Full wwPDB NMR Structure Validation Report (i)

Nov 7, 2023 – 09:33 AM EST

PDB ID	:	2RNY
Title	:	Complex Structures of CBP Bromodomain with H4 ack20 Peptide
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Deposited on	:	2008-02-03

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:

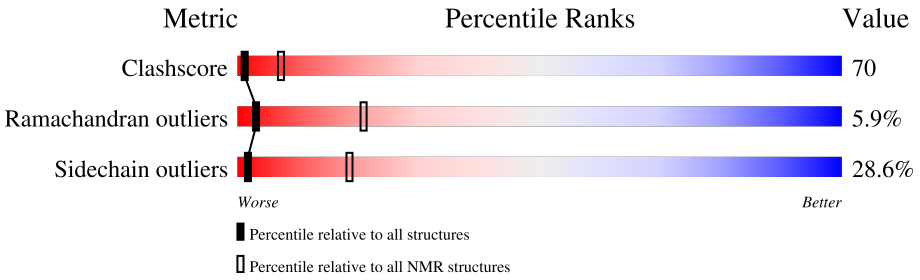
Cyrange	:	Kirchner and Güntert (2011)
NmrClust	:	Kelley et al. (1996)
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
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

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

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	121	10% 54% 17% 19%
2	B	15	100%

2 Ensemble composition and analysis

This entry contains 20 models. Model 13 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:1083-A:1112, A:1124-A:1168, A:1174-A:1196 (98)	0.39	13

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 2 single-model clusters were found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 2284 atoms, of which 1143 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 a protein called Histone H4.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	B	15	262	75	136	30	21	0

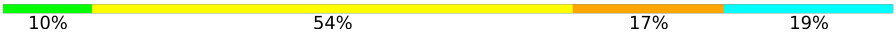
4 Residue-property plots (i)

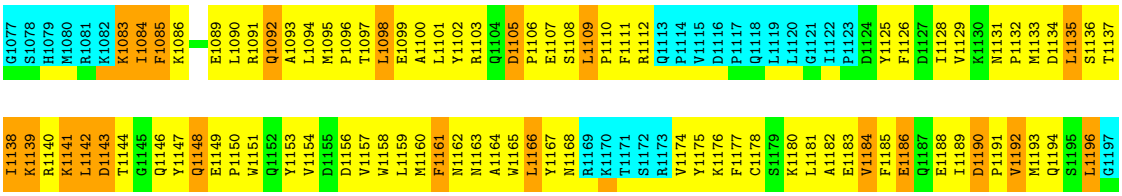
4.1 Average score per residue in the NMR ensemble

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: CREB-binding protein

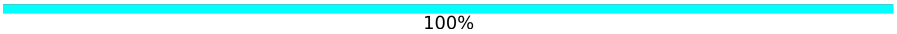
Chain A:

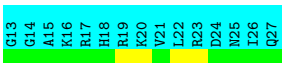




• Molecule 2: Histone H4

Chain B:





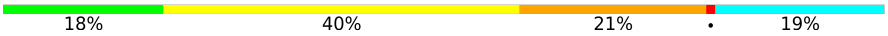
4.2 Scores per residue for each member of the ensemble

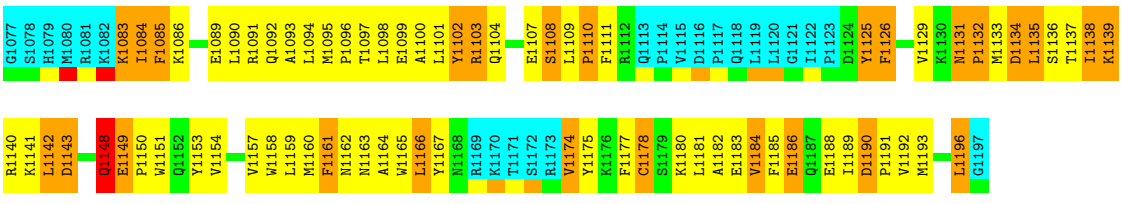
Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: CREB-binding protein

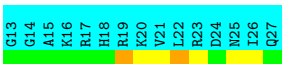
Chain A:





• Molecule 2: Histone H4

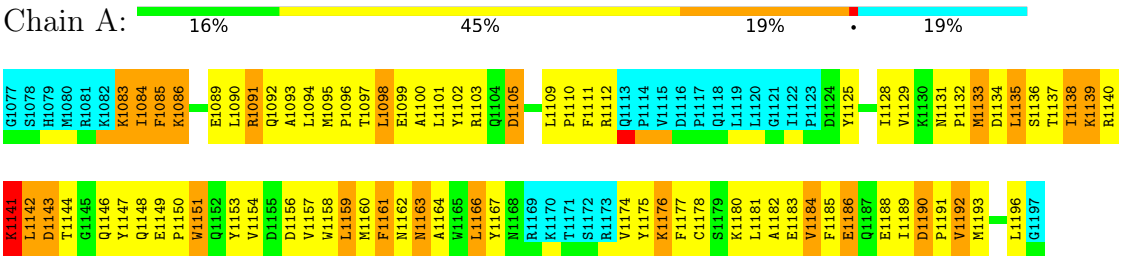
Chain B:



4.2.2 Score per residue for model 2

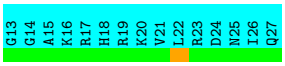
• Molecule 1: CREB-binding protein

Chain A:



• Molecule 2: Histone H4

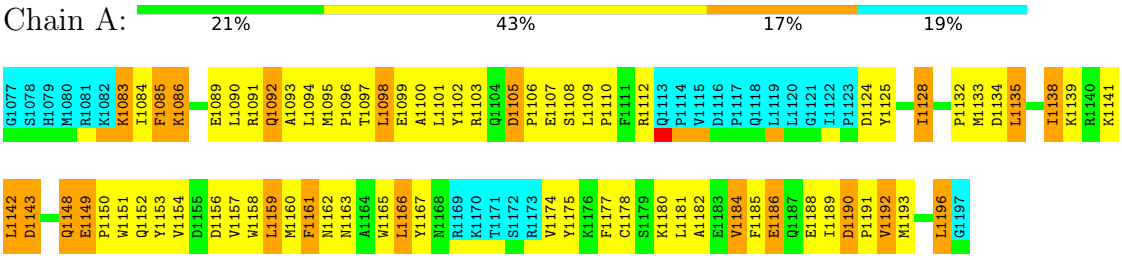
Chain B:



4.2.3 Score per residue for model 3

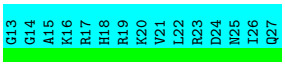
• Molecule 1: CREB-binding protein

Chain A:



• Molecule 2: Histone H4

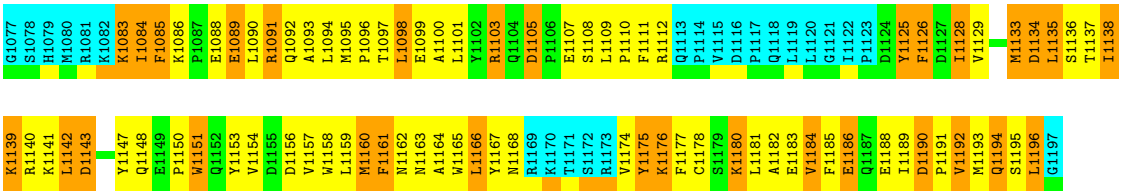
Chain B:



4.2.4 Score per residue for model 4

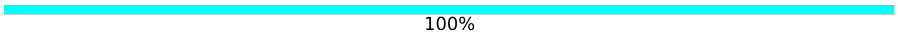
• Molecule 1: CREB-binding protein

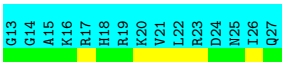
Chain A:



• Molecule 2: Histone H4

Chain B:

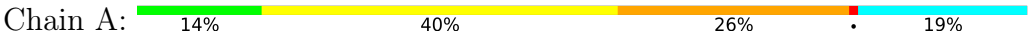


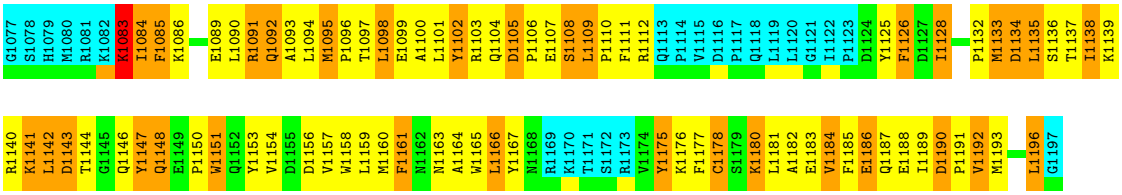


4.2.5 Score per residue for model 5

• Molecule 1: CREB-binding protein

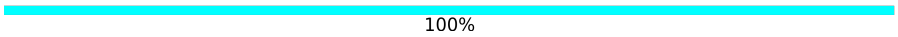
Chain A:

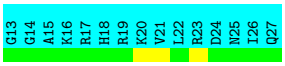




• Molecule 2: Histone H4

Chain B:

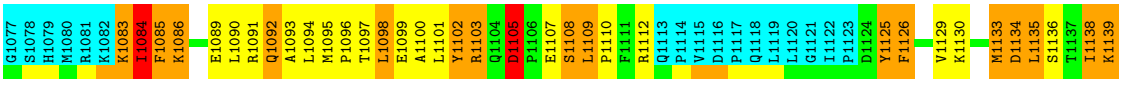




4.2.6 Score per residue for model 6

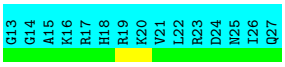
• Molecule 1: CREB-binding protein

Chain A:



• Molecule 2: Histone H4

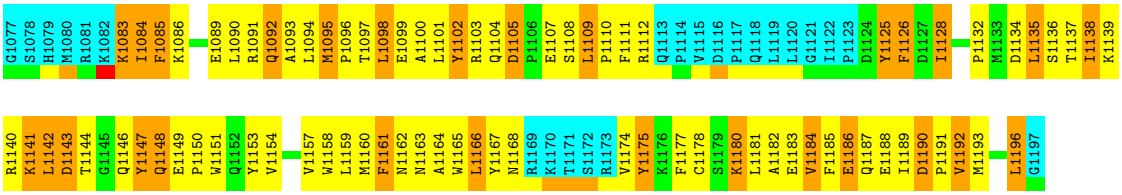
Chain B: 100%



4.2.7 Score per residue for model 7

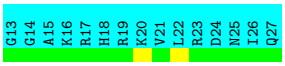
• Molecule 1: CREB-binding protein

Chain A: 14% 44% 23% 19%



• Molecule 2: Histone H4

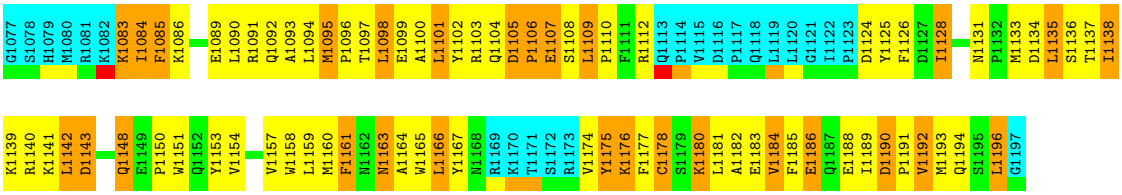
Chain B: 100%



4.2.8 Score per residue for model 8

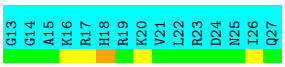
• Molecule 1: CREB-binding protein

Chain A: 17% 41% 23% 19%



• Molecule 2: Histone H4

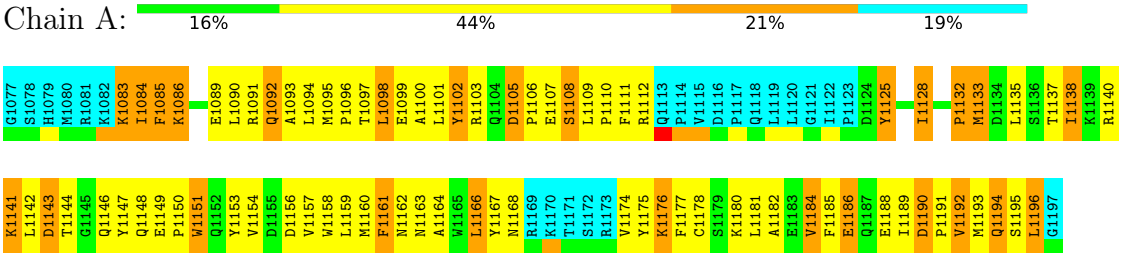
Chain B: 100%



4.2.9 Score per residue for model 9

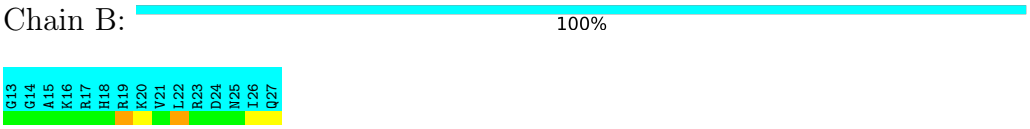
• Molecule 1: CREB-binding protein

Chain A:



• Molecule 2: Histone H4

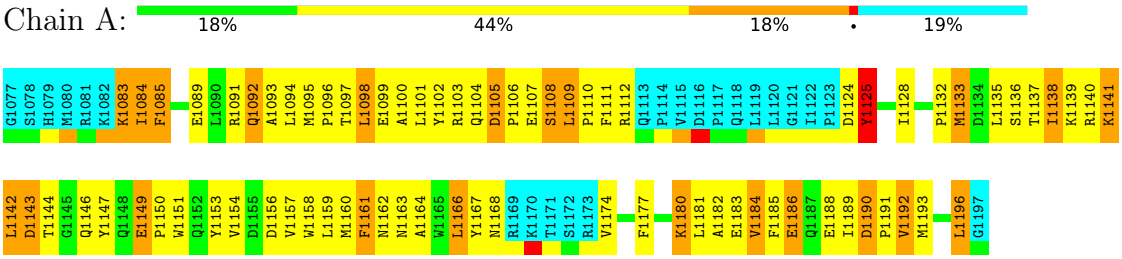
Chain B:



4.2.10 Score per residue for model 10

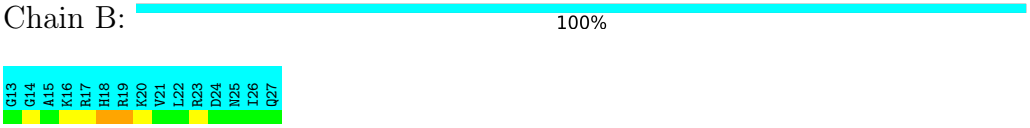
• Molecule 1: CREB-binding protein

Chain A:



• Molecule 2: Histone H4

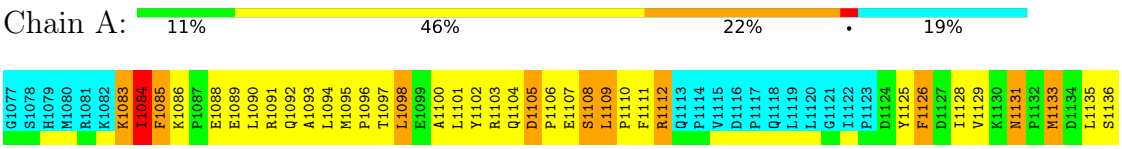
Chain B:

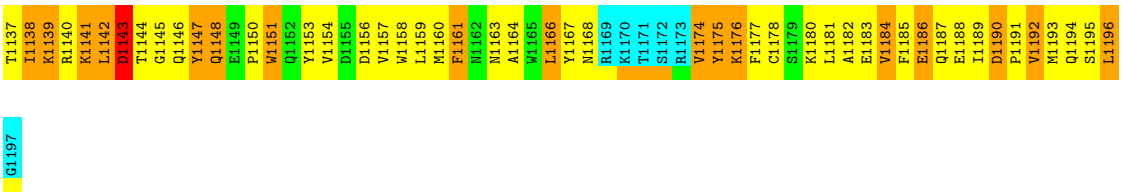


4.2.11 Score per residue for model 11

• Molecule 1: CREB-binding protein

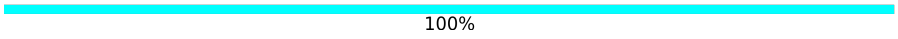
Chain A:

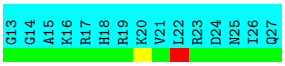




• Molecule 2: Histone H4

Chain B:

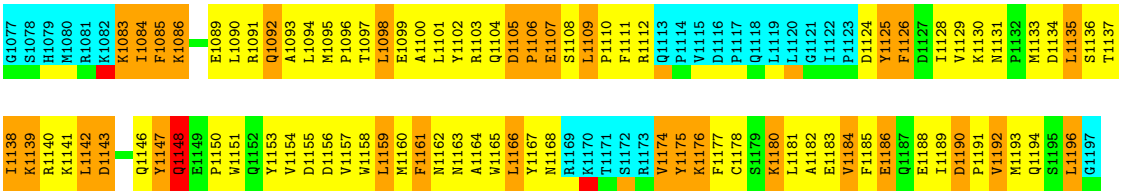




4.2.12 Score per residue for model 12

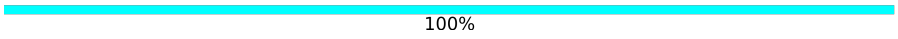
• Molecule 1: CREB-binding protein

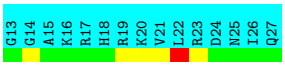
Chain A:



• Molecule 2: Histone H4

Chain B:

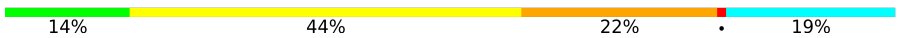


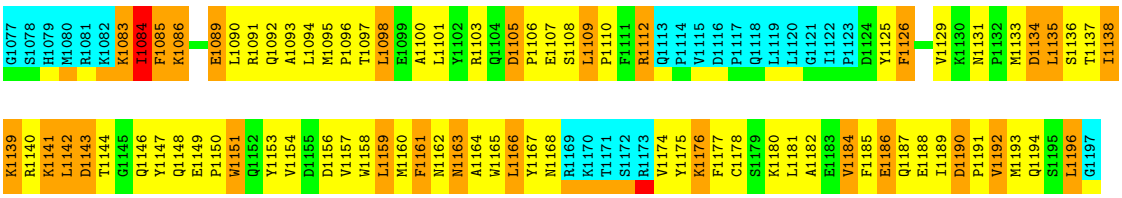


4.2.13 Score per residue for model 13 (medoid)

• Molecule 1: CREB-binding protein

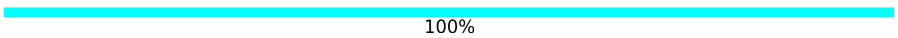
Chain A:

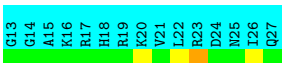




• Molecule 2: Histone H4

Chain B:

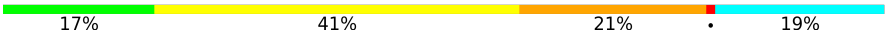


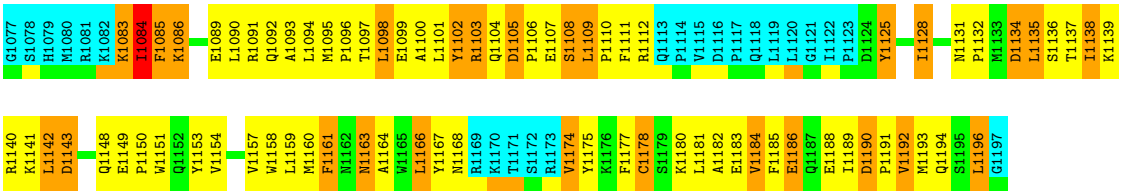


4.2.14 Score per residue for model 14

• Molecule 1: CREB-binding protein

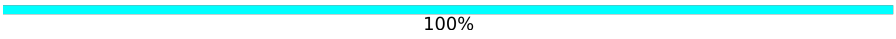
Chain A:

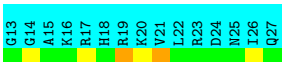




• Molecule 2: Histone H4

Chain B:

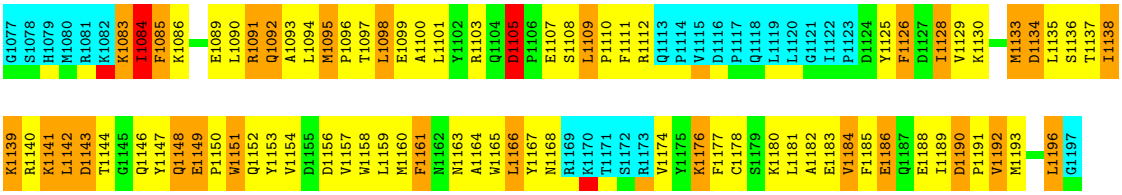




4.2.15 Score per residue for model 15

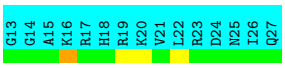
• Molecule 1: CREB-binding protein

Chain A:



• Molecule 2: Histone H4

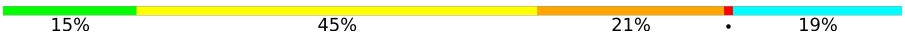
Chain B:

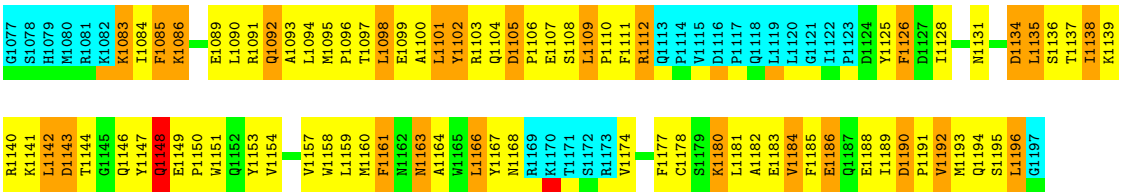


4.2.16 Score per residue for model 16

• Molecule 1: CREB-binding protein

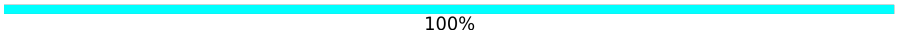
Chain A:

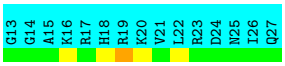




• Molecule 2: Histone H4

Chain B:

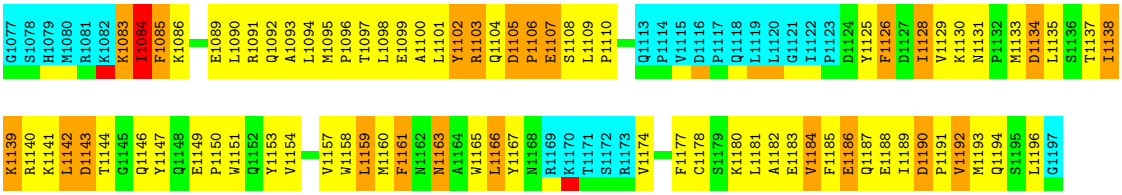




4.2.17 Score per residue for model 17

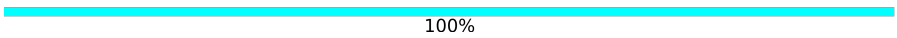
• Molecule 1: CREB-binding protein

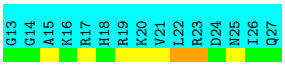
Chain A:



• Molecule 2: Histone H4

Chain B:

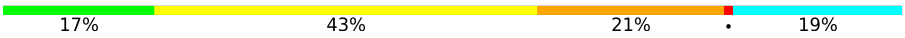


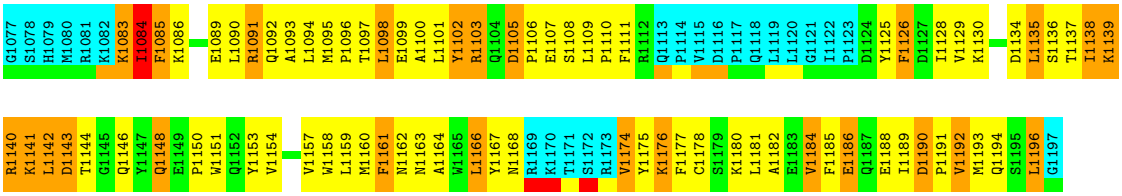


4.2.18 Score per residue for model 18

• Molecule 1: CREB-binding protein

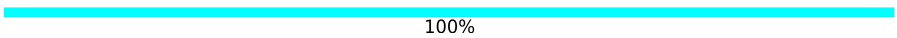
Chain A:

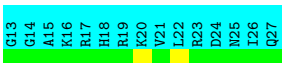




• Molecule 2: Histone H4

Chain B:

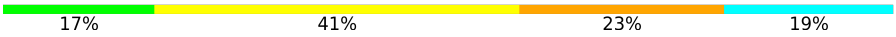


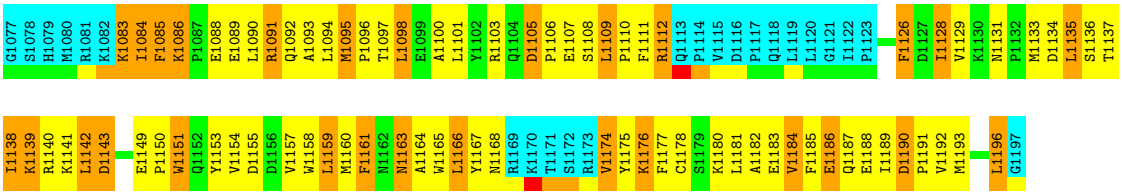


4.2.19 Score per residue for model 19

• Molecule 1: CREB-binding protein

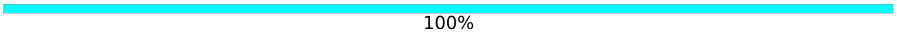
Chain A:

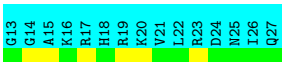




• Molecule 2: Histone H4

Chain B:

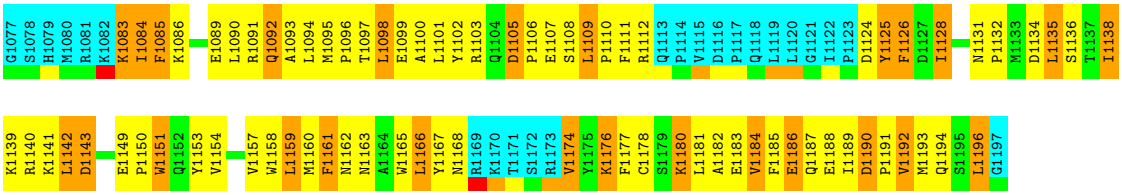




4.2.20 Score per residue for model 20

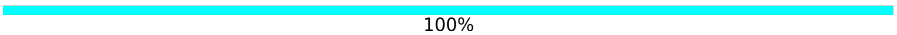
• Molecule 1: CREB-binding protein

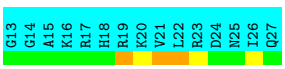
Chain A:



• Molecule 2: Histone H4

Chain B:





5 Refinement protocol and experimental data overview

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
CNS	structure solution	1.0
CNS	refinement	1.0

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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

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

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	836	814	814	116±12
2	B	0	0	0	0±0
All	All	16720	16280	16280	2323

