Full wwPDB NMR Structure Validation Report (i)

Apr 21, 2024 – 08:20 AM EDT

PDB ID	:	2L84
BMRB ID	:	17392
Title	:	Solution NMR structures of CBP bromodomain with small molecule j28
Authors	:	Borah, J.C.; Mujtaba, S.; Karakikes, I.; Zeng, L.; Muller, M.; Patel, J.; Moshkina, N.; Morohashi, K.; Zhang, W.; Gerona-Navarro, G.; Hajjar, R.J.; Zhou, M.
Deposited on	:	2011-01-03

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:

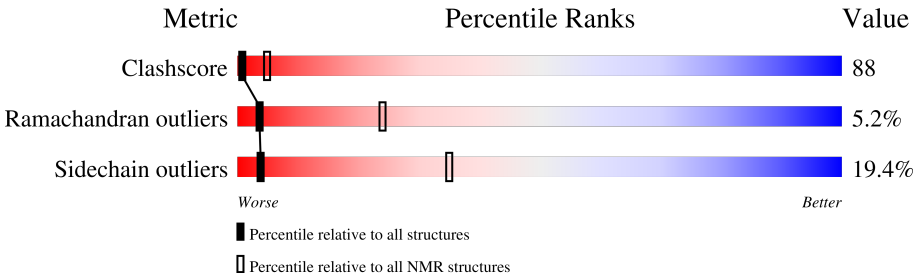
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (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 75%.

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	121	13% 59% 17% 11%

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:1084-A:1167, A:1174-A:1197 (108)	0.29	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 4 clusters and 3 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2062 atoms, of which 1024 are hydrogens and 0 are deuteriums.

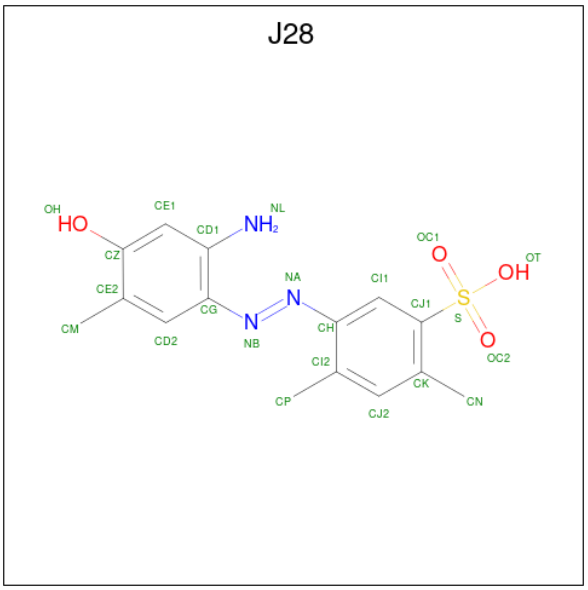
- Molecule 1 is a protein called CREB-binding protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	121	2022	655	1007	169	185	6	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1077	GLY	-	expression tag	UNP Q92793
A	1078	SER	-	expression tag	UNP Q92793
A	1079	HIS	-	expression tag	UNP Q92793
A	1080	MET	-	expression tag	UNP Q92793

- Molecule 2 is 5-[(E)-(2-amino-4-hydroxy-5-methylphenyl)diazenyl]-2,4-dimethylbenzenesulfonic acid (three-letter code: J28) (formula: $C_{15}H_{17}N_3O_4S$).



Mol	Chain	Residues	Atoms					
			Total	C	H	N	O	S
2	A	1	40	15	17	3	4	1

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: CREB-binding protein

Chain A: 13% 59% 17% 11%

G1077 S1078 H1079 M1080 R1081 K1082 K1083 I1084 F1085 K1086 E1089 L1090 R1091 Q1092 A1093 L1094 M1095 P1096 T1097 L1098 E1099 A1100 L1101 Y1102 R1103 Q1104 D1105 P1106 E1107 S1108 L1109 P1110 F1111 R1112 Q1113 P1114 V1115 D1116 P1117 Q1118 L1119 L1120 G1121 I1122 P1123 D1124 Y1125 F1126 D1127 I1128 V1129 K1130 N1131 P1132 M1133 D1134 L1135 S1136 T1137

I1138 K1139 R1140 K1141 L1142 Q1146 Y1147 Q1148 E1149 P1150 W1151 Q1152 Y1153 V1154 D1155 D1156 V1157 W1158 L1159 M1160 F1161 N1162 N1163 A1164 W1165 L1166 Y1167 N1168 R1169 K1170 T1171 S1172 R1173 V1174 Y1175 K1176 F1177 C1178 S1179 K1180 L1181 A1182 E1183 V1184 F1185 E1186 Q1187 E1188 I1189 D1190 P1191 V1192 M1193 Q1194 S1195 L1196 G1197

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: CREB-binding protein

Chain A: 19% 56% 13% • 11%

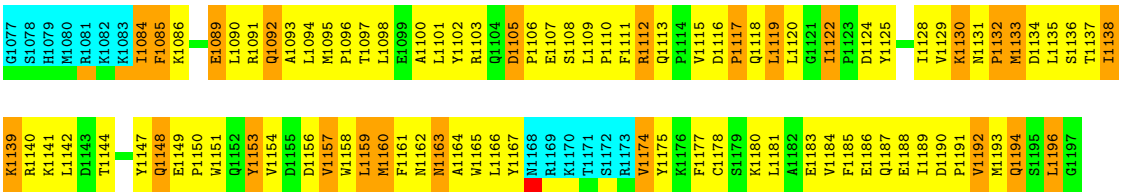
G1077 S1078 H1079 M1080 R1081 K1082 K1083 I1084 F1085 K1086 E1089 L1090 R1091 Q1092 A1093 L1094 M1095 P1096 T1097 L1098 E1099 A1100 L1101 Y1102 R1103 Q1104 D1105 P1106 E1107 S1108 L1109 P1110 F1111 R1112 Q1113 P1114 V1115 D1116 P1117 L1120 G1121 I1122 P1123 D1124 Y1125 I1128 V1129 K1130 N1131 P1132 M1133 D1134 L1135 S1136 T1137 I1138 K1139

R1140 K1141 L1142 D1143 T1144 Y1147 Q1148 E1149 P1150 W1151 Q1152 Y1153 V1154 D1155 D1156 V1157 W1158 L1159 M1160 F1161 N1162 N1163 A1164 W1165 L1166 Y1167 N1168 R1169 K1170 T1171 S1172 R1173 V1174 F1177 C1178 S1179 K1180 L1181 A1182 E1183 V1184 F1185 E1186 Q1187 E1188 I1189 D1190 P1191 V1192 M1193 Q1194 S1195 L1196 G1197

4.2.2 Score per residue for model 2

• Molecule 1: CREB-binding protein

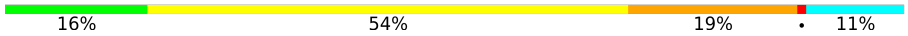
Chain A: 16% 54% 20% 11%

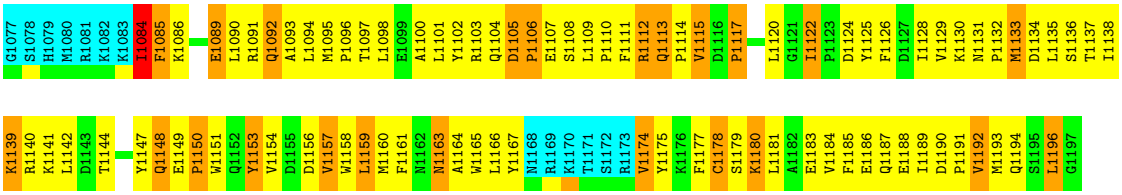


4.2.3 Score per residue for model 3

- Molecule 1: CREB-binding protein

Chain A:

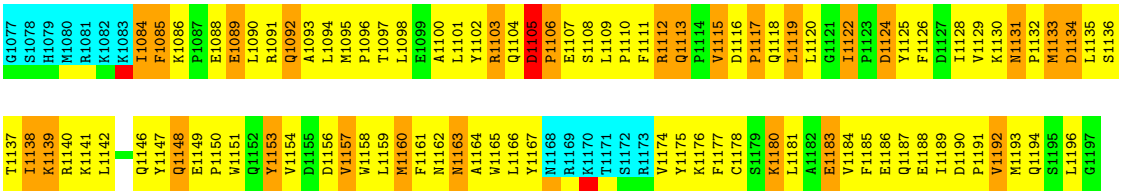




4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: CREB-binding protein

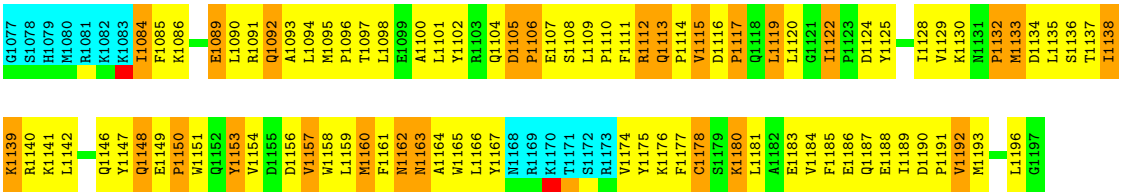
Chain A:



4.2.5 Score per residue for model 5

- Molecule 1: CREB-binding protein

Chain A:



4.2.6 Score per residue for model 6

- Molecule 1: CREB-binding protein

Chain A: 19% 52% 17% • 11%

G1077 S1078 H1079 M1080 R1081 K1082 K1083 I1084 F1085 K1086 E1089 L1090 R1091 Q1092 A1093 L1094 M1095 P1096 T1097 L1098 E1099 A1100 L1101 Y1102 R1103 Q1104 D1105 P1106 E1107 S1108 L1109 P1110 F1111 R1112 Q1113 P1114 V1115 D1116 P1117 Q1118 L1119 L1120 G1121 I1122 P1123 D1124 Y1125 F1126 D1127 I1128 V1129 K1130 N1131 P1132 M1133 D1134 L1135 S1136 T1137

I1138 K1139 R1140 K1141 L1142 Y1147 Q1148 E1149 P1150 W1151 Q1152 Y1153 V1154 D1155 D1156 V1157 W1158 L1159 M1160 F1161 N1162 N1163 A1164 W1165 L1166 Y1167 N1168 R1169 K1170 T1171 S1172 R1173 V1174 F1177 C1178 S1179 K1180 L1181 A1182 E1183 V1184 F1185 E1186 Q1187 E1188 I1189 D1190 P1191 V1192 M1193 Q1194 S1195 L1196 G1197

4.2.7 Score per residue for model 7

- Molecule 1: CREB-binding protein

Chain A: 18% 54% 16% • 11%

G1077 S1078 H1079 M1080 R1081 K1082 K1083 I1084 F1085 K1086 E1089 L1090 R1091 Q1092 A1093 L1094 M1095 P1096 T1097 L1098 E1099 A1100 L1101 Y1102 R1103 Q1104 D1105 P1106 E1107 S1108 L1109 P1110 F1111 R1112 Q1113 P1114 V1115 D1116 P1117 Q1118 L1119 L1120 G1121 I1122 P1123 D1124 Y1125 F1126 D1127 I1128 V1129 K1130 N1131 P1132 M1133 D1134 L1135 S1136 T1137

I1138 K1139 R1140 K1141 L1142 Y1147 Q1148 E1149 P1150 W1151 Q1152 Y1153 V1154 D1155 D1156 V1157 W1158 L1159 M1160 F1161 N1162 N1163 A1164 W1165 L1166 Y1167 N1168 R1169 K1170 T1171 S1172 R1173 F1177 C1178 S1179 K1180 L1181 A1182 E1183 V1184 F1185 E1186 Q1187 E1188 I1189 D1190 P1191 V1192 M1193 L1196 G1197

4.2.8 Score per residue for model 8

- Molecule 1: CREB-binding protein

Chain A: 17% 55% 18% 11%

G1077 S1078 H1079 M1080 R1081 K1082 K1083 I1084 F1085 K1086 E1089 L1090 R1091 Q1092 A1093 L1094 M1095 P1096 T1097 L1098 E1099 A1100 L1101 Y1102 R1103 Q1104 D1105 P1106 E1107 S1108 L1109 P1110 F1111 R1112 Q1113 P1114 V1115 D1116 P1117 Q1118 L1119 L1120 G1121 I1122 P1123 D1124 Y1125 F1126 D1127 I1128 V1129 K1130 N1131 P1132 M1133 D1134 L1135 S1136 T1137

I1138 K1139 R1140 K1141 L1142 D1143 T1144 G1145 Q1146 Y1147 Q1148 E1149 P1150 W1151 Q1152 Y1153 V1154 D1155 D1156 V1157 W1158 L1159 M1160 F1161 N1162 N1163 A1164 W1165 L1166 Y1167 N1168 R1169 K1170 T1171 S1172 R1173 V1174 Y1175 K1176 F1177 C1178 S1179 K1180 L1181 A1182 E1183 V1184 F1185 E1186 Q1187 E1188 I1189 D1190 P1191 V1192 M1193 L1196 G1197

4.2.9 Score per residue for model 9

- Molecule 1: CREB-binding protein

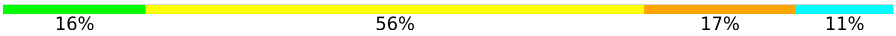
Chain A: 15% 57% 17% 11%

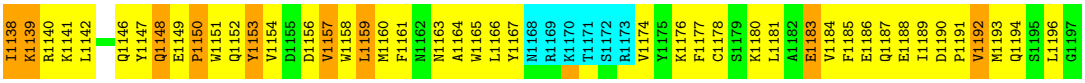
G1077 S1078 H1079 M1080 R1081 K1082 K1083 I1084 F1085 E1089 L1090 R1091 Q1092 A1093 L1094 M1095 P1096 T1097 L1098 E1099 A1100 L1101 Y1102 R1103 Q1104 D1105 P1106 E1107 S1108 L1109 P1110 F1111 R1112 V1115 D1116 P1117 Q1118 L1119 L1120 G1121 I1122 P1123 D1124 Y1125 F1126 D1127 I1128 V1129 K1130 N1131 P1132 M1133 D1134 L1135 S1136 T1137 I1138 K1139

4.2.10 Score per residue for model 10

- Molecule 1: CREB-binding protein

Chain A:

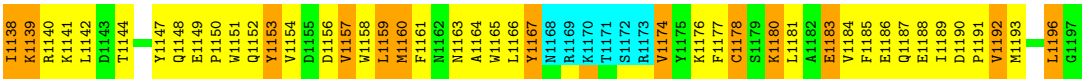




4.2.11 Score per residue for model 11

- Molecule 1: CREB-binding protein

Chain A:



4.2.12 Score per residue for model 12

- Molecule 1: CREB-binding protein

Chain A:

4.2.13 Score per residue for model 13

- Molecule 1: CREB-binding protein

Chain A: 18% 52% 19% 11%

G1077 S1078 H1079 M1080 R1081 K1082 K1083 I1084 F1085 K1086 E1089 L1090 R1091 Q1092 A1093 L1094 M1095 P1096 T1097 L1098 E1099 A1100 L1101 Y1102 R1103 Q1104 D1105 P1106 E1107 S1108 L1109 P1110 F1111 R1112 Q1113 P1114 V1115 D1116 P1117 L1120 G1121 I1122 P1123 D1124 Y1125 F1126 D1127 I1128 V1129 K1130 N1131 P1132 M1133 D1134 L1135 S1136 T1137 I1138

K1139 R1140 K1141 L1142 Q1146 Y1147 Q1148 E1149 P1150 W1151 Q1152 Y1153 V1154 D1155 D1156 V1157 W1158 L1159 M1160 F1161 N1162 N1163 A1164 W1165 L1166 Y1167 N1168 R1169 K1170 T1171 S1172 R1173 V1174 Y1175 K1176 F1177 C1178 S1179 K1180 L1181 A1182 E1183 V1184 F1185 E1186 Q1187 E1188 I1189 D1190 P1191 V1192 M1193 L1196 G1197

4.2.14 Score per residue for model 14

- Molecule 1: CREB-binding protein

Chain A: 15% 56% 18% 11%

G1077 S1078 H1079 M1080 R1081 K1082 K1083 I1084 F1085 K1086 P1087 E1088 E1089 L1090 R1091 Q1092 A1093 L1094 M1095 P1096 T1097 L1098 E1099 A1100 L1101 Y1102 R1103 Q1104 D1105 P1106 E1107 S1108 L1109 P1110 F1111 R1112 Q1113 P1114 V1115 D1116 P1117 Q1118 L1119 L1120 G1121 I1122 P1123 D1124 Y1125 I1128 V1129 K1130 N1131 P1132 M1133 D1134 L1135 S1136 T1137

I1138 K1139 R1140 K1141 L1142 Q1146 Y1147 Q1148 E1149 P1150 W1151 Q1152 Y1153 V1154 D1155 D1156 V1157 W1158 L1159 M1160 F1161 N1162 N1163 A1164 W1165 L1166 Y1167 N1168 R1169 K1170 T1171 S1172 R1173 V1174 Y1175 K1176 F1177 C1178 S1179 K1180 L1181 A1182 E1183 V1184 F1185 E1186 Q1187 E1188 I1189 D1190 P1191 V1192 M1193 L1196 G1197

4.2.15 Score per residue for model 15

- Molecule 1: CREB-binding protein

Chain A: 15% 59% 16% 11%

G1077 S1078 H1079 M1080 R1081 K1082 K1083 I1084 F1085 K1086 E1089 L1090 R1091 Q1092 A1093 L1094 M1095 P1096 T1097 L1098 E1099 A1100 L1101 Y1102 R1103 Q1104 D1105 P1106 E1107 S1108 L1109 P1110 F1111 R1112 Q1113 P1114 V1115 D1116 P1117 Q1118 L1119 L1120 G1121 I1122 P1123 D1124 Y1125 F1126 D1127 I1128 V1129 K1130 N1131 P1132 M1133 D1134 L1135 S1136 T1137

I1138 K1139 R1140 K1141 L1142 Q1146 Y1147 Q1148 E1149 P1150 W1151 Q1152 Y1153 V1154 D1155 D1156 V1157 W1158 L1159 M1160 F1161 N1162 N1163 A1164 W1165 L1166 Y1167 N1168 R1169 K1170 T1171 S1172 R1173 V1174 Y1175 K1176 F1177 C1178 S1179 K1180 L1181 A1182 E1183 V1184 F1185 E1186 Q1187 E1188 I1189 D1190 P1191 V1192 M1193 L1196 G1197

4.2.16 Score per residue for model 16

- Molecule 1: CREB-binding protein

Chain A: 15% 52% 21% • 11%

G1077 S1078 H1079 M1080 R1081 K1082 K1083 I1084 F1085 K1086 E1089 L1090 R1091 Q1092 A1093 L1094 M1095 P1096 T1097 L1098 E1099 A1100 L1101 Y1102 R1103 Q1104 D1105 P1106 E1107 S1108 L1109 P1110 F1111 R1112 Q1113 P1114 V1115 D1116 P1117 L1120 G1121 I1122 P1123 D1124 Y1125 F1126 D1127 I1128 V1129 K1130 N1131 P1132 M1133 D1134 L1135 S1136 T1137 I1138

K1139 R1140 K1141 L1142 Y1147 Q1148 E1149 P1150 W1151 Q1152 Y1153 V1154 D1155 D1156 V1157 W1158 L1159 M1160 F1161 N1162 N1163 A1164 W1165 L1166 Y1167 N1168 R1169 K1170 T1171 S1172 R1173 V1174 Y1175 K1176 F1177 C1178 S1179 K1180 L1181 A1182 E1183 V1184 F1185 E1186 Q1187 E1188 I1189 D1190 P1191 V1192 M1193 Q1194 S1195 L1196 G1197

4.2.17 Score per residue for model 17

- Molecule 1: CREB-binding protein

Chain A: 15% 55% 17% • 11%

G1077 S1078 H1079 M1080 R1081 K1082 K1083 I1084 F1085 K1086 E1089 L1090 R1091 Q1092 A1093 L1094 M1095 P1096 T1097 L1098 E1099 A1100 L1101 Y1102 R1103 Q1104 D1105 P1106 E1107 S1108 L1109 P1110 F1111 R1112 Q1113 P1114 V1115 D1116 P1117 Q1118 L1119 L1120 G1121 I1122 P1123 D1124 Y1125 I1128 V1129 K1130 N1131 P1132 M1133 D1134 L1135 S1136 T1137 I1138

K1139 R1140 K1141 L1142 Y1147 Q1148 E1149 P1150 W1151 Q1152 Y1153 V1154 D1155 D1156 V1157 W1158 L1159 M1160 F1161 N1162 N1163 A1164 W1165 L1166 Y1167 N1168 R1169 K1170 T1171 S1172 R1173 V1174 Y1175 K1176 F1177 C1178 S1179 K1180 L1181 A1182 E1183 V1184 F1185 E1186 Q1187 E1188 I1189 D1190 P1191 V1192 M1193 Q1194 S1195 L1196 G1197

4.2.18 Score per residue for model 18

- Molecule 1: CREB-binding protein

Chain A: 18% 51% 20% 11%

G1077 S1078 H1079 M1080 R1081 K1082 K1083 I1084 F1085 K1086 E1089 L1090 R1091 Q1092 A1093 L1094 M1095 P1096 T1097 L1098 E1099 A1100 L1101 Y1102 R1103 Q1104 D1105 P1106 E1107 S1108 L1109 P1110 F1111 R1112 Q1113 P1114 V1115 D1116 P1117 Q1118 L1119 L1120 G1121 I1122 P1123 D1124 Y1125 F1126 D1127 I1128 V1129 K1130 N1131 P1132 M1133 D1134 L1135 S1136 T1137

I1138 K1139 R1140 K1141 L1142 Y1147 Q1148 E1149 P1150 Y1153 V1154 D1155 D1156 V1157 W1158 L1159 M1160 F1161 N1162 N1163 A1164 W1165 L1166 Y1167 N1168 R1169 K1170 T1171 S1172 R1173 V1174 F1177 C1178 S1179 K1180 L1181 A1182 E1183 V1184 F1185 E1186 Q1187 E1188 I1189 D1190 P1191 V1192 M1193 L1196 G1197

4.2.19 Score per residue for model 19

- Molecule 1: CREB-binding protein

Chain A: 17% 52% 20% 11%

G1077 S1078 H1079 M1080 R1081 K1082 K1083 I1084 F1085 K1086 E1089 L1090 R1091 Q1092 A1093 L1094 M1095 P1096 T1097 L1098 E1099 A1100 L1101 Y1102 R1103 Q1104 D1105 P1106 E1107 S1108 L1109 P1110 F1111 R1112 Q1113 P1114 V1115 D1116 P1117 Q1118 L1119 L1120 G1121 I1122 P1123 D1124 Y1125 F1126 D1127 I1128 V1129 K1130 N1131 P1132 M1133 D1134 L1135 S1136 T1137

I1138 K1139 R1140 K1141 L1142 Q1146 Y1147 Q1148 E1149 P1150 W1151 Q1152 Y1153 V1154 D1155 D1156 V1157 W1158 L1159 M1160 F1161 N1162 N1163 A1164 W1165 L1166 Y1167 N1168 R1169 K1170 T1171 S1172 R1173 V1174 F1177 C1178 S1179 K1180 L1181 A1182 E1183 V1184 F1185 E1186 Q1187 E1188 I1189 D1190 P1191 V1192 M1193 Q1194 S1195 L1196 G1197

4.2.20 Score per residue for model 20

- Molecule 1: CREB-binding protein

Chain A: 18% 55% 16% • 11%

G1077 S1078 H1079 M1080 R1081 K1082 K1083 I1084 F1085 E1089 L1090 R1091 Q1092 A1093 L1094 M1095 P1096 T1097 L1098 E1099 A1100 L1101 Y1102 R1103 Q1104 D1105 P1106 E1107 S1108 L1109 P1110 F1111 R1112 Q1113 P1114 V1115 D1116 P1117 Q1118 L1119 L1120 G1121 I1122 P1123 D1124 Y1125 I1128 V1129 K1130 N1131 P1132 M1133 D1134 L1135 S1136 T1137 I1138 K1139

R1140
K1141
L1142
Q1146
Y1147
Q1148
E1149
P1150
W1151
Q1152
Y1153
V1154
D1155
D1156
V1157
W1158
L1159
M1160
F1161
N1162
N1163
A1164
W1165
L1166
Y1167
N1168
R1169
K1170
T1171
S1172
R1173
V1174
Y1175
K1176
F1177
C1178
S1179
K1180
L1181
A1182
E1183
V1184
F1185
E1186
Q1187
E1188
I1189
D1190
P1191
V1192
M1193
L1196
G1197

5 Refinement protocol and experimental data overview (i)

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

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
ARIA	refinement	2.2
CNS	structure solution	1.2

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	1278
Number of shifts mapped to atoms	1278
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	75%

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: J28

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	906	884	884	161±7
2	A	23	17	16	5±1
All	All	18580	18020	18000	3212

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 88.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1122:ILE:HG21	1:A:1167:TYR:OH	0.86	1.69	16	3
1:A:1120:LEU:HD11	2:A:201:J28:HPB	0.84	1.49	14	18
1:A:1161:PHE:CZ	1:A:1181:LEU:HB3	0.84	2.08	16	20
1:A:1189:ILE:HD12	1:A:1192:VAL:HG11	0.81	1.51	14	20
1:A:1135:LEU:HG	1:A:1160:MET:HE1	0.80	1.53	17	1
1:A:1115:VAL:HG23	1:A:1120:LEU:HD12	0.78	1.55	19	18
1:A:1098:LEU:HD12	1:A:1142:LEU:HD22	0.76	1.55	9	19
1:A:1162:ASN:O	1:A:1166:LEU:HD13	0.76	1.81	6	1
1:A:1120:LEU:HD13	2:A:201:J28:HD2	0.76	1.57	8	16
1:A:1093:ALA:HB1	1:A:1192:VAL:HG22	0.75	1.58	19	20
1:A:1157:VAL:O	1:A:1160:MET:SD	0.73	2.47	8	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1160:MET:SD	1:A:1161:PHE:CD1	0.73	2.82	1	13
1:A:1111:PHE:HB3	1:A:1160:MET:SD	0.72	2.23	18	6
1:A:1094:LEU:HD11	1:A:1150:PRO:HA	0.72	1.62	9	20
1:A:1192:VAL:CG1	1:A:1193:MET:N	0.72	2.52	7	20
1:A:1154:VAL:HG22	1:A:1189:ILE:HD11	0.72	1.62	18	20
1:A:1142:LEU:HA	1:A:1147:TYR:CE2	0.72	2.19	20	2
1:A:1109:LEU:HD13	2:A:201:J28:HNB	0.71	1.60	12	13
1:A:1135:LEU:HD21	1:A:1160:MET:HE3	0.71	1.62	13	1
1:A:1119:LEU:HD12	1:A:1119:LEU:O	0.70	1.87	18	13
1:A:1105:ASP:HB3	1:A:1106:PRO:HD2	0.69	1.65	10	18
1:A:1157:VAL:O	1:A:1160:MET:HE3	0.69	1.88	1	1
1:A:1135:LEU:CD2	1:A:1160:MET:HE3	0.69	2.18	13	2
1:A:1125:TYR:CE1	1:A:1129:VAL:HG11	0.68	2.23	20	18
1:A:1164:ALA:HB3	1:A:1178:CYS:SG	0.68	2.28	10	15
1:A:1175:TYR:HA	1:A:1178:CYS:SG	0.68	2.29	9	5
1:A:1090:LEU:HD12	1:A:1147:TYR:CD1	0.68	2.24	9	2
1:A:1120:LEU:HD13	2:A:201:J28:CD2	0.67	2.20	16	18
1:A:1189:ILE:O	1:A:1192:VAL:HG12	0.67	1.90	2	20
1:A:1098:LEU:CD1	1:A:1142:LEU:HD22	0.67	2.20	20	19
1:A:1135:LEU:CG	1:A:1160:MET:HE1	0.67	2.18	17	1
1:A:1110:PRO:HA	2:A:201:J28:HPA	0.66	1.67	5	9
1:A:1135:LEU:HD21	1:A:1160:MET:CE	0.66	2.21	13	2
1:A:1109:LEU:HD23	1:A:1112:ARG:NH1	0.65	2.04	17	3
1:A:1099:GLU:O	1:A:1103:ARG:HG2	0.65	1.90	16	1
1:A:1098:LEU:HD23	1:A:1101:LEU:HD12	0.65	1.68	1	18
1:A:1109:LEU:HD23	1:A:1112:ARG:HE	0.65	1.52	8	6
1:A:1192:VAL:O	1:A:1196:LEU:HD12	0.64	1.92	17	20
1:A:1161:PHE:HA	1:A:1178:CYS:SG	0.64	2.32	3	14
1:A:1133:MET:SD	1:A:1141:LYS:HE2	0.64	2.32	8	9
1:A:1138:ILE:HA	1:A:1141:LYS:HE3	0.64	1.68	13	9
1:A:1094:LEU:HD13	1:A:1153:TYR:CG	0.63	2.29	20	10
1:A:1094:LEU:HD13	1:A:1153:TYR:CD1	0.63	2.29	19	19
1:A:1160:MET:SD	1:A:1161:PHE:CE1	0.63	2.92	10	7
1:A:1101:LEU:O	1:A:1108:SER:HB3	0.62	1.94	15	17
1:A:1166:LEU:HD23	1:A:1167:TYR:N	0.62	2.09	14	1
1:A:1107:GLU:HA	1:A:1177:PHE:CG	0.62	2.29	1	20
1:A:1128:ILE:HG21	1:A:1167:TYR:HA	0.62	1.70	5	18
1:A:1115:VAL:HG23	1:A:1120:LEU:CD1	0.62	2.24	18	2
1:A:1104:GLN:CG	1:A:1184:VAL:HG11	0.62	2.25	4	6
1:A:1185:PHE:O	1:A:1189:ILE:HG22	0.62	1.95	2	20
1:A:1093:ALA:HB1	1:A:1192:VAL:CG2	0.62	2.24	14	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1154:VAL:HG22	1:A:1189:ILE:CD1	0.61	2.24	19	20
1:A:1184:VAL:O	1:A:1188:GLU:HG3	0.61	1.95	7	2
1:A:1091:ARG:HA	1:A:1142:LEU:HD11	0.61	1.72	20	2
1:A:1098:LEU:HD11	1:A:1139:LYS:HB2	0.61	1.71	17	1
1:A:1159:LEU:O	1:A:1163:ASN:ND2	0.61	2.33	11	7
1:A:1166:LEU:HD12	1:A:1167:TYR:N	0.61	2.11	17	18
1:A:1112:ARG:HA	1:A:1135:LEU:HB2	0.61	1.73	13	3
1:A:1147:TYR:O	1:A:1148:GLN:HG3	0.61	1.95	10	9
1:A:1137:THR:HG22	1:A:1141:LYS:HD3	0.60	1.73	7	18
1:A:1154:VAL:CG2	1:A:1189:ILE:HD11	0.60	2.27	19	20
1:A:1090:LEU:HD11	1:A:1149:GLU:N	0.60	2.10	12	18
1:A:1150:PRO:HG3	1:A:1196:LEU:HD22	0.60	1.73	10	19
1:A:1174:VAL:O	1:A:1178:CYS:SG	0.60	2.59	8	5
1:A:1098:LEU:HD13	1:A:1139:LYS:CG	0.60	2.27	11	19
1:A:1163:ASN:HA	1:A:1166:LEU:HG	0.60	1.73	9	18
1:A:1116:ASP:HB2	1:A:1119:LEU:HD23	0.60	1.73	7	9
1:A:1098:LEU:HD13	1:A:1139:LYS:HG3	0.60	1.72	11	19
1:A:1161:PHE:CZ	1:A:1181:LEU:CB	0.60	2.84	10	14
1:A:1157:VAL:HG22	1:A:1185:PHE:CE2	0.59	2.32	20	20
1:A:1192:VAL:HG12	1:A:1193:MET:N	0.59	2.12	19	20
1:A:1090:LEU:HD23	1:A:1090:LEU:N	0.59	2.11	20	20
1:A:1165:TRP:NE1	1:A:1178:CYS:SG	0.59	2.75	20	3
1:A:1124:ASP:O	1:A:1128:ILE:HD12	0.59	1.98	19	20
1:A:1112:ARG:CZ	1:A:1112:ARG:HB2	0.59	2.27	17	7
1:A:1131:ASN:O	1:A:1163:ASN:ND2	0.59	2.35	19	7
1:A:1104:GLN:NE2	1:A:1104:GLN:HA	0.59	2.12	4	3
1:A:1094:LEU:HD13	1:A:1153:TYR:CD2	0.58	2.32	16	1
1:A:1147:TYR:HD1	1:A:1148:GLN:N	0.58	1.96	20	2
1:A:1111:PHE:HB2	1:A:1135:LEU:HD12	0.58	1.74	11	13
1:A:1132:PRO:HA	1:A:1163:ASN:ND2	0.58	2.14	6	2
1:A:1105:ASP:O	1:A:1107:GLU:N	0.57	2.38	15	20
1:A:1154:VAL:HG12	1:A:1158:TRP:CD1	0.57	2.35	16	20
1:A:1192:VAL:HG22	1:A:1196:LEU:HD11	0.57	1.76	3	20
1:A:1109:LEU:HA	1:A:1112:ARG:HD3	0.57	1.74	7	7
1:A:1161:PHE:CE1	1:A:1181:LEU:HD23	0.57	2.34	16	1
1:A:1161:PHE:HZ	1:A:1181:LEU:HB3	0.57	1.58	10	4
1:A:1101:LEU:O	1:A:1108:SER:CB	0.57	2.52	12	17
1:A:1094:LEU:HD11	1:A:1150:PRO:CA	0.57	2.30	19	20
1:A:1104:GLN:HG3	1:A:1181:LEU:HD12	0.57	1.75	16	1
1:A:1104:GLN:HE21	1:A:1184:VAL:HG21	0.57	1.59	9	2
1:A:1117:PRO:HB3	1:A:1122:ILE:O	0.56	2.00	13	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1163:ASN:HA	1:A:1166:LEU:HD22	0.56	1.77	14	1
1:A:1186:GLU:O	1:A:1190:ASP:HB2	0.56	2.01	10	20
1:A:1165:TRP:NE1	1:A:1178:CYS:HB3	0.56	2.15	1	14
1:A:1086:LYS:H	1:A:1089:GLU:HG3	0.56	1.60	18	15
1:A:1106:PRO:HA	1:A:1109:LEU:HB2	0.56	1.76	11	1
1:A:1190:ASP:O	1:A:1194:GLN:HG2	0.56	2.01	16	2
1:A:1111:PHE:O	1:A:1134:ASP:HB2	0.56	1.99	20	4
1:A:1128:ILE:HD13	1:A:1167:TYR:CE2	0.56	2.36	1	13
1:A:1188:GLU:C	1:A:1191:PRO:HD2	0.56	2.22	7	20
1:A:1160:MET:HA	1:A:1163:ASN:ND2	0.56	2.14	19	6
1:A:1111:PHE:O	1:A:1134:ASP:HB3	0.55	2.01	5	15
1:A:1184:VAL:O	1:A:1187:GLN:HB3	0.55	2.01	7	2
1:A:1192:VAL:C	1:A:1196:LEU:HD12	0.55	2.21	1	20
1:A:1137:THR:O	1:A:1141:LYS:HE3	0.55	2.00	14	9
1:A:1164:ALA:HB1	1:A:1174:VAL:HG23	0.55	1.78	6	15
1:A:1111:PHE:O	1:A:1135:LEU:N	0.55	2.39	16	12
1:A:1100:ALA:HB1	1:A:1184:VAL:CG2	0.55	2.32	20	18
1:A:1147:TYR:C	1:A:1149:GLU:H	0.55	2.04	20	20
1:A:1154:VAL:HG12	1:A:1158:TRP:HD1	0.55	1.60	16	20
1:A:1142:LEU:HD12	1:A:1147:TYR:CE2	0.55	2.37	9	2
1:A:1160:MET:HA	1:A:1163:ASN:OD1	0.55	2.01	18	6
1:A:1184:VAL:HG13	1:A:1185:PHE:N	0.55	2.17	10	16
1:A:1156:ASP:HA	1:A:1159:LEU:HB2	0.54	1.78	18	20
1:A:1122:ILE:HD12	1:A:1125:TYR:HD2	0.54	1.62	13	1
1:A:1097:THR:HA	1:A:1188:GLU:HB3	0.54	1.79	10	20
1:A:1138:ILE:CG2	1:A:1139:LYS:N	0.54	2.70	15	19
1:A:1138:ILE:HD11	1:A:1153:TYR:O	0.54	2.02	9	1
1:A:1091:ARG:CG	1:A:1142:LEU:HG	0.54	2.33	11	19
1:A:1095:MET:O	1:A:1098:LEU:HB2	0.54	2.03	14	19
1:A:1122:ILE:HG23	1:A:1167:TYR:OH	0.54	2.03	19	11
1:A:1110:PRO:HA	2:A:201:J28:CP	0.54	2.33	9	9
1:A:1119:LEU:HD12	1:A:1119:LEU:C	0.54	2.23	10	13
1:A:1084:ILE:HG23	1:A:1148:GLN:HE22	0.54	1.63	5	5
1:A:1181:LEU:O	1:A:1185:PHE:HB2	0.53	2.03	14	17
1:A:1150:PRO:HB2	1:A:1193:MET:CE	0.53	2.33	18	20
1:A:1092:GLN:O	1:A:1096:PRO:HG2	0.53	2.04	10	20
1:A:1084:ILE:HG13	1:A:1149:GLU:HG3	0.53	1.79	9	3
1:A:1192:VAL:HG12	1:A:1193:MET:H	0.53	1.64	14	20
1:A:1095:MET:HB3	1:A:1096:PRO:HD3	0.53	1.81	7	20
1:A:1115:VAL:O	1:A:1117:PRO:HD3	0.53	2.04	18	3
1:A:1132:PRO:O	1:A:1163:ASN:ND2	0.53	2.42	12	8

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1132:PRO:O	1:A:1133:MET:O	0.53	2.26	10	19
1:A:1129:VAL:HB	1:A:1163:ASN:HB3	0.53	1.81	7	4
1:A:1106:PRO:O	1:A:1110:PRO:HD2	0.53	2.04	16	2
1:A:1111:PHE:CZ	1:A:1178:CYS:SG	0.53	3.02	6	9
1:A:1160:MET:HA	1:A:1163:ASN:HD21	0.52	1.64	11	1
1:A:1098:LEU:HD21	1:A:1135:LEU:HD22	0.52	1.80	17	1
1:A:1105:ASP:CB	1:A:1106:PRO:HD2	0.52	2.35	17	18
1:A:1160:MET:HE3	1:A:1161:PHE:CE1	0.52	2.40	17	1
1:A:1158:TRP:NE1	1:A:1185:PHE:CE2	0.52	2.77	20	20
1:A:1098:LEU:CD2	1:A:1135:LEU:HD22	0.52	2.35	17	2
1:A:1147:TYR:HD1	1:A:1148:GLN:H	0.52	1.47	9	2
1:A:1163:ASN:HA	1:A:1166:LEU:CG	0.52	2.35	1	18
1:A:1138:ILE:HD11	1:A:1157:VAL:N	0.52	2.19	4	18
1:A:1181:LEU:O	1:A:1185:PHE:CB	0.52	2.58	15	20
1:A:1100:ALA:O	1:A:1104:GLN:HG2	0.52	2.05	3	9
1:A:1147:TYR:HB2	1:A:1149:GLU:O	0.52	2.04	9	2
1:A:1132:PRO:O	1:A:1163:ASN:OD1	0.52	2.27	15	4
1:A:1090:LEU:HD22	1:A:1150:PRO:HD3	0.52	1.81	19	4
1:A:1147:TYR:CE2	1:A:1153:TYR:HB2	0.52	2.39	17	18
1:A:1180:LYS:O	1:A:1183:GLU:HB3	0.52	2.05	18	15
1:A:1192:VAL:HG12	1:A:1193:MET:HG2	0.52	1.80	20	20
1:A:1129:VAL:O	1:A:1130:LYS:HB2	0.52	2.05	7	14
1:A:1180:LYS:O	1:A:1180:LYS:HD2	0.52	2.04	15	3
1:A:1115:VAL:HG13	1:A:1120:LEU:HD12	0.52	1.81	12	1
1:A:1185:PHE:CE1	1:A:1189:ILE:HB	0.51	2.40	10	20
1:A:1189:ILE:HA	1:A:1192:VAL:HB	0.51	1.82	14	20
1:A:1115:VAL:O	1:A:1120:LEU:HG	0.51	2.05	13	11
1:A:1160:MET:CE	1:A:1161:PHE:CE1	0.51	2.93	13	1
1:A:1133:MET:HG2	1:A:1156:ASP:HB3	0.51	1.83	14	4
1:A:1106:PRO:O	1:A:1110:PRO:HD3	0.51	2.06	9	8
1:A:1150:PRO:O	1:A:1154:VAL:HG23	0.51	2.05	15	17
1:A:1190:ASP:HB3	1:A:1191:PRO:HD3	0.51	1.82	2	20
1:A:1116:ASP:O	1:A:1118:GLN:N	0.51	2.43	19	13
1:A:1107:GLU:N	1:A:1107:GLU:CD	0.51	2.64	7	1
1:A:1128:ILE:HD13	1:A:1167:TYR:CE1	0.51	2.40	5	3
1:A:1085:PHE:CD1	1:A:1090:LEU:HD21	0.51	2.40	9	19
1:A:1184:VAL:O	1:A:1187:GLN:HB2	0.51	2.06	10	18
1:A:1084:ILE:HG23	1:A:1148:GLN:NE2	0.51	2.21	9	1
1:A:1138:ILE:O	1:A:1141:LYS:N	0.51	2.44	20	1
1:A:1109:LEU:HA	1:A:1112:ARG:HH11	0.51	1.66	10	1
1:A:1147:TYR:C	1:A:1149:GLU:N	0.50	2.65	20	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1142:LEU:HD12	1:A:1147:TYR:OH	0.50	2.06	20	2
1:A:1108:SER:OG	1:A:1112:ARG:CZ	0.50	2.59	20	3
1:A:1157:VAL:HA	1:A:1160:MET:SD	0.50	2.46	15	7
1:A:1116:ASP:H	1:A:1120:LEU:HD11	0.50	1.66	18	1
1:A:1104:GLN:HG3	1:A:1184:VAL:HG11	0.50	1.83	4	6
1:A:1183:GLU:HG3	1:A:1184:VAL:N	0.50	2.21	9	7
1:A:1109:LEU:HG	1:A:1112:ARG:CZ	0.50	2.37	14	3
1:A:1115:VAL:HG21	1:A:1125:TYR:CD2	0.50	2.41	13	3
1:A:1089:GLU:O	1:A:1092:GLN:HB3	0.50	2.07	3	16
1:A:1184:VAL:HA	1:A:1187:GLN:HE21	0.50	1.67	5	3
1:A:1129:VAL:CG1	1:A:1163:ASN:HB2	0.50	2.36	6	3
1:A:1090:LEU:CD2	1:A:1150:PRO:HD3	0.50	2.36	19	5
1:A:1165:TRP:HA	1:A:1175:TYR:CE2	0.50	2.41	5	1
1:A:1151:TRP:CD2	1:A:1193:MET:SD	0.50	3.05	9	16
1:A:1153:TYR:HE1	1:A:1189:ILE:HD13	0.50	1.66	20	19
1:A:1156:ASP:O	1:A:1159:LEU:HB2	0.50	2.07	5	11
1:A:1180:LYS:HD2	1:A:1180:LYS:C	0.50	2.27	15	3
1:A:1109:LEU:HG	1:A:1112:ARG:NH1	0.50	2.21	19	1
1:A:1112:ARG:O	1:A:1136:SER:HB3	0.49	2.07	11	3
1:A:1164:ALA:CB	1:A:1178:CYS:SG	0.49	3.00	6	10
1:A:1113:GLN:NE2	2:A:201:J28:HP	0.49	2.22	5	2
1:A:1166:LEU:HD22	1:A:1167:TYR:N	0.49	2.22	6	1
1:A:1122:ILE:HD12	1:A:1125:TYR:CD2	0.49	2.42	13	1
1:A:1108:SER:O	1:A:1112:ARG:HG3	0.49	2.08	17	14
1:A:1115:VAL:HG13	1:A:1120:LEU:CD1	0.49	2.37	12	1
1:A:1162:ASN:O	1:A:1166:LEU:HB3	0.49	2.08	14	1
1:A:1110:PRO:HB3	2:A:201:J28:HPA	0.49	1.84	2	3
1:A:1138:ILE:CG2	1:A:1153:TYR:CD2	0.49	2.96	20	1
1:A:1189:ILE:CD1	1:A:1192:VAL:HG11	0.49	2.36	17	20
1:A:1163:ASN:HA	1:A:1166:LEU:CD2	0.49	2.37	6	1
1:A:1147:TYR:HA	1:A:1152:GLN:HE21	0.49	1.66	10	1
1:A:1140:ARG:C	1:A:1142:LEU:N	0.49	2.65	12	20
1:A:1154:VAL:HG21	1:A:1193:MET:SD	0.49	2.48	3	13
1:A:1113:GLN:HG2	1:A:1114:PRO:HD2	0.49	1.85	13	5
1:A:1106:PRO:HB3	1:A:1109:LEU:HD12	0.48	1.85	10	12
1:A:1116:ASP:CB	1:A:1119:LEU:HB2	0.48	2.38	15	3
1:A:1135:LEU:O	1:A:1139:LYS:HB2	0.48	2.07	9	2
1:A:1095:MET:HE3	1:A:1142:LEU:HD23	0.48	1.84	13	1
1:A:1107:GLU:O	1:A:1177:PHE:HB3	0.48	2.08	16	9
1:A:1138:ILE:HG12	1:A:1147:TYR:OH	0.48	2.08	19	16
1:A:1129:VAL:C	1:A:1131:ASN:H	0.48	2.11	11	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1157:VAL:HA	1:A:1160:MET:CE	0.48	2.38	15	10
1:A:1120:LEU:HD12	1:A:1122:ILE:HD11	0.48	1.85	8	1
1:A:1175:TYR:CA	1:A:1178:CYS:SG	0.48	3.01	20	5
1:A:1153:TYR:HE2	1:A:1189:ILE:HD13	0.48	1.68	16	1
1:A:1111:PHE:HB2	1:A:1135:LEU:CD1	0.48	2.38	11	8
1:A:1135:LEU:HG	1:A:1160:MET:HE2	0.48	1.85	8	6
1:A:1188:GLU:O	1:A:1191:PRO:HD2	0.48	2.08	7	20
1:A:1116:ASP:C	1:A:1118:GLN:H	0.48	2.11	10	13
1:A:1104:GLN:NE2	1:A:1180:LYS:HE3	0.48	2.23	5	1
1:A:1116:ASP:C	1:A:1118:GLN:N	0.48	2.67	19	13
1:A:1113:GLN:NE2	2:A:201:J28:HJ2	0.48	2.24	16	3
1:A:1163:ASN:O	1:A:1167:TYR:CB	0.48	2.62	8	4
1:A:1111:PHE:CG	1:A:1160:MET:SD	0.48	3.07	17	2
1:A:1108:SER:HB2	1:A:1112:ARG:HG2	0.48	1.85	15	1
1:A:1101:LEU:O	1:A:1108:SER:OG	0.48	2.31	11	1
1:A:1151:TRP:CE2	1:A:1193:MET:SD	0.48	3.07	20	18
1:A:1102:TYR:CE1	1:A:1135:LEU:HB3	0.48	2.44	9	16
1:A:1147:TYR:O	1:A:1148:GLN:HG2	0.48	2.08	6	6
1:A:1185:PHE:O	1:A:1189:ILE:N	0.48	2.41	17	20
1:A:1166:LEU:HD13	1:A:1166:LEU:H	0.48	1.69	6	1
1:A:1165:TRP:HA	1:A:1175:TYR:CD2	0.48	2.44	14	1
1:A:1129:VAL:HG12	1:A:1166:LEU:HD11	0.48	1.85	15	4
1:A:1148:GLN:O	1:A:1148:GLN:NE2	0.47	2.47	10	4
1:A:1109:LEU:HA	1:A:1112:ARG:HD2	0.47	1.86	19	1
1:A:1129:VAL:CG1	1:A:1163:ASN:HB3	0.47	2.39	9	7
1:A:1086:LYS:H	1:A:1089:GLU:HG2	0.47	1.69	7	2
1:A:1135:LEU:CD2	1:A:1160:MET:HE2	0.47	2.39	10	1
1:A:1147:TYR:O	1:A:1149:GLU:N	0.47	2.46	20	1
1:A:1104:GLN:NE2	1:A:1180:LYS:HE2	0.47	2.24	11	5
1:A:1138:ILE:HA	1:A:1141:LYS:CE	0.47	2.40	19	4
1:A:1095:MET:CE	1:A:1142:LEU:HD23	0.47	2.39	13	17
1:A:1138:ILE:CD1	1:A:1157:VAL:N	0.47	2.78	12	19
1:A:1098:LEU:HD21	1:A:1138:ILE:CG2	0.47	2.39	13	10
1:A:1184:VAL:CG1	1:A:1185:PHE:N	0.47	2.78	10	14
1:A:1098:LEU:HD23	1:A:1135:LEU:HD22	0.47	1.85	7	6
1:A:1167:TYR:CE2	2:A:201:J28:HMA	0.47	2.45	8	1
1:A:1147:TYR:CB	1:A:1152:GLN:HB2	0.47	2.39	9	2
1:A:1103:ARG:C	1:A:1105:ASP:H	0.47	2.12	16	1
1:A:1116:ASP:HB2	1:A:1119:LEU:HG	0.47	1.86	19	3
1:A:1108:SER:OG	1:A:1112:ARG:NH1	0.47	2.48	19	1
1:A:1098:LEU:O	1:A:1101:LEU:N	0.47	2.48	16	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1112:ARG:HB2	1:A:1112:ARG:NH1	0.47	2.25	7	3
1:A:1111:PHE:C	1:A:1113:GLN:H	0.47	2.13	18	7
1:A:1098:LEU:O	1:A:1102:TYR:N	0.47	2.48	20	14
1:A:1113:GLN:HA	1:A:1136:SER:HB2	0.47	1.86	12	2
1:A:1183:GLU:HG3	1:A:1187:GLN:HE21	0.47	1.67	4	1
1:A:1098:LEU:CD2	1:A:1101:LEU:HD12	0.47	2.40	17	1
1:A:1158:TRP:CD1	1:A:1185:PHE:CE2	0.47	3.02	17	19
1:A:1192:VAL:HG13	1:A:1196:LEU:CD1	0.47	2.40	13	20
1:A:1099:GLU:O	1:A:1102:TYR:HB2	0.47	2.10	16	1
1:A:1132:PRO:O	1:A:1160:MET:HA	0.46	2.10	6	6
1:A:1141:LYS:HG2	1:A:1146:GLN:CD	0.46	2.30	13	11
1:A:1122:ILE:HD13	2:A:201:J28:HMB	0.46	1.87	8	1
1:A:1093:ALA:HB3	1:A:1196:LEU:HD21	0.46	1.85	7	11
1:A:1177:PHE:O	1:A:1181:LEU:HD22	0.46	2.11	16	1
1:A:1174:VAL:HA	1:A:1177:PHE:HB2	0.46	1.87	11	7
1:A:1111:PHE:C	1:A:1113:GLN:N	0.46	2.68	17	8
1:A:1165:TRP:CD1	1:A:1178:CYS:SG	0.46	3.01	15	3
1:A:1147:TYR:CD1	1:A:1148:GLN:N	0.46	2.83	20	2
1:A:1134:ASP:C	1:A:1136:SER:N	0.46	2.69	2	16
1:A:1101:LEU:HD23	1:A:1188:GLU:OE2	0.46	2.11	10	2
1:A:1094:LEU:O	1:A:1097:THR:N	0.46	2.49	7	18
1:A:1098:LEU:HD13	1:A:1139:LYS:CB	0.46	2.40	19	12
1:A:1085:PHE:HD1	1:A:1090:LEU:HD21	0.46	1.69	9	4
1:A:1139:LYS:HG2	1:A:1142:LEU:HD23	0.46	1.87	9	1
1:A:1142:LEU:HB2	1:A:1147:TYR:HE2	0.46	1.71	10	17
1:A:1093:ALA:CB	1:A:1192:VAL:HG22	0.46	2.37	14	10
1:A:1151:TRP:HA	1:A:1154:VAL:CG2	0.46	2.41	19	1
1:A:1130:LYS:HD2	1:A:1130:LYS:N	0.46	2.25	9	4
1:A:1133:MET:HG3	1:A:1134:ASP:N	0.46	2.26	20	3
1:A:1151:TRP:CD1	1:A:1193:MET:HE1	0.46	2.45	11	4
1:A:1122:ILE:HD13	1:A:1125:TYR:CD2	0.45	2.46	2	2
1:A:1117:PRO:CB	1:A:1122:ILE:O	0.45	2.64	20	16
1:A:1189:ILE:HG13	1:A:1193:MET:CG	0.45	2.41	13	16
1:A:1126:PHE:CE1	1:A:1132:PRO:HG3	0.45	2.46	6	10
1:A:1098:LEU:CD1	1:A:1139:LYS:HB2	0.45	2.41	17	1
1:A:1095:MET:O	1:A:1098:LEU:N	0.45	2.49	3	18
1:A:1184:VAL:HG22	1:A:1188:GLU:OE2	0.45	2.11	7	2
1:A:1161:PHE:CD1	1:A:1161:PHE:N	0.45	2.80	15	1
1:A:1133:MET:HG2	1:A:1156:ASP:O	0.45	2.12	16	12
1:A:1160:MET:O	1:A:1163:ASN:OD1	0.45	2.34	6	1
1:A:1097:THR:HB	1:A:1188:GLU:HB2	0.45	1.89	7	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1112:ARG:HB2	1:A:1112:ARG:CZ	0.45	2.42	8	1
1:A:1141:LYS:HZ1	1:A:1156:ASP:CG	0.45	2.15	6	8
1:A:1128:ILE:CG2	1:A:1167:TYR:HA	0.45	2.42	11	3
1:A:1120:LEU:CD1	2:A:201:J28:HPB	0.45	2.41	12	1
1:A:1175:TYR:O	1:A:1179:SER:OG	0.45	2.34	16	1
1:A:1133:MET:CG	1:A:1134:ASP:N	0.45	2.80	20	3
1:A:1113:GLN:HE22	2:A:201:J28:HP	0.45	1.72	5	1
1:A:1115:VAL:C	1:A:1117:PRO:HD3	0.45	2.32	18	4
1:A:1112:ARG:O	1:A:1136:SER:HB2	0.45	2.11	12	7
1:A:1108:SER:OG	1:A:1112:ARG:HD2	0.45	2.12	7	2
1:A:1162:ASN:O	1:A:1165:TRP:HB2	0.45	2.12	6	1
1:A:1159:LEU:O	1:A:1163:ASN:OD1	0.45	2.35	2	5
1:A:1191:PRO:HA	1:A:1194:GLN:NE2	0.44	2.27	6	5
1:A:1160:MET:HE1	1:A:1161:PHE:CZ	0.44	2.48	13	1
1:A:1184:VAL:O	1:A:1188:GLU:HG2	0.44	2.11	15	14
1:A:1157:VAL:HA	1:A:1160:MET:HE2	0.44	1.90	2	3
1:A:1122:ILE:CG2	1:A:1167:TYR:OH	0.44	2.66	9	7
1:A:1140:ARG:O	1:A:1144:THR:HG23	0.44	2.12	8	5
1:A:1151:TRP:N	1:A:1193:MET:HE1	0.44	2.28	3	8
1:A:1106:PRO:O	1:A:1109:LEU:HB2	0.44	2.12	6	7
1:A:1190:ASP:O	1:A:1194:GLN:CG	0.44	2.65	16	2
1:A:1150:PRO:HB2	1:A:1193:MET:HE3	0.44	1.90	14	5
1:A:1138:ILE:HG22	1:A:1139:LYS:N	0.44	2.27	7	7
1:A:1111:PHE:CB	1:A:1160:MET:SD	0.44	3.05	17	1
1:A:1116:ASP:O	1:A:1119:LEU:N	0.44	2.49	8	3
1:A:1113:GLN:NE2	1:A:1113:GLN:O	0.44	2.51	4	1
1:A:1159:LEU:O	1:A:1163:ASN:CG	0.44	2.56	8	7
1:A:1163:ASN:HA	1:A:1166:LEU:HD21	0.44	1.90	6	1
1:A:1133:MET:HE1	1:A:1141:LYS:HE2	0.44	1.90	10	5
1:A:1101:LEU:HD12	1:A:1135:LEU:CD2	0.44	2.42	15	3
1:A:1158:TRP:O	1:A:1162:ASN:HB2	0.44	2.13	15	9
1:A:1157:VAL:HG23	1:A:1160:MET:HE1	0.44	1.90	13	1
1:A:1102:TYR:HE1	1:A:1135:LEU:HB3	0.44	1.71	17	1
1:A:1094:LEU:O	1:A:1095:MET:C	0.43	2.56	7	20
1:A:1174:VAL:HA	1:A:1177:PHE:CG	0.43	2.48	5	3
1:A:1097:THR:HB	1:A:1188:GLU:OE1	0.43	2.12	7	2
1:A:1185:PHE:HA	1:A:1188:GLU:OE1	0.43	2.13	7	2
1:A:1104:GLN:OE1	1:A:1104:GLN:HA	0.43	2.12	9	2
1:A:1099:GLU:O	1:A:1103:ARG:HB3	0.43	2.12	11	3
1:A:1097:THR:O	1:A:1101:LEU:HG	0.43	2.13	19	13
1:A:1133:MET:CE	1:A:1141:LYS:HE2	0.43	2.43	8	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1091:ARG:O	1:A:1096:PRO:HD3	0.43	2.12	13	4
1:A:1107:GLU:HA	1:A:1177:PHE:CD2	0.43	2.48	1	2
1:A:1085:PHE:CZ	1:A:1196:LEU:O	0.43	2.72	20	6
1:A:1129:VAL:HG23	1:A:1130:LYS:N	0.43	2.28	14	5
1:A:1116:ASP:HB2	1:A:1119:LEU:CD2	0.43	2.42	7	3
1:A:1093:ALA:O	1:A:1096:PRO:HD2	0.43	2.14	4	19
1:A:1189:ILE:HA	1:A:1192:VAL:CG1	0.43	2.44	10	4
1:A:1125:TYR:CE1	1:A:1132:PRO:HB3	0.43	2.49	11	3
1:A:1111:PHE:CE2	1:A:1181:LEU:CD1	0.43	3.02	5	8
1:A:1131:ASN:O	1:A:1163:ASN:CG	0.43	2.57	14	3
1:A:1133:MET:HE1	1:A:1141:LYS:HE3	0.43	1.91	9	1
1:A:1134:ASP:O	1:A:1137:THR:N	0.43	2.52	20	2
1:A:1180:LYS:C	1:A:1180:LYS:CD	0.43	2.87	15	1
1:A:1190:ASP:CB	1:A:1191:PRO:HD3	0.42	2.44	2	16
1:A:1115:VAL:HG22	1:A:1117:PRO:HD3	0.42	1.91	19	2
1:A:1105:ASP:C	1:A:1107:GLU:N	0.42	2.71	15	4
1:A:1185:PHE:CE1	1:A:1189:ILE:CB	0.42	3.02	17	19
1:A:1116:ASP:CB	1:A:1119:LEU:HD23	0.42	2.42	7	7
1:A:1125:TYR:HE1	1:A:1129:VAL:HG11	0.42	1.74	13	1
1:A:1147:TYR:O	1:A:1148:GLN:HB2	0.42	2.14	16	1
1:A:1085:PHE:HZ	1:A:1196:LEU:O	0.42	1.98	2	3
1:A:1090:LEU:HD11	1:A:1148:GLN:C	0.42	2.35	6	4
1:A:1103:ARG:O	1:A:1103:ARG:HD3	0.42	2.15	8	2
1:A:1177:PHE:O	1:A:1181:LEU:HD12	0.42	2.14	8	1
1:A:1114:PRO:O	1:A:1115:VAL:C	0.42	2.58	7	2
1:A:1086:LYS:O	1:A:1090:LEU:HG	0.42	2.14	12	1
1:A:1111:PHE:HB3	1:A:1160:MET:HG3	0.42	1.90	13	1
1:A:1135:LEU:CD2	1:A:1160:MET:HE1	0.42	2.44	17	1
1:A:1102:TYR:CE2	1:A:1112:ARG:HB3	0.42	2.49	17	3
1:A:1190:ASP:N	1:A:1191:PRO:CD	0.42	2.82	17	14
1:A:1191:PRO:O	1:A:1194:GLN:HG2	0.42	2.15	1	4
1:A:1163:ASN:O	1:A:1166:LEU:HD22	0.42	2.15	6	1
1:A:1113:GLN:HE21	2:A:201:J28:HJ2	0.42	1.75	12	1
1:A:1089:GLU:O	1:A:1092:GLN:CB	0.42	2.68	14	1
1:A:1153:TYR:CZ	1:A:1157:VAL:HG11	0.42	2.50	1	6
1:A:1130:LYS:N	1:A:1130:LYS:CD	0.42	2.83	18	1
1:A:1091:ARG:O	1:A:1096:PRO:CD	0.41	2.68	11	3
1:A:1131:ASN:O	1:A:1163:ASN:OD1	0.41	2.38	13	2
1:A:1101:LEU:HD21	1:A:1185:PHE:HB2	0.41	1.92	7	4
1:A:1161:PHE:CE1	1:A:1181:LEU:HD13	0.41	2.50	15	1
1:A:1091:ARG:HG3	1:A:1142:LEU:HG	0.41	1.92	13	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1086:LYS:O	1:A:1088:GLU:N	0.41	2.54	4	2
1:A:1163:ASN:O	1:A:1167:TYR:HB3	0.41	2.14	16	2
1:A:1094:LEU:HD23	1:A:1192:VAL:HG21	0.41	1.93	7	1
1:A:1183:GLU:CG	1:A:1184:VAL:N	0.41	2.83	8	1
1:A:1090:LEU:O	1:A:1091:ARG:C	0.41	2.57	14	1
1:A:1175:TYR:O	1:A:1178:CYS:SG	0.41	2.79	15	1
1:A:1116:ASP:H	1:A:1120:LEU:CD1	0.41	2.29	18	1
1:A:1185:PHE:HA	1:A:1188:GLU:CD	0.41	2.36	10	2
1:A:1102:TYR:O	1:A:1112:ARG:NH1	0.41	2.53	18	1
1:A:1086:LYS:C	1:A:1088:GLU:N	0.41	2.74	11	1
1:A:1111:PHE:CD2	1:A:1181:LEU:CD2	0.41	3.03	16	1
1:A:1113:GLN:HE22	2:A:201:J28:HN	0.41	1.75	16	1
1:A:1117:PRO:O	1:A:1122:ILE:O	0.41	2.38	16	1
1:A:1100:ALA:CB	1:A:1188:GLU:HG3	0.41	2.46	17	1
1:A:1157:VAL:CG1	1:A:1185:PHE:CZ	0.41	3.04	14	2
1:A:1104:GLN:CD	1:A:1180:LYS:HE2	0.41	2.36	8	1
1:A:1111:PHE:CD2	1:A:1181:LEU:CD1	0.41	3.04	8	1
1:A:1135:LEU:HD21	1:A:1160:MET:HE1	0.41	1.92	1	1
1:A:1177:PHE:CD1	1:A:1177:PHE:N	0.41	2.87	19	1
1:A:1140:ARG:C	1:A:1142:LEU:H	0.41	2.20	12	3
1:A:1125:TYR:OH	1:A:1163:ASN:ND2	0.41	2.53	6	1
1:A:1101:LEU:CD1	1:A:1135:LEU:CD2	0.41	2.99	7	3
1:A:1098:LEU:HD21	1:A:1138:ILE:HG21	0.41	1.93	10	1
1:A:1101:LEU:O	1:A:1104:GLN:HB2	0.41	2.16	11	1
1:A:1180:LYS:O	1:A:1183:GLU:N	0.41	2.54	12	1
1:A:1135:LEU:CD2	1:A:1160:MET:CE	0.41	2.98	17	2
1:A:1106:PRO:O	1:A:1110:PRO:CD	0.41	2.68	8	1
1:A:1124:ASP:HB3	1:A:1127:ASP:HB2	0.41	1.93	19	1
1:A:1093:ALA:C	1:A:1096:PRO:HD2	0.40	2.37	20	2
1:A:1100:ALA:HB3	1:A:1188:GLU:HG2	0.40	1.92	10	1
1:A:1174:VAL:O	1:A:1177:PHE:HB2	0.40	2.16	16	1
1:A:1122:ILE:HD13	1:A:1125:TYR:HD2	0.40	1.75	2	2
1:A:1086:LYS:N	1:A:1089:GLU:HG3	0.40	2.31	16	1
1:A:1177:PHE:N	1:A:1177:PHE:CD1	0.40	2.90	20	2
1:A:1100:ALA:HB1	1:A:1184:VAL:HG21	0.40	1.93	12	2
1:A:1101:LEU:O	1:A:1108:SER:HB2	0.40	2.15	12	1
1:A:1180:LYS:O	1:A:1183:GLU:HB2	0.40	2.16	14	1
1:A:1125:TYR:C	1:A:1127:ASP:H	0.40	2.19	18	1
1:A:1085:PHE:CE1	1:A:1196:LEU:HB3	0.40	2.52	3	1
1:A:1103:ARG:HD2	1:A:1103:ARG:O	0.40	2.16	14	1
1:A:1099:GLU:HA	1:A:1102:TYR:HB2	0.40	1.92	17	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1155:ASP:O	1:A:1159:LEU:HB2	0.40	2.16	18	1
1:A:1107:GLU:O	1:A:1181:LEU:HD11	0.40	2.16	20	1
1:A:1181:LEU:HA	1:A:1184:VAL:CG1	0.40	2.46	3	1
1:A:1115:VAL:HG22	1:A:1116:ASP:N	0.40	2.32	13	1
1:A:1167:TYR:HE1	2:A:201:J28:HOH	0.40	1.57	18	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	107/121 (88%)	81±2 (75±2%)	21±2 (19±2%)	6±1 (5±1%)	4	24
All	All	2140/2420 (88%)	1615 (75%)	414 (19%)	111 (5%)	4	24

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)
1	A	1084	ILE	20
1	A	1105	ASP	20
1	A	1133	MET	19
1	A	1117	PRO	18
1	A	1106	PRO	18
1	A	1132	PRO	9
1	A	1115	VAL	2
1	A	1126	PHE	2
1	A	1167	TYR	1
1	A	1104	GLN	1
1	A	1148	GLN	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	101/113 (89%)	81±3 (81±3%)	20±3 (19±3%)	4 35
All	All	2020/2260 (89%)	1628 (81%)	392 (19%)	4 35

All 47 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	1122	ILE	20
1	A	1153	TYR	20
1	A	1157	VAL	20
1	A	1192	VAL	20
1	A	1092	GLN	19
1	A	1139	LYS	19
1	A	1112	ARG	18
1	A	1089	GLU	17
1	A	1138	ILE	17
1	A	1163	ASN	16
1	A	1119	LEU	16
1	A	1160	MET	16
1	A	1115	VAL	15
1	A	1103	ARG	15
1	A	1183	GLU	13
1	A	1148	GLN	11
1	A	1176	LYS	11
1	A	1085	PHE	10
1	A	1159	LEU	10
1	A	1113	GLN	10
1	A	1196	LEU	9
1	A	1180	LYS	8
1	A	1174	VAL	7
1	A	1178	CYS	7
1	A	1105	ASP	6
1	A	1150	PRO	5
1	A	1130	LYS	4
1	A	1134	ASP	3
1	A	1125	TYR	3
1	A	1194	GLN	2
1	A	1179	SER	2
1	A	1124	ASP	2
1	A	1131	ASN	2
1	A	1162	ASN	2

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Mol	Chain	Res	Type	Models (Total)
1	A	1106	PRO	2
1	A	1166	LEU	2
1	A	1147	TYR	2
1	A	1149	GLU	2
1	A	1084	ILE	1
1	A	1107	GLU	1
1	A	1108	SER	1
1	A	1109	LEU	1
1	A	1152	GLN	1
1	A	1181	LEU	1
1	A	1190	ASP	1
1	A	1098	LEU	1
1	A	1151	TRP	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)

1 ligand 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	J28	A	201	-	23,24,24	1.63±0.03	2±0 (8±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	J28	A	201	-	31,36,36	1.75±0.02	8±0 (24±1%)

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	J28	A	201	-	-	0±0,11,11,11	0±0,2,2,2

All unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	201	J28	CG-NB	4.50	1.32	1.42	18	20
2	A	201	J28	CH-NA	4.49	1.32	1.42	18	20

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	A	201	J28	CJ2-CK-CJ1	5.09	120.50	116.94	19	20
2	A	201	J28	CN-CK-CJ1	3.82	120.42	124.16	1	20
2	A	201	J28	CI2-CH-NA	3.76	120.47	116.46	17	20
2	A	201	J28	CH-NA-NB	3.06	121.62	114.56	19	20
2	A	201	J28	CJ2-CI2-CH	2.65	121.06	118.25	13	20
2	A	201	J28	CD2-CE2-CZ	2.50	119.55	117.56	20	20
2	A	201	J28	CE1-CD1-CG	2.37	120.97	118.97	17	20
2	A	201	J28	CG-NB-NA	2.32	119.92	114.56	14	12

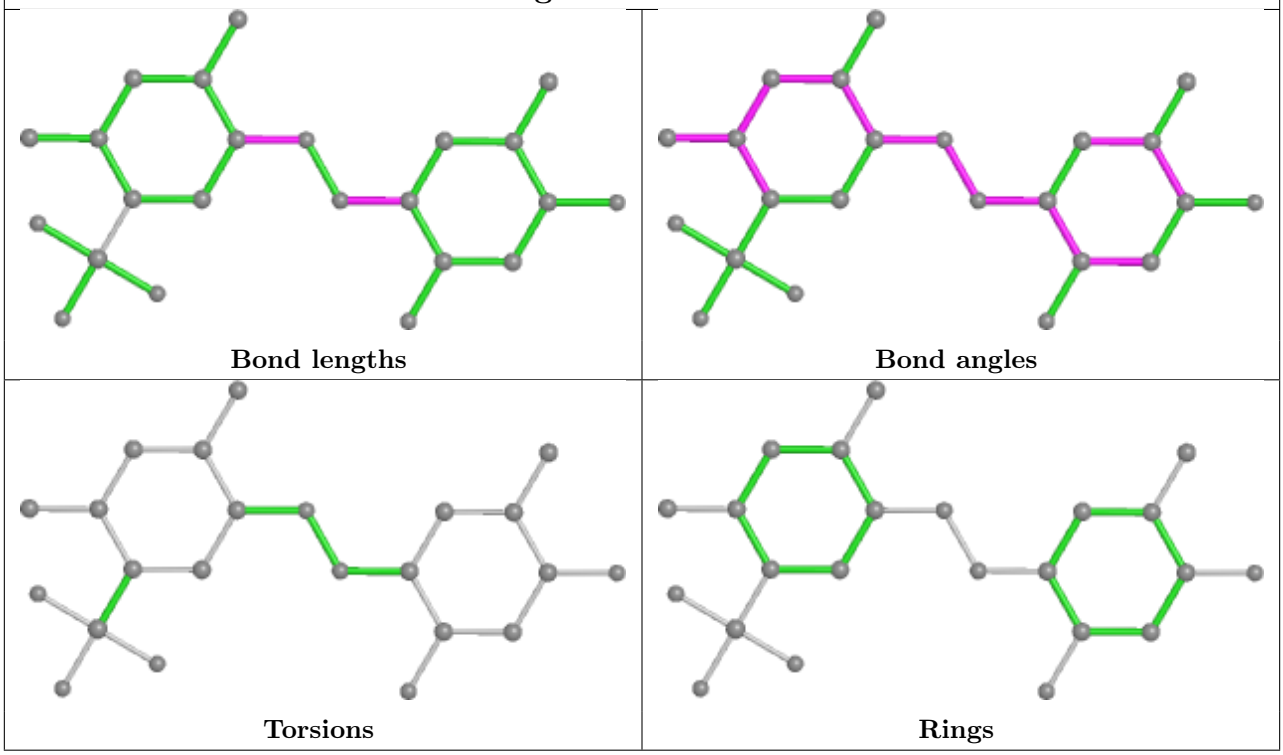
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand J28 A 201



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 75% for the well-defined parts and 73% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *ppm.str*

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	1278
Number of shifts mapped to atoms	1278
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	10

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	119	-0.42 ± 0.17	None needed (< 0.5 ppm)
$^{13}C_{\beta}$	117	0.33 ± 0.16	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	107	0.56 ± 0.34	None needed (imprecise)

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 75%, i.e. 1160 atoms were assigned a chemical shift out of a possible 1554. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	413/523 (79%)	208/209 (100%)	107/216 (50%)	98/98 (100%)
Sidechain	653/881 (74%)	394/571 (69%)	247/280 (88%)	12/30 (40%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	94/150 (63%)	48/72 (67%)	43/75 (57%)	3/3 (100%)
Overall	1160/1554 (75%)	650/852 (76%)	397/571 (70%)	113/131 (86%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 73%, i.e. 1275 atoms were assigned a chemical shift out of a possible 1753. 0 out of 20 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	455/589 (77%)	229/236 (97%)	119/242 (49%)	107/111 (96%)
Sidechain	724/1006 (72%)	436/649 (67%)	276/314 (88%)	12/43 (28%)
Aromatic	96/158 (61%)	49/76 (64%)	44/77 (57%)	3/5 (60%)
Overall	1275/1753 (73%)	714/961 (74%)	439/633 (69%)	122/159 (77%)

7.1.4 Statistically unusual chemical shifts (i)

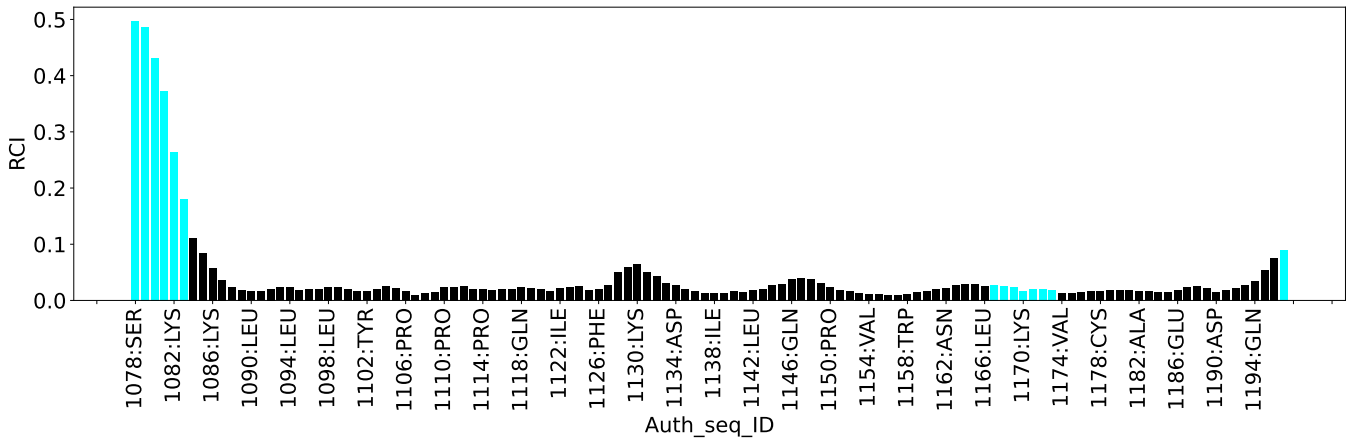
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	1103	ARG	NE	123.77	76.53 – 92.65	24.3
1	A	1091	ARG	NE	123.61	76.53 – 92.65	24.2
1	A	1112	ARG	NE	121.92	76.53 – 92.65	23.2
1	A	1151	TRP	NE1	110.67	118.53 – 139.98	-8.7
1	A	1157	VAL	HG21	-1.55	-0.58 – 2.19	-8.5
1	A	1165	TRP	HD1	4.97	5.46 – 8.81	-6.5
1	A	1115	VAL	HG21	-0.64	-0.58 – 2.19	-5.2
1	A	1141	LYS	HB2	0.54	0.58 – 2.97	-5.2
1	A	1121	GLY	N	127.93	91.59 – 127.52	5.1
1	A	1170	LYS	HA	2.14	2.15 – 6.37	-5.0

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
0.0
0.1
0.2
0.3
0.4
0.5
1078:SER
1082:LYS
1086:LYS
1090:LEU
1094:LEU
1098:LEU
1102:TYR
1106:PRO
1110:PRO
1114:PRO
1118:GLN
1122:ILE
1126:PHE
1130:LYS
1134:ASP
1138:ILE
1142:LEU
1146:GLN
1150:PRO
1154:VAL
1158:TRP
1162:ASN
1166:LEU
1170:LYS
1174:VAL
1178:CYS
1182:ALA
1186:GLU
1190:ASP
1194:GLN
Auth_seq_ID