Full wwPDB NMR Structure Validation Report (i)

Nov 7, 2023 – 09:15 AM EST

PDB ID	:	2RUI
BMRB ID	:	11570
Title	:	Solution Structure of the Bacillus anthracis Sortase A-substrate Complex
Authors	:	Chan, A.H.; Yi, S.; Jung, M.E.; Clubb, R.T.
Deposited on	:	2014-06-22

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:

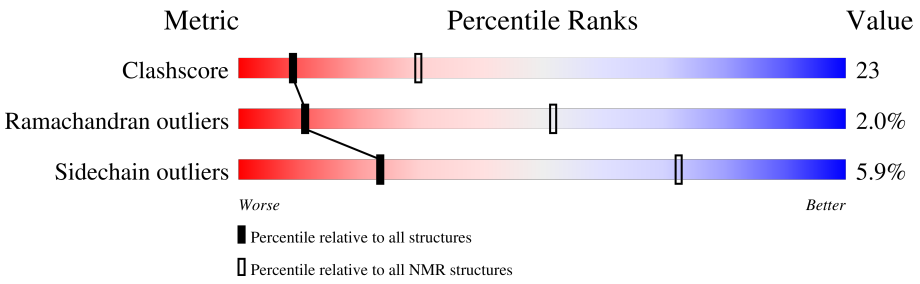
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 87%.

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	65% 30% • •
2	B	5	20% 40% 40%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 4 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:58-A:210, B:702-B:704 (156)	0.53	4

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 3 clusters. No single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2492 atoms, of which 1259 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	2417	750	1218	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 Q6I399
A	54	SER	-	expression tag	UNP Q6I399
A	55	HIS	-	expression tag	UNP Q6I399
A	56	MET	-	expression tag	UNP Q6I399

- Molecule 2 is a protein called Boc-LPAT*.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	5	75	23	41	4	6	1	0

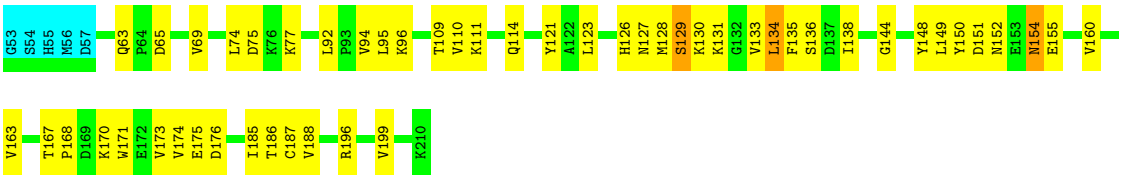
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

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

• Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 65% 30%



• Molecule 2: Boc-LPAT*

Chain B: 20% 40% 40%

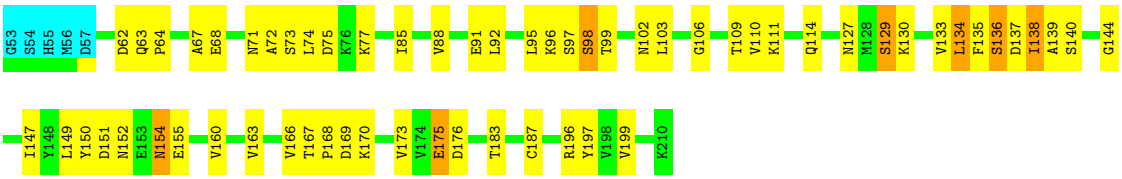
4.2 Scores per residue for each member of the ensemble

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: 58% 34%



• Molecule 2: Boc-LPAT*

Chain B: 20% 40% 40%

B0C701 L702 P703 A704 B27705

4.2.2 Score per residue for model 2

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 63% 30%

G53 S54 H55 M56 D57 Q63 P64 D65 L66 V69 L74 K77 V94 L95 S98 T99 E100 K101 N102 L103 L104 S105 G106 T109 V110 K111 Q114 A122 L123 N127 M128 S129 K130 K131 G132 V133 L134 F135 S136 D137 I138 G144 D145 K146 Y150 D151 N152 E153

N154 E155 V160 T167 P168 D169 K170 V173 V174 E175 D176 E181 I182 I185 T186 C187 V188 S189 K210

- Molecule 2: Boc-LPAT*

Chain B: 20% 40% 40%

B0C701 L702 P703 A704 B27705

4.2.3 Score per residue for model 3

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 66% 28%

G53 S54 H55 M56 D57 Q63 E68 L74 D75 S89 L90 E91 L92 L95 K96 T99 E100 G106 T109 V110 K111 Q114 V115 M116 Y121 N127 M128 S129 K130 K131 G132 V133 L134 F135 I138 G144 I147 Y150 D151 N152 E153 N154 E155 V160

V163 T167 P168 D169 K170 W171 E172 V173 V174 E175 D176 T186 C187 V188 S189 R196 V199 K210

- Molecule 2: Boc-LPAT*

Chain B: 20% 40% 40%

B0C701 L702 P703 A704 B27705

4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 59% 35%

G53 S54 H55 M56 D57 A58 S59 P64 V69 S73 L74 D75 Q78 V79 I80 I83 S84 I85 V88 S89 L92 P93 V94 L95 K96 L103 L104 T109 V110 Q114 N120 Y121 A122 L123 H126 N127 M128 S129 K130 K131 G132 V133 L134 G144 D145 K146 I147

Y148 L149 Y150 D151 N152 E153 N154 E155 V160 T167 P168 D169 K170 W171 E172 V173 V174 E175 D176 T183 L184 I185 T186 C187 V188 S189 D202 L203 K210

• Molecule 2: Boc-LPAT*

Chain B: 40% 20% 40%

B0C701 L702 P703 A704 B27705

4.2.5 Score per residue for model 5

• Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 58% 35%

G53 S54 H55 M56 D57 A58 S59 Q63 P64 D65 L66 A67 E68 V69 A70 N71 L74 D75 K76 V79 I85 V88 S89 L95 K96 L104 V110 K111 Q114 V115 M116 G117 Y121 A122 H126 N127 M128 S129 K130 K131 G132 V133 L134 I138 G144 Y148

L149 Y150 D151 N152 E153 N154 E155 V160 V163 T167 P168 D169 K170 W171 E172 V173 V174 E175 D180 E181 I182 T186 C187 V188 S189 D192 R196 V199 L203 K210

• Molecule 2: Boc-LPAT*

Chain B: 40% 20% 40%

B0C701 L702 P703 A704 B27705

4.2.6 Score per residue for model 6

• Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 54% 37% 6%

G53 S54 H55 M56 D57 A58 S59 Q63 P64 D65 E68 A72 K76 K77 Q78 V79 I83 S84 I85 P86 S87 V88 L92 L95 K96 S97 S98 T99 E100 A107 A108 T109 V110 K111 Q114 Y121 A122 L123 H126 N127 M128 S129 K130 V133 L134 F135 S136 D137

I138 G144 D145 Y148 L149 Y150 D151 N154 E155 Y156 E157 V160 V163 V166 T167 P168 D169 K170 W171 E172 V173 V174 E175 D176 E181 I182 T183 R196 Y197 V198 V199 D202 L203 V204 K210