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 70.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1138:ILE:HA	1:A:1141:LYS:HZ2	0.99	1.16	15	3
1:A:1154:VAL:HG22	1:A:1189:ILE:HD11	0.85	1.48	18	19
1:A:1083:LYS:HD3	1:A:1083:LYS:H	0.85	1.31	13	3
1:A:1091:ARG:HG2	1:A:1142:LEU:HD12	0.80	1.51	11	1
1:A:1185:PHE:CZ	1:A:1189:ILE:HD13	0.79	2.13	6	20
1:A:1101:LEU:HD21	1:A:1185:PHE:HB2	0.79	1.53	13	19
1:A:1138:ILE:HA	1:A:1141:LYS:NZ	0.78	1.94	19	15
1:A:1192:VAL:HG12	1:A:1193:MET:N	0.77	1.95	11	19
1:A:1135:LEU:HD23	1:A:1138:ILE:HD12	0.76	1.57	10	20
1:A:1093:ALA:HB1	1:A:1192:VAL:HG22	0.76	1.56	5	20
1:A:1098:LEU:HA	1:A:1101:LEU:HD12	0.75	1.56	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1163:ASN:O	1:A:1167:TYR:HB2	0.75	1.81	18	20
1:A:1142:LEU:HD23	1:A:1147:TYR:CE1	0.74	2.17	2	1
1:A:1084:ILE:HD12	1:A:1084:ILE:N	0.73	1.99	3	10
1:A:1133:MET:SD	1:A:1159:LEU:HD13	0.72	2.24	19	1
1:A:1085:PHE:CD1	1:A:1090:LEU:HD21	0.72	2.19	2	7
1:A:1084:ILE:N	1:A:1084:ILE:HD13	0.72	1.99	14	8
1:A:1085:PHE:CD1	1:A:1085:PHE:N	0.72	2.57	1	20
1:A:1133:MET:HG3	1:A:1159:LEU:HB3	0.72	1.60	19	1
1:A:1137:THR:HG22	1:A:1141:LYS:HD2	0.71	1.62	9	4
1:A:1083:LYS:N	1:A:1083:LYS:HD3	0.71	2.00	5	2
1:A:1137:THR:HG22	1:A:1141:LYS:HD3	0.71	1.63	18	3
1:A:1141:LYS:HB2	1:A:1141:LYS:NZ	0.70	2.01	7	4
1:A:1100:ALA:HB3	1:A:1188:GLU:OE2	0.70	1.86	19	3
1:A:1138:ILE:HA	1:A:1141:LYS:HZ3	0.70	1.44	18	2
1:A:1109:LEU:O	1:A:1109:LEU:HD22	0.70	1.86	6	7
1:A:1137:THR:HG22	1:A:1141:LYS:CD	0.69	2.18	18	3
1:A:1142:LEU:HD23	1:A:1147:TYR:CE2	0.69	2.23	4	6
1:A:1091:ARG:HD2	1:A:1143:ASP:HA	0.69	1.65	4	18
1:A:1106:PRO:HA	1:A:1109:LEU:HD21	0.68	1.64	19	5
1:A:1090:LEU:HD12	1:A:1147:TYR:CE1	0.68	2.23	6	6
1:A:1097:THR:CG2	1:A:1192:VAL:HG21	0.67	2.18	1	1
1:A:1108:SER:HA	1:A:1181:LEU:HD11	0.67	1.66	10	9
1:A:1109:LEU:N	1:A:1112:ARG:HD2	0.67	2.04	16	1
1:A:1163:ASN:O	1:A:1167:TYR:CB	0.67	2.43	7	19
1:A:1138:ILE:HA	1:A:1141:LYS:HZ1	0.67	1.49	14	7
1:A:1158:TRP:HA	1:A:1161:PHE:CD2	0.67	2.24	9	20
1:A:1099:GLU:O	1:A:1103:ARG:HG3	0.66	1.90	8	15
1:A:1093:ALA:CB	1:A:1192:VAL:HG22	0.66	2.21	15	20
1:A:1157:VAL:HG11	1:A:1185:PHE:CZ	0.66	2.25	17	20
1:A:1095:MET:HE1	1:A:1139:LYS:O	0.65	1.91	2	2
1:A:1100:ALA:HB3	1:A:1188:GLU:HG3	0.65	1.66	15	16
1:A:1101:LEU:HD11	1:A:1185:PHE:HB2	0.65	1.69	3	1
1:A:1094:LEU:HB2	1:A:1142:LEU:HD21	0.65	1.68	5	17
1:A:1135:LEU:HG	1:A:1160:MET:SD	0.65	2.32	2	5
1:A:1138:ILE:HD13	1:A:1157:VAL:HA	0.65	1.67	2	18
1:A:1184:VAL:O	1:A:1188:GLU:HG2	0.65	1.92	7	17
1:A:1166:LEU:HD13	1:A:1167:TYR:N	0.64	2.07	18	20
1:A:1142:LEU:HD12	1:A:1142:LEU:C	0.64	2.12	11	1
1:A:1109:LEU:H	1:A:1109:LEU:HD13	0.64	1.53	13	5
1:A:1083:LYS:HZ1	1:A:1150:PRO:HD2	0.64	1.51	13	2
1:A:1100:ALA:HA	1:A:1103:ARG:HD2	0.64	1.70	18	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1109:LEU:N	1:A:1112:ARG:HD3	0.64	2.07	20	4
1:A:1175:TYR:HA	1:A:1178:CYS:SG	0.64	2.33	7	7
1:A:1091:ARG:NE	1:A:1143:ASP:HA	0.64	2.07	18	2
1:A:1184:VAL:O	1:A:1188:GLU:HG3	0.64	1.92	17	3
1:A:1160:MET:HA	1:A:1163:ASN:HD21	0.63	1.53	5	6
1:A:1182:ALA:O	1:A:1186:GLU:HB3	0.63	1.94	10	20
1:A:1097:THR:HA	1:A:1188:GLU:HB3	0.62	1.71	17	20
1:A:1137:THR:O	1:A:1141:LYS:HB3	0.62	1.94	2	1
1:A:1175:TYR:CD1	1:A:1175:TYR:N	0.62	2.68	12	4
1:A:1091:ARG:CD	1:A:1143:ASP:HA	0.62	2.25	10	10
1:A:1094:LEU:HB3	1:A:1142:LEU:HD11	0.62	1.71	20	16
1:A:1091:ARG:HG3	1:A:1143:ASP:HA	0.62	1.70	6	1
1:A:1105:ASP:O	1:A:1110:PRO:HD3	0.62	1.94	15	3
1:A:1150:PRO:HG3	1:A:1196:LEU:HB3	0.62	1.71	4	18
1:A:1154:VAL:HG22	1:A:1189:ILE:CD1	0.61	2.25	18	19
1:A:1142:LEU:HD23	1:A:1147:TYR:HE2	0.61	1.55	9	5
1:A:1131:ASN:HB3	1:A:1159:LEU:HD11	0.61	1.73	1	2
1:A:1185:PHE:HZ	1:A:1189:ILE:HD13	0.61	1.53	20	19
1:A:1091:ARG:HG3	1:A:1142:LEU:HD22	0.61	1.71	4	10
1:A:1093:ALA:HB1	1:A:1192:VAL:CG2	0.61	2.26	5	19
1:A:1129:VAL:HG12	1:A:1166:LEU:HD11	0.61	1.72	2	3
1:A:1161:PHE:CD1	1:A:1181:LEU:HB2	0.61	2.31	17	3
1:A:1139:LYS:O	1:A:1143:ASP:HB2	0.61	1.94	13	9
1:A:1150:PRO:O	1:A:1154:VAL:HG23	0.61	1.95	14	20
1:A:1109:LEU:HD22	1:A:1109:LEU:N	0.61	2.10	19	1
1:A:1188:GLU:O	1:A:1191:PRO:HD2	0.60	1.95	14	6
1:A:1192:VAL:CG1	1:A:1193:MET:N	0.60	2.64	7	19
1:A:1109:LEU:HA	1:A:1112:ARG:CD	0.60	2.27	15	8
1:A:1107:GLU:OE1	1:A:1181:LEU:HD21	0.60	1.96	8	2
1:A:1180:LYS:O	1:A:1184:VAL:HG22	0.60	1.95	8	8
1:A:1177:PHE:O	1:A:1181:LEU:HG	0.60	1.96	6	20
1:A:1098:LEU:HD23	1:A:1153:TYR:OH	0.60	1.96	7	17
1:A:1157:VAL:O	1:A:1160:MET:HG3	0.60	1.96	4	1
1:A:1101:LEU:O	1:A:1108:SER:HB2	0.60	1.97	14	5
1:A:1092:GLN:O	1:A:1096:PRO:HG2	0.60	1.97	5	20
1:A:1083:LYS:HD3	1:A:1083:LYS:N	0.60	2.10	13	1
1:A:1128:ILE:HG23	1:A:1166:LEU:HD22	0.59	1.73	19	7
1:A:1176:LYS:HG3	1:A:1177:PHE:N	0.59	2.12	9	11
1:A:1141:LYS:HB2	1:A:1141:LYS:HZ3	0.59	1.55	7	1
1:A:1141:LYS:HB3	1:A:1146:GLN:HB2	0.59	1.75	13	2
1:A:1107:GLU:CD	1:A:1108:SER:N	0.59	2.55	8	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1109:LEU:N	1:A:1110:PRO:HD2	0.59	2.13	5	14
1:A:1161:PHE:HA	1:A:1178:CYS:SG	0.59	2.37	14	3
1:A:1084:ILE:N	1:A:1084:ILE:CD1	0.58	2.66	3	7
1:A:1094:LEU:HD23	1:A:1192:VAL:HG11	0.58	1.74	1	1
1:A:1083:LYS:C	1:A:1084:ILE:HD13	0.58	2.17	16	3
1:A:1133:MET:O	1:A:1133:MET:HE3	0.58	1.98	3	1
1:A:1129:VAL:HG11	1:A:1163:ASN:HB2	0.58	1.75	12	5
1:A:1180:LYS:O	1:A:1183:GLU:HB3	0.58	1.97	10	14
1:A:1189:ILE:HG13	1:A:1193:MET:HG2	0.58	1.76	6	18
1:A:1168:ASN:HB3	1:A:1175:TYR:CZ	0.58	2.33	12	4
1:A:1091:ARG:HA	1:A:1142:LEU:HD11	0.58	1.74	13	1
1:A:1097:THR:HG21	1:A:1192:VAL:HG21	0.58	1.75	1	1
1:A:1109:LEU:HD23	1:A:1112:ARG:NH1	0.58	2.13	8	1
1:A:1160:MET:HA	1:A:1163:ASN:ND2	0.58	2.14	9	10
1:A:1101:LEU:O	1:A:1108:SER:HB3	0.58	1.99	5	7
1:A:1107:GLU:OE2	1:A:1181:LEU:CD2	0.57	2.52	12	1
1:A:1098:LEU:HD21	1:A:1135:LEU:HD22	0.57	1.77	9	1
1:A:1109:LEU:N	1:A:1109:LEU:HD22	0.57	2.13	12	4
1:A:1129:VAL:HG11	1:A:1163:ASN:CB	0.57	2.28	2	3
1:A:1109:LEU:HD13	1:A:1110:PRO:N	0.57	2.15	7	7
1:A:1147:TYR:HD1	1:A:1148:GLN:N	0.57	1.98	7	2
1:A:1086:LYS:H	1:A:1089:GLU:HG3	0.57	1.60	16	17
1:A:1154:VAL:CG2	1:A:1189:ILE:HD11	0.57	2.27	18	14
1:A:1104:GLN:C	1:A:1107:GLU:OE2	0.56	2.44	8	2
1:A:1129:VAL:O	1:A:1129:VAL:HG23	0.56	2.00	2	1
1:A:1093:ALA:HB3	1:A:1196:LEU:HD11	0.56	1.76	2	20
1:A:1083:LYS:H	1:A:1083:LYS:CD	0.56	2.11	5	2
1:A:1181:LEU:HD23	1:A:1181:LEU:N	0.56	2.14	17	3
1:A:1189:ILE:HD12	1:A:1192:VAL:HG11	0.56	1.76	18	17
1:A:1100:ALA:HA	1:A:1103:ARG:HD3	0.56	1.76	3	7
1:A:1166:LEU:HD13	1:A:1166:LEU:C	0.56	2.22	16	14
