Full wwPDB NMR Structure Validation Report (i)

Oct 12, 2021 – 04:18 PM EDT

PDB ID	:	2ARF
Title	:	Solution structure of the Wilson ATPase N-domain in the presence of ATP
Authors	:	Dmitriev, O.; Tsivkovskii, R.; Abildgaard, F.; Morgan, C.T.; Markley, J.L.; Lutsenko, S.
Deposited on	:	2005-08-19

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

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

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

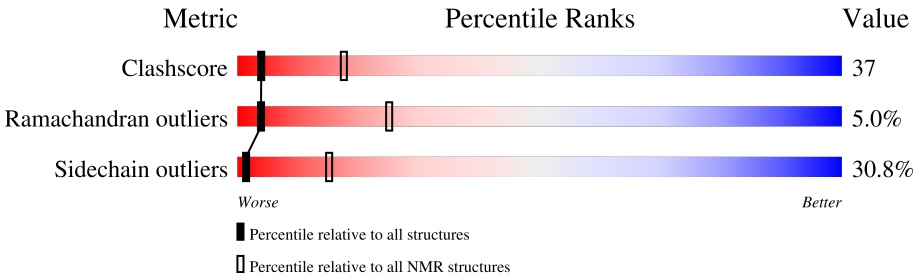
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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	165	32% 41% 6% • 21%

2 Ensemble composition and analysis

This entry contains 10 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 5 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:1037-A:1111, A:1141-A:1196 (131)	0.68	5

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters. No single-model clusters were found.

Cluster number	Models
1	3, 4, 5, 6, 8, 9
2	1, 2, 7, 10

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2437 atoms, of which 1230 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called WILSON DISEASE ATPASE.

Mol	Chain	Residues	Atoms						Trace
1	A	165	Total	C	H	N	O	S	0
			2437	753	1230	210	234	10	

There are 3 discrepancies between the modelled and reference sequences:

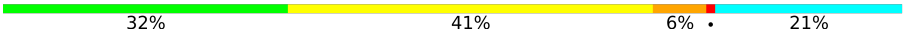
Chain	Residue	Modelled	Actual	Comment	Reference
A	1032	ALA	ILE	engineered mutation	UNP P35670
A	1033	GLY	THR	engineered mutation	UNP P35670
A	1035	MET	GLY	engineered mutation	UNP P35670

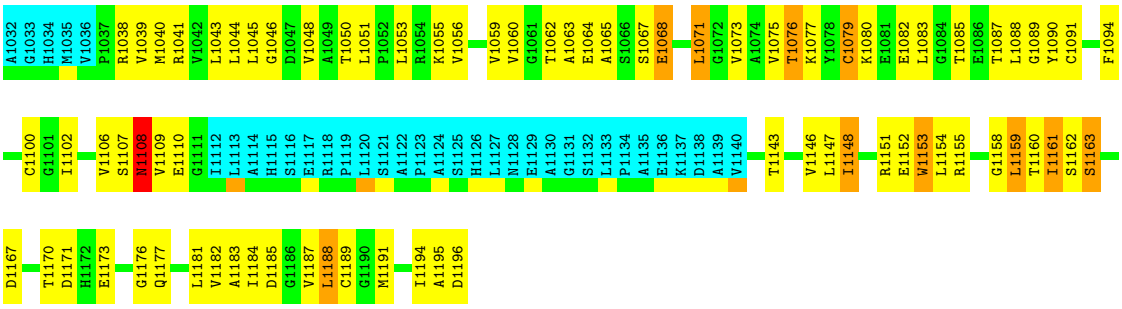
4 Residue-property plots (i)

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: WILSON DISEASE ATPASE

Chain A: 

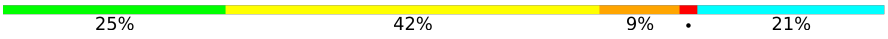


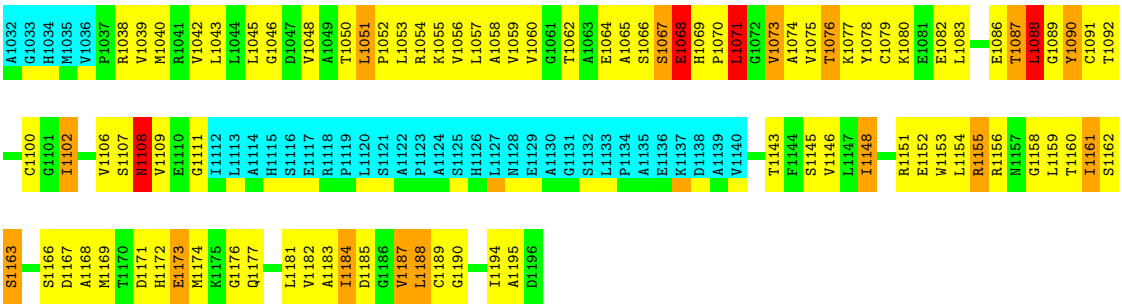
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: WILSON DISEASE ATPASE

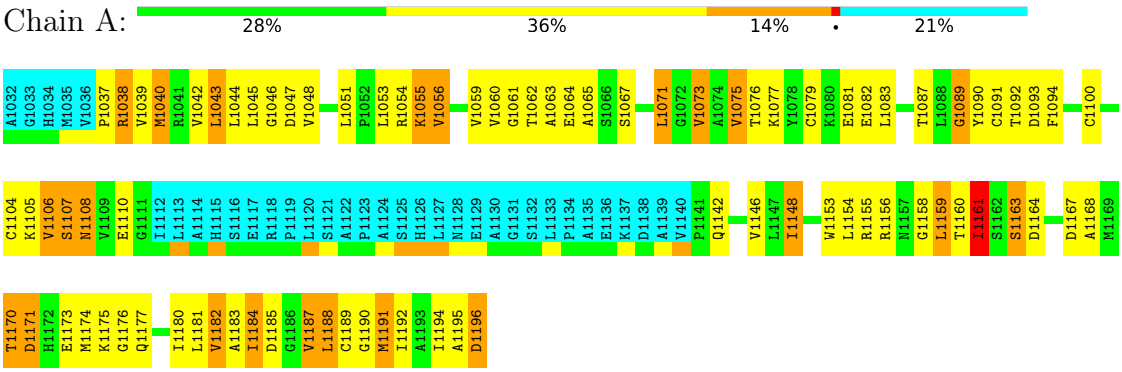
Chain A: 



4.2.2 Score per residue for model 2

• Molecule 1: WILSON DISEASE ATPASE

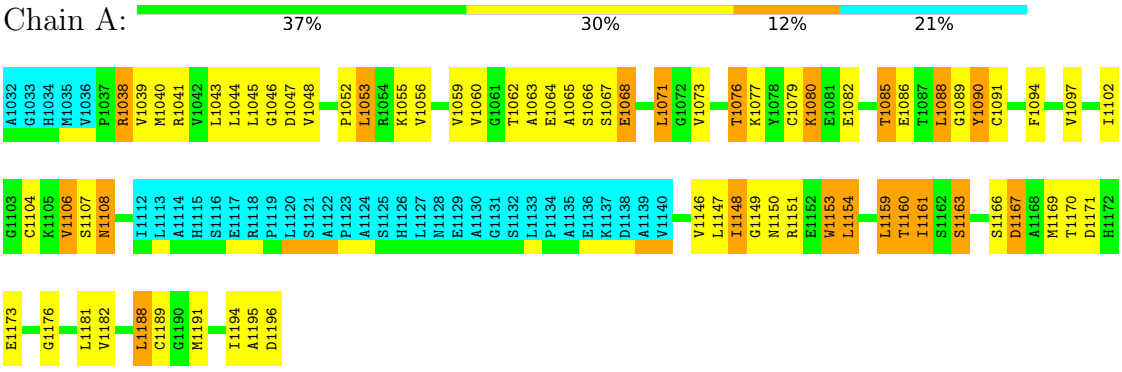
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: WILSON DISEASE ATPASE

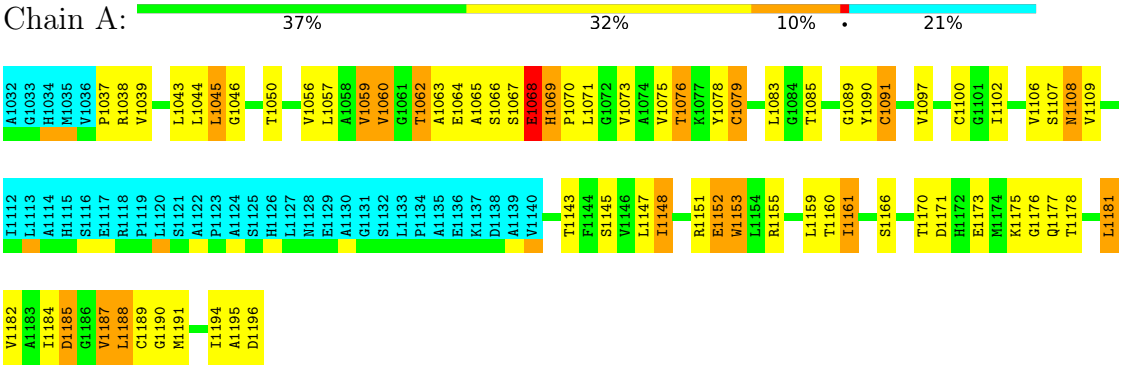
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: WILSON DISEASE ATPASE

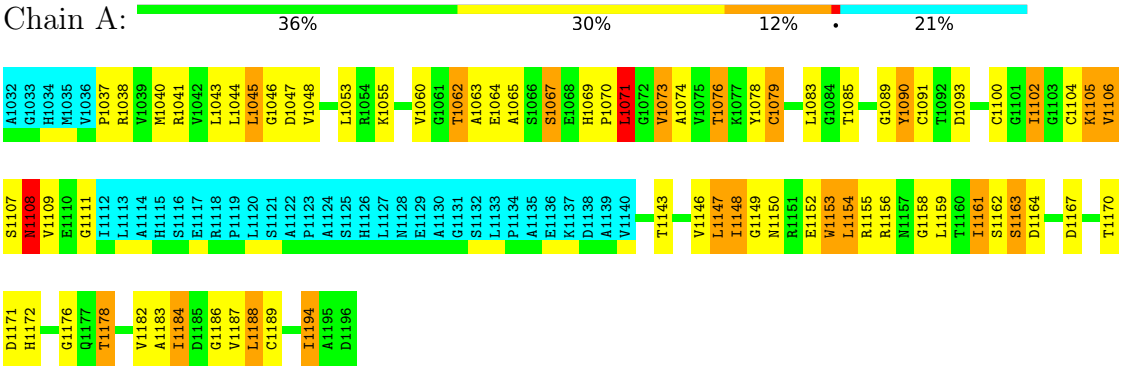
Chain A:



4.2.5 Score per residue for model 5 (medoid)

• Molecule 1: WILSON DISEASE ATPASE

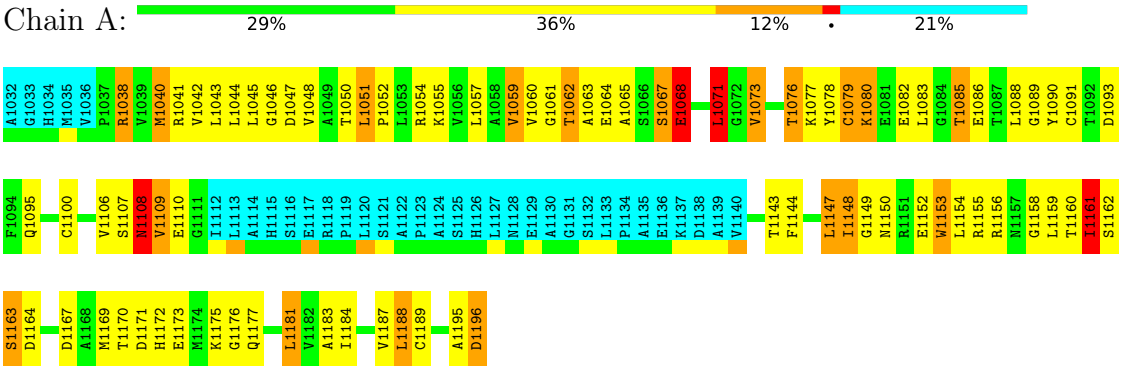
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: WILSON DISEASE ATPASE

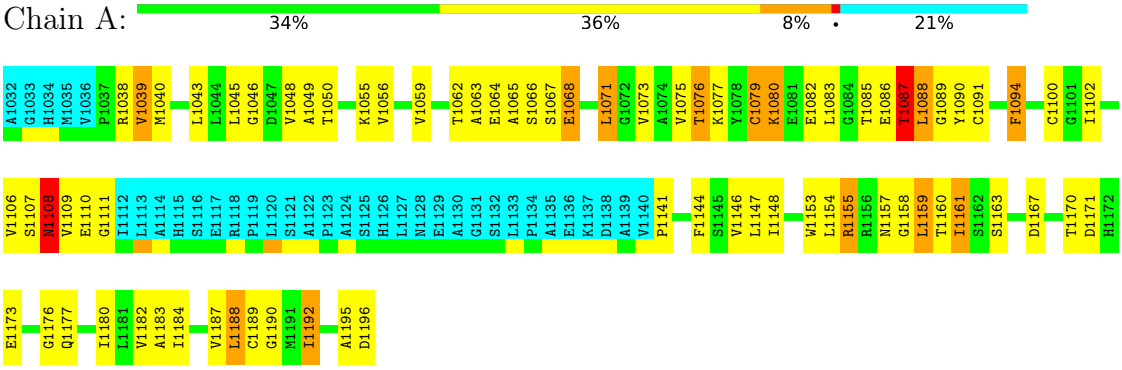
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: WILSON DISEASE ATPASE

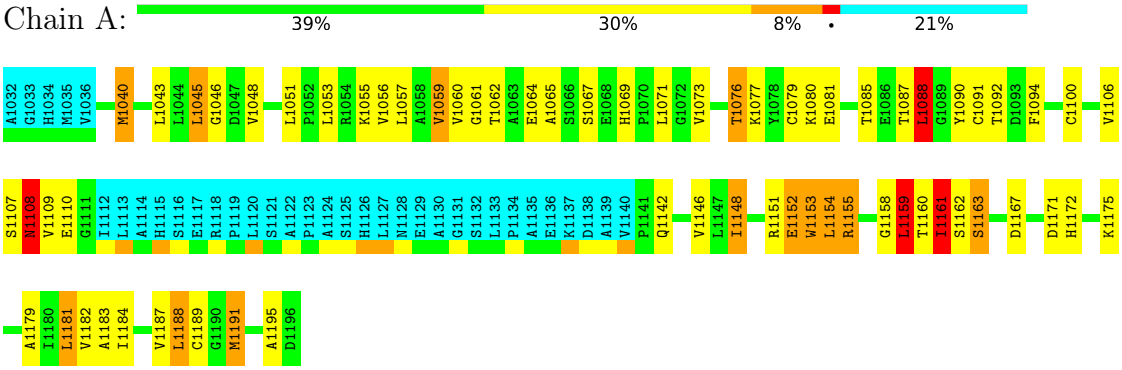
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: WILSON DISEASE ATPASE

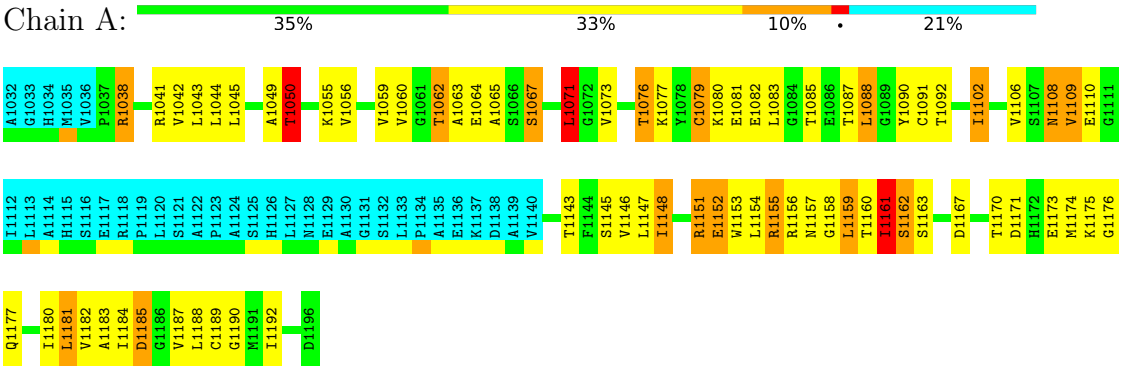
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: WILSON DISEASE ATPASE

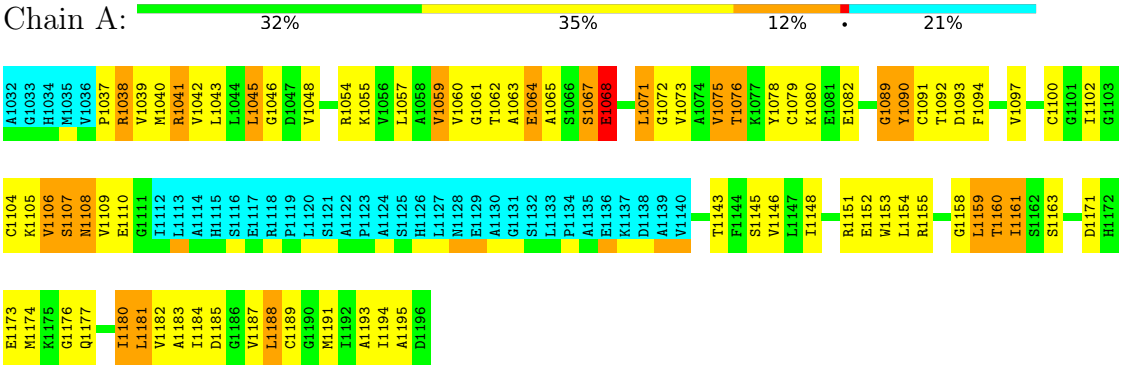
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: WILSON DISEASE ATPASE

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 10 were deposited, based on the following criterion: *target function.*

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

Software name	Classification	Version
CYANA	structure solution	1.0
CYANA	refinement	1.0

No chemical shift data was provided.

6 Model quality

6.1 Standard geometry

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	964	983	985	73±9
All	All	9640	9849	9850	730

