Full wwPDB NMR Structure Validation Report (i)

Feb 13, 2022 – 08:17 PM EST

PDB ID	:	1I6Z
Title	:	BAG DOMAIN OF BAG1 COCHAPERONE
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Deposited on	:	2001-03-06

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

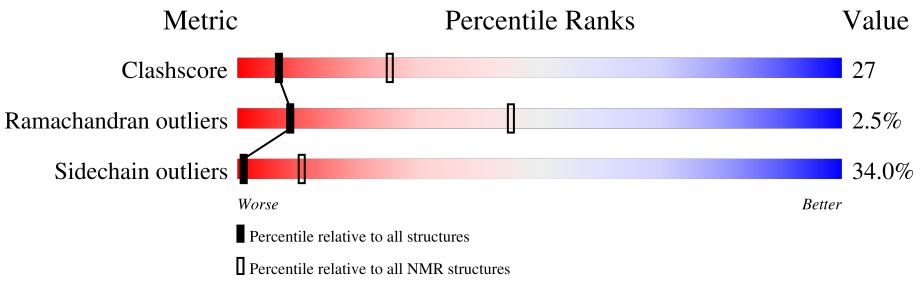
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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 was not calculated.

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	135	25% 54% • 18%

2 Ensemble composition and analysis (i)

This entry contains 25 models. Model 12 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:98-A:208 (111)	0.70	12

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 2 clusters and 1 single-model cluster was found.

Cluster number	Models
1	1, 2, 3, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 16, 17, 18, 19, 20, 21, 22, 24, 25
2	4, 23
Single-model clusters	15

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2207 atoms, of which 1123 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	135	2207	683	1123	180	215	6	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	85	GLY	-	cloning artifact	UNP Q60739
A	86	SER	-	cloning artifact	UNP Q60739
A	87	PRO	-	cloning artifact	UNP Q60739
A	88	GLU	-	cloning artifact	UNP Q60739
A	89	PHE	-	cloning artifact	UNP Q60739

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: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

Chain A: 25% 54% • 18%

G85 S86 P87 E88 F89 M90 L91 I92 G93 E94 K95 S96 N97 P98 E99 E100 E101 V102 E103 L104 K105 K106 L107 K108 D109 L110 E111 V112 S113 A114 E115 K116 I117 A118 N119 H120 L121 L124 N125 K126 E127 L128 Q132 Q133 G134 F135 L136 A137 K138 E139 L140 Q141 A142 E143 A144 L145 C146 K147

L148 D149 R150 K151 V152 K153 A154 T155 I156 E157 Q158 F159 M160 K161 I162 L163 I166 V170 L171 P172 E173 Q174 F175 K176 D177 S178 R179 L180 K181 R182 K183 N184 L185 V186 K187 K188 V189 Q190 V191 F192 L193 A194 E195 C196 D197 T198 V199 E200 Q201 Y202 I203 T207 E208 R209 L210 Q211 S212

T213 N214 L215 A216 L217 A218 E219

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: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

Chain A: 38% 32% 13% 18%

G85 S86 P87 E88 F89 M90 L91 I92 G93 E94 K95 S96 N97 P98 E99 E100 L104 K105 K106 L107 K108 D109 L110 E111 V112 S113 A114 E115 K116 I117 H120 L121 L124 N125 K126 S129 F135 L136 A137 K138 E139 L140 Q141 A142 L145 C146 K147 L148 D149 R150 K151 V152 K153

I156 E157 Q158 F159 M160 K161 I162 L163 M169 V170 L171 S178 R179 L180 K181 R182 L185 V186 K187 K188 V189 L193 A194 E195 C196 V199 E200 Q201 Y202 I203 T207 E208 R209 L210 Q211 S212 T213 N214 L215 A216 L217 A218 E219

4.2.2 Score per residue for model 2

• Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

Chain A: 30% 41% 12% 18%

G85 S86 P87 E88 F89 M90 L91 I92 G93 E94 K95 S96 N97 P98 E99 E100 L104 K105 K106 L107 K108 D109 L110 E111 V112 S113 A114 E115 K116 I117 A118 N119 H120 L121 Q122 E123 L124 N125 K126 E127 L128 S129 G130 I131 Q132 Q133 G134 F135 L136 A137 K138 Q141 A142 L145 C146 K147 L148

D149 R150 K151 V152 K153 A154 T155 I156 E157 Q158 F159 M160 K161 I162 L163 D167 T168 M169 E173 Q174 F175 K176 D177 S178 R179 L180 K181 R182 L185 V186 K187 K188 V189 Q190 V191 F192 L193 A194 E195 C196 E200 Q201 Y202 I203 T207 E208 R209 L210 Q211 S212 T213 N214 L215 A216 L217

A218 E219

4.2.3 Score per residue for model 3

• Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

Chain A: 27% 42% 13% 18%

G85 S86 P87 E88 F89 M90 L91 I92 G93 E94 K95 S96 N97 P98 E99 E100 E101 V102 E103 L104 K105 K106 L107 K108 D109 L110 E111 V112 S113 A114 E115 K116 I117 A118 N119 H120 L121 Q122 E123 L124 N125 K126 E127 L128 Q132 Q133 L136 L140 Q141 A144 L145 C146 K147 L148 D149 R150

K151 V152 K153 A154 T155 I156 E157 Q158 F159 M160 K161 I162 L163 I166 M169 V170 L171 Q174 F175 K176 D177 S178 R179 L180 K181 R182 L185 V186 K187 K188 V189 Q190 V191 F192 L193 A194 E195 C196 V199 E200 Q201 Y202 I203 C204 Q205 E206 T207 E208 R209 L210 Q211 S212 T213 N214 L215

A216 L217 A218 E219

4.2.4 Score per residue for model 4

• Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

Chain A: 31% 39% 12% 18%

G85 S86 P87 E88 F89 M90 L91 I92 G93 E94 K95 S96 N97 P98 E99 E100 E103 L104 K105 K106 L107 K108 D109 L110 E111 V112 S113 A114 E115 K116 I117 A118 N119 H120 L121 Q122 E123 L124 N125 K126 E127 L128 I131 Q132 Q133 G134 F135 L136 L140 Q141 A142 E143 A144 L145 C146 K147 L148

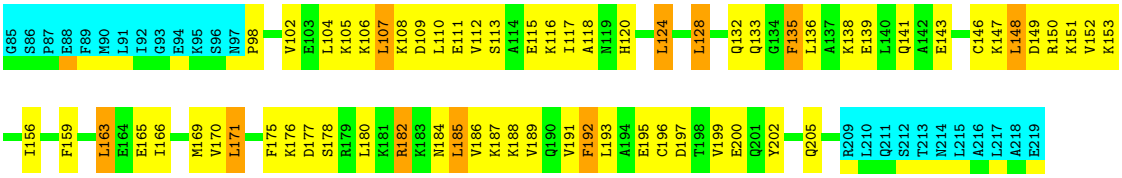
D149 R150 K151 V152 T155 I156 E157 Q158 F159 M160 K161 I162 L163 T168 M169 V170 L171 P172 E173 K176 D177 S178 R179 L180 K181 R182 L185 V186 K187 K188 V189 F192 L193 A194 E195 C196 D197 T198 V199 E200 Q201 C204 Q205 E206 T207 E208 R209 L210 Q211 S212 T213 N214 L215 A216