1:A:1109:LEU:HA	1:A:1112:ARG:NE	0.56	2.16	19	2
1:A:1108:SER:C	1:A:1110:PRO:HD2	0.55	2.22	6	5
1:A:1180:LYS:HD2	1:A:1184:VAL:HG13	0.55	1.76	12	5
1:A:1086:LYS:H	1:A:1089:GLU:HG2	0.55	1.62	4	2
1:A:1142:LEU:HA	1:A:1147:TYR:CE2	0.55	2.37	5	7
1:A:1107:GLU:OE2	1:A:1181:LEU:HD21	0.55	2.02	12	1
1:A:1128:ILE:HG21	1:A:1167:TYR:HA	0.55	1.79	7	14
1:A:1083:LYS:HE3	1:A:1084:ILE:N	0.55	2.16	8	3
1:A:1112:ARG:HA	1:A:1135:LEU:HB2	0.55	1.78	10	2
1:A:1107:GLU:OE1	1:A:1181:LEU:CD2	0.55	2.55	8	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1095:MET:HB3	1:A:1096:PRO:HD3	0.55	1.79	11	19
1:A:1166:LEU:C	1:A:1166:LEU:HD13	0.55	2.23	9	6
1:A:1175:TYR:H	1:A:1175:TYR:HD1	0.55	1.42	12	3
1:A:1091:ARG:HA	1:A:1142:LEU:HD13	0.55	1.79	11	1
1:A:1094:LEU:HD13	1:A:1153:TYR:CG	0.55	2.37	11	15
1:A:1138:ILE:O	1:A:1141:LYS:NZ	0.55	2.40	13	1
1:A:1091:ARG:HD2	1:A:1143:ASP:CA	0.54	2.33	2	7
1:A:1124:ASP:O	1:A:1125:TYR:O	0.54	2.26	10	1
1:A:1107:GLU:OE2	1:A:1108:SER:N	0.54	2.40	17	2
1:A:1164:ALA:HB3	1:A:1178:CYS:SG	0.54	2.43	9	3
1:A:1083:LYS:HG2	1:A:1084:ILE:H	0.54	1.62	13	2
1:A:1135:LEU:O	1:A:1139:LYS:HB3	0.54	2.03	19	2
1:A:1083:LYS:HD3	1:A:1085:PHE:CE1	0.54	2.38	8	1
1:A:1109:LEU:N	1:A:1110:PRO:CD	0.54	2.71	15	9
1:A:1185:PHE:CE2	1:A:1189:ILE:HB	0.54	2.38	18	7
1:A:1163:ASN:OD1	1:A:1164:ALA:N	0.53	2.40	4	3
1:A:1175:TYR:N	1:A:1175:TYR:HD1	0.53	2.01	7	1
1:A:1083:LYS:HD3	1:A:1085:PHE:CD1	0.53	2.37	8	1
1:A:1109:LEU:HA	1:A:1112:ARG:HE	0.53	1.63	19	3
1:A:1111:PHE:O	1:A:1112:ARG:C	0.53	2.47	10	4
1:A:1174:VAL:O	1:A:1177:PHE:N	0.53	2.40	1	3
1:A:1111:PHE:HB3	1:A:1135:LEU:H	0.53	1.63	12	7
1:A:1109:LEU:HA	1:A:1112:ARG:HD3	0.53	1.79	9	8
1:A:1141:LYS:NZ	1:A:1147:TYR:OH	0.53	2.36	15	3
1:A:1151:TRP:CD1	1:A:1151:TRP:N	0.53	2.77	2	4
1:A:1189:ILE:HA	1:A:1192:VAL:HB	0.53	1.80	4	17
1:A:1135:LEU:HD21	1:A:1160:MET:CE	0.53	2.34	19	8
1:A:1089:GLU:O	1:A:1092:GLN:HB2	0.53	2.04	1	2
1:A:1105:ASP:O	1:A:1107:GLU:N	0.53	2.42	17	17
1:A:1085:PHE:HD1	1:A:1085:PHE:H	0.52	1.48	3	9
1:A:1126:PHE:CD1	1:A:1126:PHE:N	0.52	2.74	13	14
1:A:1144:THR:OG1	1:A:1146:GLN:HG3	0.52	2.04	11	10
1:A:1083:LYS:C	1:A:1084:ILE:HD12	0.52	2.25	3	3
1:A:1142:LEU:HD12	1:A:1153:TYR:CE1	0.52	2.40	15	7
1:A:1109:LEU:HD13	1:A:1109:LEU:C	0.52	2.23	14	7
1:A:1095:MET:HE1	1:A:1142:LEU:HG	0.52	1.80	11	1
1:A:1083:LYS:NZ	1:A:1151:TRP:NE1	0.52	2.58	19	2
1:A:1108:SER:O	1:A:1109:LEU:C	0.52	2.47	20	4
1:A:1100:ALA:HA	1:A:1103:ARG:CD	0.52	2.34	7	10
1:A:1158:TRP:HA	1:A:1161:PHE:CE2	0.52	2.40	1	15
1:A:1128:ILE:HG23	1:A:1166:LEU:CD2	0.52	2.35	19	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1083:LYS:HG3	1:A:1085:PHE:CE1	0.52	2.40	3	13
1:A:1100:ALA:HB3	1:A:1188:GLU:CD	0.52	2.25	19	3
1:A:1091:ARG:HG2	1:A:1142:LEU:CD1	0.52	2.31	11	1
1:A:1185:PHE:HA	1:A:1188:GLU:CD	0.52	2.25	17	3
1:A:1107:GLU:OE1	1:A:1108:SER:N	0.52	2.42	12	1
1:A:1168:ASN:HB2	1:A:1175:TYR:CZ	0.52	2.40	18	1
1:A:1101:LEU:CD2	1:A:1188:GLU:OE2	0.52	2.58	6	3
1:A:1090:LEU:HD12	1:A:1147:TYR:CD1	0.51	2.40	4	3
1:A:1175:TYR:HD1	1:A:1175:TYR:H	0.51	1.46	7	1
1:A:1174:VAL:O	1:A:1178:CYS:SG	0.51	2.68	19	4
1:A:1138:ILE:HD11	1:A:1160:MET:HB2	0.51	1.81	19	7
1:A:1109:LEU:HD22	1:A:1109:LEU:C	0.51	2.26	6	7
1:A:1091:ARG:HA	1:A:1142:LEU:CD1	0.51	2.36	11	2
1:A:1141:LYS:O	1:A:1145:GLY:N	0.51	2.42	11	1
1:A:1137:THR:O	1:A:1141:LYS:HG3	0.51	2.05	7	6
1:A:1163:ASN:O	1:A:1167:TYR:HB3	0.51	2.06	11	5
1:A:1100:ALA:CB	1:A:1188:GLU:HG3	0.51	2.35	4	16
1:A:1134:ASP:O	1:A:1138:ILE:HG13	0.51	2.06	6	13
1:A:1109:LEU:N	1:A:1109:LEU:HD13	0.51	2.20	12	3
1:A:1091:ARG:HD3	1:A:1142:LEU:O	0.51	2.06	7	7
1:A:1094:LEU:CB	1:A:1142:LEU:HD21	0.51	2.35	7	16
1:A:1094:LEU:O	1:A:1097:THR:N	0.51	2.44	11	17
1:A:1133:MET:SD	1:A:1133:MET:N	0.51	2.83	19	1
1:A:1135:LEU:HA	1:A:1138:ILE:HB	0.51	1.83	2	10
1:A:1111:PHE:CE2	1:A:1181:LEU:HD12	0.51	2.41	20	6
1:A:1140:ARG:O	1:A:1141:LYS:C	0.51	2.50	5	13
1:A:1109:LEU:HD13	1:A:1109:LEU:N	0.51	2.20	13	2
1:A:1084:ILE:HG23	1:A:1148:GLN:O	0.50	2.06	3	2
1:A:1180:LYS:HE3	1:A:1184:VAL:HG22	0.50	1.83	6	8
1:A:1105:ASP:O	1:A:1109:LEU:HD23	0.50	2.06	17	3
1:A:1165:TRP:CD1	1:A:1178:CYS:SG	0.50	3.05	19	10
1:A:1149:GLU:HB3	1:A:1151:TRP:CD1	0.50	2.41	20	3
1:A:1095:MET:HE3	1:A:1142:LEU:HB3	0.50	1.82	12	1
1:A:1100:ALA:HB2	1:A:1188:GLU:CD	0.50	2.27	14	1
1:A:1108:SER:C	1:A:1112:ARG:HD2	0.50	2.26	16	1
1:A:1138:ILE:CA	1:A:1141:LYS:HZ2	0.50	2.06	15	1
1:A:1109:LEU:HD22	1:A:1110:PRO:HD2	0.50	1.83	12	3
1:A:1083:LYS:N	1:A:1083:LYS:CD	0.50	2.72	19	2
1:A:1159:LEU:HD12	1:A:1159:LEU:O	0.50	2.07	20	1
1:A:1091:ARG:HA	1:A:1142:LEU:HD22	0.50	1.82	9	2
1:A:1085:PHE:N	1:A:1085:PHE:HD1	0.50	2.03	2	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1098:LEU:HD11	1:A:1135:LEU:HD22	0.49	1.84	17	2
1:A:1133:MET:HG2	1:A:1156:ASP:O	0.49	2.06	10	10
1:A:1098:LEU:CD2	1:A:1139:LYS:HB2	0.49	2.37	1	2
1:A:1107:GLU:CG	1:A:1181:LEU:HD21	0.49	2.37	8	3
1:A:1144:THR:OG1	1:A:1146:GLN:HG2	0.49	2.07	9	1
1:A:1099:GLU:HA	1:A:1102:TYR:HB2	0.49	1.84	17	14
1:A:1150:PRO:HB3	1:A:1196:LEU:CD1	0.49	2.36	1	20
1:A:1159:LEU:O	1:A:1162:ASN:HB3	0.49	2.08	20	2
1:A:1134:ASP:O	1:A:1136:SER:N	0.49	2.45	7	14
1:A:1104:GLN:C	1:A:1107:GLU:OE1	0.49	2.51	12	1
1:A:1104:GLN:HB2	1:A:1107:GLU:CD	0.49	2.27	8	3
1:A:1142:LEU:C	1:A:1144:THR:N	0.49	2.66	11	1
1:A:1099:GLU:O	1:A:1103:ARG:HB3	0.49	2.08	17	1
1:A:1128:ILE:O	1:A:1166:LEU:HD21	0.49	2.08	18	2
1:A:1109:LEU:HD22	1:A:1110:PRO:HD3	0.49	1.84	16	1
1:A:1090:LEU:HD23	1:A:1090:LEU:N	0.49	2.22	19	17
1:A:1142:LEU:HA	1:A:1147:TYR:HE2	0.49	1.66	7	3
1:A:1135:LEU:HG	1:A:1160:MET:HE2	0.49	1.85	13	1
1:A:1190:ASP:O	1:A:1194:GLN:HG2	0.48	2.08	9	2
1:A:1140:ARG:O	1:A:1143:ASP:N	0.48	2.46	15	5
1:A:1142:LEU:C	1:A:1144:THR:H	0.48	2.12	11	1
1:A:1109:LEU:H	1:A:1109:LEU:HD22	0.48	1.67	12	4
1:A:1180:LYS:NZ	1:A:1184:VAL:HG13	0.48	2.22	16	4
1:A:1095:MET:HA	1:A:1142:LEU:HD21	0.48	1.84	11	1
1:A:1103:ARG:C	1:A:1105:ASP:H	0.48	2.11	2	9
1:A:1140:ARG:C	1:A:1142:LEU:N	0.48	2.67	6	3
1:A:1107:GLU:HA	1:A:1177:PHE:HB3	0.48	1.85	18	13
1:A:1180:LYS:O	1:A:1183:GLU:N	0.48	2.47	19	8
1:A:1157:VAL:O	1:A:1160:MET:HB3	0.48	2.09	18	13
1:A:1083:LYS:NZ	1:A:1196:LEU:O	0.48	2.43	5	1
1:A:1094:LEU:HD12	1:A:1142:LEU:HD21	0.48	1.84	9	3
1:A:1094:LEU:HD12	1:A:1147:TYR:OH	0.48	2.09	11	1
1:A:1090:LEU:O	1:A:1093:ALA:N	0.48	2.47	15	7
1:A:1100:ALA:HB3	1:A:1188:GLU:HG2	0.48	1.86	6	1
1:A:1095:MET:HB2	1:A:1142:LEU:HD11	0.48	1.85	11	1
1:A:1094:LEU:O	1:A:1097:THR:OG1	0.47	2.26	11	4
1:A:1089:GLU:O	1:A:1092:GLN:HB3	0.47	2.09	6	11
1:A:1160:MET:HA	1:A:1163:ASN:OD1	0.47	2.08	14	5
1:A:1083:LYS:HG3	1:A:1085:PHE:CZ	0.47	2.44	17	6
1:A:1138:ILE:O	1:A:1142:LEU:HB2	0.47	2.09	6	3
1:A:1108:SER:HB3	1:A:1112:ARG:HD2	0.47	1.86	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1176:LYS:HG2	1:A:1177:PHE:N	0.47	2.23	15	1
1:A:1138:ILE:HA	1:A:1141:LYS:CE	0.47	2.39	16	2
1:A:1101:LEU:CD2	1:A:1185:PHE:HB2	0.47	2.39	18	13
1:A:1104:GLN:O	1:A:1107:GLU:HG3	0.47	2.10	12	1
1:A:1098:LEU:HD23	1:A:1153:TYR:CE1	0.47	2.45	19	7
1:A:1125:TYR:OH	1:A:1132:PRO:HB3	0.47	2.10	10	2
1:A:1105:ASP:HB2	1:A:1106:PRO:CD	0.47	2.39	17	8
1:A:1091:ARG:NE	1:A:1095:MET:SD	0.47	2.88	6	1
1:A:1095:MET:HE3	1:A:1142:LEU:HD13	0.47	1.87	7	1
1:A:1137:THR:O	1:A:1141:LYS:HD3	0.47	2.09	18	1
1:A:1165:TRP:NE1	1:A:1178:CYS:SG	0.47	2.88	7	3
1:A:1083:LYS:HZ1	1:A:1150:PRO:CD	0.47	2.21	5	1
1:A:1105:ASP:CA	1:A:1109:LEU:HB3	0.47	2.39	14	5
1:A:1109:LEU:HD13	1:A:1110:PRO:CD	0.47	2.40	11	3
1:A:1133:MET:SD	1:A:1156:ASP:HB3	0.47	2.49	6	2
1:A:1129:VAL:O	1:A:1130:LYS:HB2	0.47	2.10	6	4
1:A:1109:LEU:HA	1:A:1112:ARG:HH11	0.47	1.67	8	1
1:A:1161:PHE:HB3	1:A:1178:CYS:SG	0.47	2.50	18	3
1:A:1124:ASP:HB3	1:A:1128:ILE:HD12	0.47	1.87	10	1
1:A:1106:PRO:CA	1:A:1109:LEU:HD21	0.47	2.37	19	3
1:A:1091:ARG:HG3	1:A:1095:MET:HB2	0.47	1.87	13	1
1:A:1109:LEU:C	1:A:1111:PHE:H	0.47	2.14	16	2
1:A:1101:LEU:HD23	1:A:1135:LEU:HD21	0.47	1.85	3	1
1:A:1083:LYS:CE	1:A:1084:ILE:H	0.47	2.23	5	1
1:A:1131:ASN:HB3	1:A:1159:LEU:HD21	0.47	1.87	1	1
1:A:1139:LYS:HE3	1:A:1140:ARG:N	0.47	2.25	17	2
1:A:1192:VAL:O	1:A:1196:LEU:N	0.47	2.48	9	19
1:A:1095:MET:O	1:A:1099:GLU:HG3	0.47	2.09	17	6
1:A:1097:THR:O	1:A:1101:LEU:HG	0.47	2.10	11	7
1:A:1105:ASP:O	1:A:1109:LEU:N	0.47	2.48	15	7
1:A:1104:GLN:HE21	1:A:1180:LYS:HG2	0.46	1.71	1	1
1:A:1108:SER:O	1:A:1135:LEU:HD12	0.46	2.11	6	3
1:A:1136:SER:O	1:A:1140:ARG:HB2	0.46	2.11	10	1
1:A:1135:LEU:CG	1:A:1160:MET:HE2	0.46	2.40	13	1
1:A:1134:ASP:O	1:A:1137:THR:N	0.46	2.48	19	1
1:A:1111:PHE:HB2	1:A:1135:LEU:HG	0.46	1.87	19	3
1:A:1129:VAL:HG13	1:A:1167:TYR:HD2	0.46	1.71	13	2
1:A:1105:ASP:C	1:A:1109:LEU:HD12	0.46	2.30	2	1
1:A:1105:ASP:CB	1:A:1106:PRO:CD	0.46	2.92	8	8
1:A:1084:ILE:HD13	1:A:1084:ILE:N	0.46	2.25	4	2
1:A:1086:LYS:HB2	1:A:1089:GLU:OE1	0.46	2.10	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1147:TYR:C	1:A:1147:TYR:CD1	0.46	2.89	5	3
1:A:1108:SER:HB3	1:A:1112:ARG:HG3	0.46	1.86	12	2
1:A:1184:VAL:HB	1:A:1188:GLU:OE2	0.46	2.10	19	2
1:A:1108:SER:O	1:A:1111:PHE:N	0.46	2.46	12	2
1:A:1105:ASP:O	1:A:1109:LEU:CD2	0.46	2.63	20	4
1:A:1131:ASN:HB3	1:A:1159:LEU:CD1	0.46	2.39	1	2
1:A:1138:ILE:CD1	1:A:1157:VAL:HA	0.46	2.40	3	1
1:A:1091:ARG:O	1:A:1091:ARG:HD3	0.46	2.11	6	1
1:A:1095:MET:CE	1:A:1142:LEU:HB3	0.46	2.41	12	3
1:A:1166:LEU:HD22	1:A:1166:LEU:O	0.46	2.10	12	2
1:A:1109:LEU:CD2	1:A:1110:PRO:HD3	0.46	2.40	16	1
1:A:1108:SER:O	1:A:1112:ARG:HG3	0.46	2.11	8	1
1:A:1180:LYS:HD2	1:A:1184:VAL:HG22	0.46	1.87	7	4
1:A:1149:GLU:HA	1:A:1149:GLU:OE1	0.46	2.09	10	2
1:A:1147:TYR:CZ	1:A:1153:TYR:HA	0.46	2.45	17	3
1:A:1134:ASP:C	1:A:1136:SER:N	0.46	2.69	15	9
1:A:1174:VAL:O	1:A:1175:TYR:C	0.46	2.54	19	3
1:A:1138:ILE:O	1:A:1141:LYS:HE2	0.46	2.11	2	1
1:A:1184:VAL:O	1:A:1188:GLU:N	0.46	2.49	19	4
1:A:1138:ILE:HA	1:A:1141:LYS:HD3	0.46	1.87	9	2
1:A:1105:ASP:O	1:A:1109:LEU:HD22	0.46	2.11	20	1
1:A:1147:TYR:CD2	1:A:1148:GLN:N	0.45	2.84	2	1
1:A:1140:ARG:O	1:A:1144:THR:HG23	0.45	2.11	13	1
1:A:1098:LEU:CD2	1:A:1139:LYS:CB	0.45	2.94	1	2
1:A:1180:LYS:CE	1:A:1184:VAL:HG13	0.45	2.41	3	4
1:A:1100:ALA:HB3	1:A:1188:GLU:CG	0.45	2.42	6	1
1:A:1147:TYR:CD1	1:A:1148:GLN:N	0.45	2.82	7	2
1:A:1091:ARG:CG	1:A:1143:ASP:HA	0.45	2.41	11	1
1:A:1083:LYS:CG	1:A:1085:PHE:CZ	0.45	2.99	7	5
1:A:1158:TRP:O	1:A:1162:ASN:HB2	0.45	2.12	3	6
1:A:1160:MET:SD	1:A:1161:PHE:N	0.45	2.90	15	1
1:A:1084:ILE:HG13	1:A:1149:GLU:HG3	0.45	1.88	2	1
1:A:1111:PHE:CD2	1:A:1181:LEU:CD1	0.45	2.99	15	1
1:A:1083:LYS:NZ	1:A:1151:TRP:HE1	0.45	2.10	19	1
1:A:1163:ASN:ND2	1:A:1164:ALA:N	0.45	2.65	2	2
1:A:1107:GLU:HB3	1:A:1177:PHE:O	0.45	2.12	5	4
1:A:1085:PHE:HB3	1:A:1089:GLU:HG3	0.45	1.88	8	5
1:A:1112:ARG:CA	1:A:1135:LEU:HB2	0.45	2.42	10	1
1:A:1131:ASN:HB3	1:A:1159:LEU:HD13	0.45	1.89	17	2
1:A:1109:LEU:O	1:A:1111:PHE:N	0.45	2.50	1	2
1:A:1094:LEU:HD13	1:A:1153:TYR:CD2	0.45	2.46	11	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1111:PHE:CZ	1:A:1178:CYS:SG	0.45	3.10	14	1
1:A:1160:MET:HE3	1:A:1161:PHE:CE1	0.45	2.47	3	1
1:A:1085:PHE:CZ	1:A:1196:LEU:HA	0.45	2.47	8	1
1:A:1137:THR:O	1:A:1141:LYS:HD2	0.45	2.11	15	1
1:A:1090:LEU:HB2	1:A:1147:TYR:OH	0.45	2.12	2	1
1:A:1125:TYR:N	1:A:1167:TYR:OH	0.44	2.51	4	2
1:A:1105:ASP:C	1:A:1109:LEU:HD23	0.44	2.32	9	3
1:A:1184:VAL:O	1:A:1187:GLN:HB3	0.44	2.12	7	4
1:A:1180:LYS:HD3	1:A:1183:GLU:HB3	0.44	1.89	7	1
1:A:1098:LEU:HD13	1:A:1102:TYR:CD1	0.44	2.47	9	1
1:A:1105:ASP:O	1:A:1107:GLU:OE1	0.44	2.35	12	1
1:A:1109:LEU:HA	1:A:1112:ARG:HG3	0.44	1.88	14	1
1:A:1093:ALA:O	1:A:1097:THR:HG23	0.44	2.12	19	9
1:A:1125:TYR:CZ	1:A:1132:PRO:HB3	0.44	2.47	3	3
1:A:1083:LYS:HG2	1:A:1196:LEU:O	0.44	2.12	5	1
1:A:1098:LEU:CD2	1:A:1135:LEU:HD22	0.44	2.42	9	1
1:A:1168:ASN:ND2	1:A:1174:VAL:HG11	0.44	2.26	20	1
1:A:1085:PHE:CE1	1:A:1196:LEU:O	0.44	2.70	5	1
1:A:1083:LYS:CG	1:A:1085:PHE:CE1	0.44	3.00	13	2
1:A:1164:ALA:CB	1:A:1178:CYS:SG	0.44	3.06	14	1
1:A:1109:LEU:N	1:A:1112:ARG:CD	0.44	2.79	16	1
1:A:1128:ILE:HG22	1:A:1129:VAL:N	0.44	2.27	19	2
1:A:1101:LEU:HB3	1:A:1108:SER:OG	0.44	2.13	15	2
1:A:1083:LYS:N	1:A:1084:ILE:HD12	0.44	2.27	19	1
1:A:1109:LEU:C	1:A:1111:PHE:N	0.44	2.71	1	2
1:A:1192:VAL:HG13	1:A:1196:LEU:HD12	0.44	1.89	17	6
1:A:1138:ILE:HG23	1:A:1141:LYS:NZ	0.44	2.27	6	1
1:A:1184:VAL:HG12	1:A:1187:GLN:NE2	0.44	2.27	11	1
1:A:1098:LEU:HD12	1:A:1102:TYR:CE1	0.44	2.47	6	4
1:A:1180:LYS:HE2	1:A:1184:VAL:HG13	0.44	1.89	3	1
1:A:1154:VAL:HG12	1:A:1158:TRP:CD1	0.44	2.48	13	2
1:A:1086:LYS:N	1:A:1086:LYS:HD3	0.44	2.28	3	2
1:A:1184:VAL:C	1:A:1188:GLU:HG3	0.44	2.33	19	3
1:A:1125:TYR:CD2	1:A:1126:PHE:CE1	0.44	3.05	7	1
1:A:1091:ARG:CD	1:A:1142:LEU:O	0.43	2.66	4	2
1:A:1095:MET:HE3	1:A:1139:LYS:O	0.43	2.13	19	2
1:A:1147:TYR:CD1	1:A:1147:TYR:C	0.43	2.92	9	1
1:A:1104:GLN:HB2	1:A:1107:GLU:OE2	0.43	2.12	12	1
1:A:1098:LEU:CD1	1:A:1139:LYS:HB2	0.43	2.43	2	1
1:A:1097:THR:HA	1:A:1188:GLU:CB	0.43	2.44	11	3
1:A:1192:VAL:O	1:A:1196:LEU:HB2	0.43	2.13	5	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1091:ARG:HD2	1:A:1142:LEU:O	0.43	2.12	19	1
1:A:1137:THR:C	1:A:1141:LYS:HE2	0.43	2.34	10	1
1:A:1095:MET:CE	1:A:1142:LEU:HD13	0.43	2.44	15	2
1:A:1109:LEU:HB2	1:A:1110:PRO:CD	0.43	2.44	8	1
1:A:1092:GLN:O	1:A:1096:PRO:CG	0.43	2.66	9	3
1:A:1104:GLN:O	1:A:1107:GLU:N	0.43	2.46	10	3
1:A:1090:LEU:HD12	1:A:1147:TYR:HE1	0.43	1.74	11	1
1:A:1129:VAL:HG13	1:A:1167:TYR:HD1	0.43	1.72	12	1
1:A:1180:LYS:HE3	1:A:1184:VAL:HG13	0.43	1.90	13	1
1:A:1150:PRO:HB3	1:A:1196:LEU:HD13	0.43	1.89	20	7
1:A:1133:MET:HG3	1:A:1138:ILE:HG12	0.43	1.91	8	1
1:A:1097:THR:HB	1:A:1188:GLU:HB2	0.43	1.90	17	1
1:A:1140:ARG:O	1:A:1142:LEU:N	0.43	2.51	2	2
1:A:1101:LEU:O	1:A:1108:SER:CB	0.43	2.66	5	3
1:A:1091:ARG:N	1:A:1147:TYR:OH	0.43	2.52	6	1
1:A:1097:THR:OG1	1:A:1098:LEU:N	0.43	2.52	17	2
1:A:1094:LEU:HD21	1:A:1196:LEU:HD12	0.43	1.91	20	8
1:A:1192:VAL:HG13	1:A:1196:LEU:CD1	0.43	2.44	1	1
1:A:1155:ASP:O	1:A:1159:LEU:HB2	0.43	2.13	19	2
1:A:1189:ILE:CD1	1:A:1192:VAL:HG11	0.42	2.44	6	9
1:A:1094:LEU:O	1:A:1095:MET:C	0.42	2.58	10	9
1:A:1192:VAL:O	1:A:1194:GLN:N	0.42	2.52	11	11
1:A:1105:ASP:N	1:A:1107:GLU:OE2	0.42	2.53	8	2
1:A:1137:THR:O	1:A:1141:LYS:HE2	0.42	2.14	10	1
1:A:1180:LYS:HE2	1:A:1184:VAL:HG22	0.42	1.92	19	2
1:A:1189:ILE:HG13	1:A:1193:MET:CG	0.42	2.44	1	1
1:A:1190:ASP:CB	1:A:1191:PRO:HD3	0.42	2.45	4	20
1:A:1194:GLN:HG3	1:A:1195:SER:N	0.42	2.30	11	4
1:A:1112:ARG:O	1:A:1136:SER:CB	0.42	2.68	11	2
1:A:1129:VAL:CG1	1:A:1163:ASN:HB3	0.42	2.44	18	1
1:A:1132:PRO:O	1:A:1163:ASN:ND2	0.42	2.52	5	1
1:A:1102:TYR:CZ	1:A:1112:ARG:HG2	0.42	2.49	14	2
1:A:1142:LEU:O	1:A:1144:THR:N	0.42	2.53	11	1
1:A:1101:LEU:HD23	1:A:1188:GLU:OE2	0.42	2.14	6	2
1:A:1125:TYR:O	1:A:1126:PHE:HB2	0.42	2.14	8	1
1:A:1094:LEU:CB	1:A:1142:LEU:HD11	0.42	2.43	15	4
1:A:1104:GLN:HG3	1:A:1180:LYS:HG3	0.42	1.92	16	1
1:A:1101:LEU:O	1:A:1108:SER:OG	0.42	2.38	1	1
1:A:1091:ARG:HB2	1:A:1147:TYR:OH	0.42	2.14	6	1
1:A:1161:PHE:O	1:A:1178:CYS:SG	0.42	2.77	9	1
1:A:1101:LEU:O	1:A:1107:GLU:OE2	0.42	2.37	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1137:THR:O	1:A:1141:LYS:HE3	0.42	2.14	16	1
1:A:1129:VAL:CG2	1:A:1130:LYS:N	0.42	2.83	17	1
1:A:1091:ARG:O	1:A:1091:ARG:HD2	0.42	2.15	11	1
1:A:1103:ARG:HB2	1:A:1104:GLN:HE21	0.42	1.75	16	1
1:A:1107:GLU:HB2	1:A:1181:LEU:HD21	0.42	1.90	17	1
1:A:1083:LYS:H	1:A:1084:ILE:HD12	0.42	1.74	2	1
1:A:1189:ILE:HG13	1:A:1189:ILE:O	0.42	2.15	20	2
1:A:1088:GLU:O	1:A:1092:GLN:HG3	0.42	2.15	4	3
1:A:1111:PHE:CG	1:A:1160:MET:SD	0.42	3.13	12	2
1:A:1101:LEU:O	1:A:1104:GLN:N	0.42	2.53	5	3
1:A:1105:ASP:C	1:A:1107:GLU:OE2	0.42	2.58	8	1
1:A:1085:PHE:HB2	1:A:1089:GLU:HB2	0.42	1.91	11	3
1:A:1112:ARG:O	1:A:1136:SER:HB2	0.42	2.15	15	3
1:A:1083:LYS:HE3	1:A:1084:ILE:HD13	0.42	1.91	13	1
1:A:1098:LEU:HD22	1:A:1101:LEU:HD12	0.42	1.90	13	1
1:A:1141:LYS:HA	1:A:1144:THR:OG1	0.42	2.15	13	1
1:A:1090:LEU:HD11	1:A:1148:GLN:C	0.42	2.36	16	1
1:A:1111:PHE:CB	1:A:1160:MET:SD	0.41	3.08	1	2
1:A:1190:ASP:HB3	1:A:1191:PRO:HD3	0.41	1.92	16	16
1:A:1109:LEU:HA	1:A:1112:ARG:CG	0.41	2.45	6	2
1:A:1094:LEU:CD2	1:A:1196:LEU:HD12	0.41	2.45	4	6
1:A:1107:GLU:OE1	1:A:1181:LEU:HD22	0.41	2.14	17	1
1:A:1094:LEU:HD22	1:A:1153:TYR:CD2	0.41	2.50	1	1
1:A:1111:PHE:HB3	1:A:1160:MET:SD	0.41	2.55	1	1
1:A:1124:ASP:HB2	1:A:1167:TYR:OH	0.41	2.15	8	2
1:A:1096:PRO:O	1:A:1099:GLU:HB2	0.41	2.14	14	1
1:A:1137:THR:CG2	1:A:1141:LYS:HD3	0.41	2.46	14	1
1:A:1111:PHE:CB	1:A:1135:LEU:H	0.41	2.27	20	1
1:A:1131:ASN:O	1:A:1159:LEU:HD11	0.41	2.16	20	1
1:A:1111:PHE:O	1:A:1134:ASP:HB2	0.41	2.15	16	1
1:A:1189:ILE:HD12	1:A:1192:VAL:CG1	0.41	2.44	18	1
1:A:1085:PHE:CB	1:A:1089:GLU:HG3	0.41	2.45	19	4
1:A:1161:PHE:CA	1:A:1178:CYS:SG	0.41	3.08	16	2
1:A:1109:LEU:N	1:A:1110:PRO:HD3	0.41	2.31	15	1
1:A:1149:GLU:HB2	1:A:1152:GLN:HE21	0.41	1.74	3	1
1:A:1099:GLU:O	1:A:1102:TYR:N	0.41	2.53	8	1
1:A:1094:LEU:HD23	1:A:1192:VAL:CG1	0.41	2.46	1	1
1:A:1105:ASP:O	1:A:1109:LEU:HD12	0.41	2.15	2	1
1:A:1147:TYR:C	1:A:1147:TYR:HD1	0.41	2.19	5	1
1:A:1168:ASN:CB	1:A:1175:TYR:CZ	0.41	3.04	7	1
1:A:1164:ALA:HA	1:A:1168:ASN:ND2	0.41	2.31	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1083:LYS:HG2	1:A:1085:PHE:CE1	0.41	2.51	19	1
1:A:1129:VAL:C	1:A:1131:ASN:H	0.41	2.19	11	2
1:A:1164:ALA:HA	1:A:1168:ASN:OD1	0.41	2.16	4	1
1:A:1105:ASP:C	1:A:1107:GLU:N	0.41	2.74	5	7
1:A:1191:PRO:HA	1:A:1194:GLN:NE2	0.41	2.31	13	1
1:A:1126:PHE:CD1	1:A:1132:PRO:HG3	0.41	2.51	1	1
1:A:1175:TYR:O	1:A:1178:CYS:SG	0.41	2.79	4	1
1:A:1142:LEU:HD23	1:A:1147:TYR:OH	0.41	2.16	5	1
1:A:1098:LEU:HD21	1:A:1138:ILE:CG2	0.41	2.46	6	1
1:A:1104:GLN:HE21	1:A:1180:LYS:HD2	0.41	1.76	8	1
1:A:1094:LEU:HD13	1:A:1153:TYR:HB3	0.41	1.93	9	1
1:A:1098:LEU:HD13	1:A:1102:TYR:CE1	0.41	2.51	9	1
1:A:1095:MET:HE1	1:A:1142:LEU:CG	0.41	2.46	11	1
1:A:1108:SER:C	1:A:1110:PRO:CD	0.41	2.90	16	2
1:A:1091:ARG:HA	1:A:1142:LEU:CD2	0.41	2.46	18	1
1:A:1091:ARG:O	1:A:1096:PRO:HD3	0.41	2.16	19	1
1:A:1185:PHE:HA	1:A:1188:GLU:OE1	0.41	2.15	19	1
1:A:1105:ASP:O	1:A:1108:SER:N	0.41	2.52	20	1
1:A:1133:MET:HE3	1:A:1133:MET:C	0.41	2.36	3	1
1:A:1112:ARG:N	1:A:1135:LEU:HB2	0.41	2.31	4	1
1:A:1133:MET:SD	1:A:1138:ILE:HG12	0.41	2.56	10	1
1:A:1109:LEU:HB2	1:A:1112:ARG:HD3	0.41	1.93	14	1
1:A:1104:GLN:HB2	1:A:1107:GLU:OE1	0.40	2.15	8	1
1:A:1100:ALA:O	1:A:1104:GLN:HG2	0.40	2.15	14	1
1:A:1097:THR:CG2	1:A:1192:VAL:CG2	0.40	2.96	1	1
1:A:1129:VAL:CG1	1:A:1163:ASN:HA	0.40	2.46	2	1
1:A:1088:GLU:HG3	1:A:1091:ARG:NH2	0.40	2.30	4	1
1:A:1168:ASN:O	1:A:1175:TYR:OH	0.40	2.33	4	1
1:A:1124:ASP:O	1:A:1125:TYR:C	0.40	2.59	10	1
1:A:1141:LYS:HE2	1:A:1147:TYR:CZ	0.40	2.51	13	1
1:A:1097:THR:O	1:A:1188:GLU:OE1	0.40	2.39	17	1
1:A:1140:ARG:HE	1:A:1144:THR:HG21	0.40	1.76	18	1
1:A:1138:ILE:C	1:A:1140:ARG:N	0.40	2.74	1	1
1:A:1156:ASP:O	1:A:1159:LEU:CB	0.40	2.70	3	1
1:A:1108:SER:HB3	1:A:1112:ARG:CG	0.40	2.46	12	1
1:A:1102:TYR:CE2	1:A:1112:ARG:NE	0.40	2.90	2	1
1:A:1129:VAL:O	1:A:1129:VAL:CG2	0.40	2.69	2	1
1:A:1132:PRO:O	1:A:1133:MET:C	0.40	2.60	5	1
1:A:1107:GLU:OE1	1:A:1180:LYS:HB3	0.40	2.16	5	1
1:A:1090:LEU:HD11	1:A:1148:GLN:O	0.40	2.16	12	1
1:A:1147:TYR:CE2	1:A:1153:TYR:HB2	0.40	2.52	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1180:LYS:O	1:A:1180:LYS:HD3	0.40	2.17	20	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	98/121 (81%)	70±3 (72±3%)	22±3 (22±3%)	6±1 (6±1%)	3 21
2	B	0	-	-	-	-
All	All	1960/2720 (72%)	1404 (72%)	441 (22%)	115 (6%)	3 21