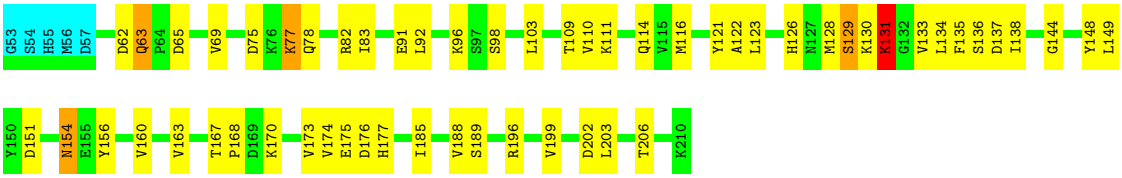
• Molecule 2: Boc-LPAT*

Chain B: 20% 40% 40%

4.2.7 Score per residue for model 7

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 61% 33%



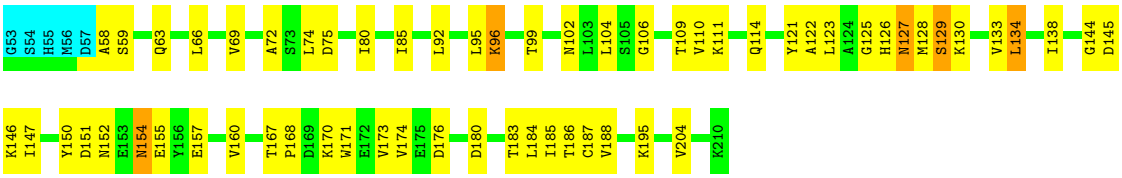
- Molecule 2: Boc-LPAT*

Chain B: 40% 20% 40%

4.2.8 Score per residue for model 8

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 59% 35%



- Molecule 2: Boc-LPAT*

Chain B: 20% 40% 40%

4.2.9 Score per residue for model 9

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 60% 34%

G53 S54 H55 M56 D57 P64 E68 A72 S73 L74 D75 K76 K77 I80 I83 V88 S89 L92 P93 V94 L95 K96 G106 T109 V110 K111 Q114 V115 K118 G119 N120 Y121 A122 L123 N127 M128 S129 K130 V133 L134 F135 S136 A139 Y148 L149

Y150 D151 N152 E153 N154 E155 V166 T167 P168 D169 K170 W171 E172 V173 D176 H177 I185 T186 C187 R196 Y197 D202 L203 V204 K210

• Molecule 2: Boc-LPAT*

Chain B: 20% 40% 40%

B0C701 L702 P703 A704 B27705

4.2.10 Score per residue for model 10

• Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 60% 31% 6%

G53 S54 H55 M56 D57 Q63 P64 D65 L66 V69 L74 D75 K76 V79 I83 S84 I85 V88 S89 L92 P93 V94 L95 K96 T109 V110 Q114 V115 M116 Y121 A122 L123 M128 S129 K130 K131 G132 V133 L134 F135 S136 D137 I138 K142 K143 G144 D145

Y148 L149 Y150 D151 N152 E153 N154 E155 V160 T167 P168 D169 K170 W171 E172 V173 V174 E175 D176 H177 E181 I182 I185 T186 Y197 D202 L203 K210

• Molecule 2: Boc-LPAT*

Chain B: 20% 40% 40%

B0C701 L702 P703 A704 B27705

4.2.11 Score per residue for model 11

• Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 65% 30%

G53 S54 H55 M56 D57 A58 S59 Q63 P64 E68 A72 K76 V79 R82 I85 V88 S89 V94 L95 K96 T109 V110 K111 Q114 V115 K118 A122 L123 A124 G125 H126 N127 M128 S129 K130 V133 L134 D137 S140 G144 Y150

N154 E155 V160 V163 T167 P168 D169 K170 W171 E172 V173 V174 E175 D176 T186 C187 V188 R196 Y197 V198 V199 K210

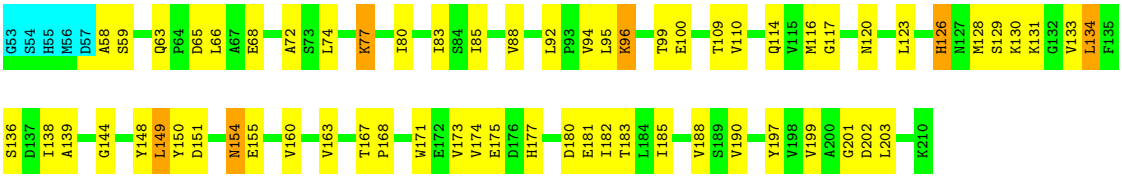
• Molecule 2: Boc-LPAT*

Chain B: 20% 40% 40%

4.2.12 Score per residue for model 12

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 56% 37%



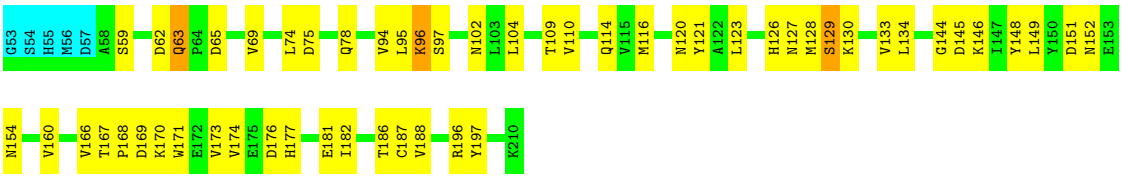
- Molecule 2: Boc-LPAT*

Chain B: 20% 40% 40%

4.2.13 Score per residue for model 13

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 63% 32%



- Molecule 2: Boc-LPAT*

Chain B: 20% 20% 20% 40%

4.2.14 Score per residue for model 14

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 62% 32%

G53 S54 H55 M56 D57 D65 L66 V69 S73 L74 D75 Q78 R82 I83 S89 L90 E91 L92 P93 V94 L95 T109 V110 K111 Q114 V115 K118 G119 N120 Y121 A122 L123 H126 N127 M128 S129 K130 V133 L134 I138 G144 Y150 D151 N154 E155

V160 V163 T167 P168 D169 K170 W171 E172 V173 V174 E175 D176 H177 L184 I185 V188 K191 D192 R196 Y197 V198 V199 K210

• Molecule 2: Boc-LPAT*

Chain B: 20% 40% 40%

B0C701 L702 P703 A704 B27705

4.2.15 Score per residue for model 15

• Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 64% 30%

G53 S54 H55 M56 D57 A58 S59 D65 E68 V69 I83 L92 L95 K96 S97 S98 T99 N102 T109 V110 K111 Q114 N120 L123 H126 N127 M128 S129 K130 K131 G132 V133 L134 F135 S136 G144 D145 K146 I147 Y148 L149 Y150 D151 N154 E155 V160

V163 T167 P168 D169 K170 W171 E172 V173 V174 E175 D176 T186 C187 V188 S189 V190 K191 D192 N193 S194 V199 K210

• Molecule 2: Boc-LPAT*

Chain B: 60% 40%

B0C701 L702 P703 A704 B27705

4.2.16 Score per residue for model 16

• Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 61% 32%

G53 S54 H55 M56 D57 A58 S59 D62 Q63 P64 D65 V69 S73 L74 D75 K76 K77 Q78 V79 I80 V94 L95 K96 S97 S98 N102 L103 L104 S105 G106 T109 V110 K111 Q114 G125 H126 N127 M128 S129 K130 V133 L134 F135 I138 G144 D145 K146 I147 Y148

L149 Y150 D151 N152 E153 N154 E155 V160 T167 P168 W171 D176 E181 I182 I185 T186 C187 R196 Y197 D202 L203 K210

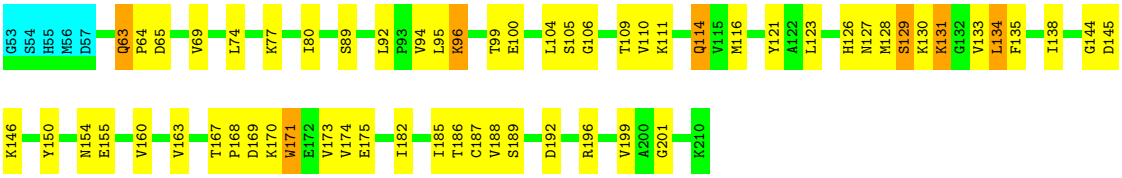
• Molecule 2: Boc-LPAT*

Chain B: 20% 40% 40%

4.2.17 Score per residue for model 17

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 59% 34%



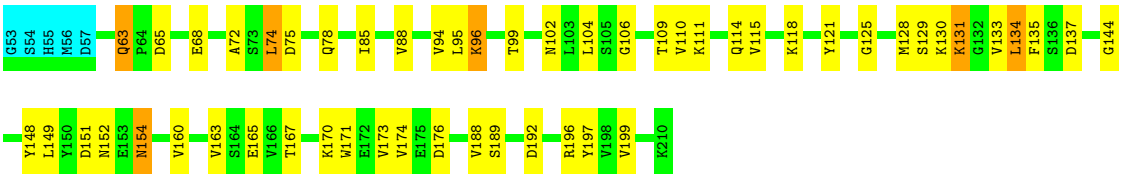
- Molecule 2: Boc-LPAT*

Chain B: 20% 40% 40%

4.2.18 Score per residue for model 18

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 63% 30%



- Molecule 2: Boc-LPAT*

Chain B: 20% 40% 40%

4.2.19 Score per residue for model 19

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 61% 32%

G53 S54 H55 M56 D57 A58 S59 D62 Q63 P64 D65 V69 D75 K76 V79 I85 V88 L92 P93 V94 L95 K96 S97 S98 T99 E100 K101 N102 S105 G106 T109 V110 K111 Q114 V115 M116 N120 Y121 M128 S129 K130 V133 L134 F135 G144 D145

K146 L149 Y150 D151 N154 E157 V160 V166 T167 P168 D169 K170 W171 E172 V173 V174 E175 D176 H177 E181 I182 I185 T186 C187 R196 V204 K210

- Molecule 2: Boc-LPAT*

Chain B: 20% 40% 40%

B0C701 L702 P703 A704 B27705

4.2.20 Score per residue for model 20

- Molecule 1: LPXTG-site transpeptidase family protein

Chain A: 61% 34%

G53 S54 H55 M56 D57 Q63 I83 S89 L92 P93 V94 L95 K96 S97 S98 T99 E100 L104 T109 V110 K111 Q114 Y121 A122 L123 H126 N127 M128 S129 K130 K131 G132 V133 L134 D137 I138 A139 G144 Y150 D151 N152 E153 N154 E155 Y156 E157 V160

V166 T167 P168 D169 K170 W171 E172 V173 V174 E175 D176 E181 I182 I185 V188 S189 V190 N193 R196 Y197 V198 D202 L203 V204 G205 T206 K210

- Molecule 2: Boc-LPAT*

Chain B: 20% 40% 40%

B0C701 L702 P703 A704 B27705

5 Refinement protocol and experimental data overview (i)

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

Of the 200 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
X-PLOR NIH	structure solution	2.25
X-PLOR NIH	refinement	2.25
TALOS	geometry optimization	
UNIO	structure solution	10

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	1798
Number of shifts mapped to atoms	1798
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	87%

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: BOC, B27

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	1163	1188	1188	54±4
2	B	20	23	23	5±2
All	All	23660	24220	24220	1111

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 23.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:66:LEU:HD21	1:A:133:VAL:HG23	0.86	1.46	10	2
1:A:130:LYS:O	1:A:133:VAL:HG12	0.81	1.75	20	20
1:A:122:ALA:C	1:A:123:LEU:HD12	0.80	1.98	4	2
1:A:134:LEU:O	1:A:136:SER:N	0.79	2.15	10	1
1:A:170:LYS:O	1:A:173:VAL:HG22	0.79	1.76	5	14
1:A:68:GLU:O	1:A:72:ALA:HB2	0.79	1.78	18	6
1:A:134:LEU:HD23	1:A:134:LEU:N	0.79	1.93	9	10
1:A:91:GLU:O	1:A:92:LEU:HD23	0.77	1.80	1	2
1:A:188:VAL:HG22	1:A:197:TYR:CE2	0.77	2.15	13	3
1:A:134:LEU:HD13	1:A:134:LEU:H	0.77	1.40	4	3
1:A:163:VAL:HG22	1:A:199:VAL:HG22	0.76	1.57	18	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:110:VAL:HG11	1:A:174:VAL:HG11	0.75	1.58	6	3
1:A:163:VAL:HG12	1:A:199:VAL:HG22	0.75	1.59	11	8
1:A:111:LYS:H	1:A:114:GLN:NE2	0.75	1.79	9	10
1:A:180:ASP:OD2	1:A:203:LEU:HD22	0.74	1.82	12	2
1:A:170:LYS:O	2:B:702:LEU:HD23	0.74	1.82	18	3
1:A:196:ARG:NH2	2:B:702:LEU:HD22	0.74	1.98	7	2
1:A:76:LYS:O	1:A:79:VAL:HG12	0.74	1.82	16	6
1:A:127:ASN:ND2	1:A:129:SER:H	0.72	1.82	20	4
1:A:139:ALA:HB2	1:A:197:TYR:OH	0.72	1.83	1	2
1:A:149:LEU:C	1:A:149:LEU:HD22	0.72	2.05	19	1
1:A:63:GLN:NE2	1:A:126:HIS:CE1	0.72	2.58	17	2
1:A:134:LEU:HD13	1:A:134:LEU:N	0.71	2.00	4	3
1:A:65:ASP:O	1:A:69:VAL:HG23	0.70	1.85	16	9
1:A:114:GLN:N	1:A:114:GLN:HE21	0.70	1.84	14	1
1:A:188:VAL:HG22	1:A:197:TYR:CD2	0.69	2.22	14	4
1:A:74:LEU:C	1:A:74:LEU:HD13	0.69	2.08	14	6
1:A:116:MET:SD	1:A:121:TYR:CZ	0.67	2.87	13	3
1:A:127:ASN:ND2	1:A:187:CYS:H	0.67	1.86	15	3
1:A:63:GLN:NE2	1:A:126:HIS:ND1	0.67	2.42	7	3
1:A:196:ARG:HH22	2:B:702:LEU:HD22	0.66	1.50	11	2
1:A:121:TYR:CE2	1:A:123:LEU:HD11	0.66	2.25	4	2
1:A:134:LEU:HD23	1:A:134:LEU:H	0.66	1.51	19	9
1:A:116:MET:SD	1:A:121:TYR:CE2	0.66	2.88	19	3
1:A:126:HIS:O	1:A:134:LEU:HD23	0.66	1.91	4	2
1:A:173:VAL:HG13	1:A:174:VAL:HG23	0.66	1.68	12	1
1:A:111:LYS:N	1:A:114:GLN:NE2	0.65	2.45	6	9
1:A:138:ILE:HD11	1:A:184:LEU:HD13	0.65	1.67	14	1
1:A:134:LEU:H	1:A:134:LEU:CD2	0.65	2.04	19	9
1:A:122:ALA:CB	1:A:174:VAL:HG12	0.65	2.21	11	3
1:A:138:ILE:HD11	1:A:197:TYR:OH	0.65	1.92	16	1
1:A:79:VAL:HG13	1:A:79:VAL:O	0.64	1.93	19	4
1:A:173:VAL:CG2	1:A:183:THR:HG21	0.63	2.22	6	1
1:A:63:GLN:HE21	1:A:63:GLN:N	0.63	1.92	11	1
1:A:188:VAL:HG23	1:A:195:LYS:O	0.63	1.93	8	1
1:A:63:GLN:NE2	1:A:63:GLN:H	0.63	1.91	11	3
1:A:122:ALA:CB	1:A:174:VAL:HG13	0.63	2.24	5	3
1:A:169:ASP:O	1:A:171:TRP:NE1	0.63	2.31	17	1
1:A:186:THR:OG1	1:A:197:TYR:CZ	0.62	2.52	10	1
1:A:63:GLN:NE2	1:A:63:GLN:N	0.62	2.47	7	3
1:A:185:ILE:HD13	2:B:702:LEU:HD21	0.62	1.70	9	11
1:A:63:GLN:O	1:A:63:GLN:NE2	0.61	2.33	6	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:80:ILE:O	1:A:152:ASN:ND2	0.61	2.33	16	1
1:A:151:ASP:OD1	1:A:152:ASN:N	0.61	2.33	20	12
1:A:128:MET:O	1:A:130:LYS:N	0.61	2.33	17	1
1:A:148:TYR:C	1:A:149:LEU:HD23	0.61	2.16	5	7
1:A:106:GLY:O	1:A:135:PHE:CE1	0.61	2.54	3	8
1:A:150:TYR:CZ	1:A:155:GLU:OE2	0.61	2.54	17	11
1:A:111:LYS:O	1:A:114:GLN:NE2	0.61	2.33	16	7
1:A:83:ILE:HG22	1:A:92:LEU:O	0.61	1.95	10	9
1:A:114:GLN:NE2	1:A:114:GLN:H	0.60	1.93	20	1
1:A:68:GLU:N	1:A:68:GLU:OE1	0.60	2.34	3	2
1:A:144:GLY:N	1:A:160:VAL:O	0.60	2.33	7	19
1:A:94:VAL:HG23	1:A:94:VAL:O	0.60	1.96	16	3
1:A:202:ASP:OD1	1:A:203:LEU:N	0.60	2.35	9	6
1:A:74:LEU:C	1:A:74:LEU:HD23	0.60	2.16	10	2
1:A:75:ASP:OD2	1:A:78:GLN:NE2	0.60	2.34	7	2
1:A:149:LEU:N	1:A:149:LEU:HD23	0.59	2.12	9	2
1:A:173:VAL:HG22	1:A:183:THR:HG21	0.59	1.74	12	3
1:A:150:TYR:CE2	1:A:155:GLU:OE1	0.59	2.56	2	3
1:A:127:ASN:ND2	1:A:186:THR:OG1	0.59	2.35	9	4
1:A:120:ASN:ND2	1:A:177:HIS:ND1	0.59	2.50	19	4
1:A:67:ALA:O	1:A:71:ASN:ND2	0.59	2.35	1	1
1:A:134:LEU:N	1:A:134:LEU:CD2	0.59	2.60	9	13
1:A:171:TRP:CZ3	1:A:175:GLU:OE2	0.59	2.56	20	3
1:A:127:ASN:O	1:A:127:ASN:ND2	0.59	2.35	8	1
1:A:186:THR:HG22	1:A:187:CYS:N	0.59	2.11	16	3
1:A:97:SER:OG	1:A:102:ASN:ND2	0.59	2.36	16	2
1:A:77:LYS:H	1:A:77:LYS:CE	0.59	2.09	7	1
1:A:116:MET:SD	1:A:151:ASP:OD1	0.59	2.60	7	2
1:A:114:GLN:HE21	1:A:114:GLN:CA	0.59	2.10	17	2
1:A:114:GLN:OE1	1:A:122:ALA:N	0.58	2.36	9	6
1:A:110:VAL:N	1:A:114:GLN:HE22	0.58	1.95	6	2
1:A:111:LYS:CE	1:A:171:TRP:HE1	0.58	2.10	9	2
1:A:63:GLN:N	1:A:63:GLN:HE21	0.58	1.97	7	1
1:A:82:ARG:NH2	1:A:91:GLU:OE1	0.58	2.35	14	1
1:A:59:SER:O	1:A:196:ARG:NH2	0.58	2.36	16	2
2:B:703:PRO:O	2:B:704:ALA:O	0.58	2.20	4	20
1:A:168:PRO:O	2:B:702:LEU:CB	0.58	2.52	6	17
1:A:171:TRP:CE3	1:A:175:GLU:OE2	0.58	2.56	15	2
1:A:122:ALA:HB1	1:A:174:VAL:HG12	0.58	1.75	14	3
1:A:193:ASN:O	1:A:196:ARG:NH1	0.58	2.37	20	1
1:A:169:ASP:O	1:A:171:TRP:CD1	0.58	2.56	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:121:TYR:CE2	1:A:123:LEU:HD21	0.57	2.34	14	7
1:A:152:ASN:HD22	1:A:152:ASN:N	0.57	1.96	16	1
1:A:99:THR:OG1	1:A:102:ASN:ND2	0.57	2.36	1	1
1:A:182:ILE:HG22	1:A:201:GLY:O	0.57	1.99	17	2
1:A:68:GLU:O	1:A:72:ALA:N	0.57	2.38	11	2
1:A:82:ARG:NH1	1:A:91:GLU:OE2	0.57	2.38	7	1
1:A:94:VAL:C	1:A:95:LEU:HD12	0.56	2.20	19	13
1:A:74:LEU:HD13	1:A:75:ASP:N	0.56	2.14	3	5
1:A:127:ASN:HD21	1:A:187:CYS:H	0.56	1.43	3	2
1:A:149:LEU:HD13	1:A:149:LEU:H	0.56	1.59	19	1
1:A:63:GLN:OE1	1:A:126:HIS:ND1	0.56	2.38	20	1
1:A:127:ASN:HD21	1:A:187:CYS:N	0.56	1.99	13	2
1:A:74:LEU:HD23	1:A:75:ASP:N	0.56	2.15	1	2
1:A:130:LYS:O	1:A:133:VAL:CG1	0.56	2.54	3	15
1:A:150:TYR:CE2	1:A:155:GLU:CD	0.56	2.79	14	6
1:A:135:PHE:CG	1:A:138:ILE:HD12	0.56	2.36	1	3
1:A:127:ASN:HD22	1:A:187:CYS:H	0.56	1.44	15	1
1:A:188:VAL:CG1	1:A:192:ASP:O	0.56	2.54	18	2
1:A:85:ILE:HG12	1:A:147:ILE:HG23	0.56	1.78	8	1
1:A:173:VAL:HG23	1:A:174:VAL:HG13	0.56	1.76	11	6
1:A:188:VAL:HG13	1:A:189:SER:N	0.56	2.16	18	8
1:A:68:GLU:O	1:A:72:ALA:CB	0.56	2.53	11	5
1:A:110:VAL:HG13	2:B:703:PRO:CD	0.56	2.31	1	8
1:A:134:LEU:CD2	1:A:134:LEU:H	0.56	2.12	3	2
1:A:157:GLU:O	1:A:204:VAL:HG12	0.56	2.00	20	2
1:A:63:GLN:H	1:A:63:GLN:CD	0.55	2.03	10	7
1:A:80:ILE:HD13	1:A:96:LYS:CE	0.55	2.31	17	5
1:A:150:TYR:CZ	1:A:155:GLU:CD	0.55	2.80	8	7
1:A:127:ASN:ND2	1:A:136:SER:OG	0.55	2.38	6	2
1:A:127:ASN:ND2	1:A:187:CYS:N	0.55	2.54	15	2
1:A:110:VAL:HG23	2:B:703:PRO:CG	0.55	2.31	20	1
1:A:114:GLN:N	1:A:114:GLN:NE2	0.55	2.54	14	1
1:A:149:LEU:HD13	1:A:149:LEU:N	0.55	2.15	19	1
1:A:171:TRP:O	1:A:174:VAL:HG22	0.55	2.02	3	8
1:A:110:VAL:HG22	2:B:703:PRO:HG2	0.55	1.77	5	5
1:A:114:GLN:HE21	1:A:114:GLN:N	0.55	1.99	17	1
1:A:99:THR:HG22	1:A:100:GLU:N	0.54	2.18	12	6
1:A:63:GLN:CD	1:A:63:GLN:N	0.54	2.60	10	2
1:A:173:VAL:HG13	1:A:174:VAL:HG13	0.54	1.79	6	1
1:A:95:LEU:N	1:A:95:LEU:HD12	0.54	2.17	12	18
1:A:133:VAL:CG1	1:A:136:SER:OG	0.54	2.55	1	4

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:166:VAL:O	1:A:196:ARG:O	0.54	2.25	1	3
1:A:64:PRO:CB	1:A:68:GLU:OE1	0.54	2.55	11	3
1:A:145:ASP:OD1	1:A:146:LYS:N	0.54	2.41	19	8
1:A:64:PRO:CG	1:A:104:LEU:HD11	0.54	2.32	17	1
1:A:96:LYS:O	1:A:109:THR:OG1	0.54	2.26	10	15
1:A:134:LEU:HD22	1:A:134:LEU:N	0.54	2.18	10	6
1:A:82:ARG:HA	1:A:94:VAL:HG23	0.54	1.79	11	1
1:A:133:VAL:HG22	1:A:134:LEU:HD22	0.54	1.78	20	3
1:A:134:LEU:H	1:A:134:LEU:CD1	0.54	2.11	20	2
1:A:130:LYS:O	1:A:131:LYS:O	0.54	2.26	3	8
1:A:173:VAL:HG22	1:A:183:THR:CG2	0.54	2.32	12	1
1:A:62:ASP:N	1:A:62:ASP:OD1	0.54	2.40	19	2
1:A:114:GLN:CD	1:A:114:GLN:H	0.54	2.06	16	1
1:A:126:HIS:O	1:A:134:LEU:O	0.54	2.26	8	8
1:A:111:LYS:NZ	1:A:175:GLU:CD	0.54	2.61	17	1
1:A:186:THR:OG1	1:A:197:TYR:CE2	0.53	2.60	10	1
1:A:63:GLN:NE2	1:A:64:PRO:O	0.53	2.41	1	1
1:A:104:LEU:HD22	1:A:104:LEU:N	0.53	2.18	17	1
1:A:110:VAL:HG13	2:B:703:PRO:CG	0.53	2.33	15	11
1:A:184:LEU:HD12	1:A:184:LEU:N	0.53	2.19	4	2
1:A:134:LEU:N	1:A:134:LEU:HD22	0.53	2.19	4	3
1:A:150:TYR:CE1	1:A:155:GLU:CD	0.53	2.82	20	3
1:A:104:LEU:N	1:A:104:LEU:CD2	0.53	2.71	17	1
1:A:175:GLU:OE1	1:A:176:ASP:O	0.53	2.27	1	1
1:A:63:GLN:CD	1:A:126:HIS:CG	0.52	2.83	8	1
1:A:94:VAL:O	1:A:94:VAL:CG2	0.52	2.57	9	3
1:A:78:GLN:N	1:A:78:GLN:CD	0.52	2.62	16	1
1:A:149:LEU:N	1:A:149:LEU:CD1	0.52	2.71	19	1
1:A:176:ASP:OD1	1:A:176:ASP:O	0.52	2.27	4	12
1:A:127:ASN:OD1	1:A:127:ASN:O	0.52	2.27	9	4
1:A:63:GLN:OE1	1:A:128:MET:CG	0.52	2.57	16	1
1:A:114:GLN:H	1:A:114:GLN:CD	0.52	2.07	20	1
1:A:92:LEU:CD1	1:A:107:ALA:HB2	0.52	2.35	6	1
1:A:114:GLN:NE2	1:A:114:GLN:CA	0.52	2.72	14	1
1:A:78:GLN:N	1:A:78:GLN:OE1	0.52	2.42	16	1
1:A:152:ASN:ND2	1:A:152:ASN:N	0.52	2.56	16	1
1:A:66:LEU:N	1:A:66:LEU:HD12	0.52	2.19	12	2
1:A:185:ILE:HD13	2:B:702:LEU:CD2	0.52	2.34	20	9
1:A:95:LEU:N	1:A:95:LEU:CD1	0.52	2.72	18	18
1:A:109:THR:HA	1:A:123:LEU:HD23	0.52	1.80	20	10
1:A:59:SER:CB	2:B:702:LEU:O	0.52	2.58	12	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:GLN:N	1:A:114:GLN:OE1	0.52	2.43	16	1
1:A:103:LEU:HD13	2:B:704:ALA:HB3	0.52	1.82	2	3
1:A:95:LEU:HD12	1:A:95:LEU:N	0.52	2.20	19	1
1:A:80:ILE:HD13	1:A:96:LYS:HE3	0.51	1.82	8	5
1:A:171:TRP:N	1:A:171:TRP:CD1	0.51	2.76	11	6
1:A:85:ILE:CG2	1:A:88:VAL:HG22	0.51	2.35	4	9
1:A:128:MET:O	1:A:129:SER:OG	0.51	2.25	18	1
1:A:157:GLU:O	1:A:204:VAL:HG22	0.51	2.05	19	2
1:A:109:THR:CG2	1:A:114:GLN:NE2	0.51	2.74	2	1
1:A:89:SER:O	1:A:89:SER:OG	0.51	2.28	11	3
1:A:171:TRP:CE2	1:A:175:GLU:OE2	0.51	2.64	3	1
1:A:183:THR:C	1:A:184:LEU:HD12	0.51	2.26	8	2
1:A:128:MET:O	1:A:129:SER:CB	0.51	2.58	20	16
1:A:138:ILE:CG1	1:A:197:TYR:OH	0.51	2.58	16	1
1:A:149:LEU:C	1:A:149:LEU:CD2	0.51	2.79	19	1
1:A:63:GLN:OE1	1:A:63:GLN:N	0.51	2.44	13	2
1:A:135:PHE:CD2	1:A:138:ILE:HD12	0.51	2.41	6	2
1:A:134:LEU:CD2	1:A:134:LEU:N	0.51	2.73	13	1
1:A:92:LEU:HD13	1:A:105:SER:O	0.51	2.04	17	1
1:A:149:LEU:HD23	1:A:149:LEU:N	0.50	2.21	5	2
1:A:148:TYR:C	1:A:149:LEU:HD22	0.50	2.26	7	4
1:A:167:THR:OG1	1:A:169:ASP:OD1	0.50	2.29	5	2
1:A:111:LYS:O	1:A:114:GLN:OE1	0.50	2.29	20	1
1:A:114:GLN:CA	1:A:114:GLN:NE2	0.50	2.72	17	1
1:A:128:MET:O	1:A:190:VAL:CG1	0.50	2.59	20	1
1:A:133:VAL:HG22	1:A:134:LEU:H	0.50	1.65	5	6
1:A:175:GLU:O	1:A:177:HIS:CE1	0.50	2.64	7	3
1:A:127:ASN:ND2	1:A:187:CYS:O	0.50	2.45	13	2
1:A:150:TYR:CD1	1:A:150:TYR:N	0.50	2.79	19	1
1:A:97:SER:CB	1:A:102:ASN:ND2	0.50	2.74	1	1
1:A:175:GLU:OE1	1:A:176:ASP:OD1	0.50	2.29	1	1
1:A:74:LEU:C	1:A:74:LEU:CD1	0.50	2.80	5	6
1:A:114:GLN:OE1	1:A:120:ASN:O	0.50	2.29	12	4
1:A:59:SER:C	1:A:196:ARG:HH22	0.50	2.10	16	1
1:A:130:LYS:O	1:A:131:LYS:C	0.50	2.50	18	11
1:A:117:GLY:O	1:A:180:ASP:OD2	0.50	2.29	5	2
2:B:702:LEU:HD23	2:B:703:PRO:HD2	0.49	1.84	19	3
1:A:63:GLN:N	1:A:63:GLN:CD	0.49	2.63	13	2
1:A:88:VAL:O	1:A:89:SER:OG	0.49	2.30	9	1
1:A:138:ILE:CD1	1:A:197:TYR:OH	0.49	2.60	16	1
1:A:121:TYR:CD2	1:A:123:LEU:HD11	0.49	2.42	4	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:172:GLU:OE1	1:A:175:GLU:OE1	0.49	2.31	6	2
1:A:68:GLU:OE1	1:A:68:GLU:N	0.49	2.43	18	1
1:A:79:VAL:O	1:A:79:VAL:CG1	0.49	2.61	19	4
1:A:173:VAL:HG23	1:A:174:VAL:HG23	0.49	1.85	4	3
1:A:186:THR:CG2	1:A:197:TYR:CZ	0.49	2.96	9	1
1:A:134:LEU:C	1:A:136:SER:N	0.48	2.67	10	1
1:A:166:VAL:HG11	1:A:173:VAL:CG1	0.48	2.38	13	1
1:A:150:TYR:CZ	1:A:155:GLU:OE1	0.48	2.67	8	1
1:A:196:ARG:NH2	2:B:702:LEU:HD13	0.48	2.23	11	1
1:A:133:VAL:HG22	1:A:134:LEU:N	0.48	2.23	1	7
1:A:187:CYS:SG	1:A:196:ARG:NH1	0.48	2.86	3	1
1:A:134:LEU:H	1:A:134:LEU:HD22	0.48	1.67	20	2
1:A:191:LYS:O	1:A:192:ASP:OD1	0.48	2.32	14	1
1:A:134:LEU:N	1:A:134:LEU:CD1	0.48	2.71	4	2
1:A:190:VAL:HG22	1:A:190:VAL:O	0.48	2.08	12	2
1:A:192:ASP:OD1	1:A:194:SER:OG	0.48	2.26	15	1
1:A:186:THR:CG2	1:A:187:CYS:N	0.48	2.77	16	2
1:A:151:ASP:OD1	1:A:152:ASN:OD1	0.48	2.31	18	1
1:A:151:ASP:N	1:A:154:ASN:O	0.48	2.45	14	11
1:A:63:GLN:OE1	1:A:63:GLN:O	0.48	2.31	5	1
1:A:62:ASP:OD1	1:A:62:ASP:O	0.48	2.32	7	2
1:A:69:VAL:HG22	1:A:104:LEU:CD1	0.48	2.39	17	1
1:A:63:GLN:N	1:A:63:GLN:NE2	0.48	2.57	11	1
1:A:64:PRO:HG3	1:A:104:LEU:HD11	0.47	1.85	17	1
1:A:171:TRP:CZ2	1:A:175:GLU:OE2	0.47	2.67	3	1
1:A:188:VAL:CG1	1:A:189:SER:N	0.47	2.77	5	5
1:A:63:GLN:OE1	1:A:128:MET:SD	0.47	2.72	16	1
1:A:128:MET:C	1:A:130:LYS:N	0.47	2.67	17	1
1:A:127:ASN:OD1	1:A:127:ASN:C	0.47	2.52	3	3
1:A:63:GLN:HE22	1:A:126:HIS:CE1	0.47	2.28	17	1
1:A:98:SER:OG	1:A:109:THR:O	0.47	2.24	6	5
1:A:137:ASP:O	1:A:140:SER:OG	0.47	2.30	11	2
1:A:152:ASN:OD1	1:A:153:GLU:N	0.47	2.48	9	1
1:A:104:LEU:HD12	1:A:104:LEU:N	0.47	2.24	18	2
1:A:69:VAL:CG1	1:A:104:LEU:O	0.47	2.63	13	2
1:A:114:GLN:CG	1:A:121:TYR:CE1	0.47	2.98	20	1
1:A:69:VAL:HG13	1:A:104:LEU:HB3	0.46	1.85	16	3
1:A:111:LYS:CB	1:A:114:GLN:NE2	0.46	2.79	14	1
1:A:175:GLU:OE1	1:A:176:ASP:N	0.46	2.48	1	1
1:A:123:LEU:HD12	1:A:123:LEU:N	0.46	2.26	4	1
1:A:63:GLN:HE21	1:A:128:MET:CE	0.46	2.23	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:114:GLN:CD	1:A:114:GLN:N	0.46	2.68	16	1
1:A:111:LYS:HB2	1:A:114:GLN:NE2	0.46	2.26	14	1
1:A:111:LYS:NZ	1:A:171:TRP:NE1	0.46	2.63	9	1
1:A:171:TRP:O	1:A:171:TRP:CG	0.46	2.69	9	1
1:A:138:ILE:CG2	1:A:139:ALA:N	0.46	2.79	12	2
1:A:128:MET:HB2	1:A:133:VAL:HG21	0.46	1.87	14	3
1:A:115:VAL:O	1:A:118:LYS:O	0.46	2.34	14	4
1:A:77:LYS:H	1:A:77:LYS:CD	0.46	2.24	2	2
1:A:168:PRO:O	2:B:702:LEU:HD12	0.46	2.11	1	1
1:A:120:ASN:ND2	1:A:177:HIS:CE1	0.46	2.84	9	1
1:A:66:LEU:N	1:A:66:LEU:CD1	0.46	2.79	12	2
1:A:135:PHE:HA	1:A:138:ILE:HD12	0.46	1.88	3	1
1:A:106:GLY:CA	1:A:134:LEU:HD13	0.45	2.41	1	1
1:A:75:ASP:OD2	1:A:78:GLN:CD	0.45	2.54	14	3
1:A:138:ILE:CD1	1:A:186:THR:OG1	0.45	2.63	8	1
1:A:63:GLN:CD	1:A:63:GLN:H	0.45	2.14	13	2
1:A:89:SER:OG	1:A:89:SER:O	0.45	2.32	14	1
1:A:63:GLN:CD	1:A:63:GLN:O	0.45	2.55	16	1
1:A:109:THR:HG22	1:A:114:GLN:NE2	0.45	2.27	2	1
1:A:63:GLN:O	1:A:63:GLN:CD	0.45	2.55	6	2
1:A:92:LEU:HD13	1:A:106:GLY:HA3	0.45	1.87	8	2
1:A:127:ASN:O	1:A:127:ASN:CG	0.45	2.54	8	1
1:A:127:ASN:OD1	1:A:187:CYS:O	0.45	2.35	5	1
1:A:138:ILE:HD11	1:A:186:THR:HG21	0.45	1.89	5	1
1:A:176:ASP:OD1	1:A:176:ASP:N	0.45	2.50	14	2
1:A:66:LEU:N	1:A:66:LEU:CD2	0.45	2.79	8	1
1:A:100:GLU:O	1:A:104:LEU:CD2	0.45	2.65	17	1
1:A:147:ILE:HD11	1:A:160:VAL:CG2	0.45	2.42	1	2
1:A:116:MET:CG	1:A:121:TYR:CZ	0.45	3.00	5	3
1:A:174:VAL:HG12	1:A:174:VAL:O	0.45	2.12	12	1
1:A:69:VAL:HG22	1:A:104:LEU:HD22	0.44	1.87	2	1
1:A:114:GLN:OE1	1:A:121:TYR:CZ	0.44	2.71	7	1
1:A:99:THR:CG2	1:A:100:GLU:N	0.44	2.79	12	2
1:A:111:LYS:H	1:A:114:GLN:HE22	0.44	1.54	9	1
1:A:65:ASP:O	1:A:68:GLU:OE1	0.44	2.35	18	1
1:A:99:THR:OG1	1:A:102:ASN:CG	0.44	2.56	18	2
1:A:128:MET:CG	1:A:133:VAL:HG21	0.44	2.42	13	2
1:A:110:VAL:HG13	2:B:703:PRO:HD3	0.44	1.89	1	1
1:A:87:SER:CB	1:A:145:ASP:OD1	0.44	2.65	6	1
1:A:120:ASN:HD22	1:A:177:HIS:CE1	0.44	2.31	14	2
1:A:142:LYS:N	1:A:145:ASP:OD2	0.44	2.46	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:126:HIS:O	1:A:134:LEU:CB	0.44	2.66	13	2
1:A:134:LEU:N	1:A:134:LEU:HD23	0.44	2.27	1	1
1:A:102:ASN:O	1:A:105:SER:OG	0.44	2.33	2	1
1:A:135:PHE:CD1	1:A:138:ILE:HD12	0.44	2.48	3	1
1:A:154:ASN:ND2	1:A:154:ASN:N	0.44	2.66	8	1
1:A:76:LYS:O	1:A:79:VAL:CG1	0.44	2.61	19	2
1:A:63:GLN:CG	1:A:126:HIS:ND1	0.44	2.81	5	2
1:A:63:GLN:CD	1:A:126:HIS:ND1	0.44	2.72	7	1
1:A:82:ARG:NH1	1:A:91:GLU:CD	0.44	2.71	7	1
1:A:166:VAL:HG11	1:A:173:VAL:HG11	0.44	1.90	13	1
1:A:184:LEU:N	1:A:184:LEU:CD1	0.43	2.81	8	2
1:A:145:ASP:OD1	1:A:145:ASP:C	0.43	2.53	19	3
1:A:169:ASP:OD1	1:A:169:ASP:C	0.43	2.56	5	4
1:A:114:GLN:OE1	1:A:122:ALA:O	0.43	2.36	6	2
1:A:66:LEU:N	1:A:66:LEU:HD22	0.43	2.27	8	1
1:A:166:VAL:HG21	1:A:198:VAL:HG21	0.43	1.90	6	1
1:A:137:ASP:N	1:A:137:ASP:OD1	0.43	2.52	7	2
1:A:202:ASP:OD1	1:A:202:ASP:O	0.43	2.37	12	2
1:A:127:ASN:HD21	1:A:187:CYS:CA	0.43	2.26	15	1
1:A:69:VAL:HG22	1:A:104:LEU:HD12	0.43	1.89	17	1
1:A:74:LEU:C	1:A:74:LEU:CD2	0.43	2.87	1	2
1:A:116:MET:SD	1:A:151:ASP:CG	0.43	2.96	12	1
1:A:180:ASP:OD1	1:A:180:ASP:O	0.43	2.37	8	1
1:A:149:LEU:HD22	1:A:149:LEU:O	0.43	2.12	19	1
1:A:100:GLU:O	1:A:104:LEU:CD1	0.43	2.67	20	1
1:A:181:GLU:HG2	1:A:182:ILE:N	0.43	2.28	16	8
1:A:168:PRO:O	2:B:702:LEU:CD1	0.43	2.67	4	1
1:A:111:LYS:HZ3	1:A:175:GLU:CD	0.43	2.15	17	1
1:A:97:SER:HB3	1:A:102:ASN:ND2	0.43	2.29	1	1
1:A:149:LEU:HD22	1:A:149:LEU:N	0.43	2.29	1	2
1:A:150:TYR:OH	1:A:155:GLU:OE2	0.43	2.35	17	1
1:A:137:ASP:OD1	1:A:137:ASP:N	0.43	2.52	20	1
1:A:63:GLN:HG3	1:A:126:HIS:ND1	0.42	2.30	8	1
1:A:63:GLN:NE2	1:A:126:HIS:CD2	0.42	2.87	8	1
1:A:103:LEU:HD13	2:B:704:ALA:CB	0.42	2.45	7	2
1:A:197:TYR:CD1	1:A:197:TYR:C	0.42	2.92	1	1
1:A:122:ALA:HB3	1:A:174:VAL:HG13	0.42	1.91	2	1
1:A:99:THR:HG1	1:A:102:ASN:CG	0.42	2.17	15	1
1:A:165:GLU:CG	1:A:197:TYR:CE2	0.42	3.02	18	1
1:A:171:TRP:NE1	2:B:702:LEU:N	0.42	2.67	19	1
1:A:128:MET:O	1:A:190:VAL:HG13	0.42	2.13	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:134:LEU:C	1:A:136:SER:H	0.42	2.16	10	1
1:A:64:PRO:HD2	1:A:104:LEU:HD21	0.42	1.90	2	1
1:A:63:GLN:NE2	1:A:128:MET:CG	0.42	2.83	3	1
1:A:174:VAL:O	1:A:174:VAL:HG12	0.42	2.14	10	2
1:A:110:VAL:H	1:A:114:GLN:HE22	0.42	1.56	6	1
1:A:186:THR:HG21	1:A:197:TYR:OH	0.42	2.14	9	1
1:A:127:ASN:ND2	1:A:186:THR:CG2	0.42	2.83	16	1
1:A:169:ASP:N	1:A:169:ASP:OD1	0.42	2.53	17	1
1:A:75:ASP:OD2	1:A:102:ASN:OD1	0.42	2.38	19	1
1:A:127:ASN:ND2	1:A:186:THR:HG22	0.42	2.30	15	1
1:A:156:TYR:CD1	1:A:206:THR:HG23	0.42	2.50	20	1
1:A:176:ASP:O	1:A:176:ASP:OD1	0.41	2.37	1	2
1:A:63:GLN:OE1	1:A:126:HIS:CD2	0.41	2.73	6	1
1:A:111:LYS:CE	1:A:171:TRP:NE1	0.41	2.82	9	1
1:A:202:ASP:OD1	1:A:202:ASP:C	0.41	2.59	9	1
1:A:168:PRO:O	2:B:702:LEU:CG	0.41	2.67	1	2
1:A:111:LYS:H	1:A:114:GLN:CD	0.41	2.17	3	1
1:A:67:ALA:O	1:A:71:ASN:N	0.41	2.53	5	1
1:A:192:ASP:OD1	1:A:192:ASP:C	0.41	2.58	5	1
1:A:63:GLN:HE21	1:A:63:GLN:C	0.41	2.18	3	1
1:A:128:MET:C	1:A:129:SER:OG	0.41	2.56	19	1
1:A:62:ASP:OD1	1:A:63:GLN:N	0.41	2.53	1	1
1:A:77:LYS:N	1:A:77:LYS:HD3	0.41	2.30	1	1
1:A:138:ILE:HD11	1:A:186:THR:HB	0.41	1.91	17	2
1:A:114:GLN:OE1	1:A:114:GLN:O	0.41	2.38	16	1
1:A:80:ILE:HG21	1:A:96:LYS:HE3	0.41	1.92	17	1
1:A:170:LYS:O	1:A:173:VAL:HG12	0.41	2.16	6	1
1:A:75:ASP:CG	1:A:78:GLN:NE2	0.41	2.74	7	1
1:A:171:TRP:CD1	1:A:171:TRP:N	0.41	2.86	16	1
1:A:181:GLU:CG	1:A:182:ILE:N	0.40	2.83	6	4
1:A:127:ASN:CB	1:A:134:LEU:O	0.40	2.69	17	1
1:A:156:TYR:CD2	1:A:206:THR:HG23	0.40	2.51	7	1
1:A:63:GLN:HE21	1:A:128:MET:HE1	0.40	1.76	10	1
1:A:128:MET:SD	1:A:133:VAL:HG21	0.40	2.56	10	1
1:A:174:VAL:O	1:A:174:VAL:CG1	0.40	2.70	10	1
1:A:127:ASN:OD1	1:A:129:SER:N	0.40	2.45	2	1
1:A:98:SER:O	1:A:98:SER:OG	0.40	2.35	7	1
1:A:166:VAL:HG21	1:A:198:VAL:CG2	0.40	2.47	20	1
1:A:63:GLN:NE2	1:A:128:MET:CE	0.40	2.84	10	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	152/158 (96%)	145±2 (96±1%)	5±2 (3±1%)	2±1 (1±1%)	18 66
2	B	3/5 (60%)	0±0 (13±16%)	1±1 (40±23%)	1±1 (47±22%)	0 0
All	All	3100/3260 (95%)	2914 (94%)	124 (4%)	62 (2%)	11 52

All 11 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	704	ALA	20
1	A	96	LYS	12
1	A	131	LYS	10
1	A	65	ASP	5
2	B	702	LEU	5
1	A	73	SER	3
2	B	703	PRO	3
1	A	64	PRO	1
1	A	72	ALA	1
1	A	135	PHE	1
1	A	129	SER	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	130/134 (97%)	123±2 (95±2%)	7±2 (5±2%)	26 75
2	B	2/2 (100%)	1±0 (65±23%)	1±0 (35±23%)	1 9
All	All	2640/2720 (97%)	2485 (94%)	155 (6%)	23 72

All 29 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	154	ASN	20
1	A	167	THR	20
1	A	129	SER	15
1	A	134	LEU	14
2	B	702	LEU	14
1	A	63	GLN	13
1	A	136	SER	7
1	A	74	LEU	7
1	A	149	LEU	7
1	A	77	LYS	6
1	A	98	SER	4
1	A	89	SER	4
1	A	126	HIS	3
1	A	114	GLN	3
1	A	138	ILE	2
1	A	187	CYS	2
1	A	186	THR	2
1	A	175	GLU	1
1	A	92	LEU	1
1	A	131	LYS	1
1	A	127	ASN	1
1	A	204	VAL	1
1	A	155	GLU	1
1	A	73	SER	1
1	A	171	TRP	1
1	A	121	TYR	1
1	A	105	SER	1
1	A	150	TYR	1
1	A	151	ASP	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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds

that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	B27	B	705	2,1	5,6,6	0.41±0.03	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	B27	B	705	2,1	2,7,7	0.11±0.06	0±0 (0±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	B27	B	705	2,1	-	0±0,4,6,6	-

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 87% for the well-defined parts and 85% 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	1798
Number of shifts mapped to atoms	1798
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
$^{13}C_{\alpha}$	152	0.19 ± 0.12	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	142	-0.04 ± 0.13	None needed (< 0.5 ppm)
$^{13}C'$	146	0.31 ± 0.13	None needed (< 0.5 ppm)
^{15}N	143	0.19 ± 0.17	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 87%, i.e. 1780 atoms were assigned a chemical shift out of a possible 2051. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	741/781 (95%)	305/318 (96%)	294/312 (94%)	142/151 (94%)
Sidechain	992/1180 (84%)	664/768 (86%)	319/376 (85%)	9/36 (25%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	47/90 (52%)	24/43 (56%)	23/44 (52%)	0/3 (0%)
Overall	1780/2051 (87%)	993/1129 (88%)	636/732 (87%)	151/190 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 85%, i.e. 1794 atoms were assigned a chemical shift out of a possible 2104. 0 out of 31 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	749/807 (93%)	308/329 (94%)	298/322 (93%)	143/156 (92%)
Sidechain	998/1200 (83%)	668/781 (86%)	321/383 (84%)	9/36 (25%)
Aromatic	47/97 (48%)	24/47 (51%)	23/46 (50%)	0/4 (0%)
Overall	1794/2104 (85%)	1000/1157 (86%)	642/751 (85%)	152/196 (78%)

7.1.4 Statistically unusual chemical shifts (i)

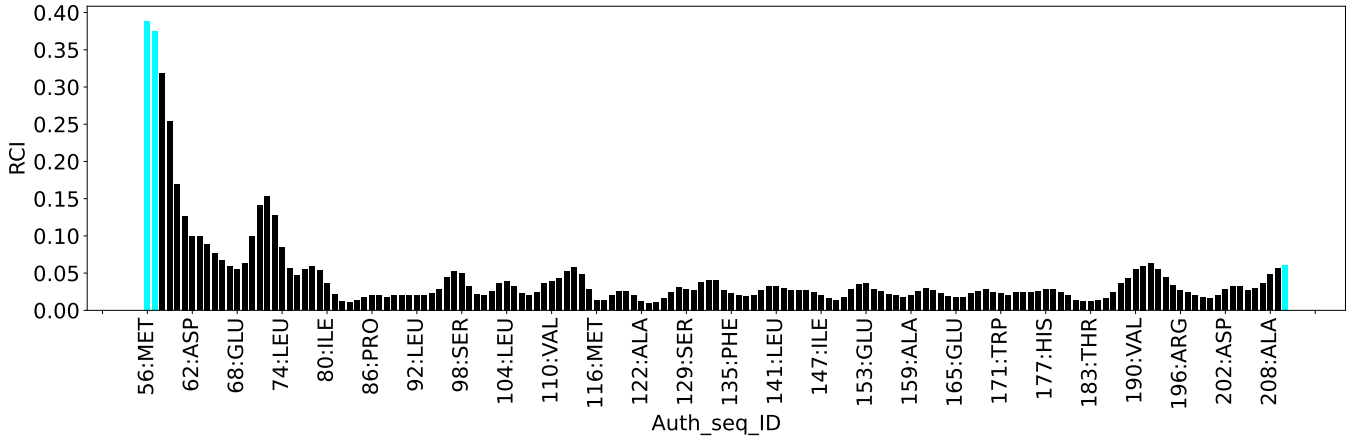
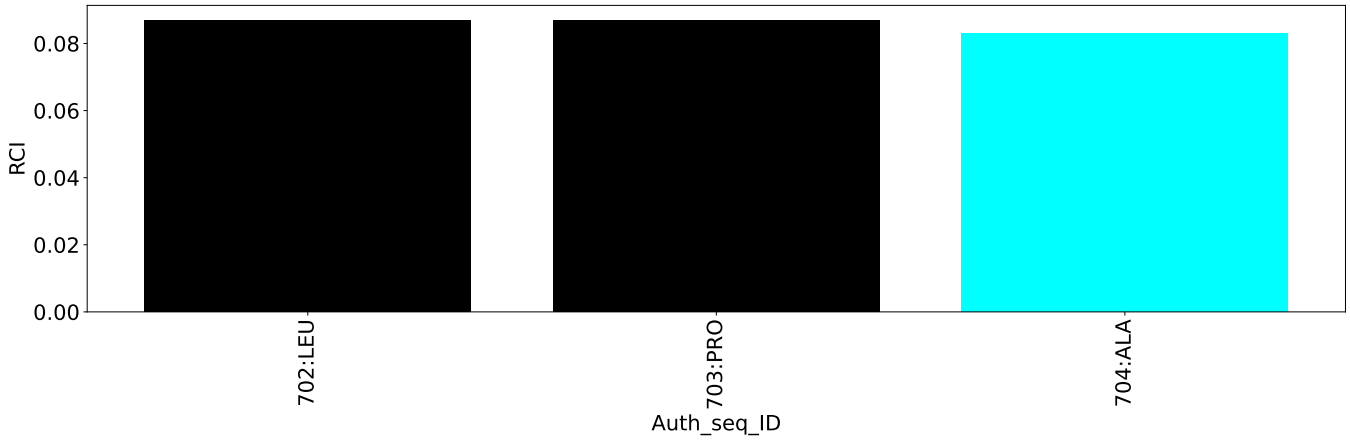
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

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	0.34	0.42 – 3.63	-5.3

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:



Random coil index (RCI) for chain B: