Full wwPDB NMR Structure Validation Report (i)

Feb 23, 2022 – 08:29 AM EST

PDB ID	:	1X3U
Title	:	Solution structure of the C-terminal transcriptional activator domain of FixJ from Sinorhizobium melilot
Authors	:	Kurashima-Ito, K.; Kasai, Y.; Hosono, K.; Tamura, K.; Oue, S.; Isogai, M.; Ito, Y.; Nakamura, H.; Shiro, Y.
Deposited on	:	2005-05-10

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:

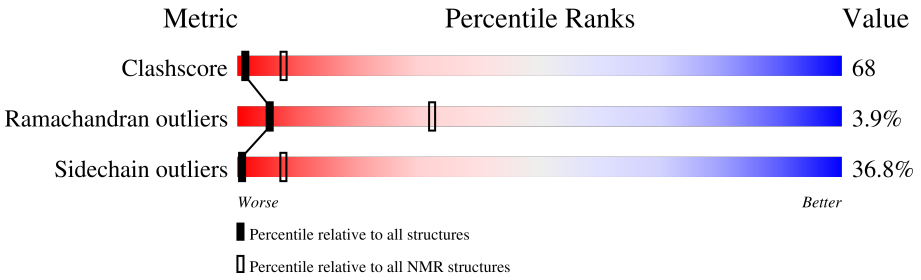
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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	79	15% 58% 16% 10%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 17 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:131-A:201 (71)	0.36	17

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, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 15, 16, 17, 19
2	14, 20
Single-model clusters	18

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1220 atoms, of which 621 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcriptional regulatory protein fixJ.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	79	1220	369	621	115	111	4	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	126	GLY	-	cloning artifact	UNP P10958
A	127	SER	-	cloning artifact	UNP P10958
A	128	HIS	-	cloning artifact	UNP P10958
A	129	MET	-	cloning artifact	UNP P10958

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: Transcriptional regulatory protein fixJ

Chain A: 15% 58% 16% 10%

G126 S127 H128 M129 D130 D131 A132 N133 D134 I135 R136 A137 R138 L139 Q140 T141 L142 S143 E144 R145 E146 R147 Q148 V149 L150 S151 A152 V153 V154 L157 K160 S161 I162 A163 Y164 D165 L166 D167 I168 S169 P170 R171 T172 V173 E174 V175 H176 R177 A178 N179 V180 M181 A182 K183 M184 K185 A186 K187

S188 L189 P190 H191 L192 V193 R194 M195 A196 L197 A198 F201 G202 P203 S204

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: Transcriptional regulatory protein fixJ

Chain A: 20% 48% 22% 10%

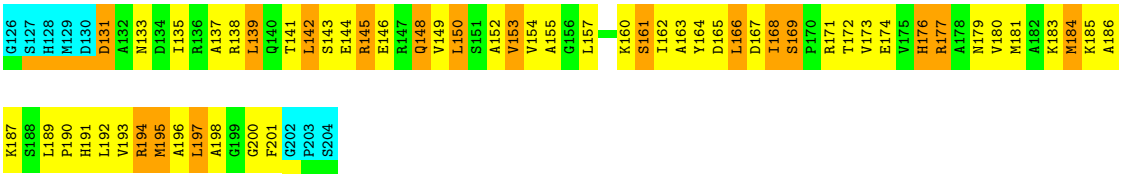
G126 S127 H128 M129 D130 D131 A132 N133 D134 I135 R136 A137 R138 L139 Q140 T141 L142 S143 E144 R145 E146 R147 Q148 V149 L150 S151 A152 V153 V154 L157 K160 S161 I162 A163 Y164 D165 L166 D167 I168 S169 P170 R171 T172 V173 E174 V175 H176 R177 A178 N179 V180 M181 A182 K183 M184 K185 A186

L189 P190 H191 L192 V193 R194 M195 A196 L197 A198 F201 G202 P203 S204

4.2.2 Score per residue for model 2

• Molecule 1: Transcriptional regulatory protein fixJ

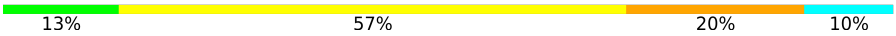
Chain A: 19% 49% 22% 10%

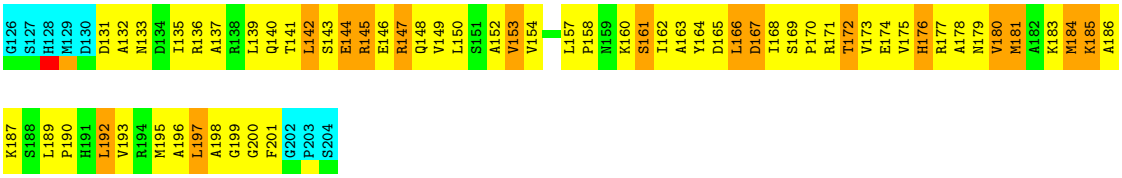


4.2.3 Score per residue for model 3

- Molecule 1: Transcriptional regulatory protein fixJ

Chain A:





4.2.4 Score per residue for model 4

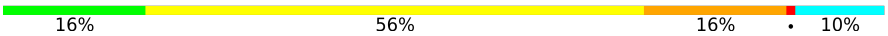
- Molecule 1: Transcriptional regulatory protein fixJ

Chain A:

4.2.5 Score per residue for model 5

- Molecule 1: Transcriptional regulatory protein fixJ

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: Transcriptional regulatory protein fixJ

Chain A: 23% 47% 20% 10%

G126 S127 H128 M129 D130 N133 D134 I135 R138 L139 Q140 T141 L142 S143 E144 R145 E146 R147 Q148 V149 L150 S151 A152 V153 V154 A155 G156 L157 K160 S161 I162 A163 Y164 D165 L166 D167 I168 S169 P170 R171 T172 V173 E174 V175 H176 R177 A178 N179 V180 M181 A182 K183 M184 K185 A186 K187 S188

L189 L192 V193 R194 M195 A196 L197 A198 F201 G202 P203 S204

4.2.7 Score per residue for model 7

- Molecule 1: Transcriptional regulatory protein fixJ

Chain A: 23% 47% 20% 10%

G126 S127 H128 M129 D130 D131 A132 N133 D134 I135 R136 A137 R138 L139 Q140 T141 L142 S143 E144 R145 E146 V149 L150 S151 A152 V153 V154 L157 K160 S161 I162 A163 Y164 D165 L166 D167 I168 S169 P170 R171 T172 V173 E174 V175 H176 R177 A178 N179 V180 M181 A182 K183 M184 K185 A186 L189

P190 H191 L192 V193 R194 M195 A196 L197 F201 G202 P203 S204

4.2.8 Score per residue for model 8

- Molecule 1: Transcriptional regulatory protein fixJ

Chain A: 20% 54% 15% 10%

G126 S127 H128 M129 D130 D131 A132 I135 R138 L139 Q140 T141 L142 S143 E144 R145 E146 R147 Q148 V149 L150 S151 A152 V153 V154 P158 N159 K160 S161 I162 A163 Y164 D165 L166 D167 I168 S169 P170 R171 T172 V173 E174 V175 H176 R177 A178 N179 V180 M181 A182 K183 M184 K185 A186 K187 S188 L189

P190 H191 L192 V193 R194 M195 A196 L197 A198 F201 G202 P203 S204

4.2.9 Score per residue for model 9

- Molecule 1: Transcriptional regulatory protein fixJ

Chain A: 16% 52% 20% • 10%

G126 S127 H128 M129 D130 D131 A132 N133 D134 I135 R136 A137 R138 L139 Q140 T141 L142 S143 E144 R145 E146 R147 Q148 V149 L150 S151 A152 V153 V154 A155 G156 L157 K160 S161 I162 A163 Y164 D165 L166 D167 I168 S169 P170 R171 T172 V173 E174 V175 H176 R177 A178 N179 V180 M181 A182 K183 M184 K185 A186

K187 S188 L189 P190 H191 L192 V193 R194 M195 A196 L197 A198 G199 G200 F201 G202 P203 S204

4.2.10 Score per residue for model 10

- Molecule 1: Transcriptional regulatory protein fixJ

Chain A: 15% 51% 23% • 10%

G126 S127 H128 M129 D130 D131 A132 N133 D134 I135 R136 A137 R138 L139 Q140 T141 L142 S143 E144 R145 E146 R147 Q148 V149 L150 S151 A152 V153 V154 P158 N159 K160 S161 I162 A163 Y164 D165 L166 D167 I168 S169 P170 R171 T172 V173 E174 V175 H176 R177 A178 N179 V180 M181 A182 K183 M184 K185 A186 K187

S188 L189 P190 H191 L192 V193 R194 M195 A196 L197 A198 G199 G200 F201 G202 P203 S204

4.2.11 Score per residue for model 11

- Molecule 1: Transcriptional regulatory protein fixJ

Chain A: 13% 57% 20% 10%

G126 S127 H128 M129 D130 D131 A132 N133 D134 I135 R136 A137 R138 L139 Q140 T141 L142 S143 E144 R145 E146 R147 Q148 V149 L150 S151 A152 V153 V154 L157 K160 S161 I162 A163 Y164 D165 L166 D167 I168 S169 P170 R171 T172 V173 E174 V175 H176 R177 A178 N179 V180 M181 A182 K183 M184 K185 A186

L189 P190 H191 L192 V193 R194 M195 A196 L197 A198 G199 G200 F201 G202 P203 S204

4.2.12 Score per residue for model 12

- Molecule 1: Transcriptional regulatory protein fixJ

Chain A: 16% 52% 22% 10%

G126 S127 H128 M129 D130 D131 A132 N133 D134 I135 R136 A137 R138 L139 Q140 T141 L142 S143 E144 R145 E146 R147 Q148 V149 L150 S151 A152 V153 V154 K160 S161 I162 A163 Y164 D165 L166 D167 I168 S169 P170 R171 T172 V173 E174 V175 H176 R177 A178 N179 V180 M181 A182 K183 M184 K185 A186 K187 S188 L189

P190 H191 L192 V193 R194 M195 A196 L197 A198 G199 G200 F201 G202 P203 S204

4.2.13 Score per residue for model 13

- Molecule 1: Transcriptional regulatory protein fixJ

Chain A: 15% 56% 19% 10%

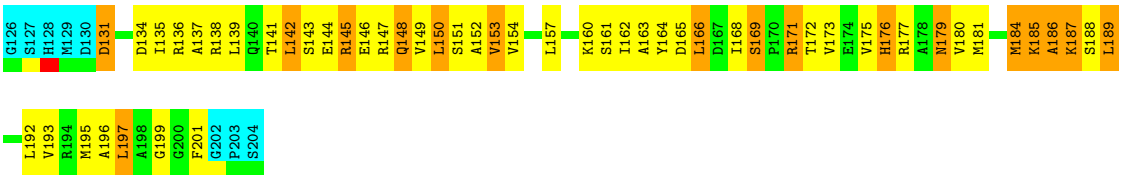
G126 S127 H128 M129 D130 D131 A132 N133 D134 I135 R136 A137 R138 L139 Q140 T141 L142 S143 E144 R145 E146 R147 Q148 V149 L150 S151 A152 V153 V154 L157 K160 S161 I162 A163 Y164 D165 L166 D167 I168 S169 P170 R171 T172 V173 E174 V175 H176 R177 A178 N179 V180 M181 A182 K183 M184 K185 A186

L189 P190 H191 L192 V193 R194 M195 A196 L197 A198 F201 G202 P203 S204

4.2.14 Score per residue for model 14

- Molecule 1: Transcriptional regulatory protein fixJ

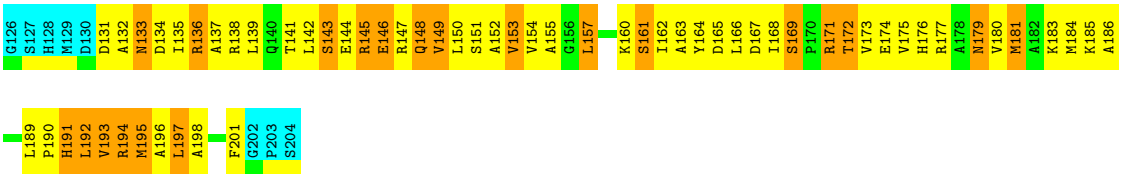
Chain A: 23% 46% 22% 10%



4.2.15 Score per residue for model 15

- Molecule 1: Transcriptional regulatory protein fixJ

Chain A: 14% 49% 27% 10%



4.2.16 Score per residue for model 16

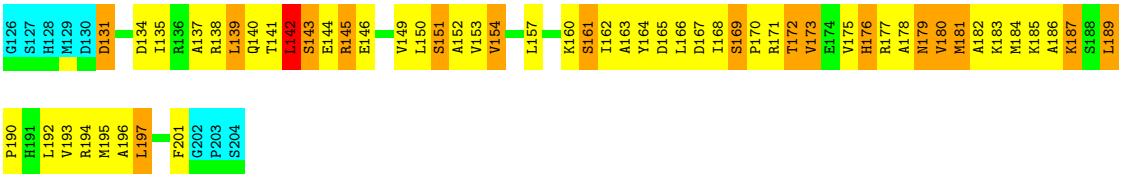
- Molecule 1: Transcriptional regulatory protein fixJ

Chain A: 19% 51% 20% 10%

4.2.17 Score per residue for model 17 (medoid)

- Molecule 1: Transcriptional regulatory protein fixJ

Chain A: 19% 48% 22% • 10%



4.2.18 Score per residue for model 18

• Molecule 1: Transcriptional regulatory protein fixJ

Chain A: 10% 57% 22% • 10%

G126 S127 H128 M129 D130 D131 A132 N133 D134 I135 R136 A137 R138 L139 Q140 T141 L142 S143 E144 R145 E146 R147 Q148 V149 L150 S151 A152 V153 V154 A155 G156 L157 P158 N159 K160 S161 I162 A163 Y164 D165 L166 D167 I168 S169 P170 R171 T172 V173 E174 V175 H176 R177 A178 N179 V180 M181 A182 K183 M184 K185

A186 K187 S188 L189 P190 H191 L192 V193 R194 M195 A196 L197 A198 G199 G200 F201 G202 P203 S204

4.2.19 Score per residue for model 19

• Molecule 1: Transcriptional regulatory protein fixJ

Chain A: 14% 54% 20% • 10%

G126 S127 H128 M129 D130 D131 A132 N133 D134 I135 R136 A137 R138 L139 Q140 T141 L142 S143 E144 R145 E146 R147 Q148 V149 L150 S151 A152 V153 V154 A155 G156 L157 P158 N159 K160 S161 I162 A163 Y164 D165 L166 D167 I168 S169 P170 R171 T172 V173 E174 V175 H176 R177 A178 N179 V180 M181 A182 K183 M184 K185

A186 L189 P190 H191 L192 V193 R194 M195 A196 L197 F201 G202 P203 S204

4.2.20 Score per residue for model 20

• Molecule 1: Transcriptional regulatory protein fixJ

Chain A: 20% 53% 15% • 10%

G126 S127 H128 M129 D130 D131 A132 N133 D134 I135 R136 A137 R138 L139 Q140 T141 L142 S143 E144 R145 E146 R147 Q148 V149 L150 S151 A152 V153 V154 L157 P158 N159 K160 S161 I162 A163 Y164 D165 L166 D167 I168 S169 P170 R171 T172 V173 H176 R177 A178 N179 V180 M181 A182 K183 M184 K185 A186 K187

S188 L189 L192 V193 R194 M195 A196 L197 A198 F201 G202 P203 S204

5 Refinement protocol and experimental data overview (i)

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

Of the 80 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
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	545	575	573	76±9
All	All	10900	11500	11460	1514

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 68.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:ALA:HB3	1:A:162:ILE:HG23	1.08	1.22	2	17
1:A:168:ILE:HD12	1:A:172:THR:HG21	1.07	1.22	2	10
1:A:152:ALA:CB	1:A:162:ILE:HG23	0.93	1.93	3	17
1:A:163:ALA:HB2	1:A:173:VAL:CG1	0.93	1.94	18	15
1:A:181:MET:CB	1:A:192:LEU:HD11	0.93	1.94	20	1
1:A:135:ILE:HG22	1:A:139:LEU:HD21	0.92	1.36	3	2
1:A:139:LEU:HD23	1:A:201:PHE:CD1	0.92	1.99	8	4
1:A:149:VAL:HG11	1:A:180:VAL:HG21	0.90	1.41	7	3
1:A:163:ALA:HB2	1:A:173:VAL:HG13	0.89	1.39	6	10
1:A:132:ALA:HB1	1:A:198:ALA:O	0.87	1.69	12	5
1:A:150:LEU:HD11	1:A:196:ALA:HB2	0.87	1.45	4	7
1:A:176:HIS:O	1:A:180:VAL:HG23	0.87	1.70	7	5
1:A:168:ILE:CD1	1:A:172:THR:HG21	0.86	2.01	2	3
1:A:150:LEU:O	1:A:154:VAL:HG22	0.86	1.68	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:142:LEU:HD11	1:A:184:MET:CG	0.86	2.01	13	6
1:A:149:VAL:O	1:A:153:VAL:HG13	0.86	1.71	16	4
1:A:150:LEU:O	1:A:154:VAL:HG23	0.85	1.71	3	2
1:A:137:ALA:O	1:A:141:THR:HG23	0.85	1.71	9	17
1:A:149:VAL:O	1:A:153:VAL:HG22	0.85	1.70	4	1
1:A:153:VAL:HG22	1:A:189:LEU:HD21	0.85	1.49	2	2
1:A:153:VAL:HG22	1:A:189:LEU:HD11	0.85	1.46	10	6
1:A:150:LEU:O	1:A:154:VAL:HG13	0.84	1.72	19	10
1:A:145:ARG:O	1:A:149:VAL:HG23	0.84	1.71	18	8
1:A:135:ILE:HG22	1:A:139:LEU:CD1	0.84	2.01	9	5
1:A:168:ILE:HD12	1:A:172:THR:CG2	0.84	2.02	2	12
1:A:138:ARG:O	1:A:141:THR:HG22	0.83	1.72	6	1
1:A:145:ARG:O	1:A:149:VAL:HG12	0.81	1.75	12	7
1:A:135:ILE:CG2	1:A:139:LEU:HD21	0.81	2.04	3	1
1:A:135:ILE:HG22	1:A:139:LEU:HD12	0.80	1.54	6	1
1:A:150:LEU:HD21	1:A:196:ALA:CB	0.80	2.06	12	1
1:A:142:LEU:HD13	1:A:146:GLU:CD	0.80	1.97	1	8
1:A:153:VAL:CG2	1:A:189:LEU:HD11	0.80	2.06	15	6
1:A:176:HIS:O	1:A:180:VAL:HG13	0.79	1.77	3	2
1:A:139:LEU:O	1:A:142:LEU:HD12	0.79	1.76	13	1
1:A:157:LEU:O	1:A:162:ILE:HD11	0.79	1.77	13	11
1:A:153:VAL:CG1	1:A:189:LEU:HD11	0.79	2.07	4	2
1:A:189:LEU:O	1:A:193:VAL:HG22	0.79	1.76	8	5
1:A:184:MET:SD	1:A:186:ALA:HB2	0.79	2.17	19	5
1:A:148:GLN:NE2	1:A:168:ILE:HD13	0.79	1.93	16	2
1:A:146:GLU:OE2	1:A:150:LEU:HD22	0.78	1.78	11	3
1:A:163:ALA:HB2	1:A:173:VAL:HG11	0.78	1.53	9	3
1:A:139:LEU:HD23	1:A:201:PHE:CG	0.78	2.13	11	3
1:A:171:ARG:O	1:A:175:VAL:HG23	0.78	1.79	12	17
1:A:176:HIS:O	1:A:180:VAL:HG12	0.78	1.77	9	1
1:A:139:LEU:HD12	1:A:150:LEU:HD22	0.78	1.53	13	3
1:A:131:ASP:O	1:A:135:ILE:HD12	0.77	1.79	10	3
1:A:142:LEU:HD11	1:A:184:MET:HG3	0.77	1.54	13	2
1:A:135:ILE:HG21	1:A:195:MET:HB3	0.77	1.56	2	13
1:A:145:ARG:O	1:A:149:VAL:HG13	0.77	1.78	6	1
1:A:142:LEU:HD12	1:A:183:LYS:HB2	0.77	1.56	16	1
1:A:135:ILE:HD13	1:A:195:MET:SD	0.76	2.21	9	2
1:A:151:SER:O	1:A:154:VAL:HG22	0.76	1.80	15	5
1:A:172:THR:HG23	1:A:176:HIS:CE1	0.75	2.15	9	10
1:A:181:MET:HB3	1:A:192:LEU:HD22	0.75	1.59	3	2
1:A:153:VAL:HG11	1:A:189:LEU:HD11	0.75	1.59	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:142:LEU:HD13	1:A:146:GLU:HG2	0.75	1.58	19	4
1:A:150:LEU:HD11	1:A:196:ALA:CB	0.75	2.12	4	4
1:A:189:LEU:O	1:A:193:VAL:HG12	0.75	1.81	7	1
1:A:138:ARG:O	1:A:142:LEU:HD12	0.74	1.82	10	10
1:A:135:ILE:HG22	1:A:139:LEU:CD2	0.74	2.12	3	6
1:A:142:LEU:HD21	1:A:184:MET:N	0.74	1.97	5	11
1:A:177:ARG:NH2	1:A:189:LEU:HD21	0.74	1.98	7	1
1:A:145:ARG:O	1:A:149:VAL:HG22	0.74	1.83	15	1
1:A:162:ILE:O	1:A:166:LEU:HD22	0.74	1.82	7	1
1:A:163:ALA:HB2	1:A:173:VAL:HG23	0.74	1.60	13	1
1:A:189:LEU:HA	1:A:192:LEU:HD23	0.73	1.60	8	1
1:A:142:LEU:HD11	1:A:184:MET:HG2	0.73	1.59	2	4
1:A:181:MET:HB3	1:A:192:LEU:HD11	0.73	1.61	20	8
1:A:196:ALA:HB1	1:A:201:PHE:CB	0.73	2.13	19	5
1:A:197:LEU:HD12	1:A:198:ALA:N	0.73	1.98	20	3
1:A:153:VAL:HG22	1:A:189:LEU:CD2	0.72	2.14	14	1
1:A:139:LEU:CD1	1:A:150:LEU:HD22	0.72	2.14	13	3
1:A:163:ALA:HB1	1:A:169:SER:O	0.72	1.83	17	11
1:A:135:ILE:HG21	1:A:195:MET:O	0.72	1.83	3	2
1:A:149:VAL:CG1	1:A:180:VAL:HG21	0.72	2.14	13	3
1:A:148:GLN:HB3	1:A:166:LEU:HD13	0.72	1.62	14	12
1:A:142:LEU:HD12	1:A:183:LYS:CB	0.72	2.15	16	1
1:A:150:LEU:O	1:A:150:LEU:HD23	0.71	1.84	12	1
1:A:139:LEU:HD23	1:A:146:GLU:OE2	0.71	1.86	6	1
1:A:165:ASP:C	1:A:166:LEU:HD13	0.71	2.06	7	1
1:A:154:VAL:HG21	1:A:201:PHE:O	0.71	1.84	6	2
1:A:196:ALA:HB1	1:A:201:PHE:HB2	0.70	1.64	14	5
1:A:142:LEU:HD13	1:A:146:GLU:CG	0.70	2.17	3	10
1:A:150:LEU:HD21	1:A:196:ALA:HB1	0.69	1.64	12	1
1:A:154:VAL:HA	1:A:193:VAL:HG12	0.69	1.64	6	4
1:A:154:VAL:HA	1:A:193:VAL:HG13	0.69	1.65	16	8
1:A:153:VAL:HG21	1:A:189:LEU:HD11	0.69	1.62	15	1
1:A:186:ALA:HB2	1:A:192:LEU:CD2	0.69	2.16	18	6
1:A:139:LEU:HG	1:A:150:LEU:HD23	0.68	1.65	8	4
1:A:150:LEU:HD23	1:A:154:VAL:HG13	0.68	1.65	17	1
1:A:181:MET:O	1:A:186:ALA:HB3	0.68	1.87	9	1
1:A:192:LEU:HA	1:A:195:MET:HE2	0.68	1.65	3	1
1:A:170:PRO:O	1:A:173:VAL:HG22	0.67	1.89	19	4
1:A:149:VAL:HG22	1:A:153:VAL:CG1	0.67	2.19	16	2
1:A:153:VAL:HG12	1:A:193:VAL:CG2	0.67	2.19	14	2
1:A:135:ILE:HG21	1:A:195:MET:CB	0.67	2.20	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:135:ILE:HG23	1:A:184:MET:HE1	0.67	1.64	11	2
1:A:149:VAL:HG21	1:A:177:ARG:HB3	0.67	1.65	3	2
1:A:152:ALA:HB1	1:A:162:ILE:HG12	0.67	1.67	1	12
1:A:146:GLU:OE2	1:A:150:LEU:HD13	0.67	1.89	12	1
1:A:181:MET:HA	1:A:186:ALA:HB3	0.66	1.68	5	1
1:A:168:ILE:HD13	1:A:172:THR:CG2	0.66	2.19	11	3
1:A:166:LEU:HD13	1:A:166:LEU:N	0.66	2.05	7	1
1:A:142:LEU:HD23	1:A:183:LYS:HB2	0.66	1.68	10	5
1:A:142:LEU:HD23	1:A:183:LYS:CB	0.66	2.21	2	9
1:A:152:ALA:HB1	1:A:162:ILE:HG23	0.66	1.67	19	4
1:A:170:PRO:O	1:A:173:VAL:HG13	0.65	1.90	11	1
1:A:135:ILE:HG23	1:A:184:MET:SD	0.65	2.32	20	2
1:A:142:LEU:HD13	1:A:146:GLU:HG3	0.65	1.68	3	8
1:A:184:MET:SD	1:A:192:LEU:HD22	0.65	2.31	10	1
1:A:197:LEU:N	1:A:197:LEU:HD23	0.65	2.07	1	14
1:A:146:GLU:HG2	1:A:180:VAL:HG13	0.65	1.66	8	7
1:A:196:ALA:HB1	1:A:201:PHE:HB3	0.64	1.68	19	4
1:A:177:ARG:HD2	1:A:189:LEU:HD13	0.64	1.69	15	1
1:A:135:ILE:HG22	1:A:139:LEU:HD11	0.64	1.69	9	3
1:A:139:LEU:HD23	1:A:201:PHE:CD2	0.64	2.26	15	3
1:A:150:LEU:HD13	1:A:153:VAL:HG12	0.64	1.69	6	3
1:A:142:LEU:HD11	1:A:184:MET:HB3	0.64	1.69	3	1
1:A:172:THR:HG23	1:A:176:HIS:NE2	0.64	2.08	1	6
1:A:135:ILE:HD12	1:A:195:MET:HB3	0.64	1.69	12	3
1:A:139:LEU:HD22	1:A:150:LEU:HD22	0.64	1.68	14	1
1:A:142:LEU:HD23	1:A:183:LYS:HB3	0.63	1.70	5	8
1:A:134:ASP:O	1:A:137:ALA:HB3	0.63	1.94	12	1
1:A:142:LEU:HD21	1:A:184:MET:HB3	0.63	1.70	19	3
1:A:154:VAL:HG11	1:A:201:PHE:O	0.63	1.93	8	2
1:A:153:VAL:HG23	1:A:193:VAL:HG22	0.63	1.70	16	3
1:A:132:ALA:HB1	1:A:198:ALA:C	0.63	2.13	12	2
1:A:193:VAL:HG12	1:A:197:LEU:HD23	0.62	1.69	20	2
1:A:181:MET:HA	1:A:192:LEU:HD21	0.62	1.69	10	4
1:A:197:LEU:HD12	1:A:197:LEU:C	0.62	2.14	20	2
1:A:149:VAL:HG21	1:A:177:ARG:HB2	0.62	1.70	19	1
1:A:148:GLN:C	1:A:166:LEU:HD13	0.62	2.15	3	3
1:A:193:VAL:O	1:A:196:ALA:HB3	0.61	1.93	3	16
1:A:167:ASP:O	1:A:168:ILE:HG23	0.61	1.95	17	16
1:A:139:LEU:CD2	1:A:150:LEU:HD22	0.61	2.25	14	1
1:A:142:LEU:HD21	1:A:184:MET:CB	0.61	2.25	19	2
1:A:172:THR:HG22	1:A:176:HIS:CE1	0.61	2.30	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:197:LEU:C	1:A:197:LEU:HD12	0.61	2.15	6	1
1:A:149:VAL:HG11	1:A:177:ARG:HA	0.61	1.72	20	2
1:A:180:VAL:HG12	1:A:181:MET:N	0.60	2.10	8	7
1:A:153:VAL:HG22	1:A:189:LEU:CD1	0.60	2.26	20	2
1:A:135:ILE:O	1:A:139:LEU:HD23	0.60	1.95	18	1
1:A:148:GLN:HE22	1:A:168:ILE:HD13	0.60	1.54	16	2
1:A:139:LEU:HD12	1:A:201:PHE:CD2	0.60	2.31	12	1
1:A:142:LEU:HD12	1:A:146:GLU:HG2	0.60	1.73	12	1
1:A:142:LEU:HD23	1:A:183:LYS:HG3	0.60	1.74	9	2
1:A:139:LEU:HD13	1:A:201:PHE:CD1	0.60	2.31	14	1
1:A:153:VAL:HB	1:A:189:LEU:HD11	0.60	1.73	16	1
1:A:139:LEU:HD22	1:A:184:MET:CE	0.59	2.27	3	1
1:A:139:LEU:HD23	1:A:146:GLU:CD	0.59	2.18	6	1
1:A:142:LEU:HD21	1:A:184:MET:HA	0.59	1.75	9	2
1:A:177:ARG:HE	1:A:189:LEU:HD21	0.59	1.56	19	1
1:A:163:ALA:CB	1:A:173:VAL:HG13	0.59	2.26	20	3
1:A:135:ILE:HG22	1:A:139:LEU:HD13	0.59	1.75	16	4
1:A:150:LEU:HD21	1:A:196:ALA:HB2	0.58	1.75	12	1
1:A:181:MET:CB	1:A:192:LEU:HD13	0.58	2.28	9	1
1:A:136:ARG:HA	1:A:139:LEU:HD22	0.58	1.73	11	3
1:A:146:GLU:HG3	1:A:180:VAL:HG22	0.58	1.76	18	1
1:A:146:GLU:OE2	1:A:150:LEU:HD23	0.58	1.97	16	3
1:A:152:ALA:O	1:A:157:LEU:HD22	0.58	1.99	15	1
1:A:163:ALA:HB1	1:A:169:SER:C	0.57	2.19	1	6
1:A:150:LEU:CD2	1:A:154:VAL:HG13	0.57	2.28	17	1
1:A:135:ILE:HD13	1:A:195:MET:HB3	0.57	1.76	6	1
1:A:139:LEU:HD11	1:A:150:LEU:CD2	0.57	2.29	11	1
1:A:150:LEU:HD22	1:A:201:PHE:CD1	0.57	2.34	12	1
1:A:153:VAL:HG13	1:A:189:LEU:CD1	0.57	2.29	3	2
1:A:186:ALA:HB1	1:A:192:LEU:HD23	0.57	1.76	9	3
1:A:148:GLN:CB	1:A:166:LEU:HD13	0.57	2.30	20	1
1:A:181:MET:SD	1:A:189:LEU:HD22	0.56	2.40	19	1
1:A:149:VAL:CG1	1:A:180:VAL:HG11	0.56	2.31	11	2
1:A:139:LEU:HD11	1:A:184:MET:HE1	0.56	1.76	5	2
1:A:136:ARG:HA	1:A:139:LEU:HD23	0.56	1.76	4	2
1:A:142:LEU:HD21	1:A:184:MET:CA	0.56	2.31	7	10
1:A:142:LEU:HD13	1:A:146:GLU:OE2	0.56	2.00	6	1
1:A:148:GLN:HA	1:A:166:LEU:HD22	0.56	1.76	20	1
1:A:186:ALA:HB2	1:A:192:LEU:HD23	0.55	1.76	2	9
1:A:153:VAL:CG1	1:A:193:VAL:HG22	0.55	2.31	3	4
1:A:181:MET:HB2	1:A:192:LEU:HD11	0.55	1.76	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:142:LEU:HD22	1:A:146:GLU:HG3	0.55	1.77	2	7
1:A:163:ALA:CA	1:A:168:ILE:HG22	0.55	2.32	2	2
1:A:135:ILE:HG23	1:A:184:MET:CE	0.55	2.32	11	1
1:A:142:LEU:HD23	1:A:183:LYS:CG	0.55	2.32	19	1
1:A:178:ALA:O	1:A:182:ALA:HB2	0.55	2.01	17	3
1:A:168:ILE:HB	1:A:172:THR:HG21	0.54	1.79	12	1
1:A:146:GLU:HG3	1:A:180:VAL:HG13	0.54	1.79	17	1
1:A:151:SER:C	1:A:154:VAL:HG22	0.54	2.23	20	6
1:A:172:THR:HG23	1:A:176:HIS:CD2	0.54	2.38	7	9
1:A:152:ALA:HB1	1:A:162:ILE:HA	0.54	1.79	13	3
1:A:153:VAL:HG12	1:A:193:VAL:HG22	0.54	1.79	19	3
1:A:168:ILE:CG2	1:A:169:SER:N	0.54	2.71	2	3
1:A:131:ASP:O	1:A:135:ILE:HD11	0.54	2.03	12	1
1:A:163:ALA:HB2	1:A:173:VAL:HG12	0.54	1.75	18	2
1:A:168:ILE:HD13	1:A:172:THR:HG22	0.53	1.79	3	3
1:A:139:LEU:CG	1:A:150:LEU:HD23	0.53	2.33	11	1
1:A:168:ILE:HD12	1:A:172:THR:HG22	0.53	1.80	8	1
1:A:181:MET:HE1	1:A:188:SER:HA	0.53	1.80	8	1
1:A:177:ARG:CZ	1:A:189:LEU:HD11	0.53	2.34	7	1
1:A:158:PRO:O	1:A:162:ILE:HD12	0.53	2.03	10	3
1:A:184:MET:SD	1:A:192:LEU:HD23	0.53	2.44	17	1
1:A:189:LEU:O	1:A:193:VAL:HG23	0.53	2.04	3	2
1:A:135:ILE:HG22	1:A:139:LEU:HD22	0.53	1.79	20	3
1:A:145:ARG:CG	1:A:176:HIS:CD2	0.52	2.92	18	3
1:A:139:LEU:CD2	1:A:150:LEU:HD23	0.52	2.34	9	1
1:A:139:LEU:CD1	1:A:201:PHE:CD2	0.52	2.91	12	1
1:A:157:LEU:N	1:A:157:LEU:HD13	0.52	2.19	15	1
1:A:180:VAL:HG22	1:A:181:MET:N	0.52	2.18	9	1
1:A:177:ARG:CZ	1:A:189:LEU:HD21	0.52	2.33	7	1
1:A:146:GLU:CD	1:A:180:VAL:HG13	0.52	2.25	5	2
1:A:176:HIS:C	1:A:180:VAL:HG23	0.52	2.23	5	2
1:A:189:LEU:N	1:A:190:PRO:CD	0.52	2.73	2	15
1:A:139:LEU:HD22	1:A:150:LEU:CD2	0.52	2.35	14	1
1:A:150:LEU:HD23	1:A:154:VAL:CG1	0.52	2.34	17	1
1:A:139:LEU:CD2	1:A:201:PHE:CG	0.52	2.92	10	3
1:A:163:ALA:HB2	1:A:173:VAL:CG2	0.52	2.31	13	1
1:A:181:MET:HB3	1:A:192:LEU:HD13	0.52	1.82	9	1
1:A:154:VAL:HG23	1:A:197:LEU:CD2	0.51	2.34	7	1
1:A:142:LEU:HD21	1:A:184:MET:HG2	0.51	1.82	13	1
1:A:155:ALA:HB3	1:A:157:LEU:CD2	0.51	2.35	15	1
1:A:150:LEU:CD1	1:A:196:ALA:HB2	0.51	2.35	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:146:GLU:OE2	1:A:180:VAL:HG13	0.51	2.06	5	1
1:A:151:SER:C	1:A:154:VAL:HG12	0.51	2.25	7	2
1:A:172:THR:CG2	1:A:176:HIS:CE1	0.51	2.93	12	2
1:A:181:MET:CA	1:A:186:ALA:HB3	0.51	2.35	5	3
1:A:146:GLU:OE1	1:A:180:VAL:HG13	0.51	2.06	11	1
1:A:139:LEU:HG	1:A:150:LEU:HD21	0.51	1.82	4	1
1:A:146:GLU:CG	1:A:180:VAL:HG13	0.51	2.35	5	1
1:A:139:LEU:CB	1:A:201:PHE:CE1	0.51	2.93	7	5
1:A:173:VAL:CG2	1:A:174:GLU:N	0.51	2.74	11	6
1:A:189:LEU:N	1:A:190:PRO:HD2	0.51	2.21	4	1
1:A:150:LEU:O	1:A:154:VAL:HG12	0.51	2.06	6	2
1:A:135:ILE:HG21	1:A:195:MET:C	0.50	2.27	3	1
1:A:168:ILE:HD13	1:A:172:THR:HG21	0.50	1.81	11	2
1:A:186:ALA:HB1	1:A:192:LEU:CD2	0.50	2.36	9	1
1:A:153:VAL:CG2	1:A:189:LEU:HD21	0.50	2.31	2	1
1:A:186:ALA:CB	1:A:192:LEU:CD2	0.50	2.89	4	9
1:A:142:LEU:CB	1:A:146:GLU:CG	0.50	2.90	9	1
1:A:149:VAL:HG23	1:A:176:HIS:CE1	0.50	2.41	11	1
1:A:149:VAL:HG13	1:A:150:LEU:N	0.50	2.21	16	3
1:A:194:ARG:O	1:A:198:ALA:HB2	0.50	2.07	1	1
1:A:153:VAL:HG23	1:A:154:VAL:N	0.50	2.22	5	4
1:A:132:ALA:HA	1:A:135:ILE:HD12	0.50	1.82	15	2
1:A:139:LEU:CD1	1:A:150:LEU:CD2	0.50	2.90	7	7
1:A:146:GLU:HA	1:A:180:VAL:HG21	0.50	1.84	15	7
1:A:149:VAL:CG2	1:A:176:HIS:CE1	0.49	2.94	11	1
1:A:153:VAL:HG11	1:A:189:LEU:CD1	0.49	2.34	4	1
1:A:177:ARG:HD2	1:A:189:LEU:HD21	0.49	1.83	12	2
1:A:151:SER:O	1:A:154:VAL:HG23	0.49	2.07	17	1
1:A:139:LEU:HD12	1:A:150:LEU:CD2	0.49	2.37	4	3
1:A:146:GLU:CD	1:A:150:LEU:HD23	0.49	2.27	15	2
1:A:149:VAL:CG2	1:A:150:LEU:N	0.49	2.76	6	1
1:A:193:VAL:HG12	1:A:197:LEU:HD21	0.49	1.85	11	1
1:A:176:HIS:O	1:A:180:VAL:N	0.49	2.46	4	2
1:A:186:ALA:CB	1:A:192:LEU:HD23	0.49	2.38	10	1
1:A:176:HIS:O	1:A:179:ASN:N	0.49	2.45	9	10
1:A:139:LEU:CD1	1:A:150:LEU:CD1	0.49	2.90	17	1
1:A:177:ARG:CG	1:A:178:ALA:N	0.49	2.75	3	4
1:A:149:VAL:HG11	1:A:180:VAL:HG11	0.49	1.85	11	1
1:A:139:LEU:HD11	1:A:196:ALA:HA	0.49	1.83	3	1
1:A:153:VAL:HG12	1:A:189:LEU:HD11	0.49	1.84	4	1
1:A:163:ALA:CB	1:A:173:VAL:CG1	0.48	2.90	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:146:GLU:HA	1:A:180:VAL:HG22	0.48	1.84	13	2
1:A:172:THR:CG2	1:A:176:HIS:CD2	0.48	2.96	10	2
1:A:150:LEU:HD13	1:A:192:LEU:HD11	0.48	1.86	3	1
1:A:180:VAL:CG2	1:A:181:MET:N	0.48	2.76	3	1
1:A:153:VAL:CG1	1:A:193:VAL:CG1	0.48	2.91	17	1
1:A:150:LEU:HA	1:A:153:VAL:CG2	0.48	2.39	4	6
1:A:187:LYS:CD	1:A:188:SER:N	0.48	2.77	14	3
1:A:139:LEU:CD2	1:A:150:LEU:HD21	0.48	2.38	16	1
1:A:150:LEU:HD13	1:A:192:LEU:CD1	0.48	2.38	3	1
1:A:139:LEU:CD1	1:A:184:MET:CE	0.48	2.92	17	3
1:A:186:ALA:HB2	1:A:192:LEU:HD21	0.48	1.85	12	1
1:A:136:ARG:HA	1:A:139:LEU:HD12	0.48	1.86	14	1
1:A:163:ALA:HB1	1:A:168:ILE:HG22	0.48	1.86	2	3
1:A:142:LEU:CD2	1:A:183:LYS:CB	0.48	2.91	5	1
1:A:150:LEU:HA	1:A:153:VAL:HG22	0.48	1.85	16	2
1:A:139:LEU:HA	1:A:142:LEU:HD12	0.48	1.85	1	4
1:A:151:SER:HA	1:A:154:VAL:CG2	0.48	2.39	17	4
1:A:145:ARG:CG	1:A:176:HIS:NE2	0.48	2.77	13	3
1:A:181:MET:CA	1:A:192:LEU:HD21	0.48	2.39	10	2
1:A:172:THR:CG2	1:A:176:HIS:NE2	0.48	2.77	9	1
1:A:131:ASP:CB	1:A:134:ASP:CB	0.48	2.92	12	1
1:A:154:VAL:CG2	1:A:197:LEU:CD2	0.48	2.92	7	1
1:A:153:VAL:CG1	1:A:193:VAL:CG2	0.47	2.92	19	4
1:A:146:GLU:N	1:A:180:VAL:CG2	0.47	2.76	11	1
1:A:178:ALA:O	1:A:182:ALA:HB3	0.47	2.07	12	1
1:A:149:VAL:CG1	1:A:150:LEU:N	0.47	2.77	11	3
1:A:133:ASN:ND2	1:A:136:ARG:NE	0.47	2.62	10	4
1:A:155:ALA:HB3	1:A:157:LEU:HD21	0.47	1.85	15	1
1:A:139:LEU:CD2	1:A:184:MET:CE	0.47	2.92	3	2
1:A:180:VAL:O	1:A:184:MET:CG	0.47	2.63	19	2
1:A:193:VAL:CG1	1:A:197:LEU:HD21	0.47	2.39	14	2
1:A:186:ALA:CB	1:A:192:LEU:CD1	0.47	2.92	19	2
1:A:153:VAL:HG13	1:A:193:VAL:CG2	0.47	2.39	2	2
1:A:145:ARG:HG3	1:A:176:HIS:CD2	0.47	2.44	18	5
1:A:173:VAL:O	1:A:177:ARG:CB	0.47	2.62	11	11
1:A:145:ARG:NE	1:A:176:HIS:NE2	0.47	2.63	2	3
1:A:139:LEU:HD22	1:A:201:PHE:CE2	0.47	2.45	6	1
1:A:166:LEU:N	1:A:166:LEU:CD1	0.47	2.76	7	1
1:A:172:THR:OG1	1:A:176:HIS:CE1	0.47	2.67	7	1
1:A:148:GLN:NE2	1:A:168:ILE:CD1	0.47	2.78	15	1
1:A:177:ARG:CZ	1:A:189:LEU:CD2	0.47	2.92	18	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:163:ALA:CB	1:A:168:ILE:HG22	0.47	2.40	2	3
1:A:168:ILE:HG23	1:A:169:SER:N	0.47	2.25	2	2
1:A:181:MET:HE3	1:A:192:LEU:HD21	0.47	1.87	16	1
1:A:163:ALA:HB2	1:A:170:PRO:HA	0.47	1.87	19	3
1:A:139:LEU:HD11	1:A:184:MET:CE	0.47	2.40	5	3
1:A:178:ALA:O	1:A:182:ALA:CB	0.47	2.63	13	8
1:A:139:LEU:CD2	1:A:150:LEU:CD2	0.47	2.93	9	1
1:A:151:SER:O	1:A:154:VAL:CG2	0.47	2.63	1	8
1:A:154:VAL:HG13	1:A:155:ALA:N	0.47	2.24	2	4
1:A:168:ILE:HD12	1:A:169:SER:O	0.47	2.10	11	3
1:A:139:LEU:HD23	1:A:184:MET:HE2	0.46	1.85	12	1
1:A:150:LEU:CD2	1:A:154:VAL:CG1	0.46	2.93	17	1
1:A:146:GLU:O	1:A:150:LEU:CB	0.46	2.64	11	11
1:A:184:MET:HE3	1:A:192:LEU:CD2	0.46	2.41	6	1
1:A:150:LEU:O	1:A:153:VAL:N	0.46	2.48	14	3
1:A:163:ALA:O	1:A:168:ILE:CG1	0.46	2.64	6	13
1:A:146:GLU:HA	1:A:180:VAL:CG2	0.46	2.40	8	8
1:A:151:SER:O	1:A:154:VAL:HG12	0.46	2.11	7	2
1:A:177:ARG:NE	1:A:189:LEU:CD2	0.46	2.79	10	1
1:A:159:ASN:ND2	1:A:173:VAL:HG21	0.46	2.26	18	1
1:A:154:VAL:HG23	1:A:155:ALA:N	0.46	2.26	19	1
1:A:149:VAL:HG21	1:A:177:ARG:CB	0.46	2.39	3	2
1:A:197:LEU:CD1	1:A:198:ALA:N	0.46	2.77	10	2
1:A:142:LEU:HB2	1:A:146:GLU:CB	0.46	2.40	20	4
1:A:150:LEU:HD23	1:A:184:MET:SD	0.46	2.51	18	1
1:A:135:ILE:CG2	1:A:184:MET:CE	0.46	2.94	10	1
1:A:153:VAL:CG1	1:A:193:VAL:HG13	0.46	2.41	17	1
1:A:157:LEU:HD22	1:A:157:LEU:H	0.46	1.71	15	1
1:A:136:ARG:CG	1:A:199:GLY:O	0.46	2.64	18	3
1:A:139:LEU:HD12	1:A:201:PHE:CG	0.46	2.46	3	1
1:A:181:MET:CB	1:A:192:LEU:CD1	0.46	2.93	9	1
1:A:154:VAL:CG1	1:A:155:ALA:N	0.45	2.79	9	3
1:A:169:SER:O	1:A:172:THR:CB	0.45	2.63	12	1
1:A:145:ARG:HD3	1:A:176:HIS:CE1	0.45	2.46	19	1
1:A:135:ILE:C	1:A:139:LEU:HD23	0.45	2.30	18	1
1:A:139:LEU:HB3	1:A:201:PHE:CE1	0.45	2.47	1	5
1:A:176:HIS:C	1:A:180:VAL:HG12	0.45	2.30	9	1
1:A:138:ARG:O	1:A:142:LEU:CD1	0.45	2.64	15	2
1:A:135:ILE:O	1:A:139:LEU:N	0.45	2.48	14	13
1:A:148:GLN:O	1:A:166:LEU:CD2	0.45	2.65	3	6
1:A:192:LEU:O	1:A:196:ALA:N	0.45	2.48	20	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:186:ALA:CB	1:A:192:LEU:HD22	0.45	2.42	9	1
1:A:142:LEU:HD22	1:A:142:LEU:N	0.45	2.27	16	1
1:A:186:ALA:CB	1:A:192:LEU:CB	0.45	2.94	3	1
1:A:143:SER:O	1:A:146:GLU:CG	0.45	2.65	20	2
1:A:139:LEU:CB	1:A:146:GLU:OE2	0.45	2.65	16	1
1:A:142:LEU:HD22	1:A:146:GLU:HG2	0.45	1.89	17	1
1:A:170:PRO:HA	1:A:173:VAL:HG22	0.45	1.88	3	1
1:A:173:VAL:O	1:A:177:ARG:N	0.45	2.50	16	10
1:A:188:SER:O	1:A:192:LEU:CD2	0.45	2.65	9	3
1:A:159:ASN:O	1:A:173:VAL:HG11	0.45	2.11	5	2
1:A:191:HIS:CD2	1:A:195:MET:SD	0.45	3.10	10	1
1:A:132:ALA:CB	1:A:198:ALA:O	0.45	2.65	18	1
1:A:150:LEU:HD12	1:A:153:VAL:CG2	0.45	2.42	16	1
1:A:145:ARG:HD2	1:A:176:HIS:CG	0.45	2.46	19	1
1:A:184:MET:O	1:A:185:LYS:CB	0.45	2.65	3	12
1:A:180:VAL:CG1	1:A:181:MET:N	0.45	2.79	4	2
1:A:177:ARG:NE	1:A:189:LEU:HD23	0.45	2.27	10	1
1:A:163:ALA:CB	1:A:169:SER:O	0.44	2.65	18	3
1:A:142:LEU:HB2	1:A:146:GLU:HB3	0.44	1.89	20	1
1:A:153:VAL:CG2	1:A:189:LEU:CD1	0.44	2.94	20	1
1:A:179:ASN:O	1:A:183:LYS:CG	0.44	2.66	13	4
1:A:148:GLN:CA	1:A:166:LEU:HD22	0.44	2.42	20	2
1:A:136:ARG:CD	1:A:199:GLY:O	0.44	2.66	9	3
1:A:173:VAL:HG23	1:A:174:GLU:N	0.44	2.28	7	2
1:A:139:LEU:HD23	1:A:201:PHE:CE1	0.44	2.45	8	1
1:A:150:LEU:HD22	1:A:201:PHE:CD2	0.44	2.47	17	1
1:A:142:LEU:CD2	1:A:184:MET:N	0.44	2.77	5	2
1:A:153:VAL:CG2	1:A:154:VAL:N	0.44	2.81	11	5
1:A:139:LEU:HD22	1:A:150:LEU:HD13	0.44	1.90	12	1
1:A:146:GLU:OE2	1:A:150:LEU:CD1	0.44	2.64	12	1
1:A:139:LEU:CD2	1:A:146:GLU:OE2	0.44	2.64	6	1
1:A:149:VAL:HB	1:A:176:HIS:CE1	0.44	2.48	11	1
1:A:149:VAL:HG21	1:A:180:VAL:HG21	0.44	1.89	18	1
1:A:161:SER:O	1:A:165:ASP:CB	0.44	2.66	5	11
1:A:145:ARG:HD3	1:A:176:HIS:CD2	0.44	2.47	15	4
1:A:189:LEU:O	1:A:193:VAL:CG2	0.44	2.66	3	1
1:A:179:ASN:O	1:A:183:LYS:N	0.44	2.51	11	2
1:A:139:LEU:O	1:A:146:GLU:CG	0.44	2.66	12	1
1:A:145:ARG:CD	1:A:145:ARG:N	0.44	2.79	14	1
1:A:186:ALA:HB3	1:A:192:LEU:HD11	0.44	1.89	17	1
1:A:145:ARG:CD	1:A:176:HIS:CG	0.44	3.01	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:190:PRO:O	1:A:194:ARG:CG	0.44	2.66	2	9
1:A:176:HIS:C	1:A:180:VAL:HG13	0.44	2.32	3	1
1:A:192:LEU:O	1:A:195:MET:N	0.44	2.51	19	2
1:A:179:ASN:O	1:A:183:LYS:CD	0.44	2.66	12	6
1:A:193:VAL:O	1:A:197:LEU:CD2	0.44	2.66	11	6
1:A:172:THR:O	1:A:175:VAL:N	0.44	2.51	3	4
1:A:192:LEU:HG	1:A:193:VAL:N	0.44	2.28	8	2
1:A:139:LEU:CA	1:A:146:GLU:OE2	0.44	2.66	16	2
1:A:150:LEU:HD13	1:A:192:LEU:HB3	0.44	1.89	11	1
1:A:177:ARG:O	1:A:181:MET:CG	0.43	2.66	9	4
1:A:135:ILE:O	1:A:138:ARG:N	0.43	2.51	12	6
1:A:154:VAL:CG1	1:A:201:PHE:O	0.43	2.66	8	1
1:A:167:ASP:O	1:A:168:ILE:CG2	0.43	2.66	4	13
1:A:181:MET:O	1:A:186:ALA:N	0.43	2.51	11	4
1:A:145:ARG:HB3	1:A:176:HIS:CD2	0.43	2.49	14	6
1:A:174:GLU:O	1:A:178:ALA:CB	0.43	2.66	13	1
1:A:172:THR:O	1:A:176:HIS:CG	0.43	2.71	17	1
1:A:144:GLU:O	1:A:148:GLN:CG	0.43	2.66	2	8
1:A:172:THR:HG1	1:A:176:HIS:CE1	0.43	2.31	4	1
1:A:150:LEU:HD12	1:A:154:VAL:HB	0.43	1.90	6	1
1:A:187:LYS:CG	1:A:188:SER:N	0.43	2.80	10	2
1:A:139:LEU:CA	1:A:142:LEU:HD12	0.43	2.44	1	3
1:A:177:ARG:HG2	1:A:178:ALA:N	0.43	2.29	13	1
1:A:135:ILE:O	1:A:139:LEU:CG	0.43	2.66	14	1
1:A:153:VAL:CG1	1:A:193:VAL:HG23	0.43	2.44	14	2
1:A:149:VAL:HG23	1:A:150:LEU:N	0.43	2.27	6	1
1:A:193:VAL:O	1:A:196:ALA:N	0.43	2.51	3	2
1:A:180:VAL:O	1:A:184:MET:N	0.43	2.49	7	2
1:A:145:ARG:HG3	1:A:176:HIS:NE2	0.43	2.29	7	4
1:A:196:ALA:O	1:A:199:GLY:N	0.43	2.52	10	1
1:A:131:ASP:O	1:A:135:ILE:CD1	0.43	2.67	12	1
1:A:196:ALA:O	1:A:201:PHE:N	0.43	2.52	14	1
1:A:146:GLU:O	1:A:150:LEU:N	0.43	2.47	16	1
1:A:161:SER:O	1:A:165:ASP:N	0.43	2.52	16	13
1:A:194:ARG:O	1:A:198:ALA:CB	0.43	2.67	1	2
1:A:149:VAL:HG22	1:A:153:VAL:HG13	0.43	1.89	5	1
1:A:170:PRO:O	1:A:173:VAL:CG2	0.43	2.67	17	2
1:A:146:GLU:OE1	1:A:146:GLU:CA	0.43	2.66	9	1
1:A:131:ASP:O	1:A:134:ASP:N	0.43	2.52	11	1
1:A:139:LEU:CD1	1:A:150:LEU:HD23	0.43	2.44	11	1
1:A:139:LEU:CD1	1:A:201:PHE:CG	0.43	3.01	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:148:GLN:NE2	1:A:168:ILE:HG13	0.43	2.29	14	1
1:A:139:LEU:HA	1:A:142:LEU:CD1	0.43	2.44	10	2
1:A:146:GLU:OE2	1:A:150:LEU:CD2	0.43	2.67	3	3
1:A:163:ALA:CB	1:A:173:VAL:HG11	0.43	2.44	3	1
1:A:163:ALA:HA	1:A:168:ILE:HG22	0.42	1.90	10	2
1:A:157:LEU:O	1:A:162:ILE:CD1	0.42	2.67	3	2
1:A:142:LEU:CD1	1:A:146:GLU:OE2	0.42	2.67	6	1
1:A:153:VAL:HG23	1:A:162:ILE:HG21	0.42	1.91	13	1
1:A:138:ARG:CD	1:A:184:MET:O	0.42	2.67	16	1
1:A:177:ARG:HG3	1:A:178:ALA:N	0.42	2.29	17	3
1:A:189:LEU:CB	1:A:190:PRO:HD3	0.42	2.43	8	2
1:A:152:ALA:O	1:A:162:ILE:HD12	0.42	2.14	5	1
1:A:148:GLN:O	1:A:166:LEU:HD22	0.42	2.14	16	1
1:A:191:HIS:CG	1:A:195:MET:SD	0.42	3.12	5	1
1:A:139:LEU:CD2	1:A:201:PHE:CD2	0.42	3.02	11	1
1:A:139:LEU:HG	1:A:150:LEU:HD13	0.42	1.91	17	1
1:A:181:MET:CE	1:A:187:LYS:O	0.42	2.68	17	1
1:A:152:ALA:O	1:A:155:ALA:N	0.42	2.53	6	2
1:A:186:ALA:HB2	1:A:195:MET:SD	0.42	2.55	10	1
1:A:140:GLN:OE1	1:A:147:ARG:CD	0.42	2.67	18	3
1:A:176:HIS:O	1:A:180:VAL:CG1	0.42	2.62	9	1
1:A:142:LEU:HD22	1:A:142:LEU:H	0.42	1.75	16	1
1:A:147:ARG:O	1:A:151:SER:CB	0.42	2.68	16	1
1:A:145:ARG:CD	1:A:176:HIS:CE1	0.42	3.03	19	1
1:A:144:GLU:CG	1:A:148:GLN:OE1	0.42	2.68	19	2
1:A:150:LEU:CD2	1:A:201:PHE:CD1	0.42	3.02	12	1
1:A:142:LEU:CD1	1:A:146:GLU:HB2	0.42	2.44	14	1
1:A:131:ASP:OD1	1:A:134:ASP:CB	0.42	2.68	15	1
1:A:172:THR:O	1:A:176:HIS:ND1	0.42	2.53	17	1
1:A:158:PRO:O	1:A:160:LYS:N	0.42	2.53	19	1
1:A:158:PRO:O	1:A:161:SER:N	0.42	2.53	19	1
1:A:136:ARG:O	1:A:140:GLN:NE2	0.42	2.53	11	3
1:A:189:LEU:CB	1:A:190:PRO:CD	0.42	2.98	8	1
1:A:153:VAL:CG2	1:A:189:LEU:CD2	0.42	2.92	14	1
1:A:148:GLN:O	1:A:166:LEU:CD1	0.42	2.68	16	1
1:A:195:MET:O	1:A:199:GLY:N	0.42	2.53	18	1
1:A:163:ALA:O	1:A:168:ILE:N	0.42	2.53	8	3
1:A:136:ARG:NE	1:A:199:GLY:O	0.42	2.53	9	2
1:A:135:ILE:HG23	1:A:184:MET:HE2	0.42	1.92	10	1
1:A:146:GLU:OE2	1:A:150:LEU:CB	0.42	2.68	12	1
1:A:135:ILE:O	1:A:139:LEU:HD12	0.42	2.14	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:142:LEU:CB	1:A:146:GLU:HG2	0.42	2.44	17	1
1:A:151:SER:CA	1:A:154:VAL:CG2	0.42	2.98	17	1
1:A:199:GLY:O	1:A:201:PHE:N	0.42	2.53	18	1
1:A:135:ILE:CG2	1:A:139:LEU:CD2	0.42	2.91	13	1
1:A:150:LEU:O	1:A:154:VAL:N	0.42	2.53	13	2
1:A:133:ASN:O	1:A:136:ARG:N	0.42	2.53	18	1
1:A:181:MET:CB	1:A:186:ALA:HB3	0.42	2.45	5	1
1:A:142:LEU:O	1:A:143:SER:CB	0.42	2.67	9	2
1:A:138:ARG:NH1	1:A:184:MET:O	0.42	2.53	14	1
1:A:176:HIS:O	1:A:180:VAL:CG2	0.42	2.68	15	1
1:A:135:ILE:O	1:A:139:LEU:CD2	0.42	2.68	18	1
1:A:150:LEU:O	1:A:154:VAL:CG1	0.41	2.67	7	3
1:A:142:LEU:HB2	1:A:146:GLU:CG	0.41	2.45	9	1
1:A:142:LEU:CB	1:A:146:GLU:HB3	0.41	2.45	14	1
1:A:149:VAL:O	1:A:153:VAL:N	0.41	2.51	15	2
1:A:144:GLU:O	1:A:148:GLN:CB	0.41	2.68	2	1
1:A:159:ASN:OD1	1:A:173:VAL:CG2	0.41	2.69	10	1
1:A:133:ASN:O	1:A:136:ARG:CG	0.41	2.67	15	1
1:A:193:VAL:O	1:A:197:LEU:HG	0.41	2.15	17	2
1:A:138:ARG:NH1	1:A:185:LYS:CD	0.41	2.83	6	1
1:A:151:SER:O	1:A:154:VAL:CG1	0.41	2.68	7	1
1:A:196:ALA:CB	1:A:201:PHE:HB2	0.41	2.44	19	1
1:A:149:VAL:N	1:A:166:LEU:HD13	0.41	2.30	3	1
1:A:139:LEU:HB3	1:A:201:PHE:CZ	0.41	2.50	7	1
1:A:181:MET:CB	1:A:192:LEU:HD21	0.41	2.45	10	1
1:A:187:LYS:HG3	1:A:188:SER:N	0.41	2.31	10	1
1:A:132:ALA:O	1:A:199:GLY:CA	0.41	2.67	12	1
1:A:135:ILE:CG2	1:A:195:MET:O	0.41	2.67	13	1
1:A:181:MET:HE1	1:A:188:SER:C	0.41	2.35	6	1
1:A:142:LEU:CD2	1:A:183:LYS:HB2	0.41	2.46	11	2
1:A:193:VAL:HA	1:A:196:ALA:HB3	0.41	1.92	6	1
1:A:140:GLN:OE1	1:A:147:ARG:NE	0.41	2.53	9	1
1:A:158:PRO:O	1:A:162:ILE:CD1	0.41	2.68	10	1
1:A:136:ARG:HG2	1:A:199:GLY:CA	0.41	2.45	11	1
1:A:173:VAL:HA	1:A:176:HIS:ND1	0.41	2.31	11	1
1:A:145:ARG:HD2	1:A:176:HIS:CE1	0.41	2.50	14	1
1:A:140:GLN:OE1	1:A:147:ARG:NH1	0.41	2.53	16	1
1:A:134:ASP:O	1:A:138:ARG:NH1	0.41	2.52	17	1
1:A:193:VAL:O	1:A:196:ALA:CB	0.41	2.68	3	1
1:A:193:VAL:HG23	1:A:197:LEU:HD21	0.41	1.93	7	1
1:A:145:ARG:HB3	1:A:176:HIS:CG	0.41	2.51	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:191:HIS:O	1:A:195:MET:CG	0.41	2.69	15	1
1:A:193:VAL:HG23	1:A:194:ARG:N	0.41	2.30	1	1
1:A:142:LEU:CD1	1:A:146:GLU:HG3	0.41	2.45	4	1
1:A:191:HIS:O	1:A:195:MET:N	0.41	2.52	13	1
1:A:135:ILE:C	1:A:139:LEU:HD13	0.41	2.36	16	1
1:A:142:LEU:CB	1:A:146:GLU:HB2	0.41	2.46	16	1
1:A:145:ARG:HD2	1:A:176:HIS:CD2	0.41	2.51	10	2
1:A:163:ALA:CA	1:A:173:VAL:HG11	0.41	2.46	3	1
1:A:194:ARG:O	1:A:198:ALA:N	0.41	2.51	8	1
1:A:177:ARG:HA	1:A:180:VAL:CG1	0.41	2.45	9	1
1:A:181:MET:HB2	1:A:192:LEU:CD1	0.41	2.46	9	1
1:A:184:MET:SD	1:A:192:LEU:CD2	0.41	3.09	11	1
1:A:131:ASP:HB3	1:A:134:ASP:CB	0.41	2.45	12	1
1:A:181:MET:SD	1:A:192:LEU:CD1	0.41	3.09	14	1
1:A:152:ALA:O	1:A:157:LEU:CD2	0.41	2.67	15	1
1:A:197:LEU:HD23	1:A:197:LEU:N	0.41	2.31	16	1
1:A:143:SER:N	1:A:146:GLU:OE1	0.41	2.53	17	1
1:A:152:ALA:CB	1:A:162:ILE:CG2	0.41	2.93	19	1
1:A:186:ALA:CB	1:A:192:LEU:HD11	0.41	2.46	19	1
1:A:162:ILE:O	1:A:165:ASP:N	0.41	2.54	20	1
1:A:157:LEU:HB3	1:A:158:PRO:CD	0.41	2.46	3	3
1:A:138:ARG:NH1	1:A:185:LYS:HD3	0.41	2.31	6	1
1:A:184:MET:HE1	1:A:195:MET:CE	0.41	2.46	10	1
1:A:169:SER:O	1:A:172:THR:HB	0.41	2.16	14	1
1:A:137:ALA:O	1:A:141:THR:CG2	0.41	2.69	16	1
1:A:181:MET:HE1	1:A:187:LYS:O	0.41	2.15	20	1
1:A:142:LEU:CB	1:A:146:GLU:HG3	0.40	2.46	7	2
1:A:180:VAL:O	1:A:184:MET:HG2	0.40	2.16	3	1
1:A:197:LEU:N	1:A:197:LEU:CD2	0.40	2.77	8	2
1:A:197:LEU:C	1:A:197:LEU:CD1	0.40	2.86	6	1
1:A:187:LYS:HD2	1:A:188:SER:CB	0.40	2.46	8	1
1:A:133:ASN:ND2	1:A:136:ARG:CD	0.40	2.85	10	1
1:A:146:GLU:CA	1:A:180:VAL:CG2	0.40	2.98	11	1
1:A:181:MET:HB2	1:A:192:LEU:CD2	0.40	2.46	4	1
1:A:184:MET:SD	1:A:195:MET:HE1	0.40	2.56	5	1
1:A:136:ARG:HG3	1:A:137:ALA:N	0.40	2.31	13	1
1:A:148:GLN:NE2	1:A:168:ILE:CG1	0.40	2.84	14	1
1:A:172:THR:HG22	1:A:173:VAL:N	0.40	2.30	15	1
1:A:148:GLN:O	1:A:166:LEU:HD13	0.40	2.16	16	1
1:A:180:VAL:O	1:A:184:MET:CB	0.40	2.69	19	1
1:A:136:ARG:HG3	1:A:199:GLY:O	0.40	2.16	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:146:GLU:HA	1:A:180:VAL:HG11	0.40	1.92	3	1
1:A:184:MET:SD	1:A:195:MET:CE	0.40	3.10	3	1
1:A:197:LEU:O	1:A:200:GLY:N	0.40	2.53	3	1
1:A:131:ASP:CB	1:A:134:ASP:HB3	0.40	2.46	12	1
1:A:143:SER:O	1:A:146:GLU:CB	0.40	2.68	20	1
1:A:162:ILE:N	1:A:162:ILE:HD13	0.40	2.30	13	1
1:A:136:ARG:CZ	1:A:199:GLY:O	0.40	2.70	14	1
1:A:145:ARG:CD	1:A:176:HIS:CD2	0.40	3.05	15	1
1:A:150:LEU:O	1:A:152:ALA:N	0.40	2.55	17	1
1:A:136:ARG:HG2	1:A:199:GLY:O	0.40	2.16	18	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	71/79 (90%)	54±2 (76±3%)	14±2 (20±3%)	3±1 (4±1%)	5 32
All	All	1420/1580 (90%)	1074 (76%)	290 (20%)	56 (4%)	5 32

All 17 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	142	LEU	14
1	A	131	ASP	8
1	A	143	SER	8
1	A	186	ALA	4
1	A	192	LEU	3
1	A	180	VAL	3
1	A	185	LYS	3
1	A	200	GLY	2
1	A	170	PRO	2
1	A	132	ALA	2
1	A	201	PHE	1
1	A	158	PRO	1

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Mol	Chain	Res	Type	Models (Total)
1	A	146	GLU	1
1	A	150	LEU	1
1	A	151	SER	1
1	A	149	VAL	1
1	A	159	ASN	1

6.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	58/64 (91%)	37±3 (63±5%)	21±3 (37±5%)	1 7
All	All	1160/1280 (91%)	733 (63%)	427 (37%)	1 7

All 51 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	164	TYR	20
1	A	166	LEU	20
1	A	169	SER	20
1	A	160	LYS	19
1	A	179	ASN	18
1	A	197	LEU	17
1	A	133	ASN	14
1	A	145	ARG	14
1	A	176	HIS	14
1	A	131	ASP	14
1	A	172	THR	13
1	A	139	LEU	12
1	A	184	MET	12
1	A	189	LEU	11
1	A	143	SER	11
1	A	153	VAL	10
1	A	177	ARG	10
1	A	171	ARG	10
1	A	187	LYS	10
1	A	161	SER	9

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Mol	Chain	Res	Type	Models (Total)
1	A	185	LYS	9
1	A	144	GLU	8
1	A	157	LEU	8
1	A	181	MET	8
1	A	194	ARG	8
1	A	180	VAL	8
1	A	174	GLU	7
1	A	148	GLN	7
1	A	147	ARG	7
1	A	138	ARG	6
1	A	183	LYS	6
1	A	140	GLN	5
1	A	192	LEU	5
1	A	134	ASP	5
1	A	201	PHE	5
1	A	142	LEU	5
1	A	135	ILE	4
1	A	150	LEU	4
1	A	193	VAL	4
1	A	146	GLU	4
1	A	191	HIS	3
1	A	195	MET	3
1	A	154	VAL	3
1	A	136	ARG	3
1	A	165	ASP	3
1	A	167	ASP	2
1	A	168	ILE	2
1	A	141	THR	2
1	A	151	SER	2
1	A	173	VAL	2
1	A	149	VAL	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