All 16 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	1138	ILE	20
1	A	1105	ASP	18
1	A	1084	ILE	16
1	A	1135	LEU	15
1	A	1128	ILE	13
1	A	1133	MET	10
1	A	1148	GLN	8
1	A	1132	PRO	4
1	A	1106	PRO	3
1	A	1141	LYS	2
1	A	1110	PRO	1
1	A	1083	LYS	1
1	A	1125	TYR	1
1	A	1112	ARG	1
1	A	1143	ASP	1
1	A	1124	ASP	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	93/113 (82%)	66±3 (71±4%)	27±3 (29±4%)	2 18
2	B	0	-	-	-
All	All	1860/2480 (75%)	1328 (71%)	532 (29%)	2 18

All 50 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	1083	LYS	20
1	A	1085	PHE	20
1	A	1143	ASP	20
1	A	1151	TRP	20
1	A	1161	PHE	20
1	A	1166	LEU	20
1	A	1184	VAL	20
1	A	1186	GLU	20
1	A	1190	ASP	20
1	A	1139	LYS	19
1	A	1142	LEU	19
1	A	1159	LEU	19
1	A	1196	LEU	18
1	A	1098	LEU	18
1	A	1192	VAL	18
1	A	1125	TYR	16
1	A	1174	VAL	16
1	A	1126	PHE	14
1	A	1109	LEU	13
1	A	1148	GLN	12
1	A	1176	LYS	12
1	A	1102	TYR	11
1	A	1141	LYS	10
1	A	1092	GLN	10
1	A	1134	ASP	9
1	A	1149	GLU	9
1	A	1086	LYS	9
1	A	1084	ILE	9

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Mol	Chain	Res	Type	Models (Total)
1	A	1103	ARG	8
1	A	1175	TYR	8
1	A	1180	LYS	8
1	A	1108	SER	7
1	A	1131	ASN	7
1	A	1163	ASN	7
1	A	1091	ARG	6
1	A	1178	CYS	5
1	A	1095	MET	5
1	A	1147	TYR	4
1	A	1105	ASP	3
1	A	1187	GLN	3
1	A	1162	ASN	3
1	A	1107	GLU	3
1	A	1112	ARG	3
1	A	1089	GLU	2
1	A	1194	GLN	2
1	A	1140	ARG	2
1	A	1101	LEU	2
1	A	1160	MET	1
1	A	1124	ASP	1
1	A	1152	GLN	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	ALY	B	20	2	10,11,12	0.60±0.04	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	ALY	B	20	2	7,12,14	0.95±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	ALY	B	20	2	-	0±0,9,10,12	-

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

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided