Full wwPDB NMR Structure Validation Report (i)

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PDB ID	:	2KW8
BMRB ID	:	16811
Title	:	Solution Structure of Bacillus anthracis Sortase A (SrtA) Transpeptidase
Authors	:	Weiner, E.M.; Robson, S.A.; Marohn, M.; Clubb, R.T.
Deposited on	:	2010-03-31

This is a Full wwPDB NMR Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

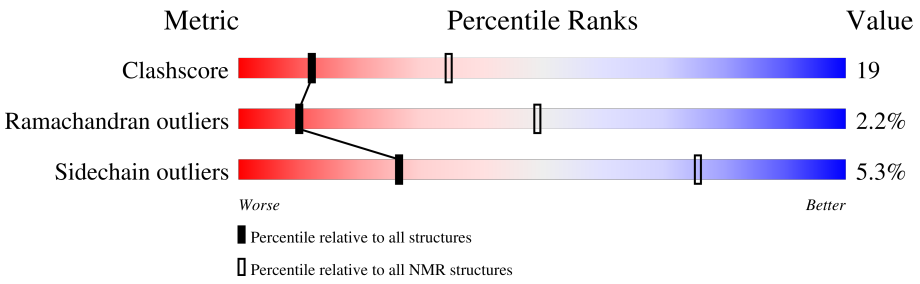
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The overall completeness of chemical shifts assignment is 88%.

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	158	60% 25% • 13%

2 Ensemble composition and analysis (i)

This entry contains 40 models. Model 8 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:64-A:186, A:196-A:210 (138)	0.50	8

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 5 clusters and 9 single-model clusters were found.

Cluster number	Models
1	1, 3, 6, 7, 8, 13, 14, 15, 19, 23, 25, 27, 29, 31, 36, 38, 39, 40
2	11, 16, 22, 35
3	18, 26, 34, 37
4	20, 21, 30
5	17, 24
Single-model clusters	2; 4; 5; 9; 10; 12; 28; 32; 33

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2418 atoms, of which 1219 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called LPXTG-site transpeptidase family protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	158	2418	750	1219	201	244	4	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	GLY	-	expression tag	UNP Q81V16
A	54	SER	-	expression tag	UNP Q81V16
A	55	HIS	-	expression tag	UNP Q81V16
A	56	MET	-	expression tag	UNP Q81V16

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: LPXTG-site transpeptidase family protein

Chain A: 60% 25% • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 L66 A67 E68 A72 S73 L74 D75 K76 R82 I83 V88 S89 L92 S97 S98 T99 N102 H126 N127 M128 S129 K130 V133 L134 F135 S136 D137 K142 D145 D151 N152 E153 N154 T161 P168

D169 K170 W171 E172 V173 V174 E175 D176 H177 D180 T183 L184 I185 T186 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 A200 G201 D202 K210

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: LPXTG-site transpeptidase family protein

Chain A: 68% 18% • 13%

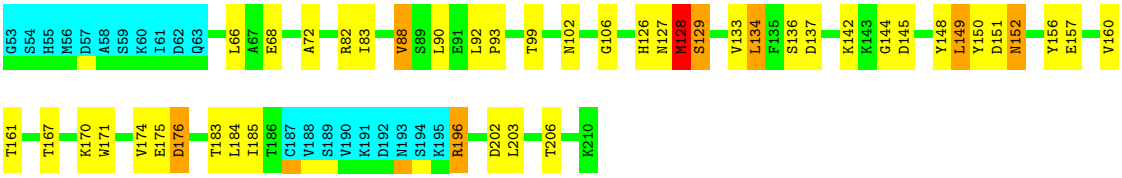
G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 P64 E68 A72 D75 K76 K77 Q78 V79 R82 I83 V88 S97 N102 N120 H126 N127 M128 S129 V133 L134 K146 I147 Y148 D151 N152 E153 N154 E157 D169 K170 V173 T183 L184

C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 K210

4.2.2 Score per residue for model 2

• Molecule 1: LPXTG-site transpeptidase family protein

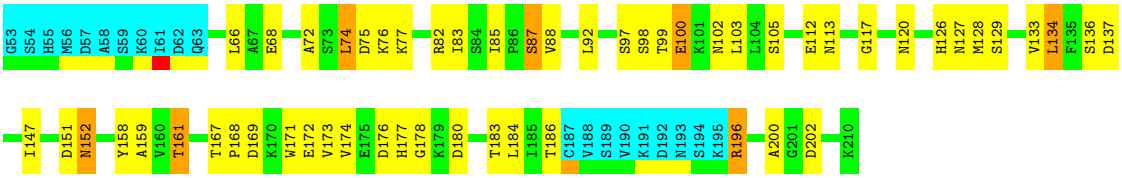
Chain A: 59% 23% • • 13%



4.2.3 Score per residue for model 3

- Molecule 1: LPXTG-site transpeptidase family protein

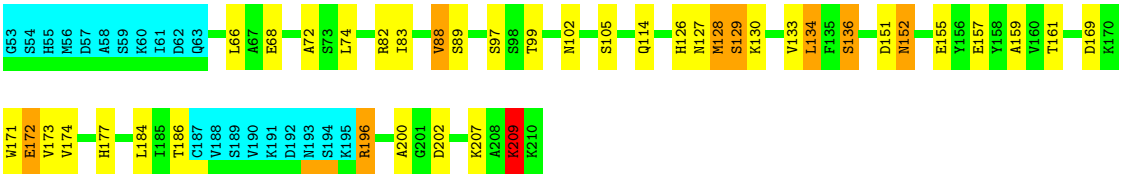
Chain A:



4.2.4 Score per residue for model 4

- Molecule 1: LPXTG-site transpeptidase family protein

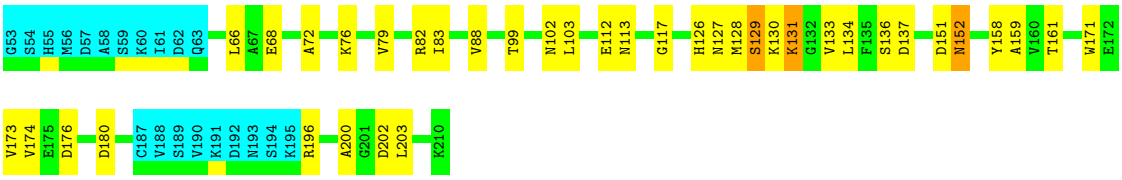
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 60% 25% • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 P64 D65 E68 V69 A72 S73 L74 Q78 R82 I83 V88 L92 K96 S97 S98 T99 N102 Q114 G119 N120 Y121 N127 M128 S129 V133 L134 F135 S136 D137 K142 D145 D151 N152

V163 V173 D176 H177 G178 K179 D180 T183 L184 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 D202 L203 A208 K209 K210

4.2.7 Score per residue for model 7

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 61% 23% • • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 L66 A67 E68 A72 S73 L74 D75 K76 K77 R82 I83 V88 T99 N102 E112 N113 Q114 Y121 N127 M128 S129 V133 L134 F135 S136 D137 S140 K146 D151 N152 E153 N154 T167 P168 D169

E172 V173 D176 H177 T183 L184 I185 T186 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 D202 L203 V204 K210

4.2.8 Score per residue for model 8 (medoid)

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 60% 24% • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 L66 A67 E68 A72 D75 K76 K77 Q78 R82 I83 V88 L92 P93 E112 N113 G117 H126 N127 M128 S129 V133 L134 F135 S136 D137 K142 D145 K146 D151 N152 E153 N154 E155 Y156 T161

T167 P168 D169 K170 W171 E172 V173 V174 D180 T183 L184 I185 T186 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 A200 T206 K210

4.2.9 Score per residue for model 9

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 55% 28% • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 P64 D65 L66 A67 E68 N71 A72 R82 V88 S89 L90 E91 I92 P93 S97 S98 T99 N102 A107 G117 H126 N127 M128 S129 K130 L134 F135 S136 D137 K142 D145 K146 I147 Y148 L149 Y150 D151 N152

Y158 V166 T167 P168 D169 K170 W171 E172 V173 V174 E175 D176 H177 D180 T183 L184 I185 T186 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 Y197 D202 L203 K210

4.2.10 Score per residue for model 10

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 59% 23% • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 L66 A67 E68 N71 A72 K76 R82 I83 V88 S89 L90 E91 L92 N102 E112 G117 N127 M128 S129 K130 V133 L134 F135 S136 D137 S140 L141 K142 D145 L149 Y150 D151 N152 Y156 E157

Y158 V166 T167 P168 D169 K170 V173 D180 T183 L184 I185 T186 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 D202 L203 T206 K210

4.2.11 Score per residue for model 11

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 52% 31% • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 L66 A67 E68 N71 A72 D75 K76 K77 Q78 V79 R82 I85 P86 S87 V88 S89 L92 L95 T99 E100 K101 N102 A107 N120 N127 M128 S129 K130 V133 L134 F135 S136 D137 L141 Y148

D151 N152 E153 N154 T161 E165 P168 D169 K170 W171 E172 E175 D176 H177 T183 L184 I185 T186 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 Y197 V198 V199 A200 G201 D202 L203 A208 K209 K210

4.2.12 Score per residue for model 12

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 59% 25% • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 P64 D65 L66 V69 A70 N71 L74 D75 K76 V79 R82 I83 S87 V88 S89 L92 L95 K96 S97 E100 K101 N102 L103 L104 N113 M116 N120 H126 N127 M128 S129 V133 L134 L141 K142

D145 D151 N152 T161 P168 D169 K170 W171 E172 V173 V174 E175 D176 T183 L184 I185 T186 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 A200 K210

4.2.13 Score per residue for model 13

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 53% 31% • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 E68 N71 A72 S73 L74 D75 K76 K77 Q78 V79 R82 I83 V88 S89 L90 E91 L92 K96 S97 S98 T99 N102 G106 E112 N113 Q114 V115 M116 G119 N120 Y121 A122 G125 H126 N127 M128 S129 V133

L134 F135 S136 D137 K142 D145 D151 N152 E153 N154 P168 D169 K170 W171 E172 V173 V174 E175 D176 H177 G178 K179 D180 T183 L184 I185 T186 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 K209 K210

4.2.14 Score per residue for model 14

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 62% 24% • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 L66 A67 E68 A72 K76 K77 Q78 V79 R82 V88 S97 S98 T99 N102 Q114 V115 M116 N120 Y121 A122 N127 M128 S129 V133 L134 K142 D145 D151 N152 E153 N154 E155 Y156 E165

K170 W171 E172 V173 V174 T183 L184 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 Y197 D202 T206 K207 K210

4.2.15 Score per residue for model 15

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 58% 26% • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 L66 A67 E68 A72 S73 L74 D75 K76 K77 Q78 R82 V88 S89 L90 E91 L92 P93 S97 S98 S105 G106 E112 G117 N127 M128 S129 K130 V133 L134 F135 S136 D137 K142 D145 K146 I147

D151 N152 Y158 T161 P168 W171 E172 V173 V174 D180 T183 L184 I185 T186 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 A200 G201 D202 L203 K210

4.2.16 Score per residue for model 16

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 59% 24% • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 L66 L74 D75 K76 K77 Q78 V79 I80 G81 R82 S89 V94 S98 T99 N102 T109 G117 H126 N127 M128 S129 K130 K131 G132 V133 L134 F135 S136 D137 I138 D151 N152 E157 Y158 A159 V160 T161

E165 W171 E172 V173 G178 K179 D180 T183 L184 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 Y197 A200 G201 D202 K207 K210

4.2.17 Score per residue for model 17

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 56% 26% • • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 E68 A72 S73 L74 D75 K76 K77 Q78 V79 R82 I83 V88 S89 L90 E91 L92 K96 S97 S98 N102 S105 G106 T109 E112 N120 H126 N127 M128 S129 V133 L134 F135 S136 D137 D151 N152

E153 N154 T161 T167 P168 D169 K170 W171 E172 V173 V174 E175 D176 H177 T183 L184 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 A200 G201 D202 K210

4.2.18 Score per residue for model 18

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 59% 24% • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 E68 A72 Q78 R82 I83 S87 V88 S89 L90 E91 L92 P93 K96 S97 S98 T99 N102 E112 N113 Q114 G119 N120 Y121 N127 M128 S129 K130 V133 L134 F135 S136 L141 K142 D145 D151

N152 E153 N154 E157 P168 W171 E172 V173 H177 G178 K179 D180 T183 L184 I185 T186 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 V204 K210

4.2.19 Score per residue for model 19

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 60% 23% • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 P64 D65 L66 A67 E68 A72 R82 I83 V88 L92 P93 T99 N102 M116 G117 N120 N127 M128 S129 V133 L134 K142 D145 K146 I147 Y148 L149 Y150 D151 N152 E153 N154 Y158 T161

T167 P168 D169 V173 D180 T183 L184 I185 T186 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 A200 G201 D202 K209 K210

4.2.20 Score per residue for model 20

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 52% 32% • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 L66 A67 E68 N71 A72 R82 I83 V88 S89 L90 E91 L92 P93 V94 L95 T99 N102 V115 M116 G119 H126 N127 M128 S129 K130 V133 L134 F135 S136 D137 S140 L141 K142 D145 K146 L149

Y150 D151 N152 E157 T161 T167 P168 D169 K170 W171 E172 V173 V174 E175 D176 K179 D180 T183 L184 I185 T186 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 A200 G201 D202 L203 V204 K209 K210

4.2.21 Score per residue for model 21

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 59% 25% • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 E68 A72 Q78 R82 I83 S84 V88 S89 K96 S97 S98 T99 N102 A108 E112 N113 M116 N127 M128 S129 K130 V133 L134 F135 S136 D137 K142 D145 K146 I147 Y150 D151 N152

Y158 T167 P168 D169 K170 W171 E172 V173 V174 E175 D176 K179 D180 E181 I182 T183 L184 I185 T186 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 K210

4.2.22 Score per residue for model 22

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 63% 22% • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 E68 A72 K76 V79 R82 I83 S84 V88 S89 T99 E100 K101 N102 Q114 G117 N120 Y121 N127 M128 S129 K130 V133 L134 F135 S136 D137 Y148 D151 N152 E153 N154 E157 T161

K170 W171 E172 V173 D180 T183 L184 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 A200 G201 D202 L203 K210

4.2.23 Score per residue for model 23

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 52% 30% 6% 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 E68 A72 S73 L74 D75 K76 K77 Q78 V79 R82 I83 S87 V88 S89 L90 E91 L92 P93 T99 E100 K101 N102 S105 Q114 V115 M116 N120 Y121 A122 N127 M128 S129 V133 L134 D137 S140 L141

D145 K146 I147 Y148 L149 Y150 D151 N152 E153 N154 Y158 T161 T167 P168 D169 K170 W171 E172 E175 D176 H177 G178 K179 D180 T183 L184 I185 T186 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 D202 L203 K210

4.2.24 Score per residue for model 24

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 54% 30% • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 P64 E68 A72 K76 V79 R82 I83 V88 L92 P93 A107 E112 N113 Q114 N120 N127 M128 S129 K130 L134 F135 S136 D137 L141 K142 K143 G144 D145 L149 Y150 D151 N152 E153 N154 E155

Y156 E157 V160 V163 P168 W171 E172 V173 V174 E175 D176 H177 T183 L184 I185 T186 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 V199 D202 L203 V204 K207 A208 K209 K210

4.2.25 Score per residue for model 25

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 63% 21% • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 L66 A67 E68 A72 S73 L74 D75 K76 K77 Q78 V79 R82 I83 V88 L92 P93 S97 S98 T99 N102 N127 M128 S129 K130 K131 G132 V133 L134 F135 S136 Y150 D151 N152 E153 N154 E155 V166 T167 P168

D169 K170 W171 E172 V173 V174 T183 L184 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 K210

4.2.26 Score per residue for model 26

• Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 61% 23% • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 E68 A72 S73 L74 R82 V88 S89 L90 E91 L92 S97 S98 T99 N102 E112 M116 H126 N127 M128 S129 V133 L134 K142 D145 K146 L149 Y150 D151 N152 E153 T161 W171 E172 V173

K179 T183 L184 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 A200 G201 D202 L203 A208 K209 K210

4.2.27 Score per residue for model 27

• Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 53% 29% • • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 L66 A67 E68 A72 S73 L74 D75 K76 K77 Q78 V79 I80 G81 R82 I83 S84 V88 E91 L92 L95 S98 T99 N102 Q114 V115 M116 N120 H126 N127 M128 S129 K130 V133 L134 F135 S136 D137

S140 Y150 D151 N152 E153 N154 E155 T161 T167 P168 D169 E172 V173 D176 H177 G178 K179 D180 E181 I182 T183 L184 I185 T186 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 A208 K209 K210

4.2.28 Score per residue for model 28

• Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 58% 27% • 13%

G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 L66 A67 E68 A72 I80 G81 R82 V88 S89 S97 S98 T99 E100 K101 N102 L103 L104 G119 N127 M128 S129 V133 L134 F135 S136 D137 I138 K142 D145 K146 I147 D151 N152 Y156 E157 Y158

T161 T167 P168 D169 K170 W171 E172 V173 V174 E175 D176 H177 G178 K179 D180 T183 L184 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 Y197 A200 T206 K210

4.2.29 Score per residue for model 29

• Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 54% 30% • 13%

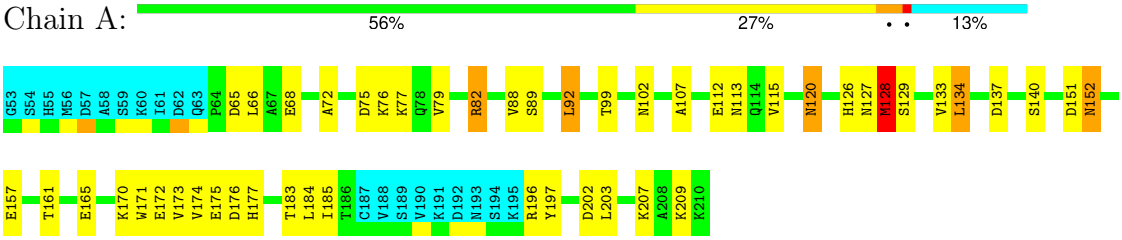
G53 S54 H55 M56 D57 A58 S59 K60 I61 D62 Q63 E68 A72 S73 L74 Q78 R82 I83 V88 E91 L92 P93 S97 S98 T99 N102 A108 N113 M116 G117 K118 G119 N120 H126 N127 M128 S129 V133 L134 F135 S136 D137 I138 L141 K142

D145 K146 I147 D151 N152 E153 N154 E155 Y156 E157 Y158 T161 G162 V163 P168 W171 E172 V173 K179 D180 T183 L184 I185 T186 C187 V188 S189 V190 K191 D192 N193 S194 K195 R196 A200 T206 K209 K210

4.2.30 Score per residue for model 30

- Molecule 1: LPXTG-site transpeptidase family protein

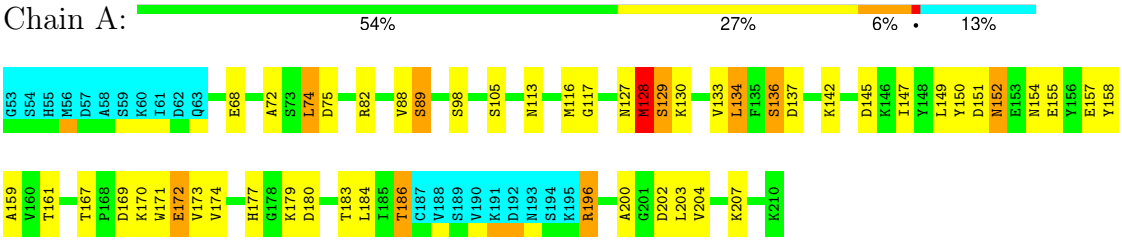
Chain A:



4.2.31 Score per residue for model 31

- Molecule 1: LPXTG-site transpeptidase family protein

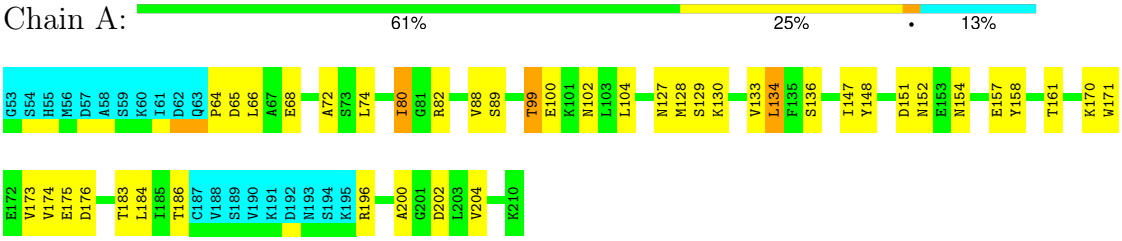
Chain A:



4.2.32 Score per residue for model 32

- Molecule 1: LPXTG-site transpeptidase family protein

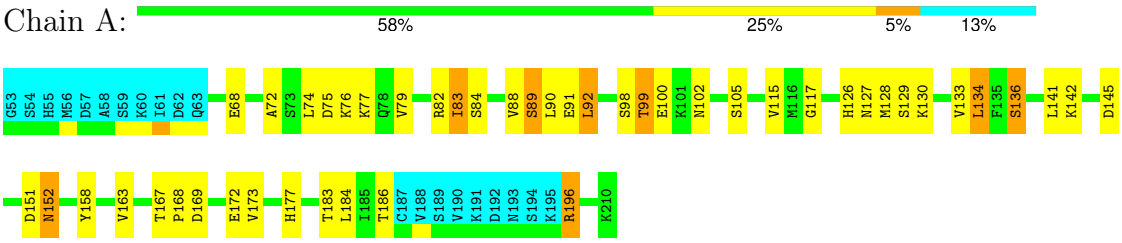
Chain A:



4.2.33 Score per residue for model 33

- Molecule 1: LPXTG-site transpeptidase family protein

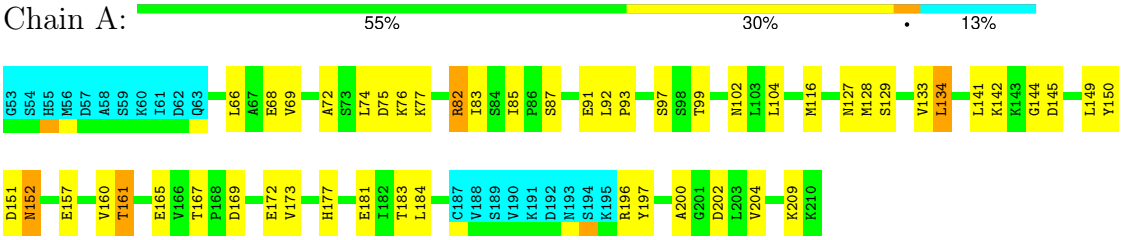
Chain A:



4.2.34 Score per residue for model 34

- Molecule 1: LPXTG-site transpeptidase family protein

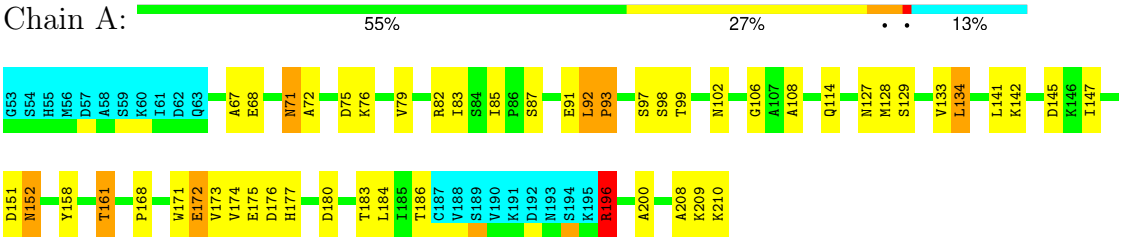
Chain A:



4.2.35 Score per residue for model 35

- Molecule 1: LPXTG-site transpeptidase family protein

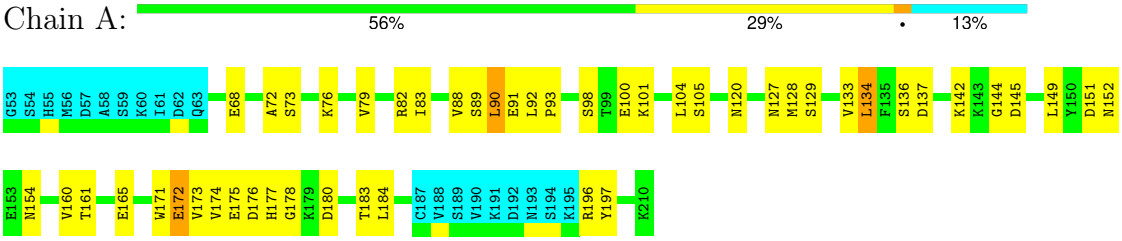
Chain A:



4.2.36 Score per residue for model 36

- Molecule 1: LPXTG-site transpeptidase family protein

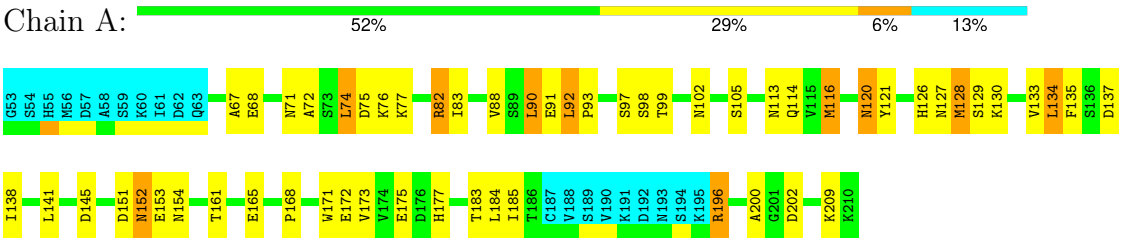
Chain A:



4.2.37 Score per residue for model 37

- Molecule 1: LPXTG-site transpeptidase family protein

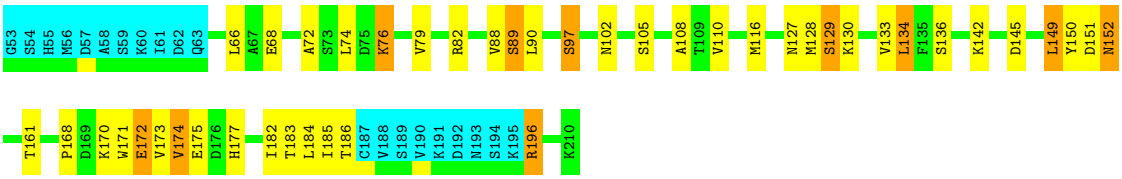
Chain A:



4.2.38 Score per residue for model 38

- Molecule 1: LPXTG-site transpeptidase family protein

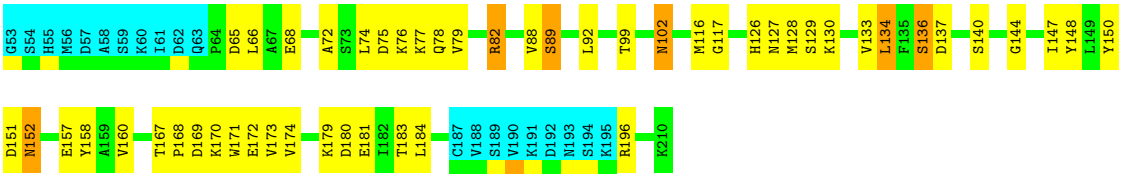
Chain A: 59% 22% 6% 13%



4.2.39 Score per residue for model 39

- Molecule 1: LPXTG-site transpeptidase family protein

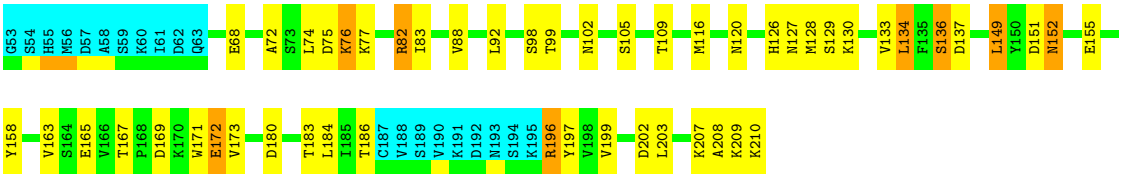
Chain A: 55% 28% • 13%



4.2.40 Score per residue for model 40

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 55% 27% 5% 13%



5 Refinement protocol and experimental data overview (i)

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

Of the 100 calculated structures, 40 were deposited, based on the following criterion: *structures with the least restraint violations*.

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

Software name	**Classification**	**Version**
X-PLOR NIH	refinement	
ProcheckNMR	geometry optimization	
TALOS	geometry optimization	

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

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1700
Number of shifts mapped to atoms	1700
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	88%

6 Model quality (i)

6.1 Standard geometry (i)

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	2.0±0.0
All	All	0	80

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	82	ARG	Sidechain	40
1	A	196	ARG	Sidechain	40

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	1052	1074	1074	41±6
All	All	42080	42960	42960	1640

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 19.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:173:VAL:O	1:A:183:THR:HG21	0.77	1.80	27	15
1:A:134:LEU:HD23	1:A:134:LEU:N	0.74	1.97	23	14
1:A:91:GLU:O	1:A:92:LEU:HD22	0.71	1.85	13	4
1:A:133:VAL:HG12	1:A:134:LEU:H	0.70	1.46	17	38
1:A:133:VAL:HG12	1:A:134:LEU:N	0.70	2.01	4	36
1:A:69:VAL:HG22	1:A:104:LEU:HD22	0.68	1.63	34	1
1:A:82:ARG:O	1:A:149:LEU:HD23	0.68	1.88	19	2
1:A:146:LYS:HZ1	1:A:204:VAL:HG11	0.67	1.48	20	1
1:A:134:LEU:HD23	1:A:134:LEU:H	0.67	1.48	9	2
1:A:134:LEU:N	1:A:134:LEU:HD23	0.66	2.05	18	25
1:A:87:SER:OG	1:A:141:LEU:HD23	0.64	1.93	11	4
1:A:82:ARG:NH1	1:A:209:LYS:NZ	0.64	2.45	13	3
1:A:82:ARG:NH1	1:A:209:LYS:HZ1	0.63	1.91	13	1
1:A:68:GLU:O	1:A:72:ALA:HB2	0.63	1.93	13	38
1:A:99:THR:OG1	1:A:102:ASN:ND2	0.63	2.32	33	23
1:A:173:VAL:HG23	1:A:174:VAL:HG13	0.63	1.71	13	3
1:A:66:LEU:HD23	1:A:66:LEU:N	0.63	2.09	9	2
1:A:71:ASN:ND2	1:A:72:ALA:N	0.62	2.46	35	1
1:A:91:GLU:O	1:A:92:LEU:HD12	0.62	1.94	27	6
1:A:97:SER:O	1:A:102:ASN:ND2	0.62	2.33	35	7
1:A:66:LEU:HD23	1:A:66:LEU:O	0.61	1.94	7	2
1:A:149:LEU:HD13	1:A:150:TYR:N	0.61	2.10	2	2
1:A:82:ARG:HH12	1:A:209:LYS:NZ	0.61	1.91	13	1
1:A:82:ARG:HH22	1:A:209:LYS:NZ	0.61	1.93	34	2
1:A:92:LEU:CD1	1:A:107:ALA:H	0.61	2.08	11	2
1:A:104:LEU:HD12	1:A:104:LEU:N	0.61	2.10	32	3
1:A:170:LYS:O	1:A:173:VAL:HG22	0.61	1.95	39	7
1:A:137:ASP:CG	1:A:140:SER:HG	0.61	1.99	7	2
1:A:170:LYS:O	1:A:171:TRP:CD1	0.60	2.55	32	4
1:A:74:LEU:HD13	1:A:75:ASP:N	0.60	2.12	16	5
1:A:82:ARG:NH1	1:A:209:LYS:HZ3	0.60	1.94	30	1
1:A:74:LEU:HD23	1:A:105:SER:OG	0.60	1.96	31	3
1:A:186:THR:O	1:A:196:ARG:NH1	0.59	2.34	15	14
1:A:102:ASN:HD22	1:A:102:ASN:N	0.59	1.95	10	6
1:A:174:VAL:HG11	1:A:185:ILE:HD13	0.59	1.73	21	5
1:A:151:ASP:OD2	1:A:156:TYR:CE1	0.59	2.55	29	1
1:A:168:PRO:O	1:A:171:TRP:NE1	0.58	2.36	9	15
1:A:74:LEU:H	1:A:74:LEU:HD23	0.58	1.56	4	4
1:A:151:ASP:O	1:A:152:ASN:C	0.58	2.40	9	40
1:A:172:GLU:O	1:A:177:HIS:NE2	0.58	2.37	37	19
1:A:82:ARG:NH2	1:A:209:LYS:NZ	0.58	2.51	13	2
1:A:82:ARG:HH22	1:A:209:LYS:HZ1	0.57	1.42	34	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:ILE:HG22	1:A:92:LEU:O	0.57	1.98	36	19
1:A:78:GLN:NE2	1:A:102:ASN:OD1	0.57	2.37	39	3
1:A:127:ASN:O	1:A:129:SER:N	0.57	2.37	5	40
1:A:202:ASP:OD1	1:A:203:LEU:N	0.57	2.38	10	14
1:A:90:LEU:HD13	1:A:91:GLU:N	0.57	2.15	36	5
1:A:97:SER:OG	1:A:102:ASN:ND2	0.57	2.38	34	7
1:A:180:ASP:OD2	1:A:203:LEU:HD22	0.57	2.00	23	1
1:A:120:ASN:ND2	1:A:183:THR:OG1	0.56	2.38	22	13
1:A:114:GLN:NE2	1:A:122:ALA:N	0.56	2.53	14	3
1:A:104:LEU:N	1:A:104:LEU:CD1	0.56	2.69	32	3
1:A:74:LEU:HD11	1:A:78:GLN:NE2	0.56	2.15	13	2
1:A:80:ILE:H	1:A:80:ILE:HD13	0.56	1.61	32	4
1:A:65:ASP:OD1	1:A:66:LEU:N	0.56	2.39	30	5
1:A:82:ARG:NH2	1:A:209:LYS:HZ1	0.56	1.98	34	1
1:A:133:VAL:CG1	1:A:134:LEU:N	0.55	2.70	21	36
1:A:134:LEU:H	1:A:134:LEU:CD2	0.55	2.12	24	2
1:A:91:GLU:N	1:A:91:GLU:OE1	0.55	2.39	15	1
1:A:173:VAL:O	1:A:173:VAL:HG12	0.55	1.99	34	4
1:A:148:TYR:CE2	1:A:157:GLU:OE1	0.55	2.60	1	4
1:A:167:THR:O	1:A:196:ARG:NH2	0.55	2.40	2	1
1:A:78:GLN:N	1:A:78:GLN:OE1	0.55	2.39	18	4
1:A:151:ASP:OD1	1:A:151:ASP:N	0.54	2.39	29	1
1:A:155:GLU:OE1	1:A:207:LYS:NZ	0.54	2.39	14	4
1:A:166:VAL:O	1:A:196:ARG:NH1	0.54	2.41	10	1
1:A:74:LEU:N	1:A:74:LEU:HD23	0.54	2.17	32	3
1:A:88:VAL:HG12	1:A:88:VAL:O	0.54	2.02	37	1
1:A:134:LEU:N	1:A:134:LEU:CD2	0.54	2.65	23	28
1:A:142:LYS:N	1:A:145:ASP:OD2	0.54	2.41	8	22
1:A:116:MET:SD	1:A:150:TYR:O	0.54	2.66	34	7
1:A:114:GLN:OE1	1:A:121:TYR:CE1	0.54	2.61	37	1
1:A:170:LYS:O	1:A:171:TRP:CG	0.54	2.61	2	4
1:A:165:GLU:OE2	1:A:197:TYR:CZ	0.54	2.60	30	5
1:A:82:ARG:CZ	1:A:209:LYS:HZ1	0.54	2.14	13	1
1:A:150:TYR:CE2	1:A:155:GLU:OE2	0.54	2.61	25	1
1:A:133:VAL:CG1	1:A:134:LEU:H	0.54	2.15	4	33
1:A:165:GLU:N	1:A:165:GLU:OE1	0.54	2.41	16	2
1:A:68:GLU:O	1:A:71:ASN:ND2	0.54	2.41	35	1
1:A:114:GLN:OE1	1:A:121:TYR:CG	0.53	2.61	18	1
1:A:76:LYS:O	1:A:79:VAL:HG12	0.53	2.04	24	13
1:A:126:HIS:O	1:A:134:LEU:O	0.53	2.26	16	18
1:A:175:GLU:O	1:A:177:HIS:CE1	0.53	2.61	38	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:ILE:HD13	1:A:84:SER:N	0.53	2.18	33	3
1:A:152:ASN:N	1:A:152:ASN:OD1	0.53	2.41	37	6
1:A:88:VAL:HG22	1:A:88:VAL:O	0.53	2.03	1	16
1:A:165:GLU:OE2	1:A:197:TYR:CE1	0.53	2.61	30	2
1:A:170:LYS:HZ1	1:A:196:ARG:NH2	0.53	2.01	17	1
1:A:90:LEU:HD11	1:A:92:LEU:HD12	0.53	1.79	36	2
1:A:186:THR:OG1	1:A:196:ARG:NH1	0.53	2.41	18	3
1:A:74:LEU:HD23	1:A:74:LEU:N	0.53	2.19	4	4
1:A:74:LEU:HD22	1:A:105:SER:HB3	0.53	1.80	17	3
1:A:68:GLU:N	1:A:68:GLU:OE1	0.53	2.41	1	2
1:A:167:THR:O	1:A:169:ASP:N	0.53	2.42	7	16
1:A:99:THR:O	1:A:102:ASN:OD1	0.53	2.27	21	6
1:A:100:GLU:CD	1:A:100:GLU:N	0.53	2.62	3	1
1:A:185:ILE:HG22	1:A:198:VAL:HG22	0.53	1.80	11	1
1:A:78:GLN:NE2	1:A:97:SER:OG	0.53	2.42	15	1
1:A:175:GLU:O	1:A:176:ASP:O	0.53	2.27	2	3
1:A:66:LEU:N	1:A:66:LEU:HD12	0.52	2.19	28	7
1:A:117:GLY:N	1:A:158:TYR:OH	0.52	2.42	5	7
1:A:156:TYR:CD2	1:A:206:THR:OG1	0.52	2.61	29	4
1:A:146:LYS:NZ	1:A:157:GLU:OE2	0.52	2.40	1	2
1:A:155:GLU:CD	1:A:207:LYS:HZ1	0.52	2.08	24	1
1:A:136:SER:OG	1:A:137:ASP:N	0.52	2.43	36	2
1:A:114:GLN:OE1	1:A:121:TYR:CZ	0.52	2.63	22	1
1:A:183:THR:C	1:A:184:LEU:HD12	0.52	2.25	20	35
1:A:74:LEU:HD22	1:A:105:SER:OG	0.52	2.05	4	2
1:A:172:GLU:H	1:A:172:GLU:CD	0.52	2.08	4	4
1:A:179:LYS:NZ	1:A:181:GLU:OE1	0.52	2.40	27	2
1:A:120:ASN:CB	1:A:175:GLU:O	0.52	2.57	23	3
1:A:150:TYR:CZ	1:A:155:GLU:OE2	0.52	2.63	25	1
1:A:151:ASP:N	1:A:154:ASN:O	0.52	2.39	7	1
1:A:148:TYR:CD2	1:A:157:GLU:OE1	0.52	2.63	22	2
1:A:71:ASN:OD1	1:A:72:ALA:N	0.51	2.43	9	2
1:A:76:LYS:O	1:A:79:VAL:HG23	0.51	2.06	33	1
1:A:175:GLU:O	1:A:177:HIS:NE2	0.51	2.43	17	1
1:A:150:TYR:CD2	1:A:155:GLU:OE2	0.51	2.63	25	1
1:A:150:TYR:CE2	1:A:155:GLU:OE1	0.51	2.63	27	1
1:A:114:GLN:OE1	1:A:121:TYR:CD1	0.51	2.63	18	1
1:A:141:LEU:HD22	1:A:145:ASP:OD2	0.51	2.06	23	1
1:A:96:LYS:NZ	1:A:112:GLU:O	0.51	2.42	18	3
1:A:147:ILE:N	1:A:158:TYR:O	0.51	2.43	15	12
1:A:89:SER:OG	1:A:89:SER:O	0.51	2.29	23	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:83:ILE:HG23	1:A:83:ILE:O	0.50	2.05	35	7
1:A:171:TRP:O	1:A:173:VAL:N	0.50	2.44	20	20
1:A:166:VAL:CG2	1:A:196:ARG:HH21	0.50	2.19	25	1
1:A:149:LEU:HD21	1:A:182:ILE:CD1	0.50	2.36	38	1
1:A:171:TRP:C	1:A:173:VAL:H	0.50	2.10	31	17
1:A:208:ALA:O	1:A:210:LYS:N	0.50	2.44	11	6
1:A:79:VAL:HG13	1:A:79:VAL:O	0.50	2.07	25	5
1:A:170:LYS:NZ	1:A:196:ARG:NH2	0.50	2.59	17	1
1:A:66:LEU:N	1:A:66:LEU:CD2	0.50	2.74	12	9
1:A:157:GLU:OE1	1:A:157:GLU:N	0.50	2.45	4	1
1:A:172:GLU:O	1:A:177:HIS:CE1	0.50	2.65	17	5
1:A:66:LEU:HD23	1:A:66:LEU:H	0.50	1.66	9	3
1:A:114:GLN:NE2	1:A:122:ALA:H	0.50	2.05	23	1
1:A:71:ASN:ND2	1:A:72:ALA:H	0.50	2.04	35	1
1:A:161:THR:HG22	1:A:200:ALA:O	0.50	2.06	15	9
1:A:179:LYS:NZ	1:A:181:GLU:CD	0.50	2.65	39	2
1:A:76:LYS:O	1:A:79:VAL:CG1	0.49	2.60	25	4
1:A:165:GLU:OE2	1:A:197:TYR:CE2	0.49	2.65	30	1
1:A:171:TRP:C	1:A:173:VAL:N	0.49	2.66	30	22
1:A:85:ILE:CG2	1:A:141:LEU:HD21	0.49	2.36	11	1
1:A:100:GLU:CG	1:A:101:LYS:N	0.49	2.75	11	1
1:A:82:ARG:HH12	1:A:209:LYS:HZ3	0.49	1.48	13	1
1:A:150:TYR:CG	1:A:155:GLU:OE2	0.49	2.66	25	1
1:A:155:GLU:CD	1:A:207:LYS:NZ	0.49	2.66	24	1
1:A:180:ASP:OD1	1:A:180:ASP:O	0.49	2.31	9	9
1:A:150:TYR:CE1	1:A:155:GLU:OE2	0.49	2.66	25	1
1:A:68:GLU:C	1:A:71:ASN:ND2	0.49	2.65	35	1
1:A:186:THR:O	1:A:196:ARG:CZ	0.49	2.61	38	2
1:A:116:MET:SD	1:A:149:LEU:HD22	0.49	2.48	20	3
1:A:169:ASP:OD1	1:A:170:LYS:N	0.49	2.46	10	3
1:A:99:THR:N	1:A:102:ASN:OD1	0.49	2.43	28	1
1:A:186:THR:HG23	1:A:196:ARG:HE	0.49	1.67	40	1
1:A:112:GLU:N	1:A:112:GLU:CD	0.49	2.66	15	2
1:A:90:LEU:CD2	1:A:92:LEU:HD23	0.49	2.38	26	1
1:A:150:TYR:CD2	1:A:155:GLU:OE1	0.49	2.66	27	1
1:A:165:GLU:OE2	1:A:197:TYR:CD1	0.49	2.66	30	1
1:A:101:LYS:CG	1:A:102:ASN:N	0.48	2.76	22	2
1:A:88:VAL:O	1:A:88:VAL:CG2	0.48	2.61	21	19
1:A:126:HIS:O	1:A:135:PHE:O	0.48	2.30	9	1
1:A:175:GLU:O	1:A:176:ASP:C	0.48	2.51	13	7
1:A:75:ASP:C	1:A:77:LYS:N	0.48	2.67	1	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:176:ASP:OD1	1:A:176:ASP:O	0.48	2.32	23	10
1:A:66:LEU:N	1:A:66:LEU:HD22	0.48	2.23	14	7
1:A:82:ARG:CZ	1:A:209:LYS:NZ	0.48	2.76	13	1
1:A:91:GLU:C	1:A:92:LEU:HD22	0.48	2.29	26	1
1:A:112:GLU:CG	1:A:113:ASN:N	0.48	2.76	30	4
1:A:80:ILE:CD1	1:A:80:ILE:N	0.48	2.76	32	4
1:A:74:LEU:H	1:A:74:LEU:CD2	0.48	2.21	32	4
1:A:173:VAL:O	1:A:173:VAL:CG1	0.48	2.62	34	1
1:A:65:ASP:O	1:A:69:VAL:HG23	0.48	2.08	6	2
1:A:68:GLU:O	1:A:71:ASN:OD1	0.48	2.30	9	2
1:A:127:ASN:C	1:A:129:SER:N	0.48	2.67	27	40
1:A:130:LYS:O	1:A:136:SER:CB	0.48	2.61	9	17
1:A:152:ASN:ND2	1:A:154:ASN:OD1	0.48	2.46	37	1
1:A:88:VAL:HG23	1:A:90:LEU:HD23	0.48	1.85	10	1
1:A:87:SER:CB	1:A:141:LEU:HD23	0.48	2.39	23	1
1:A:130:LYS:N	1:A:136:SER:OG	0.48	2.44	10	4
1:A:130:LYS:O	1:A:136:SER:OG	0.48	2.31	40	12
1:A:157:GLU:OE2	1:A:207:LYS:CE	0.48	2.62	16	2
1:A:120:ASN:HD21	1:A:183:THR:CB	0.48	2.21	40	1
1:A:66:LEU:H	1:A:66:LEU:CD2	0.47	2.21	9	1
1:A:67:ALA:O	1:A:71:ASN:ND2	0.47	2.47	35	1
1:A:169:ASP:O	1:A:169:ASP:OD1	0.47	2.31	9	9
1:A:88:VAL:CG2	1:A:88:VAL:O	0.47	2.62	17	4
1:A:174:VAL:HG11	1:A:185:ILE:HG21	0.47	1.84	13	1
1:A:180:ASP:OD1	1:A:180:ASP:N	0.47	2.46	28	2
1:A:74:LEU:N	1:A:74:LEU:CD2	0.47	2.77	4	7
1:A:168:PRO:O	1:A:171:TRP:CD1	0.47	2.67	28	3
1:A:107:ALA:HB2	1:A:135:PHE:CE1	0.47	2.44	24	1
1:A:119:GLY:CA	1:A:179:LYS:O	0.47	2.63	20	6
1:A:71:ASN:O	1:A:71:ASN:OD1	0.47	2.33	12	3
1:A:75:ASP:OD1	1:A:76:LYS:N	0.47	2.47	35	2
1:A:185:ILE:CG2	1:A:196:ARG:NH1	0.47	2.78	37	1
1:A:66:LEU:N	1:A:66:LEU:CD1	0.47	2.78	28	7
1:A:151:ASP:OD1	1:A:152:ASN:N	0.47	2.46	11	11
1:A:112:GLU:H	1:A:112:GLU:CD	0.47	2.11	10	1
1:A:100:GLU:O	1:A:104:LEU:CD1	0.47	2.63	28	3
1:A:74:LEU:HD11	1:A:78:GLN:HE22	0.47	1.70	13	1
1:A:75:ASP:O	1:A:77:LYS:N	0.47	2.48	37	9
1:A:150:TYR:CZ	1:A:155:GLU:OE1	0.47	2.67	27	1
1:A:119:GLY:C	1:A:179:LYS:O	0.47	2.53	28	1
1:A:186:THR:CG2	1:A:196:ARG:HE	0.47	2.22	40	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:97:SER:OG	1:A:102:ASN:OD1	0.47	2.33	13	1
1:A:102:ASN:ND2	1:A:102:ASN:N	0.47	2.63	39	3
1:A:150:TYR:CD1	1:A:155:GLU:OE2	0.47	2.67	25	1
1:A:96:LYS:CG	1:A:97:SER:N	0.46	2.78	6	1
1:A:99:THR:OG1	1:A:102:ASN:OD1	0.46	2.32	22	1
1:A:150:TYR:CE2	1:A:155:GLU:CD	0.46	2.89	25	1
1:A:129:SER:OG	1:A:129:SER:O	0.46	2.34	20	5
1:A:80:ILE:CD1	1:A:94:VAL:O	0.46	2.63	16	1
1:A:116:MET:N	1:A:121:TYR:CE1	0.46	2.83	37	2
1:A:157:GLU:O	1:A:204:VAL:HG12	0.46	2.11	31	5
1:A:142:LYS:O	1:A:145:ASP:OD2	0.46	2.32	8	2
1:A:76:LYS:N	1:A:76:LYS:CD	0.46	2.78	38	4
1:A:80:ILE:H	1:A:80:ILE:CD1	0.46	2.23	32	4
1:A:168:PRO:CB	1:A:196:ARG:HH21	0.46	2.23	19	1
1:A:82:ARG:NH1	1:A:92:LEU:C	0.46	2.68	39	1
1:A:136:SER:O	1:A:137:ASP:OD1	0.46	2.34	16	16
1:A:100:GLU:CD	1:A:100:GLU:H	0.46	2.14	3	1
1:A:169:ASP:N	1:A:169:ASP:OD1	0.46	2.46	34	1
1:A:133:VAL:C	1:A:136:SER:OG	0.46	2.54	8	2
1:A:129:SER:O	1:A:129:SER:OG	0.46	2.34	9	7
1:A:77:LYS:N	1:A:77:LYS:CD	0.46	2.79	11	1
1:A:88:VAL:O	1:A:89:SER:CB	0.46	2.64	11	9
1:A:74:LEU:HD13	1:A:74:LEU:C	0.46	2.30	16	1
1:A:174:VAL:HG12	1:A:183:THR:CG2	0.46	2.41	30	1
1:A:88:VAL:O	1:A:88:VAL:HG22	0.46	2.10	26	6
1:A:209:LYS:O	1:A:209:LYS:CG	0.46	2.64	4	2
1:A:120:ASN:ND2	1:A:173:VAL:O	0.46	2.45	17	1
1:A:82:ARG:HH11	1:A:209:LYS:NZ	0.46	2.09	24	1
1:A:74:LEU:HD11	1:A:78:GLN:OE1	0.46	2.10	29	2
1:A:137:ASP:OD1	1:A:140:SER:OG	0.46	2.34	30	7
1:A:92:LEU:HD22	1:A:106:GLY:HA2	0.46	1.87	2	3
1:A:102:ASN:OD1	1:A:102:ASN:N	0.46	2.48	11	1
1:A:78:GLN:OE1	1:A:102:ASN:OD1	0.46	2.34	23	2
1:A:82:ARG:HH11	1:A:150:TYR:CB	0.46	2.24	34	1
1:A:88:VAL:O	1:A:88:VAL:CG1	0.46	2.64	37	1
1:A:202:ASP:OD1	1:A:202:ASP:O	0.45	2.34	23	9
1:A:161:THR:OG1	1:A:200:ALA:O	0.45	2.34	37	11
1:A:71:ASN:N	1:A:71:ASN:HD22	0.45	2.07	35	1
1:A:165:GLU:OE1	1:A:197:TYR:CE1	0.45	2.69	40	1
1:A:152:ASN:OD1	1:A:153:GLU:N	0.45	2.47	29	3
1:A:144:GLY:N	1:A:160:VAL:O	0.45	2.44	24	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:184:LEU:HD12	1:A:184:LEU:N	0.45	2.27	4	4
1:A:114:GLN:NE2	1:A:121:TYR:CG	0.45	2.85	6	1
1:A:158:TYR:CZ	1:A:203:LEU:HD13	0.45	2.46	40	2
1:A:127:ASN:O	1:A:127:ASN:OD1	0.45	2.34	14	1
1:A:98:SER:OG	1:A:109:THR:O	0.45	2.28	17	3
1:A:88:VAL:HG21	1:A:137:ASP:O	0.45	2.11	28	3
1:A:172:GLU:CG	1:A:173:VAL:N	0.45	2.79	37	1
1:A:112:GLU:O	1:A:113:ASN:ND2	0.45	2.50	3	2
1:A:176:ASP:OD1	1:A:176:ASP:N	0.45	2.49	32	8
1:A:102:ASN:HD21	1:A:108:ALA:HB2	0.45	1.72	29	3
1:A:79:VAL:O	1:A:79:VAL:CG1	0.45	2.65	24	4
1:A:152:ASN:CG	1:A:153:GLU:N	0.45	2.71	7	1
1:A:87:SER:OG	1:A:145:ASP:OD1	0.45	2.34	23	1
1:A:141:LEU:O	1:A:163:VAL:HG21	0.45	2.12	33	2
1:A:167:THR:C	1:A:169:ASP:H	0.45	2.16	17	3
1:A:76:LYS:O	1:A:79:VAL:HG22	0.45	2.12	16	3
1:A:74:LEU:HD13	1:A:102:ASN:OD1	0.45	2.11	12	1
1:A:135:PHE:CD2	1:A:138:ILE:HD13	0.45	2.47	28	4
1:A:158:TYR:OH	1:A:180:ASP:OD2	0.45	2.35	23	1
1:A:152:ASN:OD1	1:A:152:ASN:N	0.45	2.48	26	1
1:A:165:GLU:OE2	1:A:197:TYR:CD2	0.45	2.70	30	1
1:A:167:THR:C	1:A:169:ASP:N	0.44	2.70	7	9
1:A:80:ILE:HD13	1:A:80:ILE:N	0.44	2.26	32	2
1:A:127:ASN:O	1:A:129:SER:OG	0.44	2.35	37	1
1:A:102:ASN:O	1:A:102:ASN:OD1	0.44	2.35	38	1
1:A:102:ASN:N	1:A:102:ASN:ND2	0.44	2.64	10	2
1:A:165:GLU:OE2	1:A:197:TYR:CG	0.44	2.71	30	1
1:A:110:VAL:HG21	1:A:185:ILE:HD11	0.44	1.89	38	1
1:A:69:VAL:HG22	1:A:104:LEU:CD2	0.44	2.37	34	1
1:A:106:GLY:CA	1:A:134:LEU:HD13	0.44	2.43	35	1
1:A:165:GLU:N	1:A:165:GLU:CD	0.44	2.71	40	1
1:A:83:ILE:O	1:A:83:ILE:CG2	0.44	2.65	24	11
1:A:98:SER:OG	1:A:98:SER:O	0.44	2.34	3	2
1:A:74:LEU:HD13	1:A:105:SER:CB	0.44	2.42	15	1
1:A:75:ASP:C	1:A:77:LYS:H	0.44	2.16	16	6
1:A:103:LEU:O	1:A:126:HIS:CD2	0.44	2.71	5	1
1:A:149:LEU:HD13	1:A:150:TYR:H	0.44	1.73	24	1
1:A:113:ASN:O	1:A:113:ASN:OD1	0.44	2.35	37	3
1:A:156:TYR:CE2	1:A:206:THR:HG21	0.43	2.48	8	2
1:A:92:LEU:HD22	1:A:105:SER:O	0.43	2.13	23	1
1:A:116:MET:SD	1:A:151:ASP:OD1	0.43	2.75	29	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:68:GLU:C	1:A:71:ASN:HD21	0.43	2.16	35	1
1:A:159:ALA:O	1:A:202:ASP:OD1	0.43	2.36	16	3
1:A:117:GLY:O	1:A:180:ASP:OD2	0.43	2.36	5	3
1:A:133:VAL:HG12	1:A:134:LEU:CD2	0.43	2.43	5	1
1:A:163:VAL:HG13	1:A:199:VAL:HG22	0.43	1.89	40	2
1:A:116:MET:SD	1:A:121:TYR:OH	0.43	2.71	37	1
1:A:151:ASP:CG	1:A:152:ASN:H	0.43	2.16	2	12
1:A:92:LEU:HD23	1:A:93:PRO:HD2	0.43	1.89	9	1
1:A:66:LEU:CD2	1:A:66:LEU:H	0.43	2.26	10	1
1:A:92:LEU:O	1:A:93:PRO:O	0.43	2.36	35	2
1:A:74:LEU:CD2	1:A:105:SER:OG	0.43	2.67	31	2
1:A:98:SER:O	1:A:98:SER:OG	0.43	2.35	36	3
1:A:74:LEU:HD22	1:A:105:SER:CB	0.43	2.43	40	2
1:A:150:TYR:CD1	1:A:150:TYR:N	0.43	2.86	31	1
1:A:102:ASN:ND2	1:A:108:ALA:HB2	0.43	2.29	38	1
1:A:75:ASP:H	1:A:78:GLN:NE2	0.43	2.11	11	1
1:A:112:GLU:CD	1:A:112:GLU:H	0.43	2.17	15	1
1:A:73:SER:O	1:A:101:LYS:NZ	0.43	2.39	36	1
1:A:71:ASN:HD22	1:A:72:ALA:H	0.43	1.54	35	1
1:A:184:LEU:CD1	1:A:184:LEU:N	0.43	2.82	36	1
1:A:92:LEU:O	1:A:93:PRO:C	0.43	2.57	29	12
1:A:152:ASN:CG	1:A:153:GLU:H	0.43	2.16	37	3
1:A:85:ILE:HG21	1:A:141:LEU:HD21	0.43	1.91	35	2
1:A:102:ASN:OD1	1:A:102:ASN:C	0.43	2.56	38	1
1:A:68:GLU:N	1:A:68:GLU:CD	0.43	2.71	19	2
1:A:150:TYR:CG	1:A:155:GLU:OE1	0.43	2.72	27	1
1:A:171:TRP:O	1:A:174:VAL:HG22	0.43	2.14	32	1
1:A:175:GLU:O	1:A:177:HIS:CD2	0.42	2.72	17	2
1:A:181:GLU:OE1	1:A:202:ASP:OD1	0.42	2.37	34	1
1:A:116:MET:SD	1:A:149:LEU:HD12	0.42	2.55	38	1
1:A:67:ALA:O	1:A:71:ASN:OD1	0.42	2.37	11	2
1:A:112:GLU:O	1:A:113:ASN:OD1	0.42	2.37	21	1
1:A:167:THR:OG1	1:A:169:ASP:OD1	0.42	2.36	34	1
1:A:184:LEU:N	1:A:184:LEU:CD1	0.42	2.82	8	5
1:A:102:ASN:HD21	1:A:108:ALA:CB	0.42	2.27	29	3
1:A:186:THR:O	1:A:196:ARG:NH2	0.42	2.51	33	1
1:A:79:VAL:CG1	1:A:79:VAL:O	0.42	2.67	23	1
1:A:176:ASP:OD1	1:A:177:HIS:N	0.42	2.52	6	2
1:A:76:LYS:C	1:A:78:GLN:N	0.42	2.73	15	1
1:A:184:LEU:N	1:A:184:LEU:HD12	0.42	2.28	36	1
1:A:85:ILE:CG2	1:A:87:SER:OG	0.42	2.68	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:163:VAL:O	1:A:163:VAL:HG13	0.42	2.15	6	1
1:A:92:LEU:HD12	1:A:106:GLY:CA	0.42	2.45	13	1
1:A:102:ASN:HD22	1:A:102:ASN:H	0.42	1.57	13	1
1:A:96:LYS:NZ	1:A:112:GLU:OE2	0.42	2.52	21	1
1:A:74:LEU:HD23	1:A:74:LEU:H	0.42	1.74	26	2
1:A:117:GLY:O	1:A:180:ASP:CG	0.42	2.59	8	7
1:A:159:ALA:O	1:A:202:ASP:N	0.42	2.51	5	2
1:A:180:ASP:OD2	1:A:203:LEU:HD23	0.42	2.15	31	1
1:A:88:VAL:O	1:A:89:SER:OG	0.42	2.37	32	1
1:A:103:LEU:O	1:A:134:LEU:HD12	0.42	2.15	3	1
1:A:131:LYS:N	1:A:131:LYS:HD3	0.42	2.30	5	1
1:A:99:THR:OG1	1:A:102:ASN:CG	0.42	2.58	6	4
1:A:172:GLU:OE1	1:A:172:GLU:N	0.42	2.45	26	1
1:A:127:ASN:ND2	1:A:186:THR:OG1	0.41	2.53	32	1
1:A:141:LEU:CD2	1:A:145:ASP:OD2	0.41	2.68	37	1
1:A:74:LEU:HD23	1:A:105:SER:HG	0.41	1.75	3	1
1:A:146:LYS:NZ	1:A:204:VAL:HG11	0.41	2.30	7	1
1:A:85:ILE:HG22	1:A:141:LEU:HD21	0.41	1.90	11	1
1:A:74:LEU:CD2	1:A:95:LEU:HD13	0.41	2.45	12	2
1:A:68:GLU:OE1	1:A:68:GLU:CA	0.41	2.68	1	1
1:A:142:LYS:O	1:A:145:ASP:CG	0.41	2.59	14	4
1:A:158:TYR:OH	1:A:180:ASP:OD1	0.41	2.39	23	1
1:A:165:GLU:OE2	1:A:197:TYR:OH	0.41	2.35	36	1
1:A:75:ASP:CB	1:A:78:GLN:NE2	0.41	2.84	8	1
1:A:107:ALA:HB2	1:A:135:PHE:CZ	0.41	2.50	9	1
1:A:131:LYS:O	1:A:131:LYS:CG	0.41	2.68	16	1
1:A:152:ASN:OD1	1:A:154:ASN:OD1	0.41	2.38	29	1
1:A:148:TYR:CD1	1:A:148:TYR:N	0.41	2.88	11	1
1:A:209:LYS:O	1:A:210:LYS:OXT	0.41	2.39	20	1
1:A:88:VAL:HG11	1:A:90:LEU:HD12	0.41	1.91	38	1
1:A:79:VAL:O	1:A:79:VAL:HG13	0.41	2.14	23	2
1:A:150:TYR:CE1	1:A:155:GLU:OE1	0.41	2.74	27	1
1:A:113:ASN:OD1	1:A:113:ASN:C	0.41	2.59	29	1
1:A:127:ASN:O	1:A:127:ASN:CG	0.41	2.58	40	2
1:A:114:GLN:NE2	1:A:121:TYR:CE1	0.41	2.88	7	1
1:A:166:VAL:O	1:A:196:ARG:N	0.41	2.51	9	1
1:A:95:LEU:CD1	1:A:102:ASN:O	0.41	2.69	11	2
1:A:130:LYS:H	1:A:136:SER:HG	0.41	1.58	38	1
1:A:127:ASN:O	1:A:128:MET:C	0.41	2.60	2	1
1:A:170:LYS:C	1:A:171:TRP:CD1	0.41	2.94	2	2
1:A:92:LEU:HD12	1:A:106:GLY:HA2	0.41	1.92	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:102:ASN:N	1:A:102:ASN:OD1	0.41	2.52	19	1
1:A:113:ASN:C	1:A:113:ASN:OD1	0.41	2.60	31	1
1:A:67:ALA:O	1:A:71:ASN:CG	0.41	2.59	37	1
1:A:74:LEU:HD13	1:A:105:SER:OG	0.41	2.16	38	1
1:A:149:LEU:C	1:A:150:TYR:CD1	0.41	2.94	9	1
1:A:127:ASN:C	1:A:129:SER:H	0.41	2.19	22	2
1:A:83:ILE:O	1:A:83:ILE:HG23	0.40	2.15	29	1
1:A:141:LEU:O	1:A:163:VAL:CG2	0.40	2.69	29	1
1:A:88:VAL:CG2	1:A:90:LEU:HD23	0.40	2.47	10	1
1:A:167:THR:C	1:A:196:ARG:HH12	0.40	2.20	10	1
1:A:76:LYS:O	1:A:79:VAL:HG13	0.40	2.15	39	1
1:A:120:ASN:HD22	1:A:177:HIS:CE1	0.40	2.33	13	1
1:A:74:LEU:C	1:A:74:LEU:CD1	0.40	2.89	16	1
1:A:88:VAL:O	1:A:88:VAL:HG12	0.40	2.16	28	1
1:A:100:GLU:O	1:A:104:LEU:HD21	0.40	2.15	36	1
1:A:82:ARG:CG	1:A:83:ILE:N	0.40	2.84	7	1
1:A:171:TRP:O	1:A:174:VAL:HG23	0.40	2.16	17	1
1:A:82:ARG:O	1:A:149:LEU:HD12	0.40	2.17	23	1
1:A:148:TYR:CD2	1:A:157:GLU:OE2	0.40	2.74	32	1
1:A:130:LYS:HB3	1:A:130:LYS:HZ3	0.40	1.76	37	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	137/158 (87%)	123±2 (90±2%)	11±3 (8±2%)	3±1 (2±1%)	10	49
All	All	5480/6320 (87%)	4905 (90%)	456 (8%)	119 (2%)	10	49

All 10 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	128	MET	40
1	A	152	ASN	29

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Mol	Chain	Res	Type	Models (Total)
1	A	172	GLU	12
1	A	209	LYS	9
1	A	168	PRO	8
1	A	93	PRO	6
1	A	178	GLY	5
1	A	76	LYS	4
1	A	176	ASP	3
1	A	97	SER	3

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	116/134 (87%)	110±2 (95±2%)	6±2 (5±2%)	26 75
All	All	4640/5360 (87%)	4395 (95%)	245 (5%)	26 75

All 44 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	134	LEU	39
1	A	154	ASN	17
1	A	136	SER	16
1	A	89	SER	14
1	A	129	SER	13
1	A	174	VAL	13
1	A	161	THR	12
1	A	90	LEU	10
1	A	149	LEU	9
1	A	128	MET	7
1	A	92	LEU	7
1	A	99	THR	6
1	A	98	SER	6
1	A	74	LEU	5
1	A	87	SER	5
1	A	102	ASN	5
1	A	116	MET	5

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Mol	Chain	Res	Type	Models (Total)
1	A	88	VAL	4
1	A	114	GLN	4
1	A	80	ILE	4
1	A	168	PRO	3
1	A	76	LYS	3
1	A	115	VAL	3
1	A	83	ILE	3
1	A	196	ARG	3
1	A	179	LYS	3
1	A	68	GLU	2
1	A	209	LYS	2
1	A	66	LEU	2
1	A	131	LYS	2
1	A	146	LYS	2
1	A	197	TYR	2
1	A	170	LYS	2
1	A	120	ASN	2
1	A	100	GLU	1
1	A	78	GLN	1
1	A	82	ARG	1
1	A	185	ILE	1
1	A	183	THR	1
1	A	84	SER	1
1	A	127	ASN	1
1	A	186	THR	1
1	A	71	ASN	1
1	A	105	SER	1

6.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

There are no ligands in this entry.

6.7 Other polymers (i)

There are no such molecules in this entry.

6.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

7 Chemical shift validation (i)

The completeness of assignment taking into account all chemical shift lists is 88% for the well-defined parts and 82% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

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

Total number of shifts	1700
Number of shifts mapped to atoms	1700
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	147	0.18 ± 0.09	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	135	-0.05 ± 0.06	None needed (< 0.5 ppm)
$^{13}C'$	135	0.34 ± 0.14	None needed (< 0.5 ppm)
^{15}N	140	0.29 ± 0.13	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 88%, i.e. 1605 atoms were assigned a chemical shift out of a possible 1824. 0 out of 28 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	677/693 (98%)	280/283 (99%)	266/276 (96%)	131/134 (98%)
Sidechain	874/1041 (84%)	603/678 (89%)	266/332 (80%)	5/31 (16%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	54/90 (60%)	27/43 (63%)	26/44 (59%)	1/3 (33%)
Overall	1605/1824 (88%)	910/1004 (91%)	558/652 (86%)	137/168 (82%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 82%, i.e. 1699 atoms were assigned a chemical shift out of a possible 2065. 0 out of 30 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	720/794 (91%)	298/324 (92%)	282/316 (89%)	140/154 (91%)
Sidechain	925/1174 (79%)	636/763 (83%)	284/375 (76%)	5/36 (14%)
Aromatic	54/97 (56%)	27/47 (57%)	26/46 (57%)	1/4 (25%)
Overall	1699/2065 (82%)	961/1134 (85%)	592/737 (80%)	146/194 (75%)

7.1.4 Statistically unusual chemical shifts (i)

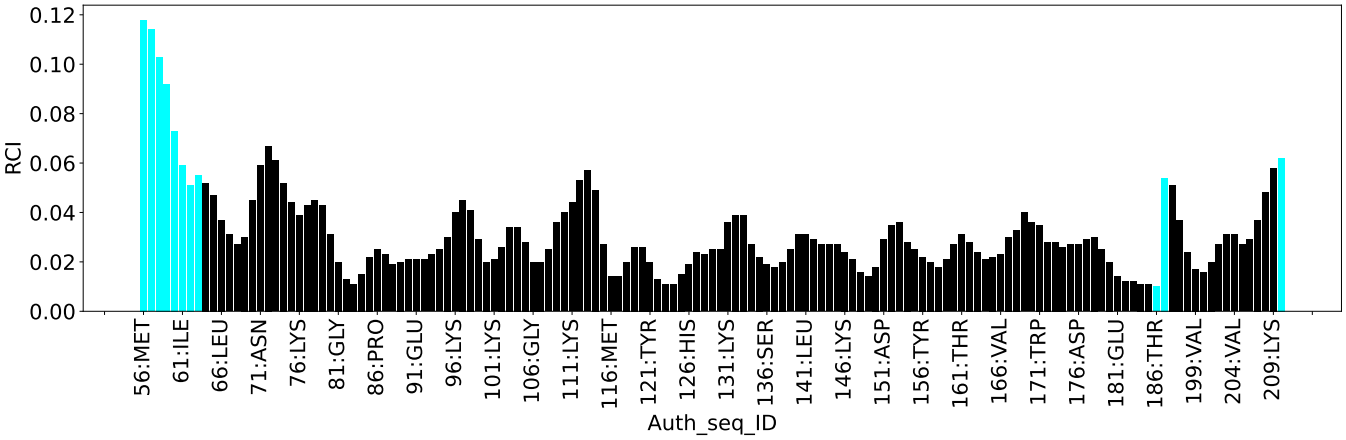
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	182	ILE	HB	0.04	0.35 – 3.22	-6.1
1	A	116	MET	HB2	0.30	0.42 – 3.63	-5.4

7.1.5 Random Coil Index (RCI) plots (i)

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

Random coil index (RCI) for chain A:


RCI
0.12
0.10
0.08
0.06
0.04
0.02
0.00
56:MET
61:ILE
66:LEU
71:ASN
76:LYS
81:GLY
86:PRO
91:GLU
96:LYS
101:LYS
106:GLY
111:LYS
116:MET
121:TYR
126:HIS
131:LYS
136:SER
141:LEU
146:LYS
151:ASP
156:TYR
161:THR
166:VAL
171:TRP
176:ASP
181:GLU
186:THR
199:VAL
204:VAL
209:LYS
Auth_seq_ID