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 37.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1153:TRP:CH2	1:A:1154:LEU:HD23	1.05	1.86	5	2
1:A:1148:ILE:HG23	1:A:1182:VAL:HG13	1.05	1.18	3	2
1:A:1059:VAL:HG23	1:A:1109:VAL:HG11	1.03	1.22	10	1
1:A:1154:LEU:HD11	1:A:1183:ALA:HB2	1.03	1.25	8	3
1:A:1090:TYR:CE2	1:A:1092:THR:HG22	1.00	1.92	10	1
1:A:1153:TRP:CH2	1:A:1154:LEU:HD13	0.97	1.94	6	1
1:A:1196:ASP:OXT	1:A:1196:ASP:OD1	0.96	1.84	6	1
1:A:1044:LEU:C	1:A:1045:LEU:HD22	0.91	1.86	2	1
1:A:1184:ILE:O	1:A:1187:VAL:HG12	0.91	1.66	9	4
1:A:1158:GLY:O	1:A:1159:LEU:HD23	0.91	1.66	8	1
1:A:1166:SER:O	1:A:1170:THR:HG23	0.90	1.67	4	2
1:A:1148:ILE:HG22	1:A:1182:VAL:HG13	0.88	1.44	8	1
1:A:1038:ARG:O	1:A:1194:ILE:HG23	0.85	1.71	10	4
1:A:1059:VAL:HG22	1:A:1106:VAL:CG1	0.84	2.02	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1148:ILE:CG2	1:A:1182:VAL:HG13	0.84	2.00	3	3
1:A:1153:TRP:CZ2	1:A:1154:LEU:HD23	0.82	2.08	5	2
1:A:1146:VAL:HG13	1:A:1183:ALA:O	0.81	1.75	2	3
1:A:1044:LEU:O	1:A:1045:LEU:HD22	0.81	1.76	6	2
1:A:1064:GLU:O	1:A:1073:VAL:HG22	0.80	1.76	10	3
1:A:1065:ALA:O	1:A:1073:VAL:HG13	0.80	1.77	3	5
1:A:1090:TYR:CD2	1:A:1106:VAL:HG21	0.79	2.12	2	1
1:A:1050:THR:O	1:A:1051:LEU:HD12	0.78	1.77	1	2
1:A:1062:THR:CG2	1:A:1106:VAL:HG21	0.78	2.09	6	1
1:A:1059:VAL:HG23	1:A:1109:VAL:CG1	0.77	2.06	10	1
1:A:1063:ALA:HB2	1:A:1106:VAL:HG21	0.77	1.57	9	2
1:A:1059:VAL:HG13	1:A:1106:VAL:CG1	0.77	2.09	9	1
1:A:1146:VAL:HG22	1:A:1184:ILE:HG13	0.76	1.54	1	1
1:A:1059:VAL:HG23	1:A:1090:TYR:CD2	0.76	2.16	1	1
1:A:1062:THR:HG22	1:A:1090:TYR:CB	0.76	2.10	10	2
1:A:1079:CYS:O	1:A:1083:LEU:HD12	0.75	1.81	1	6
1:A:1087:THR:O	1:A:1088:LEU:HD12	0.75	1.82	1	1
1:A:1154:LEU:HD11	1:A:1183:ALA:CB	0.75	2.09	8	4
1:A:1153:TRP:CZ3	1:A:1154:LEU:HD13	0.74	2.16	6	1
1:A:1146:VAL:HG23	1:A:1183:ALA:O	0.74	1.83	9	1
1:A:1063:ALA:CB	1:A:1090:TYR:CE2	0.73	2.71	2	1
1:A:1038:ARG:HA	1:A:1071:LEU:HD13	0.73	1.59	6	2
1:A:1062:THR:HG21	1:A:1090:TYR:HB2	0.72	1.59	1	2
1:A:1037:PRO:HB2	1:A:1194:ILE:HD11	0.72	1.59	5	1
1:A:1065:ALA:HB2	1:A:1076:THR:CG2	0.72	2.14	4	3
1:A:1090:TYR:OH	1:A:1109:VAL:HG12	0.72	1.84	6	1
1:A:1059:VAL:HG13	1:A:1106:VAL:HG11	0.72	1.62	9	2
1:A:1062:THR:HG21	1:A:1090:TYR:CG	0.72	2.20	6	3
1:A:1148:ILE:HG23	1:A:1182:VAL:HG22	0.71	1.62	4	1
1:A:1088:LEU:HD22	1:A:1088:LEU:O	0.71	1.85	7	1
1:A:1088:LEU:O	1:A:1088:LEU:HD13	0.71	1.85	7	1
1:A:1065:ALA:O	1:A:1073:VAL:HG22	0.70	1.86	4	2
1:A:1153:TRP:CZ2	1:A:1154:LEU:HD13	0.70	2.21	6	1
1:A:1062:THR:HG22	1:A:1090:TYR:HB3	0.70	1.61	10	2
1:A:1154:LEU:HD12	1:A:1183:ALA:CB	0.70	2.16	9	1
1:A:1153:TRP:CZ3	1:A:1154:LEU:HD23	0.70	2.22	3	2
1:A:1195:ALA:O	1:A:1196:ASP:OXT	0.69	2.09	2	4
1:A:1059:VAL:HG23	1:A:1090:TYR:CD1	0.69	2.22	3	1
1:A:1045:LEU:CD1	1:A:1188:LEU:HD21	0.69	2.18	6	1
1:A:1038:ARG:HA	1:A:1071:LEU:HD21	0.69	1.63	9	2
1:A:1063:ALA:HB2	1:A:1090:TYR:CE2	0.68	2.22	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1153:TRP:CH2	1:A:1154:LEU:CD1	0.68	2.76	6	1
1:A:1154:LEU:HD11	1:A:1183:ALA:HB3	0.68	1.64	1	2
1:A:1045:LEU:CD2	1:A:1181:LEU:HD21	0.67	2.19	4	1
1:A:1091:CYS:O	1:A:1106:VAL:HA	0.67	1.90	7	10
1:A:1107:SER:O	1:A:1108:ASN:CB	0.67	2.43	2	6
1:A:1146:VAL:HG22	1:A:1184:ILE:HD12	0.67	1.67	7	3
1:A:1090:TYR:CD2	1:A:1106:VAL:HG22	0.67	2.25	6	1
1:A:1148:ILE:HB	1:A:1182:VAL:HG22	0.66	1.67	8	1
1:A:1153:TRP:CH2	1:A:1154:LEU:CD2	0.66	2.74	5	2
1:A:1148:ILE:N	1:A:1153:TRP:CZ2	0.66	2.63	3	3
1:A:1161:ILE:HG23	1:A:1162:SER:N	0.66	2.06	8	2
1:A:1048:VAL:HG12	1:A:1048:VAL:O	0.66	1.91	6	3
1:A:1152:GLU:H	1:A:1170:THR:HG21	0.66	1.50	9	2
1:A:1039:VAL:HG21	1:A:1075:VAL:HG21	0.65	1.66	7	2
1:A:1063:ALA:HB2	1:A:1106:VAL:CG2	0.65	2.21	9	1
1:A:1159:LEU:N	1:A:1159:LEU:HD22	0.65	2.06	9	1
1:A:1154:LEU:HD21	1:A:1183:ALA:HB2	0.65	1.68	6	2
1:A:1154:LEU:CD2	1:A:1181:LEU:HD12	0.65	2.22	10	1
1:A:1059:VAL:CG2	1:A:1106:VAL:HG21	0.64	2.21	1	1
1:A:1158:GLY:C	1:A:1159:LEU:HD13	0.64	2.12	9	1
1:A:1151:ARG:HG2	1:A:1181:LEU:HD13	0.64	1.68	1	1
1:A:1048:VAL:HG13	1:A:1051:LEU:O	0.64	1.93	8	1
1:A:1065:ALA:HB2	1:A:1076:THR:HG21	0.64	1.68	4	1
1:A:1090:TYR:CD1	1:A:1106:VAL:HG22	0.63	2.27	1	1
1:A:1148:ILE:HB	1:A:1182:VAL:HG23	0.63	1.70	2	1
1:A:1151:ARG:HD2	1:A:1170:THR:HG22	0.63	1.70	3	1
1:A:1040:MET:HG3	1:A:1195:ALA:HB3	0.63	1.71	8	3
1:A:1184:ILE:HD13	1:A:1189:CYS:SG	0.62	2.33	1	1
1:A:1045:LEU:O	1:A:1188:LEU:HD12	0.62	1.94	5	3
1:A:1147:LEU:N	1:A:1147:LEU:HD12	0.62	2.09	5	1
1:A:1065:ALA:HB2	1:A:1076:THR:HB	0.62	1.72	7	3
1:A:1059:VAL:HG22	1:A:1106:VAL:HG11	0.62	1.70	4	3
1:A:1046:GLY:N	1:A:1189:CYS:O	0.62	2.33	2	9
1:A:1090:TYR:CD2	1:A:1106:VAL:CG2	0.62	2.82	2	1
1:A:1048:VAL:HG11	1:A:1053:LEU:CB	0.62	2.25	3	1
1:A:1065:ALA:HB2	1:A:1076:THR:HG22	0.61	1.72	9	2
1:A:1039:VAL:CG1	1:A:1071:LEU:HD12	0.61	2.25	2	1
1:A:1148:ILE:N	1:A:1148:ILE:HD12	0.61	2.10	6	1
1:A:1102:ILE:HD12	1:A:1148:ILE:O	0.61	1.96	9	2
1:A:1196:ASP:OXT	1:A:1196:ASP:CG	0.61	2.37	6	1
1:A:1148:ILE:HD11	1:A:1180:ILE:HB	0.61	1.70	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1045:LEU:O	1:A:1188:LEU:HD23	0.61	1.95	8	1
1:A:1066:SER:O	1:A:1067:SER:CB	0.60	2.48	1	1
1:A:1040:MET:SD	1:A:1195:ALA:HB2	0.60	2.36	10	1
1:A:1148:ILE:CG2	1:A:1182:VAL:HG22	0.60	2.26	4	2
1:A:1148:ILE:CA	1:A:1153:TRP:CH2	0.60	2.85	3	3
1:A:1100:CYS:SG	1:A:1153:TRP:CZ3	0.60	2.95	8	1
1:A:1148:ILE:HD12	1:A:1181:LEU:O	0.60	1.97	2	1
1:A:1062:THR:HG21	1:A:1090:TYR:CB	0.60	2.27	3	3
1:A:1090:TYR:OH	1:A:1109:VAL:HG23	0.59	1.98	8	3
1:A:1040:MET:CG	1:A:1195:ALA:HB3	0.59	2.27	6	5
1:A:1079:CYS:C	1:A:1083:LEU:HD12	0.59	2.17	1	4
1:A:1059:VAL:HG22	1:A:1106:VAL:HG12	0.59	1.74	4	1
1:A:1178:THR:HB	1:A:1194:ILE:HG23	0.59	1.73	5	1
1:A:1090:TYR:CE2	1:A:1106:VAL:HG21	0.59	2.32	2	1
1:A:1153:TRP:O	1:A:1153:TRP:CE3	0.59	2.56	4	3
1:A:1061:GLY:HA2	1:A:1076:THR:HG22	0.58	1.74	2	3
1:A:1041:ARG:O	1:A:1193:ALA:HB3	0.58	1.98	10	1
1:A:1045:LEU:O	1:A:1188:LEU:CG	0.58	2.51	3	8
1:A:1039:VAL:HG11	1:A:1075:VAL:HG13	0.58	1.74	4	1
1:A:1042:VAL:HG23	1:A:1191:MET:O	0.58	1.98	10	1
1:A:1062:THR:HG21	1:A:1090:TYR:CD2	0.58	2.33	6	1
1:A:1158:GLY:O	1:A:1159:LEU:CD2	0.58	2.49	8	1
1:A:1149:GLY:CA	1:A:1153:TRP:CE3	0.58	2.86	3	3
1:A:1064:GLU:HB2	1:A:1076:THR:HG21	0.58	1.75	10	6
1:A:1090:TYR:CE1	1:A:1092:THR:HG22	0.58	2.33	2	1
1:A:1040:MET:HB2	1:A:1195:ALA:HB3	0.58	1.76	7	3
1:A:1168:ALA:O	1:A:1172:HIS:CD2	0.58	2.57	1	1
1:A:1189:CYS:SG	1:A:1190:GLY:N	0.57	2.77	9	1
1:A:1059:VAL:HG23	1:A:1090:TYR:CE2	0.57	2.34	1	1
1:A:1154:LEU:HD12	1:A:1183:ALA:HB2	0.57	1.74	9	1
1:A:1090:TYR:CE2	1:A:1106:VAL:CG2	0.57	2.87	2	1
1:A:1178:THR:CB	1:A:1194:ILE:HG23	0.57	2.30	5	1
1:A:1065:ALA:N	1:A:1076:THR:HG21	0.57	2.14	4	3
1:A:1045:LEU:O	1:A:1188:LEU:CB	0.57	2.52	6	8
1:A:1045:LEU:HB3	1:A:1188:LEU:HD22	0.57	1.75	2	1
1:A:1155:ARG:NH2	1:A:1161:ILE:HD12	0.57	2.14	1	1
1:A:1039:VAL:HG12	1:A:1071:LEU:HD12	0.56	1.77	2	1
1:A:1147:LEU:HD13	1:A:1157:ASN:HD21	0.56	1.61	7	1
1:A:1152:GLU:N	1:A:1170:THR:HG21	0.56	2.16	9	1
1:A:1091:CYS:CB	1:A:1107:SER:O	0.56	2.53	2	4
1:A:1062:THR:CG2	1:A:1090:TYR:CG	0.56	2.89	6	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1044:LEU:O	1:A:1045:LEU:HD12	0.55	2.02	5	1
1:A:1091:CYS:O	1:A:1106:VAL:HG23	0.55	2.00	7	1
1:A:1159:LEU:O	1:A:1160:THR:OG1	0.55	2.24	8	1
1:A:1148:ILE:HA	1:A:1153:TRP:CH2	0.55	2.36	5	2
1:A:1063:ALA:HB2	1:A:1106:VAL:HG11	0.55	1.77	5	1
1:A:1045:LEU:O	1:A:1188:LEU:HB3	0.55	2.02	2	6
1:A:1062:THR:CG2	1:A:1106:VAL:CG2	0.55	2.85	6	1
1:A:1067:SER:O	1:A:1068:GLU:CB	0.54	2.55	10	4
1:A:1039:VAL:CG2	1:A:1075:VAL:HG21	0.54	2.30	7	1
1:A:1071:LEU:O	1:A:1075:VAL:HG23	0.54	2.01	4	3
1:A:1037:PRO:O	1:A:1071:LEU:HD13	0.54	2.02	10	1
1:A:1178:THR:HG22	1:A:1194:ILE:CG2	0.54	2.33	5	1
1:A:1059:VAL:CG2	1:A:1106:VAL:CG2	0.54	2.86	1	1
1:A:1161:ILE:CG2	1:A:1162:SER:N	0.54	2.70	9	4
1:A:1184:ILE:N	1:A:1187:VAL:O	0.54	2.41	9	9
1:A:1089:GLY:O	1:A:1108:ASN:CG	0.53	2.47	2	2
1:A:1048:VAL:HG11	1:A:1053:LEU:HB2	0.53	1.80	5	3
1:A:1147:LEU:HD13	1:A:1186:GLY:H	0.53	1.64	5	1
1:A:1158:GLY:O	1:A:1159:LEU:HD13	0.53	2.03	9	1
1:A:1168:ALA:O	1:A:1172:HIS:CG	0.53	2.62	1	1
1:A:1149:GLY:C	1:A:1153:TRP:CE3	0.53	2.81	3	3
1:A:1049:ALA:O	1:A:1050:THR:CB	0.53	2.57	7	2
1:A:1151:ARG:HG2	1:A:1181:LEU:HD23	0.53	1.80	10	1
1:A:1163:SER:O	1:A:1167:ASP:CB	0.53	2.55	9	8
1:A:1090:TYR:HE1	1:A:1092:THR:HG22	0.53	1.63	2	1
1:A:1100:CYS:O	1:A:1153:TRP:CD2	0.53	2.62	8	2
1:A:1102:ILE:HD12	1:A:1148:ILE:HD12	0.53	1.80	3	1
1:A:1109:VAL:HG11	1:A:1144:PHE:CE2	0.53	2.38	7	1
1:A:1090:TYR:OH	1:A:1109:VAL:CG1	0.53	2.57	1	3
1:A:1178:THR:CG2	1:A:1194:ILE:HG23	0.53	2.33	5	1
1:A:1045:LEU:O	1:A:1189:CYS:N	0.53	2.42	5	10
1:A:1066:SER:O	1:A:1094:PHE:CZ	0.53	2.62	3	1
1:A:1059:VAL:CG2	1:A:1106:VAL:HG12	0.53	2.33	4	1
1:A:1090:TYR:HD2	1:A:1106:VAL:HG22	0.53	1.61	6	1
1:A:1060:VAL:O	1:A:1064:GLU:CG	0.53	2.57	1	3
1:A:1065:ALA:CB	1:A:1076:THR:HG21	0.53	2.32	4	1
1:A:1061:GLY:O	1:A:1065:ALA:CB	0.53	2.57	8	2
1:A:1100:CYS:SG	1:A:1153:TRP:CH2	0.52	3.02	8	2
1:A:1040:MET:O	1:A:1041:ARG:CG	0.52	2.57	5	1
1:A:1146:VAL:CG2	1:A:1184:ILE:HD12	0.52	2.33	7	2
1:A:1151:ARG:HB2	1:A:1170:THR:HG22	0.52	1.81	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1062:THR:HG23	1:A:1088:LEU:CB	0.52	2.34	3	1
1:A:1184:ILE:HD13	1:A:1185:ASP:N	0.52	2.18	2	1
1:A:1149:GLY:N	1:A:1153:TRP:CZ3	0.52	2.77	3	1
1:A:1064:GLU:CB	1:A:1076:THR:HG21	0.52	2.35	2	5
1:A:1178:THR:CG2	1:A:1194:ILE:CG2	0.52	2.87	5	1
1:A:1059:VAL:O	1:A:1062:THR:HG22	0.52	2.04	7	2
1:A:1090:TYR:CZ	1:A:1092:THR:HG22	0.52	2.37	10	1
1:A:1045:LEU:HD21	1:A:1181:LEU:HD21	0.52	1.82	4	1
1:A:1055:LYS:O	1:A:1059:VAL:HG23	0.52	2.05	2	1
1:A:1102:ILE:HD12	1:A:1102:ILE:N	0.52	2.20	5	1
1:A:1045:LEU:O	1:A:1188:LEU:CD1	0.52	2.58	3	3
1:A:1080:LYS:CG	1:A:1085:THR:O	0.52	2.58	6	2
1:A:1091:CYS:O	1:A:1106:VAL:CG2	0.52	2.58	7	1
1:A:1090:TYR:CE2	1:A:1106:VAL:HB	0.51	2.39	2	1
1:A:1107:SER:O	1:A:1108:ASN:HB2	0.51	2.04	10	6
1:A:1087:THR:HG23	1:A:1088:LEU:N	0.51	2.21	7	1
1:A:1063:ALA:O	1:A:1067:SER:N	0.51	2.44	6	6
1:A:1154:LEU:CD2	1:A:1183:ALA:HB2	0.51	2.35	10	1
1:A:1148:ILE:CG1	1:A:1182:VAL:HG13	0.51	2.35	4	1
1:A:1090:TYR:OH	1:A:1109:VAL:CG2	0.51	2.58	7	3
1:A:1104:CYS:SG	1:A:1146:VAL:CG1	0.51	2.98	3	1
1:A:1037:PRO:O	1:A:1071:LEU:CD2	0.51	2.59	4	1
1:A:1090:TYR:CE1	1:A:1091:CYS:O	0.51	2.64	10	1
1:A:1181:LEU:HD22	1:A:1191:MET:CB	0.51	2.36	8	1
1:A:1154:LEU:HD12	1:A:1183:ALA:HB3	0.51	1.83	9	1
1:A:1089:GLY:O	1:A:1108:ASN:CB	0.51	2.58	10	1
1:A:1059:VAL:CG2	1:A:1106:VAL:CG1	0.51	2.85	4	1
1:A:1154:LEU:HD21	1:A:1183:ALA:HB3	0.51	1.82	5	1
1:A:1148:ILE:HG22	1:A:1182:VAL:HG22	0.51	1.83	10	1
1:A:1051:LEU:HD23	1:A:1052:PRO:HD2	0.50	1.81	6	2
1:A:1089:GLY:O	1:A:1108:ASN:ND2	0.50	2.44	10	1
1:A:1154:LEU:HD22	1:A:1181:LEU:HB3	0.50	1.81	10	1
1:A:1100:CYS:HB3	1:A:1153:TRP:CH2	0.50	2.41	2	2
1:A:1059:VAL:CG2	1:A:1090:TYR:CE1	0.50	2.93	3	1
1:A:1067:SER:O	1:A:1073:VAL:CG2	0.50	2.59	8	1
1:A:1093:ASP:O	1:A:1105:LYS:CG	0.50	2.60	10	1
1:A:1181:LEU:HD12	1:A:1191:MET:HB3	0.50	1.83	4	1
1:A:1160:THR:O	1:A:1161:ILE:CG1	0.50	2.60	9	1
1:A:1107:SER:HB3	1:A:1143:THR:HG23	0.50	1.81	4	1
1:A:1160:THR:O	1:A:1161:ILE:CB	0.50	2.59	9	1
1:A:1148:ILE:N	1:A:1153:TRP:CH2	0.50	2.79	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1100:CYS:O	1:A:1153:TRP:CG	0.50	2.65	4	4
1:A:1065:ALA:O	1:A:1073:VAL:CG2	0.50	2.60	5	2
1:A:1154:LEU:CD1	1:A:1183:ALA:CB	0.50	2.88	1	2
1:A:1182:VAL:HG12	1:A:1190:GLY:O	0.50	2.07	2	1
1:A:1059:VAL:HG23	1:A:1090:TYR:CE1	0.50	2.41	3	1
1:A:1149:GLY:HA3	1:A:1153:TRP:CD2	0.50	2.42	6	3
1:A:1063:ALA:HA	1:A:1090:TYR:CD2	0.49	2.42	10	2
1:A:1107:SER:CB	1:A:1143:THR:OG1	0.49	2.59	5	3
1:A:1155:ARG:NH1	1:A:1163:SER:N	0.49	2.60	2	1
1:A:1094:PHE:C	1:A:1094:PHE:CD1	0.49	2.86	7	1
1:A:1062:THR:CG2	1:A:1090:TYR:CB	0.49	2.89	4	3
1:A:1064:GLU:O	1:A:1073:VAL:CG2	0.49	2.57	10	2
1:A:1075:VAL:CG1	1:A:1076:THR:N	0.49	2.75	10	2
1:A:1059:VAL:HG21	1:A:1144:PHE:HD2	0.49	1.67	6	1
1:A:1088:LEU:O	1:A:1088:LEU:CD1	0.49	2.60	7	1
1:A:1037:PRO:O	1:A:1071:LEU:CD1	0.49	2.61	10	1
1:A:1048:VAL:CG1	1:A:1051:LEU:O	0.49	2.61	8	1
1:A:1038:ARG:HG3	1:A:1071:LEU:HD11	0.49	1.84	9	1
1:A:1040:MET:CB	1:A:1195:ALA:HB3	0.49	2.38	7	2
1:A:1156:ARG:CZ	1:A:1163:SER:OG	0.49	2.61	9	1
1:A:1067:SER:O	1:A:1068:GLU:CG	0.49	2.61	1	1
1:A:1059:VAL:HG21	1:A:1144:PHE:CD2	0.49	2.43	6	1
1:A:1147:LEU:HD22	1:A:1147:LEU:N	0.49	2.22	6	1
1:A:1052:PRO:O	1:A:1056:VAL:HG23	0.48	2.08	3	1
1:A:1080:LYS:CD	1:A:1085:THR:O	0.48	2.61	3	1
1:A:1045:LEU:HD12	1:A:1188:LEU:HD21	0.48	1.80	6	1
1:A:1094:PHE:CB	1:A:1104:CYS:HA	0.48	2.38	2	2
1:A:1088:LEU:O	1:A:1088:LEU:CD2	0.48	2.60	7	1
1:A:1070:PRO:O	1:A:1071:LEU:CB	0.48	2.61	5	1
1:A:1048:VAL:O	1:A:1048:VAL:CG1	0.48	2.61	6	1
1:A:1073:VAL:CG1	1:A:1074:ALA:N	0.48	2.77	5	2
1:A:1155:ARG:NE	1:A:1159:LEU:O	0.48	2.47	2	1
1:A:1164:ASP:O	1:A:1168:ALA:CB	0.48	2.62	2	1
1:A:1150:ASN:O	1:A:1153:TRP:N	0.48	2.47	5	3
1:A:1065:ALA:CA	1:A:1076:THR:HG21	0.48	2.37	4	1
1:A:1040:MET:CE	1:A:1193:ALA:HB1	0.48	2.38	10	1
1:A:1045:LEU:CD1	1:A:1188:LEU:CD2	0.48	2.91	6	1
1:A:1155:ARG:HH12	1:A:1163:SER:N	0.48	2.06	2	1
1:A:1059:VAL:CG2	1:A:1090:TYR:CE2	0.48	2.96	1	1
1:A:1195:ALA:O	1:A:1196:ASP:C	0.48	2.51	2	2
1:A:1065:ALA:CB	1:A:1076:THR:CG2	0.48	2.91	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1153:TRP:CZ3	1:A:1154:LEU:HD22	0.48	2.43	6	1
1:A:1146:VAL:HG22	1:A:1184:ILE:HG12	0.47	1.85	2	1
1:A:1183:ALA:HB1	1:A:1187:VAL:O	0.47	2.09	2	1
1:A:1088:LEU:HD13	1:A:1088:LEU:C	0.47	2.28	7	1
1:A:1155:ARG:CD	1:A:1160:THR:O	0.47	2.62	10	1
1:A:1100:CYS:HB3	1:A:1153:TRP:CZ2	0.47	2.44	4	1
1:A:1151:ARG:O	1:A:1155:ARG:CG	0.47	2.62	8	1
1:A:1154:LEU:HD22	1:A:1181:LEU:HD12	0.47	1.85	10	1
1:A:1195:ALA:C	1:A:1196:ASP:OXT	0.47	2.52	2	2
1:A:1091:CYS:N	1:A:1108:ASN:HD22	0.47	2.08	5	3
1:A:1071:LEU:O	1:A:1071:LEU:HD13	0.47	2.09	2	1
1:A:1045:LEU:O	1:A:1188:LEU:CD2	0.47	2.61	8	1
1:A:1059:VAL:HG22	1:A:1106:VAL:HG21	0.47	1.85	1	1
1:A:1180:ILE:HD13	1:A:1180:ILE:N	0.47	2.24	10	1
1:A:1045:LEU:CB	1:A:1190:GLY:HA2	0.47	2.38	4	3
1:A:1039:VAL:HG23	1:A:1192:ILE:HG23	0.47	1.86	2	1
1:A:1148:ILE:C	1:A:1153:TRP:CH2	0.47	2.88	3	1
1:A:1067:SER:O	1:A:1069:HIS:N	0.47	2.48	4	1
1:A:1090:TYR:CE1	1:A:1106:VAL:HB	0.47	2.45	10	1
1:A:1160:THR:HG22	1:A:1161:ILE:H	0.47	1.70	8	8
1:A:1038:ARG:C	1:A:1194:ILE:HG23	0.47	2.29	10	2
1:A:1148:ILE:HB	1:A:1182:VAL:HG13	0.46	1.87	9	1
1:A:1064:GLU:CB	1:A:1076:THR:OG1	0.46	2.64	1	2
1:A:1152:GLU:OE2	1:A:1156:ARG:CZ	0.46	2.63	6	1
1:A:1062:THR:CG2	1:A:1090:TYR:HB2	0.46	2.41	9	3
1:A:1065:ALA:O	1:A:1073:VAL:HG23	0.46	2.10	5	1
1:A:1067:SER:HA	1:A:1094:PHE:CZ	0.46	2.45	8	1
1:A:1090:TYR:CZ	1:A:1109:VAL:HG12	0.46	2.45	6	1
1:A:1048:VAL:HG21	1:A:1053:LEU:HB2	0.46	1.88	8	1
1:A:1087:THR:O	1:A:1088:LEU:CB	0.46	2.63	8	3
1:A:1090:TYR:CE2	1:A:1106:VAL:CB	0.46	2.98	2	1
1:A:1148:ILE:N	1:A:1148:ILE:CD1	0.46	2.76	6	1
1:A:1090:TYR:CD1	1:A:1106:VAL:HB	0.46	2.45	10	1
1:A:1056:VAL:CG1	1:A:1189:CYS:SG	0.46	3.04	4	1
1:A:1059:VAL:CG1	1:A:1060:VAL:N	0.46	2.78	4	2
1:A:1045:LEU:HD13	1:A:1188:LEU:HD21	0.46	1.87	6	1
1:A:1045:LEU:HD13	1:A:1181:LEU:HD11	0.46	1.88	10	1
1:A:1059:VAL:HB	1:A:1090:TYR:CE2	0.46	2.45	3	2
1:A:1067:SER:OG	1:A:1073:VAL:N	0.46	2.49	4	1
1:A:1150:ASN:ND2	1:A:1170:THR:CG2	0.46	2.79	5	1
1:A:1155:ARG:NH2	1:A:1159:LEU:HD12	0.46	2.26	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1067:SER:O	1:A:1073:VAL:HG21	0.46	2.11	8	1
1:A:1092:THR:HG22	1:A:1106:VAL:HG22	0.46	1.87	9	1
1:A:1062:THR:HG23	1:A:1088:LEU:HA	0.45	1.87	1	1
1:A:1043:LEU:HB3	1:A:1045:LEU:HD21	0.45	1.87	2	1
1:A:1153:TRP:CZ2	1:A:1154:LEU:CD2	0.45	2.94	5	2
1:A:1152:GLU:OE2	1:A:1153:TRP:N	0.45	2.49	8	1
1:A:1145:SER:O	1:A:1185:ASP:N	0.45	2.47	9	4
1:A:1092:THR:HB	1:A:1094:PHE:CE1	0.45	2.45	8	1
1:A:1102:ILE:HD11	1:A:1148:ILE:HB	0.45	1.87	4	1
1:A:1152:GLU:OE2	1:A:1153:TRP:CA	0.45	2.65	8	1
1:A:1056:VAL:O	1:A:1059:VAL:HG12	0.45	2.12	3	2
1:A:1043:LEU:HD13	1:A:1191:MET:CE	0.45	2.41	2	1
1:A:1064:GLU:CB	1:A:1076:THR:CG2	0.45	2.95	8	5
1:A:1110:GLU:CD	1:A:1111:GLY:N	0.45	2.70	7	1
1:A:1072:GLY:O	1:A:1076:THR:OG1	0.45	2.35	10	1
1:A:1045:LEU:HD22	1:A:1045:LEU:N	0.45	2.25	2	1
1:A:1066:SER:O	1:A:1067:SER:C	0.45	2.54	4	1
1:A:1079:CYS:O	1:A:1083:LEU:CD1	0.45	2.62	1	2
1:A:1050:THR:HG21	1:A:1187:VAL:HG21	0.45	1.88	4	1
1:A:1180:ILE:CG1	1:A:1192:ILE:CG2	0.45	2.95	7	1
1:A:1040:MET:SD	1:A:1195:ALA:CB	0.45	3.05	10	1
1:A:1070:PRO:O	1:A:1071:LEU:HB2	0.45	2.12	1	1
1:A:1067:SER:O	1:A:1068:GLU:C	0.44	2.55	4	1
1:A:1079:CYS:O	1:A:1083:LEU:N	0.44	2.50	7	1
1:A:1091:CYS:HB2	1:A:1108:ASN:ND2	0.44	2.28	10	1
1:A:1063:ALA:HA	1:A:1090:TYR:CG	0.44	2.48	2	2
1:A:1108:ASN:C	1:A:1110:GLU:N	0.44	2.71	2	1
1:A:1045:LEU:C	1:A:1188:LEU:HD12	0.44	2.33	5	2
1:A:1146:VAL:HG22	1:A:1184:ILE:CD1	0.44	2.42	8	2
1:A:1069:HIS:CD2	1:A:1070:PRO:HD2	0.44	2.47	4	2
1:A:1074:ALA:O	1:A:1078:TYR:CB	0.44	2.66	1	1
1:A:1086:GLU:O	1:A:1087:THR:O	0.44	2.35	7	1
1:A:1102:ILE:CG1	1:A:1148:ILE:O	0.44	2.65	4	1
1:A:1158:GLY:C	1:A:1159:LEU:CG	0.44	2.86	8	1
1:A:1045:LEU:O	1:A:1188:LEU:HB2	0.44	2.13	10	1
1:A:1151:ARG:O	1:A:1155:ARG:CD	0.44	2.65	1	2
1:A:1045:LEU:HB3	1:A:1188:LEU:CD2	0.44	2.43	2	1
1:A:1056:VAL:O	1:A:1060:VAL:HG23	0.44	2.13	2	2
1:A:1090:TYR:CD2	1:A:1108:ASN:HB3	0.44	2.48	4	1
1:A:1152:GLU:OE2	1:A:1156:ARG:NH2	0.44	2.51	6	1
1:A:1093:ASP:O	1:A:1105:LYS:CB	0.44	2.65	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1044:LEU:O	1:A:1045:LEU:HD13	0.44	2.12	2	1
1:A:1178:THR:HB	1:A:1194:ILE:CG1	0.44	2.43	4	1
1:A:1104:CYS:SG	1:A:1105:LYS:N	0.44	2.91	5	1
1:A:1062:THR:HG23	1:A:1106:VAL:HG21	0.44	1.86	6	1
1:A:1039:VAL:HG23	1:A:1069:HIS:CD2	0.44	2.47	1	1
1:A:1151:ARG:HB2	1:A:1170:THR:CG2	0.44	2.43	3	1
1:A:1155:ARG:NE	1:A:1166:SER:OG	0.43	2.51	1	1
1:A:1170:THR:CG2	1:A:1171:ASP:N	0.43	2.80	2	1
1:A:1075:VAL:HG12	1:A:1076:THR:N	0.43	2.28	10	1
1:A:1184:ILE:HG22	1:A:1187:VAL:HG12	0.43	1.90	1	1
1:A:1086:GLU:O	1:A:1087:THR:C	0.43	2.57	1	1
1:A:1108:ASN:O	1:A:1111:GLY:N	0.43	2.51	5	2
1:A:1180:ILE:HG13	1:A:1192:ILE:HG22	0.43	1.91	7	1
1:A:1151:ARG:CZ	1:A:1179:ALA:CB	0.43	2.97	8	1
1:A:1159:LEU:N	1:A:1159:LEU:CD2	0.43	2.76	9	1
1:A:1173:GLU:O	1:A:1177:GLN:O	0.43	2.37	6	7
1:A:1148:ILE:C	1:A:1153:TRP:CZ2	0.43	2.92	3	2
1:A:1102:ILE:O	1:A:1148:ILE:O	0.43	2.37	5	2
1:A:1087:THR:O	1:A:1088:LEU:CD1	0.43	2.61	1	1
1:A:1064:GLU:HB2	1:A:1076:THR:CG2	0.43	2.44	8	3
1:A:1160:THR:HG22	1:A:1161:ILE:N	0.43	2.28	8	1
1:A:1038:ARG:CG	1:A:1071:LEU:HD21	0.43	2.44	10	1
1:A:1045:LEU:N	1:A:1190:GLY:HA2	0.43	2.29	7	2
1:A:1155:ARG:NH2	1:A:1161:ILE:CD1	0.43	2.80	1	1
1:A:1147:LEU:N	1:A:1147:LEU:CD1	0.43	2.80	5	1
1:A:1155:ARG:NE	1:A:1161:ILE:O	0.43	2.48	6	1
1:A:1066:SER:O	1:A:1067:SER:OG	0.43	2.37	1	1
1:A:1110:GLU:CD	1:A:1142:GLN:O	0.43	2.58	2	1
1:A:1159:LEU:O	1:A:1160:THR:O	0.43	2.37	10	2
1:A:1180:ILE:CG1	1:A:1192:ILE:O	0.43	2.66	9	1
1:A:1048:VAL:CG1	1:A:1053:LEU:HB2	0.42	2.44	2	3
1:A:1062:THR:OG1	1:A:1090:TYR:CD1	0.42	2.52	4	1
1:A:1090:TYR:HA	1:A:1108:ASN:CB	0.42	2.44	7	3
1:A:1153:TRP:CH2	1:A:1157:ASN:ND2	0.42	2.87	9	1
1:A:1148:ILE:HG22	1:A:1182:VAL:HA	0.42	1.89	10	1
1:A:1069:HIS:CG	1:A:1070:PRO:HD2	0.42	2.49	5	1
1:A:1100:CYS:O	1:A:1153:TRP:CE3	0.42	2.72	7	1
1:A:1044:LEU:O	1:A:1045:LEU:HD23	0.42	2.14	3	1
1:A:1089:GLY:O	1:A:1108:ASN:OD1	0.42	2.37	7	1
1:A:1067:SER:C	1:A:1069:HIS:N	0.42	2.72	4	1
1:A:1107:SER:O	1:A:1108:ASN:ND2	0.42	2.49	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1087:THR:O	1:A:1088:LEU:CG	0.42	2.67	9	1
1:A:1180:ILE:HG13	1:A:1192:ILE:CG2	0.42	2.44	7	1
1:A:1090:TYR:CZ	1:A:1109:VAL:HB	0.42	2.50	8	2
1:A:1064:GLU:HB3	1:A:1076:THR:CB	0.42	2.44	1	2
1:A:1065:ALA:O	1:A:1073:VAL:CG1	0.42	2.61	10	1
1:A:1100:CYS:CB	1:A:1153:TRP:CH2	0.42	3.03	2	1
1:A:1151:ARG:HH21	1:A:1155:ARG:HH12	0.42	1.57	4	1
1:A:1067:SER:OG	1:A:1068:GLU:N	0.42	2.50	7	1
1:A:1045:LEU:C	1:A:1188:LEU:HD23	0.42	2.34	8	1
1:A:1062:THR:HG23	1:A:1088:LEU:HB2	0.42	1.91	3	1
1:A:1045:LEU:HD22	1:A:1181:LEU:HD21	0.42	1.91	4	1
1:A:1062:THR:HG21	1:A:1090:TYR:CD1	0.42	2.50	5	1
1:A:1184:ILE:HG23	1:A:1184:ILE:O	0.42	2.15	10	2
1:A:1110:GLU:OE1	1:A:1142:GLN:O	0.41	2.37	2	1
1:A:1045:LEU:CD1	1:A:1191:MET:HB3	0.41	2.44	3	1
1:A:1173:GLU:O	1:A:1177:GLN:N	0.41	2.51	4	1
1:A:1040:MET:C	1:A:1040:MET:SD	0.41	2.99	6	1
1:A:1151:ARG:CZ	1:A:1179:ALA:HB1	0.41	2.44	8	1
1:A:1090:TYR:CE2	1:A:1109:VAL:HG12	0.41	2.49	6	1
1:A:1154:LEU:CD1	1:A:1183:ALA:HB3	0.41	2.45	9	1
1:A:1064:GLU:HB3	1:A:1076:THR:CG2	0.41	2.44	7	1
1:A:1151:ARG:CG	1:A:1181:LEU:HD13	0.41	2.44	1	1
1:A:1154:LEU:HD21	1:A:1183:ALA:CB	0.41	2.46	5	1
1:A:1063:ALA:HB2	1:A:1090:TYR:CD2	0.41	2.50	2	1
1:A:1065:ALA:HA	1:A:1073:VAL:CG2	0.41	2.45	2	1
1:A:1151:ARG:NE	1:A:1179:ALA:HB1	0.41	2.30	8	1
1:A:1160:THR:O	1:A:1161:ILE:O	0.41	2.39	8	1
1:A:1045:LEU:HD23	1:A:1188:LEU:HG	0.41	1.93	4	1
1:A:1045:LEU:O	1:A:1188:LEU:C	0.41	2.59	3	2
1:A:1044:LEU:HD11	1:A:1046:GLY:O	0.41	2.16	4	1
1:A:1184:ILE:O	1:A:1187:VAL:CG1	0.41	2.68	4	1
1:A:1056:VAL:HG13	1:A:1184:ILE:HD13	0.41	1.93	9	1
1:A:1050:THR:O	1:A:1051:LEU:CD1	0.41	2.62	1	1
1:A:1053:LEU:HG	1:A:1057:LEU:HD12	0.41	1.92	1	1
1:A:1061:GLY:HA2	1:A:1076:THR:CG2	0.41	2.46	10	2
1:A:1153:TRP:CZ3	1:A:1181:LEU:O	0.41	2.74	6	1
1:A:1148:ILE:CA	1:A:1153:TRP:CZ2	0.40	3.04	5	1
1:A:1167:ASP:OD1	1:A:1167:ASP:C	0.40	2.59	5	1
1:A:1045:LEU:HD22	1:A:1181:LEU:HD11	0.40	1.93	8	1
1:A:1108:ASN:C	1:A:1108:ASN:OD1	0.40	2.59	2	1
1:A:1184:ILE:HD13	1:A:1189:CYS:CB	0.40	2.47	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:1059:VAL:HG22	1:A:1106:VAL:HG13	0.40	1.93	6	1
1:A:1062:THR:HG22	1:A:1106:VAL:HG21	0.40	1.87	6	1
1:A:1151:ARG:O	1:A:1155:ARG:CB	0.40	2.70	8	1
1:A:1155:ARG:O	1:A:1159:LEU:C	0.40	2.59	9	1
1:A:1110:GLU:C	1:A:1110:GLU:CD	0.40	2.80	10	1
1:A:1058:ALA:O	1:A:1062:THR:OG1	0.40	2.36	1	1
1:A:1094:PHE:HA	1:A:1104:CYS:CB	0.40	2.47	3	1
1:A:1054:ARG:CB	1:A:1055:LYS:HE2	0.40	2.46	6	1
1:A:1154:LEU:HB2	1:A:1181:LEU:HD13	0.40	1.94	9	1
1:A:1067:SER:O	1:A:1068:GLU:OE1	0.40	2.40	1	1
1:A:1063:ALA:CA	1:A:1090:TYR:CD2	0.40	3.05	2	1
1:A:1164:ASP:O	1:A:1168:ALA:HB2	0.40	2.17	2	1
1:A:1059:VAL:HB	1:A:1090:TYR:CZ	0.40	2.51	3	1
1:A:1060:VAL:O	1:A:1064:GLU:CB	0.40	2.70	4	1
1:A:1052:PRO:HG2	1:A:1055:LYS:CG	0.40	2.47	6	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	130/165 (79%)	112±2 (86±1%)	11±1 (9±1%)	6±2 (5±1%)	4	25
All	All	1300/1650 (79%)	1122 (86%)	113 (9%)	65 (5%)	4	25

All 14 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	1108	ASN	10
1	A	1161	ILE	10
1	A	1176	GLY	9
1	A	1089	GLY	7
1	A	1071	LEU	6
1	A	1158	GLY	6
1	A	1068	GLU	4

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Mol	Chain	Res	Type	Models (Total)
1	A	1067	SER	3
1	A	1087	THR	3
1	A	1088	LEU	2
1	A	1160	THR	2
1	A	1048	VAL	1
1	A	1159	LEU	1
1	A	1050	THR	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	106/131 (81%)	73±5 (69±4%)	33±5 (31±4%)	1 15
All	All	1060/1310 (81%)	733 (69%)	327 (31%)	1 15

All 88 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	1043	LEU	10
1	A	1159	LEU	10
1	A	1171	ASP	10
1	A	1188	LEU	10
1	A	1076	THR	9
1	A	1148	ILE	9
1	A	1055	LYS	8
1	A	1079	CYS	8
1	A	1071	LEU	7
1	A	1077	LYS	7
1	A	1080	LYS	7
1	A	1082	GLU	7
1	A	1163	SER	7
1	A	1038	ARG	7
1	A	1068	GLU	6
1	A	1088	LEU	6
1	A	1152	GLU	6
1	A	1085	THR	6

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Mol	Chain	Res	Type	Models (Total)
1	A	1181	LEU	6
1	A	1108	ASN	5
1	A	1155	ARG	5
1	A	1175	LYS	5
1	A	1060	VAL	5
1	A	1147	LEU	5
1	A	1153	TRP	5
1	A	1042	VAL	4
1	A	1073	VAL	4
1	A	1090	TYR	4
1	A	1102	ILE	4
1	A	1174	MET	4
1	A	1047	ASP	4
1	A	1106	VAL	4
1	A	1161	ILE	4
1	A	1041	ARG	4
1	A	1045	LEU	4
1	A	1057	LEU	4
1	A	1059	VAL	4
1	A	1062	THR	4
1	A	1078	TYR	4
1	A	1051	LEU	3
1	A	1054	ARG	3
1	A	1156	ARG	3
1	A	1169	MET	3
1	A	1182	VAL	3
1	A	1184	ILE	3
1	A	1187	VAL	3
1	A	1040	MET	3
1	A	1067	SER	3
1	A	1081	GLU	3
1	A	1093	ASP	3
1	A	1170	THR	3
1	A	1097	VAL	3
1	A	1154	LEU	3
1	A	1172	HIS	3
1	A	1173	GLU	2
1	A	1056	VAL	2
1	A	1075	VAL	2
1	A	1105	LYS	2
1	A	1107	SER	2
1	A	1191	MET	2

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Mol	Chain	Res	Type	Models (Total)
1	A	1196	ASP	2
1	A	1039	VAL	2
1	A	1086	GLU	2
1	A	1069	HIS	2
1	A	1185	ASP	2
1	A	1100	CYS	2
1	A	1164	ASP	2
1	A	1109	VAL	2
1	A	1110	GLU	2
1	A	1143	THR	2
1	A	1092	THR	1
1	A	1053	LEU	1
1	A	1167	ASP	1
1	A	1091	CYS	1
1	A	1178	THR	1
1	A	1194	ILE	1
1	A	1095	GLN	1
1	A	1066	SER	1
1	A	1087	THR	1
1	A	1094	PHE	1
1	A	1192	ILE	1
1	A	1142	GLN	1
1	A	1044	LEU	1
1	A	1050	THR	1
1	A	1151	ARG	1
1	A	1162	SER	1
1	A	1064	GLU	1
1	A	1180	ILE	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

There are no ligands in this entry.

6.7 Other polymers

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