L217 A218 E219

4.2.5 Score per residue for model 5

• Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

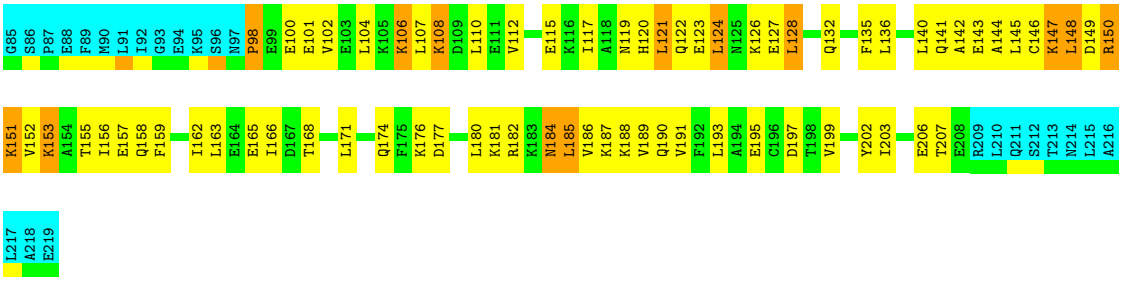
Chain A: 34% 41% 7% 18%



4.2.6 Score per residue for model 6

- Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

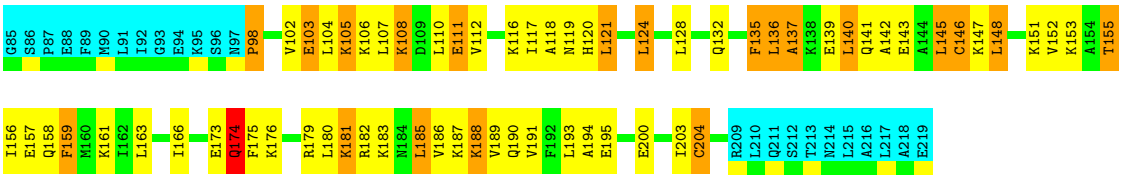
Chain A: 30% 43% 10% 18%



4.2.7 Score per residue for model 7

- Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

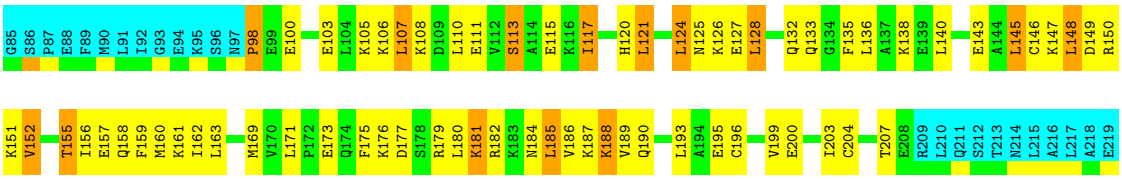
Chain A: 34% 33% 15% • 18%



4.2.8 Score per residue for model 8

- Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

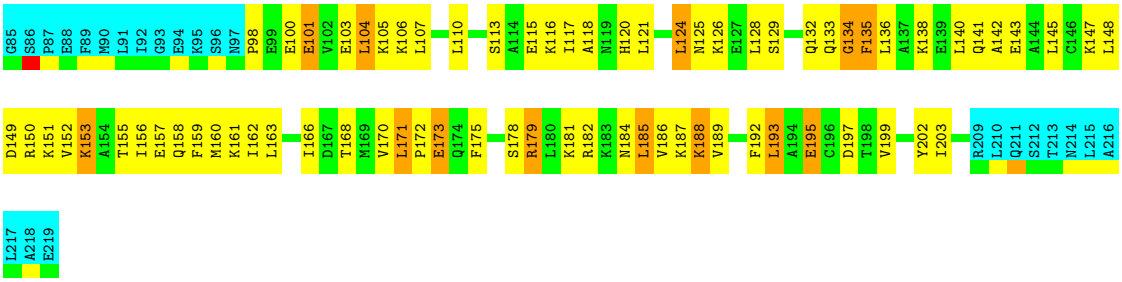
Chain A: 32% 40% 10% 18%



4.2.9 Score per residue for model 9

• Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

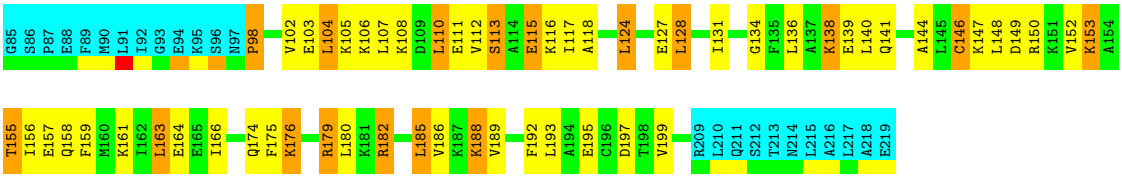
Chain A: 29% 44% 10% 18%



4.2.10 Score per residue for model 10

• Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

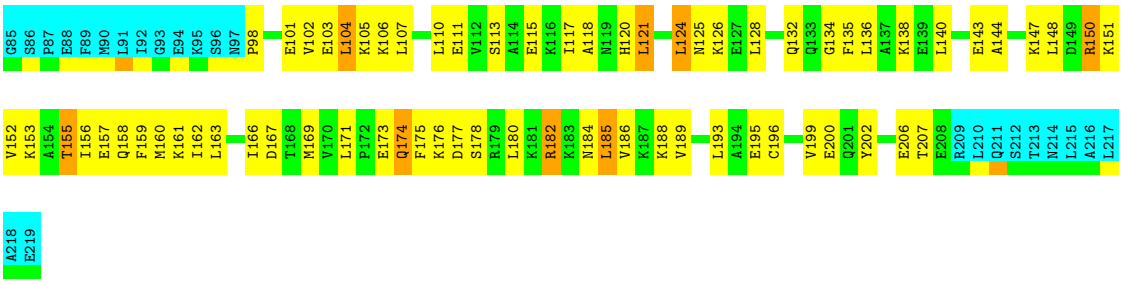
Chain A: 39% 30% 13% 18%



4.2.11 Score per residue for model 11

• Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

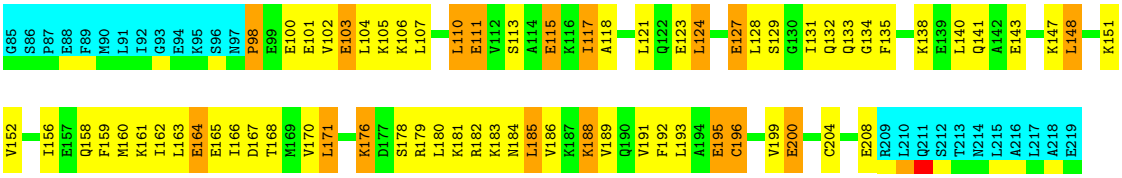
Chain A: 32% 44% 6% 18%



4.2.12 Score per residue for model 12 (medoid)

• Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

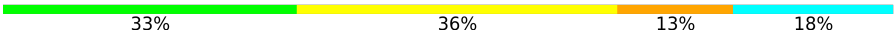
Chain A: 31% 39% 13% 18%

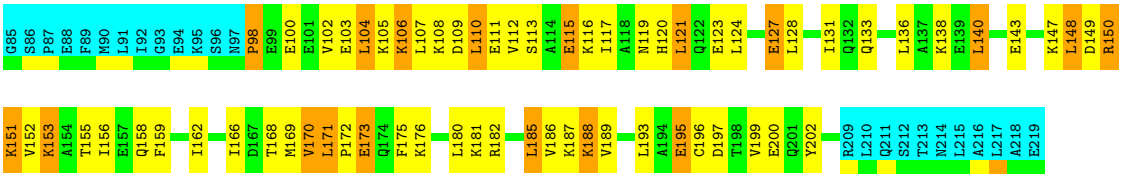


4.2.13 Score per residue for model 13

- Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

Chain A:

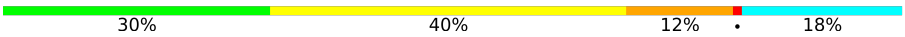


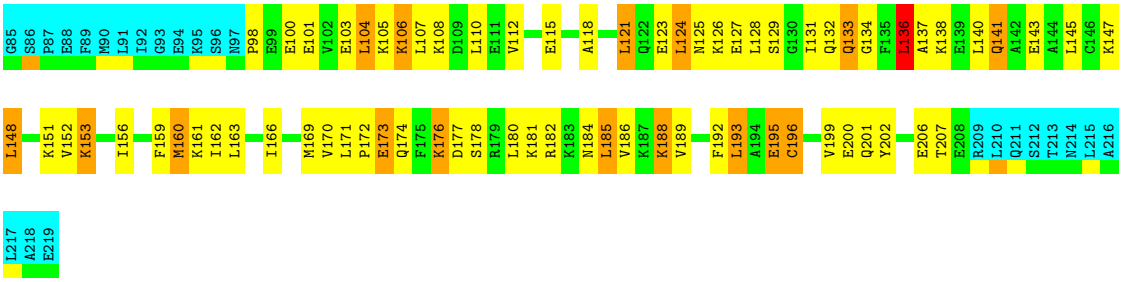


4.2.14 Score per residue for model 14

- Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

Chain A:

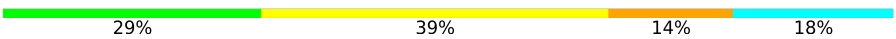


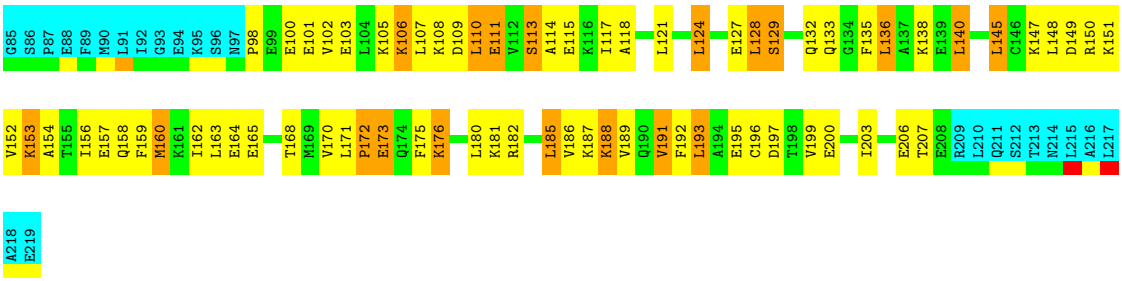


4.2.15 Score per residue for model 15

- Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

Chain A:

