG	10	0.14
(1,1814)	1:A:92:ASN:HA	1:A:93:LEU:HG	8	0.14
(1,1814)	1:A:92:ASN:HA	1:A:93:LEU:HG	17	0.14
(1,1652)	1:A:136:LEU:HG	1:A:137:TYR:H	8	0.14
(1,142)	1:A:144:ASN:H	1:A:145:PHE:HD1	12	0.14
(1,142)	1:A:144:ASN:H	1:A:145:PHE:HD2	12	0.14
(1,2651)	1:A:73:ASP:H	1:A:73:ASP:HB2	7	0.13
(1,2651)	1:A:73:ASP:H	1:A:73:ASP:HB3	7	0.13
(1,1814)	1:A:92:ASN:HA	1:A:93:LEU:HG	4	0.13
(1,1814)	1:A:92:ASN:HA	1:A:93:LEU:HG	9	0.13
(1,1814)	1:A:92:ASN:HA	1:A:93:LEU:HG	18	0.13
(1,1814)	1:A:92:ASN:HA	1:A:93:LEU:HG	20	0.13
(1,2651)	1:A:73:ASP:H	1:A:73:ASP:HB2	12	0.12
(1,2651)	1:A:73:ASP:H	1:A:73:ASP:HB3	12	0.12
(1,2391)	1:A:36:LEU:HD11	1:A:38:VAL:HG11	2	0.12
(1,2391)	1:A:36:LEU:HD11	1:A:38:VAL:HG12	2	0.12
(1,2391)	1:A:36:LEU:HD11	1:A:38:VAL:HG13	2	0.12
(1,2391)	1:A:36:LEU:HD11	1:A:38:VAL:HG21	2	0.12
(1,2391)	1:A:36:LEU:HD11	1:A:38:VAL:HG22	2	0.12
(1,2391)	1:A:36:LEU:HD11	1:A:38:VAL:HG23	2	0.12
(1,2391)	1:A:36:LEU:HD12	1:A:38:VAL:HG11	2	0.12
(1,2391)	1:A:36:LEU:HD12	1:A:38:VAL:HG12	2	0.12
(1,2391)	1:A:36:LEU:HD12	1:A:38:VAL:HG13	2	0.12
(1,2391)	1:A:36:LEU:HD12	1:A:38:VAL:HG21	2	0.12
(1,2391)	1:A:36:LEU:HD12	1:A:38:VAL:HG22	2	0.12
(1,2391)	1:A:36:LEU:HD12	1:A:38:VAL:HG23	2	0.12
(1,2391)	1:A:36:LEU:HD13	1:A:38:VAL:HG11	2	0.12
(1,2391)	1:A:36:LEU:HD13	1:A:38:VAL:HG12	2	0.12
(1,2391)	1:A:36:LEU:HD13	1:A:38:VAL:HG13	2	0.12
(1,2391)	1:A:36:LEU:HD13	1:A:38:VAL:HG21	2	0.12
(1,2391)	1:A:36:LEU:HD13	1:A:38:VAL:HG22	2	0.12
(1,2391)	1:A:36:LEU:HD13	1:A:38:VAL:HG23	2	0.12
(1,2391)	1:A:36:LEU:HD21	1:A:38:VAL:HG11	2	0.12

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Key	Atom-1	Atom-2	Model ID	Violation (Å)
(1,2391)	1:A:36:LEU:HD21	1:A:38:VAL:HG12	2	0.12
(1,2391)	1:A:36:LEU:HD21	1:A:38:VAL:HG13	2	0.12
(1,2391)	1:A:36:LEU:HD21	1:A:38:VAL:HG21	2	0.12
(1,2391)	1:A:36:LEU:HD21	1:A:38:VAL:HG22	2	0.12
(1,2391)	1:A:36:LEU:HD21	1:A:38:VAL:HG23	2	0.12
(1,2391)	1:A:36:LEU:HD22	1:A:38:VAL:HG11	2	0.12
(1,2391)	1:A:36:LEU:HD22	1:A:38:VAL:HG12	2	0.12
(1,2391)	1:A:36:LEU:HD22	1:A:38:VAL:HG13	2	0.12
(1,2391)	1:A:36:LEU:HD22	1:A:38:VAL:HG21	2	0.12
(1,2391)	1:A:36:LEU:HD22	1:A:38:VAL:HG22	2	0.12
(1,2391)	1:A:36:LEU:HD22	1:A:38:VAL:HG23	2	0.12
(1,2391)	1:A:36:LEU:HD23	1:A:38:VAL:HG11	2	0.12
(1,2391)	1:A:36:LEU:HD23	1:A:38:VAL:HG12	2	0.12
(1,2391)	1:A:36:LEU:HD23	1:A:38:VAL:HG13	2	0.12
(1,2391)	1:A:36:LEU:HD23	1:A:38:VAL:HG21	2	0.12
(1,2391)	1:A:36:LEU:HD23	1:A:38:VAL:HG22	2	0.12
(1,2391)	1:A:36:LEU:HD23	1:A:38:VAL:HG23	2	0.12
(1,1814)	1:A:92:ASN:HA	1:A:93:LEU:HG	11	0.12
(1,1814)	1:A:92:ASN:HA	1:A:93:LEU:HG	15	0.12
(1,142)	1:A:144:ASN:H	1:A:145:PHE:HD1	19	0.12
(1,142)	1:A:144:ASN:H	1:A:145:PHE:HD2	19	0.12
(1,815)	1:A:13:ASN:HA	1:A:17:LEU:H	14	0.11
(1,1814)	1:A:92:ASN:HA	1:A:93:LEU:HG	16	0.11
(1,1409)	1:A:3:THR:HG21	1:A:4:LEU:H	17	0.11
(1,1409)	1:A:3:THR:HG22	1:A:4:LEU:H	17	0.11
(1,1409)	1:A:3:THR:HG23	1:A:4:LEU:H	17	0.11
(1,1033)	1:A:36:LEU:H	1:A:36:LEU:HG	2	0.11

10 Dihedral-angle violation analysis (i)

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