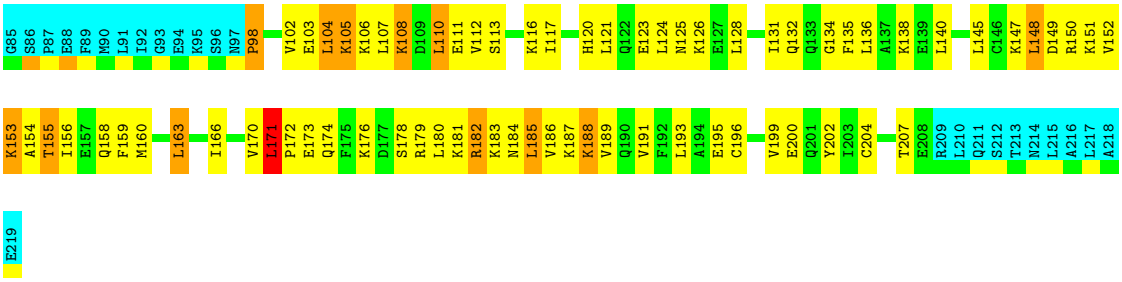




4.2.16 Score per residue for model 16

• Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

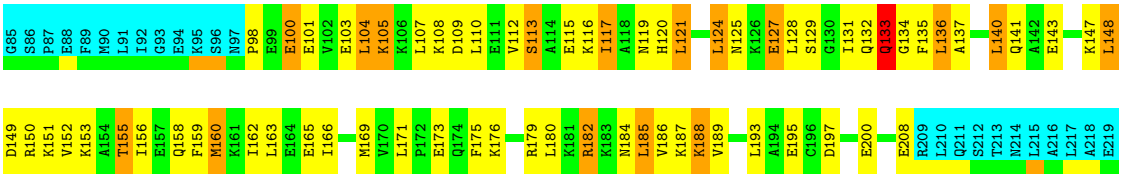
Chain A: 30% 43% 9% • 18%



4.2.17 Score per residue for model 17

• Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

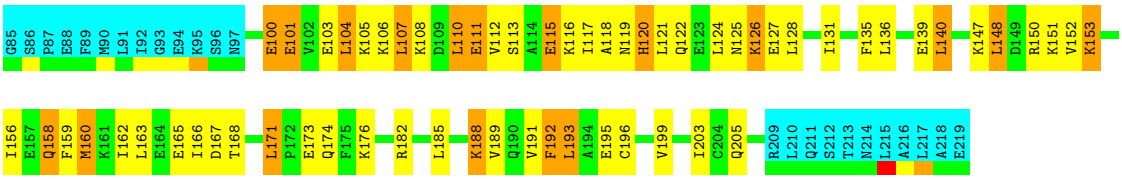
Chain A: 32% 38% 12% • 18%



4.2.18 Score per residue for model 18

• Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

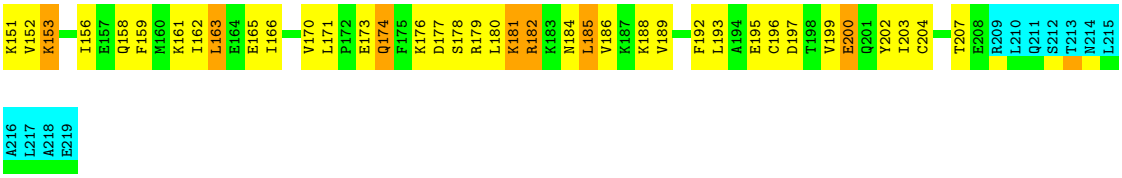
Chain A: 36% 33% 13% 18%



4.2.19 Score per residue for model 19

• Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

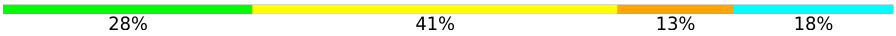
Chain A: 26% 46% 10% 18%

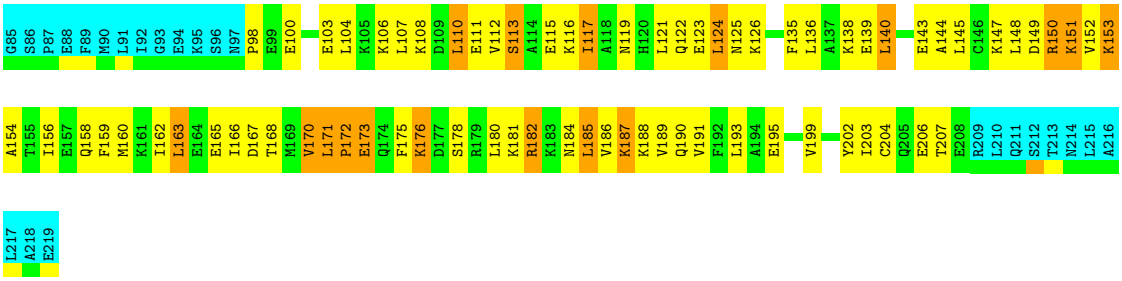


4.2.20 Score per residue for model 20

- Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

Chain A:

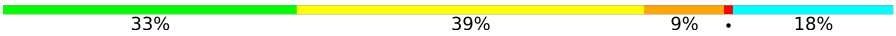


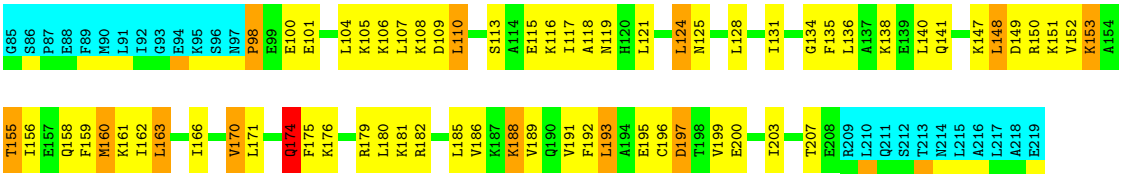


4.2.21 Score per residue for model 21

- Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

Chain A:

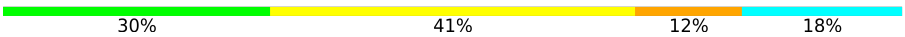


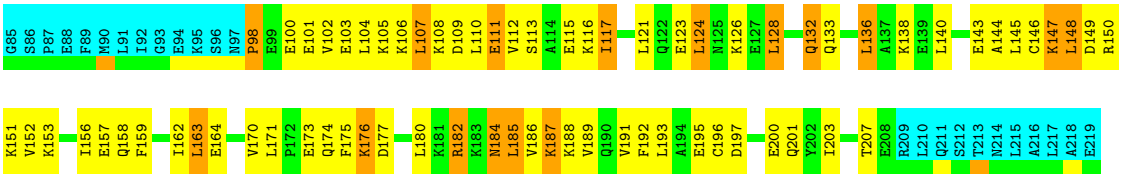


4.2.22 Score per residue for model 22

- Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

Chain A:

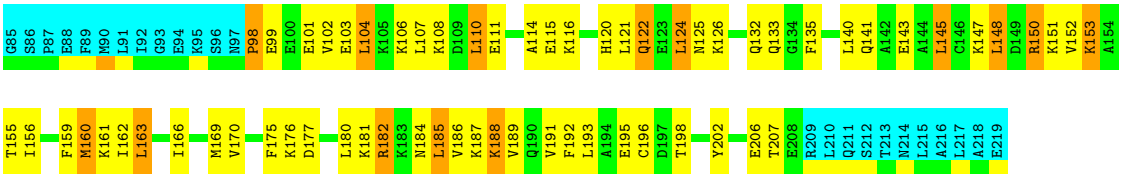




4.2.23 Score per residue for model 23

• Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

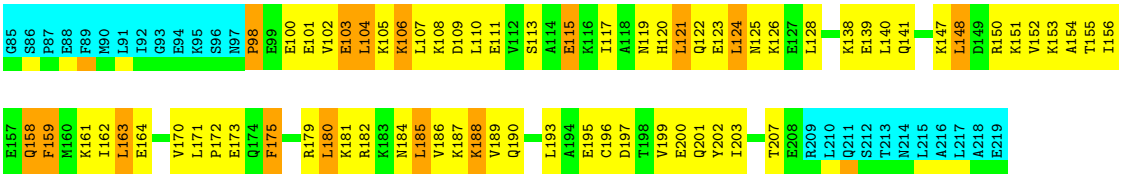
Chain A: 35% 37% 10% 18%



4.2.24 Score per residue for model 24

• Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

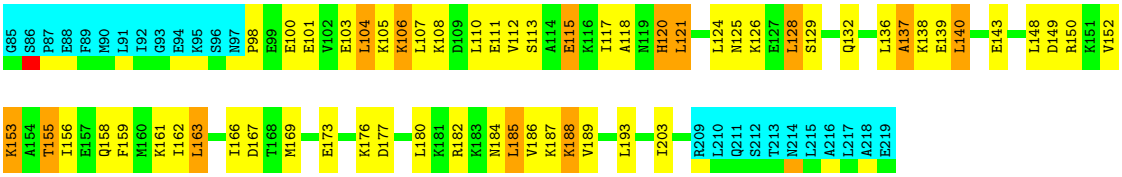
Chain A: 30% 41% 11% 18%



4.2.25 Score per residue for model 25

• Molecule 1: BAG-FAMILY MOLECULAR CHAPERONE REGULATOR-1

Chain A: 39% 33% 10% 18%



5 Refinement protocol and experimental data overview (i)

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

Of the 25 calculated structures, 25 were deposited, based on the following criterion: *all calculated structures submitted*.

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

Software name	Classification	Version
CNS	structure solution	1.0
CNS	refinement	1.0

No chemical shift data was provided.

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	902	939	938	50±7
All	All	22550	23475	23450	1260

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 27.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:LEU:HD12	1:A:155:THR:HG21	1.06	1.26	7	5
1:A:163:LEU:HD21	1:A:186:VAL:HG13	1.03	1.30	19	6
1:A:128:LEU:HD13	1:A:131:ILE:HD11	0.97	1.35	4	5
1:A:159:PHE:CG	1:A:193:LEU:HD21	0.93	1.98	2	1
1:A:128:LEU:HD23	1:A:148:LEU:HD23	0.90	1.39	11	2
1:A:110:LEU:HD21	1:A:162:ILE:HG21	0.90	1.39	17	2
1:A:121:LEU:HD11	1:A:152:VAL:HG13	0.89	1.43	3	4
1:A:185:LEU:O	1:A:189:VAL:HG23	0.88	1.68	16	23
1:A:156:ILE:HG23	1:A:193:LEU:HD11	0.88	1.44	7	2
1:A:156:ILE:HA	1:A:193:LEU:HD21	0.88	1.46	24	2
1:A:156:ILE:HG23	1:A:193:LEU:HD21	0.87	1.44	8	5
1:A:182:ARG:O	1:A:186:VAL:HG23	0.84	1.72	19	24
1:A:110:LEU:HD21	1:A:162:ILE:CG2	0.83	2.02	17	12
1:A:107:LEU:HD21	1:A:185:LEU:HD23	0.81	1.53	5	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:108:LYS:O	1:A:112:VAL:HG23	0.80	1.75	25	15
1:A:156:ILE:HA	1:A:193:LEU:HD12	0.80	1.54	2	1
1:A:107:LEU:HD12	1:A:108:LYS:N	0.79	1.91	15	6
1:A:178:SER:O	1:A:181:LYS:HG2	0.79	1.78	19	1
1:A:145:LEU:HD13	1:A:146:CYS:N	0.79	1.92	7	1
1:A:121:LEU:HD12	1:A:155:THR:CG2	0.79	2.07	7	1
1:A:156:ILE:CG2	1:A:193:LEU:HD23	0.78	2.07	3	5
1:A:152:VAL:HG11	1:A:200:GLU:OE2	0.78	1.78	11	1
1:A:195:GLU:O	1:A:198:THR:HG22	0.78	1.77	23	1
1:A:148:LEU:O	1:A:152:VAL:HG23	0.78	1.79	4	23
1:A:189:VAL:O	1:A:193:LEU:HD12	0.77	1.78	15	4
1:A:124:LEU:HD12	1:A:128:LEU:HD23	0.77	1.56	4	3
1:A:195:GLU:O	1:A:199:VAL:HG23	0.76	1.78	13	19
1:A:107:LEU:HD22	1:A:107:LEU:O	0.76	1.79	2	7
1:A:145:LEU:HD21	1:A:204:CYS:HA	0.76	1.57	7	2
1:A:98:PRO:O	1:A:102:VAL:HG23	0.76	1.80	6	14
1:A:125:ASN:OD1	1:A:199:VAL:HG11	0.75	1.81	14	1
1:A:144:ALA:O	1:A:148:LEU:HD13	0.75	1.80	20	1
1:A:124:LEU:HD12	1:A:125:ASN:N	0.75	1.95	16	2
1:A:152:VAL:HG21	1:A:200:GLU:CG	0.75	2.11	2	3
1:A:156:ILE:HG22	1:A:193:LEU:HD23	0.75	1.58	4	5
1:A:163:LEU:CD2	1:A:186:VAL:HG13	0.75	2.12	14	6
1:A:124:LEU:CD1	1:A:128:LEU:HD22	0.75	2.12	11	1
1:A:171:LEU:HD23	1:A:175:PHE:CZ	0.74	2.17	13	1
1:A:128:LEU:HD12	1:A:148:LEU:HG	0.74	1.59	15	1
1:A:135:PHE:O	1:A:136:LEU:HD12	0.74	1.82	11	1
1:A:144:ALA:O	1:A:148:LEU:HD12	0.74	1.83	19	3
1:A:128:LEU:HD23	1:A:148:LEU:CD2	0.74	2.13	11	2
1:A:171:LEU:HD13	1:A:172:PRO:HD2	0.74	1.60	16	1
1:A:153:LYS:HA	1:A:156:ILE:HD12	0.73	1.60	21	15
1:A:185:LEU:HA	1:A:188:LYS:HD3	0.73	1.61	8	21
1:A:189:VAL:HG12	1:A:193:LEU:HD12	0.73	1.59	14	5
1:A:171:LEU:HD23	1:A:175:PHE:CE2	0.73	2.18	13	1
1:A:144:ALA:C	1:A:148:LEU:HD12	0.73	2.04	19	3
1:A:118:ALA:HB1	1:A:192:PHE:CZ	0.73	2.18	14	1
1:A:107:LEU:HD13	1:A:108:LYS:N	0.73	1.99	18	7
1:A:145:LEU:HD21	1:A:203:ILE:O	0.73	1.83	3	4
1:A:156:ILE:HG23	1:A:193:LEU:CD2	0.73	2.14	12	9
1:A:145:LEU:HD21	1:A:203:ILE:HG22	0.72	1.61	19	3
1:A:103:GLU:O	1:A:107:LEU:HD13	0.72	1.84	17	2
1:A:124:LEU:HD12	1:A:128:LEU:HD13	0.72	1.60	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:LEU:HD23	1:A:125:ASN:OD1	0.72	1.84	2	2
1:A:189:VAL:O	1:A:193:LEU:HD23	0.72	1.84	2	1
1:A:110:LEU:CD1	1:A:166:ILE:HD11	0.72	2.14	5	4
1:A:121:LEU:HD13	1:A:196:CYS:SG	0.72	2.24	8	3
1:A:107:LEU:CD2	1:A:185:LEU:HD22	0.72	2.15	1	1
1:A:117:ILE:HD13	1:A:158:GLN:HB2	0.71	1.62	18	2
1:A:121:LEU:HD21	1:A:196:CYS:SG	0.71	2.26	2	2
1:A:148:LEU:HD12	1:A:203:ILE:HD13	0.71	1.62	25	3
1:A:104:LEU:HA	1:A:107:LEU:HD12	0.71	1.60	7	9
1:A:145:LEU:HD11	1:A:204:CYS:O	0.70	1.85	4	1
1:A:121:LEU:HB2	1:A:155:THR:HG21	0.70	1.62	23	2
1:A:148:LEU:CD1	1:A:203:ILE:HD13	0.70	2.17	9	4
1:A:159:PHE:CD2	1:A:193:LEU:HD21	0.70	2.22	2	1
1:A:117:ILE:HD11	1:A:159:PHE:CE1	0.70	2.21	6	6
1:A:118:ALA:HB1	1:A:192:PHE:CE1	0.70	2.21	14	5
1:A:164:GLU:O	1:A:168:THR:HG23	0.70	1.86	12	2
1:A:145:LEU:HD12	1:A:203:ILE:CG2	0.69	2.17	9	1
1:A:152:VAL:HG21	1:A:200:GLU:OE1	0.69	1.87	11	2
1:A:121:LEU:HD21	1:A:152:VAL:HG22	0.69	1.61	25	2
1:A:111:GLU:HB3	1:A:185:LEU:HD11	0.69	1.65	22	1
1:A:128:LEU:HD11	1:A:148:LEU:HD21	0.69	1.61	24	2
1:A:145:LEU:HD11	1:A:203:ILE:O	0.69	1.88	8	1
1:A:189:VAL:HG12	1:A:193:LEU:CD1	0.69	2.18	1	5
1:A:152:VAL:HG13	1:A:196:CYS:SG	0.68	2.28	14	2
1:A:176:LYS:O	1:A:180:LEU:HD13	0.68	1.88	22	10
1:A:127:GLU:O	1:A:131:ILE:HG23	0.68	1.88	17	6
1:A:152:VAL:HG11	1:A:196:CYS:O	0.68	1.89	14	7
1:A:171:LEU:HD22	1:A:172:PRO:HD3	0.68	1.66	16	1
1:A:145:LEU:O	1:A:145:LEU:HD22	0.68	1.88	7	1
1:A:111:GLU:CB	1:A:185:LEU:HD11	0.67	2.18	22	3
1:A:160:MET:HG2	1:A:193:LEU:HD11	0.67	1.64	8	6
1:A:128:LEU:HD21	1:A:148:LEU:CG	0.67	2.19	24	1
1:A:166:ILE:HG21	1:A:186:VAL:HG22	0.67	1.66	13	3
1:A:188:LYS:HD3	1:A:189:VAL:N	0.67	2.05	3	2
1:A:121:LEU:CD1	1:A:155:THR:HG21	0.67	2.14	7	2
1:A:148:LEU:HD13	1:A:203:ILE:HD13	0.67	1.67	21	2
1:A:136:LEU:HD23	1:A:140:LEU:HB3	0.67	1.65	14	2
1:A:121:LEU:HD13	1:A:125:ASN:OD1	0.67	1.89	21	1
1:A:128:LEU:CD2	1:A:148:LEU:HD22	0.66	2.20	19	2
1:A:176:LYS:O	1:A:180:LEU:HD12	0.66	1.90	15	4
1:A:121:LEU:HD23	1:A:124:LEU:HD11	0.66	1.66	16	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:163:LEU:HD23	1:A:189:VAL:HB	0.66	1.68	23	3
1:A:185:LEU:HD13	1:A:188:LYS:HD2	0.66	1.68	15	2
1:A:163:LEU:HB2	1:A:189:VAL:HG11	0.65	1.67	15	12
1:A:122:GLN:HA	1:A:125:ASN:ND2	0.65	2.05	23	5
1:A:145:LEU:HD23	1:A:207:THR:OG1	0.65	1.91	22	1
1:A:187:LYS:O	1:A:191:VAL:HG23	0.65	1.91	16	4
1:A:156:ILE:CA	1:A:193:LEU:HD21	0.65	2.22	24	2
1:A:163:LEU:HD23	1:A:189:VAL:CB	0.65	2.22	10	2
1:A:110:LEU:CD2	1:A:162:ILE:HG23	0.65	2.21	1	4
1:A:128:LEU:HD22	1:A:148:LEU:HD23	0.65	1.68	3	1
1:A:107:LEU:HD22	1:A:182:ARG:HB3	0.65	1.67	7	2
1:A:124:LEU:CD1	1:A:128:LEU:HD13	0.65	2.22	24	2
1:A:121:LEU:HD11	1:A:196:CYS:SG	0.64	2.32	24	4
1:A:145:LEU:CD2	1:A:203:ILE:HG22	0.64	2.22	19	4
1:A:128:LEU:HG	1:A:148:LEU:HD21	0.64	1.68	16	3
1:A:152:VAL:HG21	1:A:200:GLU:HB2	0.64	1.67	8	1
1:A:103:GLU:OE1	1:A:171:LEU:HD11	0.64	1.92	18	1
1:A:160:MET:HG3	1:A:193:LEU:HD21	0.64	1.69	9	2
1:A:163:LEU:HD11	1:A:190:GLN:OE1	0.64	1.92	20	2
1:A:124:LEU:O	1:A:124:LEU:HD12	0.64	1.93	5	13
1:A:124:LEU:HD11	1:A:148:LEU:HD11	0.64	1.68	5	2
1:A:128:LEU:HD22	1:A:128:LEU:O	0.63	1.92	5	2
1:A:185:LEU:HD13	1:A:188:LYS:CD	0.63	2.24	9	1
1:A:110:LEU:HD13	1:A:166:ILE:HD11	0.63	1.70	21	2
1:A:136:LEU:HG	1:A:140:LEU:HD13	0.63	1.70	14	4
1:A:124:LEU:HD12	1:A:128:LEU:HD22	0.63	1.70	11	1
1:A:118:ALA:HB2	1:A:159:PHE:CZ	0.63	2.29	2	3
1:A:107:LEU:O	1:A:185:LEU:HD21	0.63	1.94	11	4
1:A:170:VAL:O	1:A:171:LEU:HD12	0.63	1.94	4	4
1:A:128:LEU:HD21	1:A:147:LYS:HE2	0.62	1.71	22	2
1:A:122:GLN:HA	1:A:125:ASN:OD1	0.62	1.95	3	1
1:A:145:LEU:HD13	1:A:207:THR:OG1	0.62	1.95	20	5
1:A:100:GLU:O	1:A:104:LEU:HB2	0.62	1.94	21	5
1:A:112:VAL:HG13	1:A:115:GLU:OE2	0.62	1.95	18	2
1:A:128:LEU:HB3	1:A:148:LEU:HD21	0.61	1.71	4	1
1:A:200:GLU:O	1:A:203:ILE:HG22	0.61	1.95	8	1
1:A:152:VAL:HG11	1:A:200:GLU:CD	0.61	2.16	11	1
1:A:128:LEU:CD1	1:A:148:LEU:HD21	0.61	2.25	2	1
1:A:145:LEU:HD22	1:A:145:LEU:C	0.61	2.16	7	1
1:A:136:LEU:HD13	1:A:140:LEU:HD22	0.61	1.71	22	2
1:A:163:LEU:HD11	1:A:190:GLN:HG2	0.60	1.72	24	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:124:LEU:C	1:A:124:LEU:HD12	0.60	2.17	23	2
1:A:156:ILE:CG2	1:A:193:LEU:HD11	0.60	2.21	7	1
1:A:136:LEU:HD13	1:A:140:LEU:HB3	0.60	1.71	10	2
1:A:103:GLU:O	1:A:106:LYS:HG2	0.60	1.97	4	8
1:A:147:LYS:CD	1:A:148:LEU:N	0.60	2.65	6	1
1:A:124:LEU:HD12	1:A:124:LEU:O	0.60	1.96	24	3
1:A:163:LEU:HG	1:A:186:VAL:HG13	0.60	1.74	5	3
1:A:156:ILE:HA	1:A:193:LEU:CD2	0.60	2.26	24	2
1:A:104:LEU:HD12	1:A:107:LEU:HD11	0.59	1.71	6	1
1:A:117:ILE:HG22	1:A:155:THR:HG22	0.59	1.73	25	4
1:A:136:LEU:HG	1:A:140:LEU:HD22	0.59	1.73	19	1
1:A:110:LEU:CD2	1:A:166:ILE:HD11	0.59	2.27	7	3
1:A:148:LEU:HD12	1:A:203:ILE:HG21	0.59	1.74	9	1
1:A:156:ILE:HG23	1:A:193:LEU:HD23	0.59	1.73	9	9
1:A:121:LEU:HD11	1:A:196:CYS:HA	0.59	1.75	13	1
1:A:152:VAL:HG21	1:A:200:GLU:CB	0.59	2.27	24	1
1:A:128:LEU:CD2	1:A:148:LEU:HD21	0.59	2.27	2	2
1:A:193:LEU:C	1:A:193:LEU:HD23	0.59	2.18	8	8
1:A:110:LEU:HD21	1:A:166:ILE:HD11	0.59	1.74	7	5
1:A:136:LEU:HD22	1:A:140:LEU:HG	0.59	1.74	10	2
1:A:107:LEU:HD23	1:A:185:LEU:CD2	0.59	2.27	18	1
1:A:107:LEU:C	1:A:107:LEU:HD13	0.59	2.17	19	4
1:A:121:LEU:HD12	1:A:196:CYS:SG	0.59	2.38	23	1
1:A:163:LEU:HD21	1:A:186:VAL:CG1	0.59	2.20	19	4
1:A:148:LEU:HD12	1:A:200:GLU:OE1	0.59	1.97	24	1
1:A:136:LEU:HD22	1:A:140:LEU:HD13	0.59	1.74	13	2
1:A:163:LEU:HD13	1:A:163:LEU:O	0.59	1.98	6	1
1:A:111:GLU:CA	1:A:185:LEU:HD11	0.58	2.27	5	1
1:A:185:LEU:O	1:A:188:LYS:HD3	0.58	1.99	24	9
1:A:156:ILE:HG22	1:A:160:MET:HG3	0.58	1.75	2	1
1:A:171:LEU:HD22	1:A:172:PRO:CD	0.58	2.28	16	1
1:A:110:LEU:HD22	1:A:185:LEU:CD2	0.58	2.29	18	1
1:A:163:LEU:HD12	1:A:189:VAL:HB	0.58	1.74	7	3
1:A:156:ILE:HB	1:A:193:LEU:HD23	0.58	1.75	14	1
1:A:124:LEU:HD11	1:A:148:LEU:HD21	0.58	1.74	15	1
1:A:152:VAL:HG21	1:A:200:GLU:HB3	0.58	1.74	14	2
1:A:171:LEU:HD11	1:A:182:ARG:NH1	0.58	2.13	8	1
1:A:107:LEU:HD23	1:A:185:LEU:HD22	0.57	1.74	18	1
1:A:128:LEU:HD21	1:A:148:LEU:CD2	0.57	2.29	24	2
1:A:132:GLN:O	1:A:134:GLY:N	0.57	2.37	14	2
1:A:128:LEU:HD21	1:A:148:LEU:HG	0.57	1.75	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:178:SER:O	1:A:181:LYS:HG3	0.57	1.99	2	1
1:A:110:LEU:HD23	1:A:110:LEU:N	0.57	2.14	20	4
1:A:110:LEU:HD22	1:A:185:LEU:HD23	0.57	1.76	18	1
1:A:128:LEU:HD21	1:A:148:LEU:HD22	0.57	1.76	19	1
1:A:179:ARG:CD	1:A:180:LEU:HD12	0.57	2.29	4	1
1:A:111:GLU:HB2	1:A:185:LEU:HD21	0.57	1.76	24	2
1:A:152:VAL:HG21	1:A:200:GLU:HG2	0.57	1.75	2	2
1:A:107:LEU:HD22	1:A:182:ARG:HG2	0.57	1.75	14	1
1:A:152:VAL:O	1:A:156:ILE:HD12	0.57	1.99	8	1
1:A:145:LEU:HD22	1:A:207:THR:CB	0.57	2.30	23	2
1:A:185:LEU:HD13	1:A:188:LYS:HE2	0.56	1.75	13	1
1:A:124:LEU:CD1	1:A:128:LEU:HD23	0.56	2.30	4	1
1:A:170:VAL:HG13	1:A:170:VAL:O	0.56	1.99	21	3
1:A:135:PHE:O	1:A:136:LEU:HD22	0.56	2.00	16	3
1:A:110:LEU:HD11	1:A:166:ILE:HD11	0.56	1.74	5	4
1:A:107:LEU:HD21	1:A:185:LEU:HD21	0.56	1.76	8	1
1:A:128:LEU:HD13	1:A:148:LEU:HD23	0.56	1.76	9	1
1:A:110:LEU:HD21	1:A:162:ILE:HG23	0.56	1.76	4	5
1:A:120:HIS:O	1:A:124:LEU:HG	0.56	2.00	19	3
1:A:114:ALA:HB1	1:A:159:PHE:CE1	0.56	2.35	2	1
1:A:145:LEU:HD23	1:A:203:ILE:CG2	0.56	2.31	7	1
1:A:118:ALA:HB2	1:A:159:PHE:HZ	0.55	1.61	7	7
1:A:162:ILE:HG22	1:A:166:ILE:CD1	0.55	2.32	20	4
1:A:111:GLU:CG	1:A:185:LEU:HD22	0.55	2.31	8	1
1:A:101:GLU:O	1:A:105:LYS:N	0.55	2.38	18	5
1:A:107:LEU:HD22	1:A:107:LEU:C	0.55	2.22	1	7
1:A:110:LEU:HD22	1:A:162:ILE:HG23	0.55	1.79	1	2
1:A:160:MET:CG	1:A:193:LEU:HD21	0.55	2.32	4	8
1:A:185:LEU:HD13	1:A:188:LYS:CE	0.55	2.32	9	4
1:A:110:LEU:HD22	1:A:185:LEU:HD12	0.55	1.79	3	1
1:A:107:LEU:HD13	1:A:107:LEU:C	0.55	2.22	5	3
1:A:129:SER:O	1:A:132:GLN:CG	0.54	2.55	14	2
1:A:128:LEU:HD11	1:A:148:LEU:HG	0.54	1.79	8	1
1:A:148:LEU:C	1:A:148:LEU:HD13	0.54	2.23	25	3
1:A:121:LEU:O	1:A:125:ASN:OD1	0.54	2.26	3	1
1:A:107:LEU:HD21	1:A:185:LEU:CD2	0.54	2.30	5	2
1:A:128:LEU:HD23	1:A:148:LEU:HG	0.54	1.79	22	1
1:A:128:LEU:HD21	1:A:148:LEU:HD21	0.54	1.79	24	1
1:A:159:PHE:CB	1:A:193:LEU:HG	0.54	2.33	15	25
1:A:173:GLU:O	1:A:175:PHE:CD2	0.54	2.61	13	2
1:A:193:LEU:HD23	1:A:193:LEU:O	0.54	2.03	12	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:156:ILE:HG23	1:A:193:LEU:CD1	0.54	2.25	7	1
1:A:136:LEU:HD22	1:A:140:LEU:HD22	0.54	1.79	13	1
1:A:148:LEU:O	1:A:148:LEU:HD13	0.53	2.03	3	3
1:A:163:LEU:HD23	1:A:189:VAL:CG1	0.53	2.33	19	2
1:A:114:ALA:HB1	1:A:159:PHE:HE1	0.53	1.62	2	1
1:A:165:GLU:O	1:A:168:THR:HG22	0.53	2.03	18	2
1:A:185:LEU:HD12	1:A:186:VAL:HG23	0.53	1.79	8	1
1:A:160:MET:CG	1:A:193:LEU:HD11	0.53	2.33	8	3
1:A:179:ARG:HD2	1:A:180:LEU:HD12	0.53	1.80	4	1
1:A:162:ILE:HG22	1:A:166:ILE:HD11	0.53	1.78	3	5
1:A:118:ALA:HB2	1:A:192:PHE:CE1	0.53	2.38	15	1
1:A:180:LEU:C	1:A:180:LEU:HD13	0.53	2.24	16	3
1:A:152:VAL:HG11	1:A:197:ASP:HA	0.53	1.80	24	1
1:A:129:SER:O	1:A:132:GLN:HG3	0.52	2.04	2	2
1:A:172:PRO:HG2	1:A:175:PHE:CD1	0.52	2.39	20	1
1:A:159:PHE:CB	1:A:193:LEU:HD21	0.52	2.34	2	1
1:A:150:ARG:O	1:A:153:LYS:HB2	0.52	2.04	11	2
1:A:152:VAL:HG21	1:A:200:GLU:CD	0.52	2.24	16	2
1:A:131:ILE:HD13	1:A:148:LEU:HD23	0.52	1.80	13	1
1:A:171:LEU:HD23	1:A:175:PHE:HB3	0.52	1.80	8	1
1:A:110:LEU:HD23	1:A:188:LYS:NZ	0.52	2.19	18	2
1:A:145:LEU:HD22	1:A:207:THR:OG1	0.52	2.04	2	2
1:A:152:VAL:HG13	1:A:156:ILE:HD13	0.52	1.81	8	1
1:A:132:GLN:HE22	1:A:207:THR:HG21	0.52	1.65	4	1
1:A:124:LEU:CD1	1:A:148:LEU:HD21	0.52	2.35	15	1
1:A:111:GLU:HA	1:A:185:LEU:HD11	0.52	1.80	5	1
1:A:111:GLU:HB2	1:A:185:LEU:HD11	0.52	1.81	5	1
1:A:188:LYS:CE	1:A:189:VAL:HG23	0.52	2.34	10	1
1:A:121:LEU:O	1:A:125:ASN:ND2	0.51	2.43	16	4
1:A:163:LEU:HD23	1:A:163:LEU:O	0.51	2.05	9	1
1:A:163:LEU:HD23	1:A:189:VAL:HG11	0.51	1.83	19	2
1:A:120:HIS:ND1	1:A:124:LEU:HD23	0.51	2.21	16	2
1:A:117:ILE:HG22	1:A:155:THR:CG2	0.51	2.35	17	2
1:A:121:LEU:HG	1:A:155:THR:HG21	0.51	1.81	11	1
1:A:128:LEU:O	1:A:128:LEU:HD23	0.51	2.06	7	1
1:A:148:LEU:HD12	1:A:200:GLU:OE2	0.51	2.06	8	1
1:A:185:LEU:CA	1:A:188:LYS:HD3	0.51	2.36	7	8
1:A:128:LEU:HD13	1:A:148:LEU:CD2	0.51	2.35	9	1
1:A:149:ASP:OD1	1:A:150:ARG:N	0.51	2.44	10	2
1:A:193:LEU:HD23	1:A:193:LEU:C	0.51	2.27	19	4
1:A:113:SER:O	1:A:117:ILE:HG13	0.50	2.06	17	15

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:163:LEU:C	1:A:163:LEU:HD23	0.50	2.27	2	1
1:A:124:LEU:HD11	1:A:128:LEU:HD22	0.50	1.82	24	1
1:A:145:LEU:HD12	1:A:203:ILE:HG23	0.50	1.83	9	1
1:A:110:LEU:CD1	1:A:162:ILE:HG23	0.50	2.36	13	1
1:A:107:LEU:HD23	1:A:182:ARG:CZ	0.50	2.37	12	1
1:A:182:ARG:O	1:A:185:LEU:HG	0.50	2.07	8	1
1:A:117:ILE:HD13	1:A:158:GLN:CB	0.50	2.35	18	2
1:A:110:LEU:HD11	1:A:162:ILE:HG23	0.50	1.82	14	2
1:A:132:GLN:NE2	1:A:144:ALA:HB1	0.50	2.22	22	1
1:A:142:ALA:HB1	1:A:207:THR:HG23	0.50	1.83	1	1
1:A:189:VAL:O	1:A:193:LEU:HB2	0.50	2.07	10	2
1:A:103:GLU:HG2	1:A:172:PRO:CA	0.50	2.36	15	1
1:A:107:LEU:HD12	1:A:181:LYS:HD2	0.50	1.84	19	1
1:A:121:LEU:O	1:A:121:LEU:HD23	0.50	2.07	23	1
1:A:163:LEU:C	1:A:163:LEU:HD13	0.50	2.27	18	2
1:A:146:CYS:HA	1:A:149:ASP:OD2	0.49	2.06	10	3
1:A:128:LEU:HD22	1:A:131:ILE:HD11	0.49	1.83	12	2
1:A:189:VAL:HG12	1:A:193:LEU:HD11	0.49	1.82	15	1
1:A:110:LEU:HD12	1:A:166:ILE:HD11	0.49	1.82	10	1
1:A:171:LEU:HD13	1:A:172:PRO:CD	0.49	2.34	16	1
1:A:184:ASN:O	1:A:188:LYS:CD	0.49	2.59	16	2
1:A:136:LEU:O	1:A:137:ALA:HB2	0.49	2.07	25	3
1:A:149:ASP:O	1:A:152:VAL:HG12	0.49	2.07	8	1
1:A:145:LEU:CG	1:A:203:ILE:HG22	0.49	2.37	19	2
1:A:142:ALA:HA	1:A:207:THR:HG21	0.49	1.83	2	1
1:A:141:GLN:O	1:A:145:LEU:HB3	0.49	2.08	7	1
1:A:114:ALA:O	1:A:117:ILE:HG13	0.49	2.08	2	1
1:A:159:PHE:HB3	1:A:193:LEU:HG	0.49	1.84	2	7
1:A:107:LEU:HD13	1:A:181:LYS:HB3	0.49	1.84	4	1
1:A:135:PHE:C	1:A:136:LEU:HD12	0.49	2.28	11	1
1:A:163:LEU:HD11	1:A:186:VAL:CG1	0.48	2.38	15	1
1:A:144:ALA:O	1:A:147:LYS:HG3	0.48	2.08	6	1
1:A:121:LEU:HD23	1:A:125:ASN:ND2	0.48	2.22	9	2
1:A:110:LEU:HD12	1:A:166:ILE:HG12	0.48	1.85	20	1
1:A:159:PHE:CB	1:A:193:LEU:CG	0.48	2.92	2	1
1:A:159:PHE:HB3	1:A:193:LEU:CG	0.48	2.39	23	10
1:A:105:LYS:O	1:A:108:LYS:CG	0.48	2.61	7	2
1:A:171:LEU:HD22	1:A:179:ARG:CD	0.48	2.37	9	1
1:A:117:ILE:HD11	1:A:159:PHE:CD1	0.48	2.43	6	4
1:A:148:LEU:HD11	1:A:203:ILE:HD13	0.48	1.85	9	1
1:A:193:LEU:C	1:A:193:LEU:CD2	0.48	2.82	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:LEU:C	1:A:121:LEU:HD13	0.48	2.29	15	2
1:A:173:GLU:CG	1:A:175:PHE:CZ	0.48	2.96	24	1
1:A:118:ALA:HB2	1:A:192:PHE:CZ	0.48	2.44	18	1
1:A:117:ILE:CD1	1:A:159:PHE:CE1	0.48	2.97	19	3
1:A:166:ILE:HG21	1:A:186:VAL:CG2	0.48	2.39	16	3
1:A:107:LEU:HD22	1:A:182:ARG:CB	0.48	2.39	16	1
1:A:102:VAL:HG12	1:A:106:LYS:HE2	0.48	1.85	11	2
1:A:160:MET:N	1:A:193:LEU:HD11	0.48	2.24	9	1
1:A:156:ILE:CG2	1:A:193:LEU:HD21	0.48	2.38	12	2
1:A:163:LEU:HD11	1:A:186:VAL:HG13	0.48	1.86	15	1
1:A:193:LEU:C	1:A:193:LEU:HD13	0.48	2.29	24	1
1:A:135:PHE:CD1	1:A:135:PHE:N	0.48	2.82	7	1
1:A:117:ILE:CD1	1:A:162:ILE:HD11	0.48	2.39	15	1
1:A:148:LEU:HD13	1:A:148:LEU:C	0.47	2.29	15	2
1:A:128:LEU:C	1:A:128:LEU:HD13	0.47	2.28	5	2
1:A:124:LEU:O	1:A:128:LEU:HD23	0.47	2.09	16	1
1:A:125:ASN:OD1	1:A:126:LYS:N	0.47	2.47	24	2
1:A:107:LEU:HD21	1:A:185:LEU:HG	0.47	1.84	2	2
1:A:149:ASP:OD1	1:A:203:ILE:HB	0.47	2.08	22	2
1:A:160:MET:CA	1:A:193:LEU:HD11	0.47	2.39	9	1
1:A:111:GLU:O	1:A:114:ALA:HB3	0.47	2.10	23	2
1:A:188:LYS:O	1:A:191:VAL:HG12	0.47	2.09	21	3
1:A:163:LEU:CG	1:A:186:VAL:HG13	0.47	2.38	5	1
1:A:152:VAL:HG11	1:A:200:GLU:HB3	0.47	1.85	4	1
1:A:142:ALA:HA	1:A:207:THR:HG23	0.47	1.85	6	1
1:A:140:LEU:O	1:A:140:LEU:HD13	0.47	2.09	7	1
1:A:128:LEU:O	1:A:131:ILE:CG1	0.47	2.62	14	1
1:A:153:LYS:O	1:A:156:ILE:CG1	0.47	2.63	14	2
1:A:136:LEU:HD12	1:A:140:LEU:HD22	0.47	1.87	16	1
1:A:141:GLN:O	1:A:145:LEU:HD13	0.47	2.09	1	2
1:A:170:VAL:O	1:A:170:VAL:HG13	0.47	2.10	13	2
1:A:184:ASN:O	1:A:188:LYS:CE	0.47	2.63	16	1
1:A:172:PRO:CG	1:A:175:PHE:CE1	0.47	2.98	20	1
1:A:128:LEU:HD22	1:A:148:LEU:HD22	0.47	1.86	10	2
1:A:179:ARG:HG3	1:A:180:LEU:N	0.47	2.25	16	3
1:A:128:LEU:HD23	1:A:129:SER:N	0.47	2.24	15	1
1:A:156:ILE:HD11	1:A:197:ASP:HA	0.47	1.85	5	4
1:A:110:LEU:HD22	1:A:182:ARG:NH2	0.47	2.25	12	1
1:A:128:LEU:HD13	1:A:148:LEU:HG	0.47	1.86	25	2
1:A:152:VAL:HG12	1:A:156:ILE:HD11	0.46	1.87	25	2
1:A:156:ILE:HA	1:A:193:LEU:HD11	0.46	1.87	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:LEU:HD12	1:A:148:LEU:HD22	0.46	1.88	4	1
1:A:142:ALA:HA	1:A:145:LEU:HB3	0.46	1.87	7	1
1:A:145:LEU:HD23	1:A:203:ILE:HG22	0.46	1.86	7	1
1:A:156:ILE:HG23	1:A:196:CYS:HB3	0.46	1.86	14	2
1:A:156:ILE:HG23	1:A:193:LEU:CA	0.46	2.40	15	1
1:A:159:PHE:CZ	1:A:192:PHE:CG	0.46	3.04	21	1
1:A:128:LEU:HD21	1:A:147:LYS:CE	0.46	2.39	22	1
1:A:128:LEU:HD13	1:A:148:LEU:CG	0.46	2.40	25	1
1:A:159:PHE:HA	1:A:162:ILE:HD12	0.46	1.87	22	2
1:A:104:LEU:HD12	1:A:107:LEU:HD12	0.46	1.87	1	1
1:A:120:HIS:CE1	1:A:124:LEU:HD23	0.46	2.46	16	1
1:A:185:LEU:HD13	1:A:188:LYS:HZ3	0.46	1.70	4	1
1:A:100:GLU:CG	1:A:175:PHE:CD1	0.46	2.99	2	1
1:A:158:GLN:O	1:A:162:ILE:HD12	0.46	2.11	2	1
1:A:140:LEU:HD22	1:A:143:GLU:OE1	0.46	2.11	20	1
1:A:174:GLN:NE2	1:A:175:PHE:CE2	0.46	2.84	21	1
1:A:185:LEU:HA	1:A:188:LYS:HG2	0.46	1.86	16	2
1:A:153:LYS:HA	1:A:156:ILE:HG12	0.46	1.87	11	1
1:A:105:LYS:O	1:A:108:LYS:HG3	0.46	2.11	16	1
1:A:160:MET:CG	1:A:193:LEU:CD2	0.45	2.94	1	4
1:A:107:LEU:HG	1:A:181:LYS:HD3	0.45	1.89	2	1
1:A:111:GLU:O	1:A:115:GLU:N	0.45	2.50	13	7
1:A:122:GLN:O	1:A:125:ASN:OD1	0.45	2.34	18	2
1:A:163:LEU:HD13	1:A:190:GLN:OE1	0.45	2.12	8	2
1:A:152:VAL:HG13	1:A:156:ILE:CD1	0.45	2.41	8	1
1:A:190:GLN:O	1:A:194:ALA:HB3	0.45	2.10	2	2
1:A:125:ASN:HA	1:A:148:LEU:HD21	0.45	1.87	3	1
1:A:188:LYS:HE2	1:A:189:VAL:HG23	0.45	1.88	10	1
1:A:153:LYS:O	1:A:156:ILE:HG12	0.45	2.11	11	1
1:A:124:LEU:HD12	1:A:124:LEU:C	0.45	2.31	16	1
1:A:166:ILE:HG23	1:A:182:ARG:HD3	0.45	1.88	18	1
1:A:148:LEU:HD12	1:A:200:GLU:CD	0.45	2.32	24	1
1:A:136:LEU:HD22	1:A:140:LEU:HB2	0.45	1.88	3	1
1:A:184:ASN:O	1:A:188:LYS:HD2	0.45	2.11	20	5
1:A:191:VAL:O	1:A:195:GLU:CB	0.45	2.65	2	2
1:A:181:LYS:O	1:A:185:LEU:CD2	0.45	2.65	8	1
1:A:185:LEU:CD1	1:A:186:VAL:HG23	0.45	2.41	8	1
1:A:118:ALA:CB	1:A:192:PHE:CE1	0.45	3.00	3	1
1:A:132:GLN:HG2	1:A:144:ALA:HB1	0.45	1.88	3	1
1:A:145:LEU:HD13	1:A:145:LEU:C	0.45	2.32	7	1
1:A:103:GLU:OE1	1:A:175:PHE:CE2	0.45	2.70	23	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:159:PHE:CD2	1:A:193:LEU:HD11	0.44	2.47	2	1
1:A:189:VAL:O	1:A:193:LEU:CB	0.44	2.66	13	2
1:A:166:ILE:CG2	1:A:186:VAL:HG22	0.44	2.40	14	1
1:A:168:THR:HG22	1:A:168:THR:O	0.44	2.13	4	1
1:A:128:LEU:CG	1:A:148:LEU:HD21	0.44	2.41	16	2
1:A:136:LEU:CG	1:A:140:LEU:HD13	0.44	2.41	14	1
1:A:159:PHE:HB2	1:A:193:LEU:HG	0.44	1.89	15	2
1:A:122:GLN:HA	1:A:125:ASN:HD21	0.44	1.72	24	3
1:A:135:PHE:CE2	1:A:141:GLN:NE2	0.44	2.85	17	1
1:A:163:LEU:HD12	1:A:189:VAL:CG1	0.44	2.43	22	2
1:A:128:LEU:O	1:A:132:GLN:N	0.44	2.47	3	3
1:A:111:GLU:HG3	1:A:112:VAL:N	0.44	2.26	22	2
1:A:170:VAL:HG12	1:A:170:VAL:O	0.44	2.12	9	1
1:A:136:LEU:CD2	1:A:140:LEU:HD22	0.44	2.42	13	1
1:A:157:GLU:HG3	1:A:158:GLN:N	0.44	2.27	2	1
1:A:159:PHE:CB	1:A:193:LEU:CD2	0.44	2.95	2	1
1:A:180:LEU:HD22	1:A:180:LEU:O	0.44	2.12	3	1
1:A:171:LEU:HB3	1:A:175:PHE:CD2	0.44	2.48	13	1
1:A:190:GLN:O	1:A:194:ALA:CB	0.44	2.65	2	1
1:A:191:VAL:O	1:A:195:GLU:N	0.44	2.49	23	2
1:A:110:LEU:N	1:A:110:LEU:CD2	0.44	2.81	20	1
1:A:103:GLU:OE2	1:A:175:PHE:CG	0.44	2.70	23	2
1:A:107:LEU:HD12	1:A:181:LYS:HE2	0.44	1.88	2	1
1:A:186:VAL:O	1:A:189:VAL:HB	0.44	2.13	20	5
1:A:182:ARG:HA	1:A:185:LEU:HD21	0.44	1.89	8	1
1:A:160:MET:HA	1:A:193:LEU:HD11	0.44	1.89	9	1
1:A:128:LEU:HB2	1:A:148:LEU:HD21	0.44	1.90	18	1
1:A:181:LYS:O	1:A:185:LEU:HB2	0.43	2.13	4	2
1:A:117:ILE:HD12	1:A:162:ILE:HD11	0.43	1.89	15	1
1:A:121:LEU:CD1	1:A:152:VAL:HG13	0.43	2.30	3	1
1:A:145:LEU:HD22	1:A:207:THR:CG2	0.43	2.43	23	1
1:A:145:LEU:HG	1:A:203:ILE:HG23	0.43	1.90	2	1
1:A:110:LEU:CD2	1:A:162:ILE:CG2	0.43	2.96	4	2
1:A:150:ARG:O	1:A:153:LYS:CG	0.43	2.66	20	1
1:A:201:GLN:O	1:A:205:GLN:HG2	0.43	2.14	4	1
1:A:185:LEU:HA	1:A:188:LYS:CD	0.43	2.43	22	2
1:A:103:GLU:HG2	1:A:172:PRO:HA	0.43	1.90	15	1
1:A:199:VAL:HG12	1:A:203:ILE:CD1	0.43	2.43	20	2
1:A:173:GLU:HB3	1:A:175:PHE:CE1	0.43	2.49	9	1
1:A:152:VAL:HG11	1:A:200:GLU:HB2	0.43	1.90	12	1
1:A:170:VAL:HG22	1:A:171:LEU:N	0.43	2.29	24	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:131:ILE:CD1	1:A:148:LEU:HD23	0.43	2.43	13	1
1:A:152:VAL:CG2	1:A:200:GLU:HG2	0.43	2.41	2	1
1:A:199:VAL:HG12	1:A:203:ILE:HD11	0.43	1.90	9	2
1:A:128:LEU:HD13	1:A:128:LEU:O	0.43	2.13	10	1
1:A:178:SER:O	1:A:181:LYS:HD2	0.43	2.13	2	1
1:A:106:LYS:CG	1:A:107:LEU:N	0.43	2.82	4	6
1:A:100:GLU:CG	1:A:175:PHE:CE2	0.43	3.02	20	1
1:A:110:LEU:HD23	1:A:110:LEU:O	0.43	2.14	3	2
1:A:103:GLU:OE2	1:A:175:PHE:CD2	0.43	2.71	10	1
1:A:172:PRO:HG2	1:A:175:PHE:CE1	0.43	2.49	20	1
1:A:107:LEU:CD2	1:A:185:LEU:CD2	0.43	2.92	1	1
1:A:153:LYS:HG3	1:A:154:ALA:N	0.43	2.28	20	2
1:A:108:LYS:O	1:A:111:GLU:CG	0.43	2.67	25	1
1:A:127:GLU:O	1:A:131:ILE:HD12	0.42	2.14	2	1
1:A:170:VAL:HG12	1:A:171:LEU:N	0.42	2.29	5	1
1:A:102:VAL:O	1:A:106:LYS:HG3	0.42	2.14	12	2
1:A:128:LEU:HD23	1:A:128:LEU:C	0.42	2.34	7	1
1:A:140:LEU:O	1:A:144:ALA:N	0.42	2.50	11	1
1:A:173:GLU:O	1:A:175:PHE:CE2	0.42	2.72	15	1
1:A:186:VAL:O	1:A:190:GLN:N	0.42	2.50	6	1
1:A:145:LEU:HG	1:A:207:THR:HG21	0.42	1.90	14	1
1:A:147:LYS:HD2	1:A:148:LEU:N	0.42	2.30	6	1
1:A:121:LEU:HD23	1:A:125:ASN:HD21	0.42	1.74	8	1
1:A:107:LEU:HD12	1:A:107:LEU:C	0.42	2.35	15	3
1:A:104:LEU:HD12	1:A:181:LYS:HD2	0.42	1.90	19	1
1:A:145:LEU:HD22	1:A:207:THR:HG21	0.42	1.90	23	1
1:A:103:GLU:HA	1:A:106:LYS:CD	0.42	2.44	15	8
1:A:156:ILE:HG22	1:A:196:CYS:HB2	0.42	1.92	11	1
1:A:100:GLU:HA	1:A:172:PRO:HB2	0.42	1.91	15	1
1:A:159:PHE:C	1:A:193:LEU:HD12	0.42	2.35	16	2
1:A:204:CYS:O	1:A:208:GLU:CB	0.42	2.68	4	1
1:A:185:LEU:O	1:A:188:LYS:CD	0.42	2.67	15	1
1:A:149:ASP:HA	1:A:200:GLU:CG	0.42	2.44	16	1
1:A:122:GLN:O	1:A:126:LYS:HB2	0.42	2.15	18	1
1:A:111:GLU:HG3	1:A:185:LEU:HD11	0.42	1.90	24	1
1:A:197:ASP:HA	1:A:200:GLU:HG2	0.42	1.91	4	2
1:A:174:GLN:OE1	1:A:175:PHE:CZ	0.42	2.73	7	1
1:A:136:LEU:HB2	1:A:140:LEU:HD22	0.42	1.91	3	1
1:A:117:ILE:CD1	1:A:159:PHE:CD1	0.42	3.03	7	1
1:A:128:LEU:HD13	1:A:132:GLN:HG3	0.42	1.91	12	1
1:A:196:CYS:O	1:A:200:GLU:HG2	0.42	2.14	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:132:GLN:O	1:A:133:GLN:C	0.42	2.58	17	1
1:A:150:ARG:HG3	1:A:151:LYS:N	0.42	2.30	6	5
1:A:149:ASP:O	1:A:152:VAL:HB	0.42	2.14	10	1
1:A:104:LEU:HA	1:A:107:LEU:HD21	0.42	1.91	23	1
1:A:173:GLU:O	1:A:174:GLN:CB	0.41	2.68	14	1
1:A:203:ILE:O	1:A:206:GLU:HG2	0.41	2.15	15	2
1:A:180:LEU:O	1:A:180:LEU:HD22	0.41	2.15	7	1
1:A:188:LYS:HG2	1:A:189:VAL:N	0.41	2.30	23	3
1:A:103:GLU:OE2	1:A:175:PHE:CD1	0.41	2.74	13	1
1:A:141:GLN:O	1:A:145:LEU:HD23	0.41	2.14	14	1
1:A:145:LEU:CD2	1:A:207:THR:OG1	0.41	2.68	16	1
1:A:200:GLU:HG3	1:A:201:GLN:N	0.41	2.30	14	2
1:A:111:GLU:HA	1:A:188:LYS:NZ	0.41	2.30	13	1
1:A:134:GLY:O	1:A:135:PHE:CD2	0.41	2.74	9	1
1:A:152:VAL:HB	1:A:200:GLU:HG3	0.41	1.91	11	1
1:A:145:LEU:HD22	1:A:207:THR:HB	0.41	1.93	23	1
1:A:197:ASP:O	1:A:201:GLN:N	0.41	2.48	24	1
1:A:118:ALA:HB2	1:A:159:PHE:CE2	0.41	2.50	2	1
1:A:142:ALA:CB	1:A:207:THR:CG2	0.41	2.99	2	1
1:A:121:LEU:HD12	1:A:155:THR:CB	0.41	2.45	3	1
1:A:163:LEU:CD2	1:A:186:VAL:CG1	0.41	2.98	24	1
1:A:193:LEU:HD13	1:A:193:LEU:C	0.41	2.35	7	1
1:A:191:VAL:HG22	1:A:195:GLU:OE1	0.41	2.16	21	1
1:A:122:GLN:O	1:A:125:ASN:ND2	0.41	2.53	23	1
1:A:173:GLU:HG2	1:A:175:PHE:CZ	0.41	2.51	24	1
1:A:103:GLU:HA	1:A:106:LYS:HD2	0.41	1.92	3	2
1:A:159:PHE:HD2	1:A:193:LEU:HD23	0.41	1.75	24	1
1:A:159:PHE:HD2	1:A:193:LEU:HD11	0.41	1.75	2	1
1:A:163:LEU:CB	1:A:189:VAL:HG11	0.41	2.44	3	1
1:A:174:GLN:O	1:A:176:LYS:N	0.41	2.53	3	1
1:A:152:VAL:CG1	1:A:196:CYS:O	0.41	2.69	5	1
1:A:185:LEU:HD12	1:A:186:VAL:N	0.41	2.31	8	1
1:A:171:LEU:HD22	1:A:179:ARG:NE	0.41	2.31	9	1
1:A:153:LYS:HG2	1:A:154:ALA:N	0.41	2.31	16	1
1:A:104:LEU:O	1:A:107:LEU:HG	0.41	2.16	23	1
1:A:110:LEU:HD21	1:A:162:ILE:HG22	0.41	1.91	24	1
1:A:202:TYR:O	1:A:206:GLU:CG	0.41	2.68	23	3
1:A:105:LYS:HA	1:A:108:LYS:CD	0.41	2.46	7	1
1:A:132:GLN:O	1:A:135:PHE:CE1	0.41	2.74	8	1
1:A:175:PHE:O	1:A:179:ARG:CG	0.41	2.69	10	1
1:A:136:LEU:HD22	1:A:140:LEU:CD1	0.41	2.46	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:197:ASP:O	1:A:200:GLU:HG2	0.41	2.15	13	1
1:A:118:ALA:CB	1:A:192:PHE:CZ	0.41	2.98	14	1
1:A:156:ILE:CG2	1:A:196:CYS:HB3	0.41	2.45	14	1
1:A:156:ILE:O	1:A:193:LEU:HD21	0.41	2.16	18	1
1:A:124:LEU:C	1:A:124:LEU:CD1	0.41	2.88	23	1
1:A:104:LEU:HD11	1:A:108:LYS:CE	0.41	2.45	24	1
1:A:145:LEU:HG	1:A:203:ILE:CG2	0.41	2.46	3	1
1:A:173:GLU:HB2	1:A:175:PHE:CZ	0.41	2.51	9	1
1:A:114:ALA:O	1:A:117:ILE:CG1	0.41	2.69	19	1
1:A:103:GLU:OE1	1:A:175:PHE:CZ	0.40	2.74	11	1
1:A:134:GLY:O	1:A:135:PHE:CD1	0.40	2.74	12	1
1:A:191:VAL:O	1:A:195:GLU:HB2	0.40	2.16	12	1
1:A:98:PRO:HD2	1:A:101:GLU:CG	0.40	2.46	15	1
1:A:128:LEU:HD22	1:A:128:LEU:C	0.40	2.37	5	1
1:A:193:LEU:CD2	1:A:193:LEU:C	0.40	2.89	12	1
1:A:145:LEU:HG	1:A:203:ILE:HG22	0.40	1.93	15	1
1:A:107:LEU:CB	1:A:182:ARG:NH1	0.40	2.85	21	1
1:A:197:ASP:O	1:A:201:GLN:HG3	0.40	2.16	24	1
1:A:121:LEU:HD22	1:A:125:ASN:HD21	0.40	1.75	11	1
1:A:136:LEU:HB3	1:A:140:LEU:CB	0.40	2.47	17	1
1:A:145:LEU:HD21	1:A:203:ILE:C	0.40	2.37	20	1
1:A:148:LEU:O	1:A:148:LEU:HD22	0.40	2.15	21	1
1:A:154:ALA:O	1:A:158:GLN:CG	0.40	2.69	24	1
1:A:159:PHE:CE1	1:A:192:PHE:HB3	0.40	2.52	4	1
1:A:136:LEU:HD13	1:A:140:LEU:HG	0.40	1.93	7	1
1:A:136:LEU:CB	1:A:140:LEU:HD13	0.40	2.45	17	1
1:A:178:SER:O	1:A:181:LYS:CG	0.40	2.69	2	1
1:A:156:ILE:HD13	1:A:196:CYS:HB2	0.40	1.94	4	1
1:A:152:VAL:O	1:A:156:ILE:CD1	0.40	2.69	8	1
1:A:103:GLU:HG3	1:A:172:PRO:N	0.40	2.32	15	1
1:A:149:ASP:O	1:A:200:GLU:CG	0.40	2.70	19	1
1:A:148:LEU:C	1:A:148:LEU:CD2	0.40	2.89	22	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	111/135 (82%)	105±2 (94±2%)	3±2 (3±1%)	3±1 (3±1%)	9 45
All	All	2775/3375 (82%)	2618 (94%)	87 (3%)	70 (3%)	9 45

All 12 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	98	PRO	20
1	A	174	GLN	10
1	A	134	GLY	6
1	A	172	PRO	6
1	A	135	PHE	5
1	A	170	VAL	5
1	A	133	GLN	4
1	A	173	GLU	4
1	A	175	PHE	3
1	A	171	LEU	3
1	A	137	ALA	3
1	A	136	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	102/122 (84%)	67±4 (66±4%)	35±4 (34±4%)	1 10
All	All	2550/3050 (84%)	1684 (66%)	866 (34%)	1 10

All 90 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	147	LYS	24
1	A	115	GLU	23
1	A	185	LEU	23
1	A	151	LYS	22
1	A	150	ARG	20
1	A	158	GLN	20

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Mol	Chain	Res	Type	Models (Total)
1	A	124	LEU	19
1	A	188	LYS	19
1	A	104	LEU	18
1	A	153	LYS	18
1	A	105	LYS	17
1	A	148	LEU	17
1	A	138	LYS	16
1	A	140	LEU	16
1	A	181	LYS	16
1	A	116	LYS	15
1	A	120	HIS	15
1	A	126	LYS	15
1	A	171	LEU	15
1	A	187	LYS	15
1	A	143	GLU	15
1	A	136	LEU	14
1	A	106	LYS	13
1	A	163	LEU	13
1	A	173	GLU	13
1	A	121	LEU	13
1	A	100	GLU	12
1	A	110	LEU	12
1	A	113	SER	12
1	A	133	GLN	12
1	A	155	THR	12
1	A	161	LYS	12
1	A	176	LYS	12
1	A	157	GLU	11
1	A	169	MET	11
1	A	178	SER	11
1	A	202	TYR	11
1	A	123	GLU	11
1	A	182	ARG	11
1	A	101	GLU	11
1	A	132	GLN	11
1	A	179	ARG	10
1	A	109	ASP	10
1	A	177	ASP	10
1	A	111	GLU	10
1	A	141	GLN	10
1	A	184	ASN	10
1	A	160	MET	9

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Mol	Chain	Res	Type	Models (Total)
1	A	200	GLU	9
1	A	149	ASP	9
1	A	193	LEU	8
1	A	135	PHE	8
1	A	127	GLU	8
1	A	139	GLU	8
1	A	119	ASN	8
1	A	107	LEU	7
1	A	195	GLU	7
1	A	128	LEU	7
1	A	117	ILE	6
1	A	129	SER	6
1	A	167	ASP	6
1	A	146	CYS	6
1	A	165	GLU	6
1	A	180	LEU	5
1	A	174	GLN	5
1	A	145	LEU	5
1	A	192	PHE	5
1	A	197	ASP	5
1	A	204	CYS	5
1	A	103	GLU	4
1	A	164	GLU	4
1	A	159	PHE	3
1	A	205	GLN	3
1	A	108	LYS	3
1	A	122	GLN	3
1	A	183	LYS	3
1	A	168	THR	3
1	A	196	CYS	3
1	A	208	GLU	2
1	A	125	ASN	1
1	A	156	ILE	1
1	A	175	PHE	1
1	A	152	VAL	1
1	A	191	VAL	1
1	A	170	VAL	1
1	A	206	GLU	1
1	A	207	THR	1
1	A	201	GLN	1
1	A	99	GLU	1
1	A	203	ILE	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)

No chemical shift data were provided