Full wwPDB NMR Structure Validation Report (i)

Feb 19, 2022 – 08:29 PM EST

PDB ID	:	1UB1
Title	:	Solution structure of the matrix attachment region-binding domain of chicken MeCP2
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Deposited on	:	2003-03-27

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:

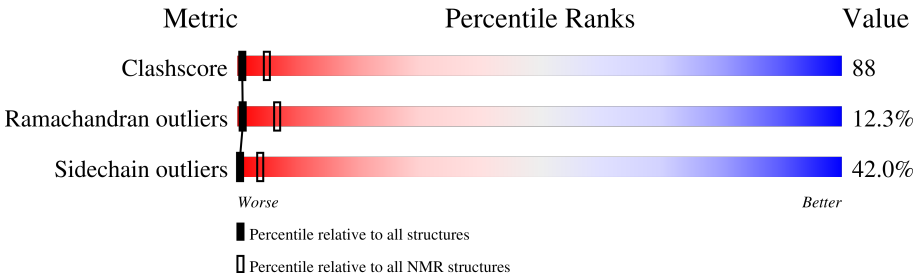
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

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	133	5% 24% 17% 48% 6%

2 Ensemble composition and analysis

This entry contains 10 models. Model 1 is the overall representative, medoid model (most similar to other models).

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:104-A:164 (61)	0.99	1

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

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

The models can be grouped into 3 clusters and 2 single-model clusters were found.

Cluster number	Models
1	1, 2, 4, 10
2	8, 9
3	5, 6
Single-model clusters	3; 7

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1969 atoms, of which 998 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called attachment region binding protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	125	1969	601	998	190	179	1	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	MET	-	expression tag	UNP O42403
A	65	GLY	-	expression tag	UNP O42403
A	66	HIS	-	expression tag	UNP O42403
A	67	HIS	-	expression tag	UNP O42403
A	68	HIS	-	expression tag	UNP O42403
A	69	HIS	-	expression tag	UNP O42403
A	70	HIS	-	expression tag	UNP O42403
A	71	HIS	-	expression tag	UNP O42403

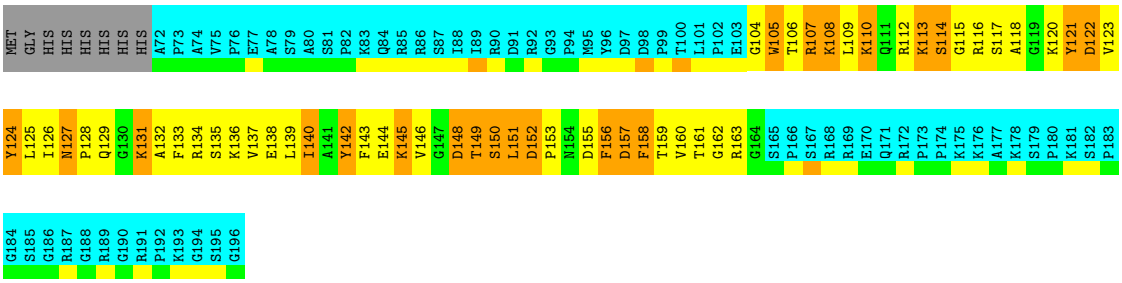
4 Residue-property plots (i)

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: attachment region binding protein

Chain A: 



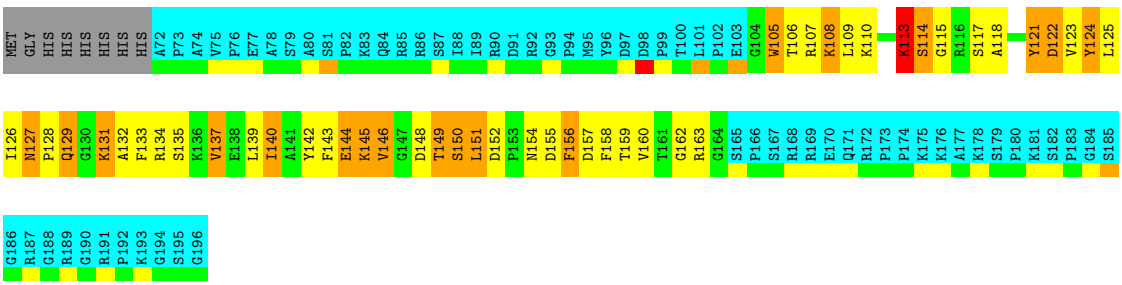
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1 (medoid)

• Molecule 1: attachment region binding protein

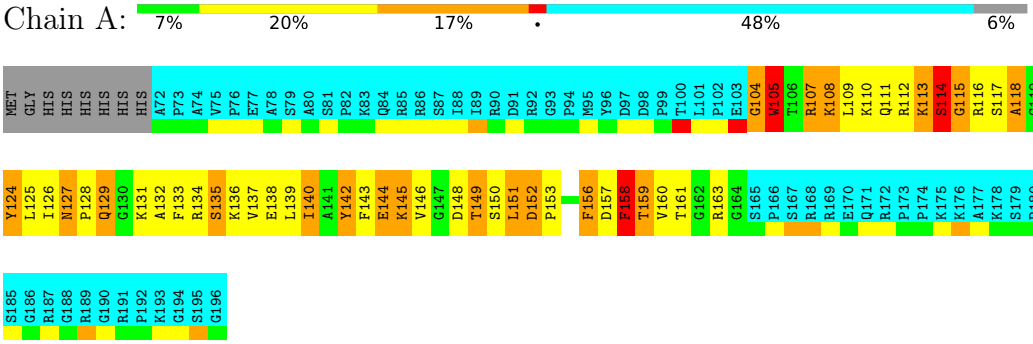
Chain A: 



4.2.2 Score per residue for model 2

• Molecule 1: attachment region binding protein

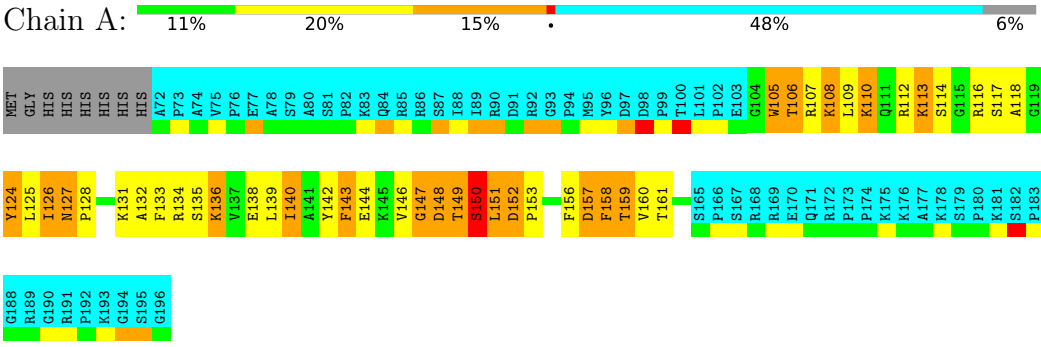
Chain A:



4.2.3 Score per residue for model 3

• Molecule 1: attachment region binding protein

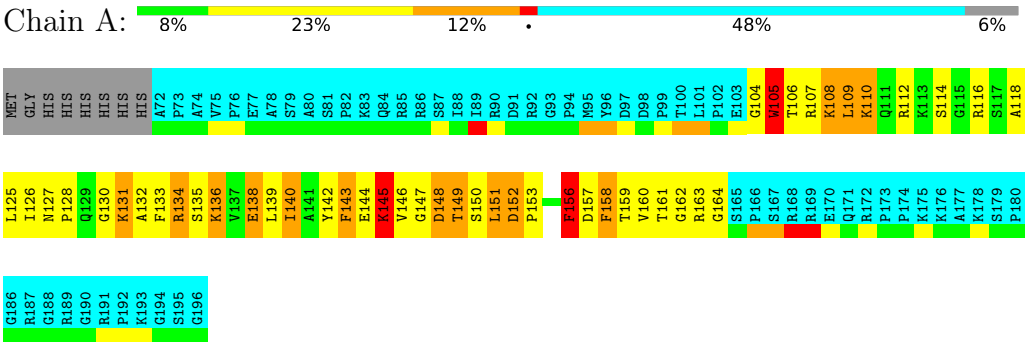
Chain A:



4.2.4 Score per residue for model 4

• Molecule 1: attachment region binding protein

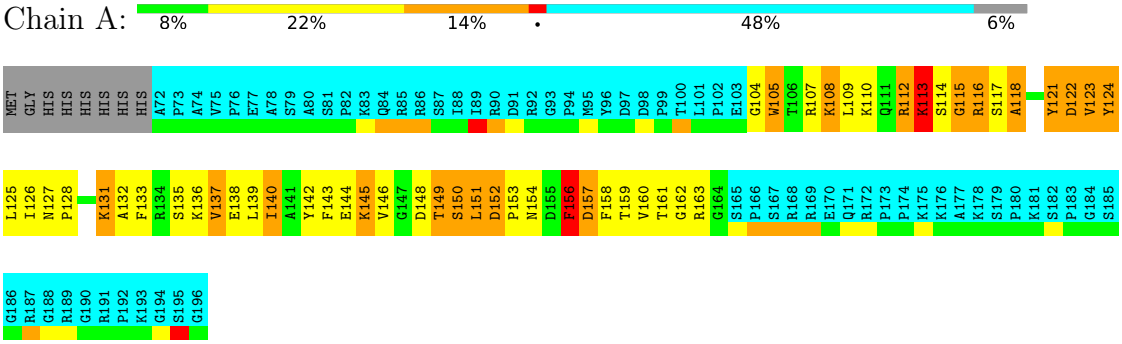
Chain A:



4.2.5 Score per residue for model 5

• Molecule 1: attachment region binding protein

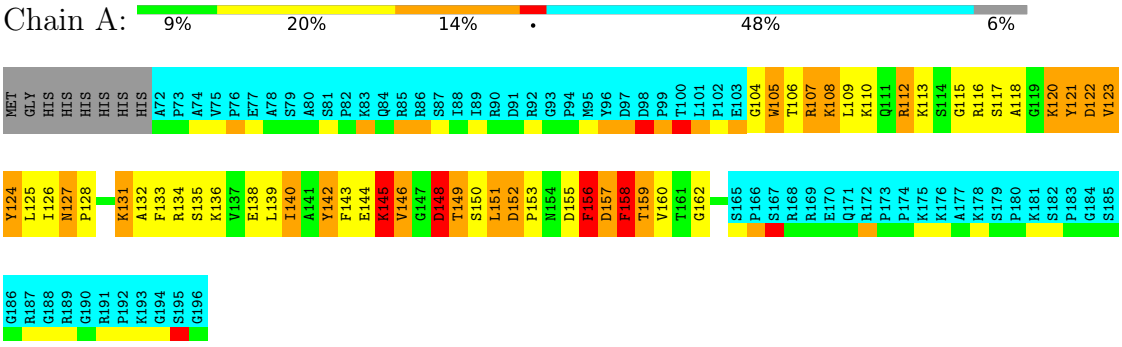
Chain A:



4.2.6 Score per residue for model 6

• Molecule 1: attachment region binding protein

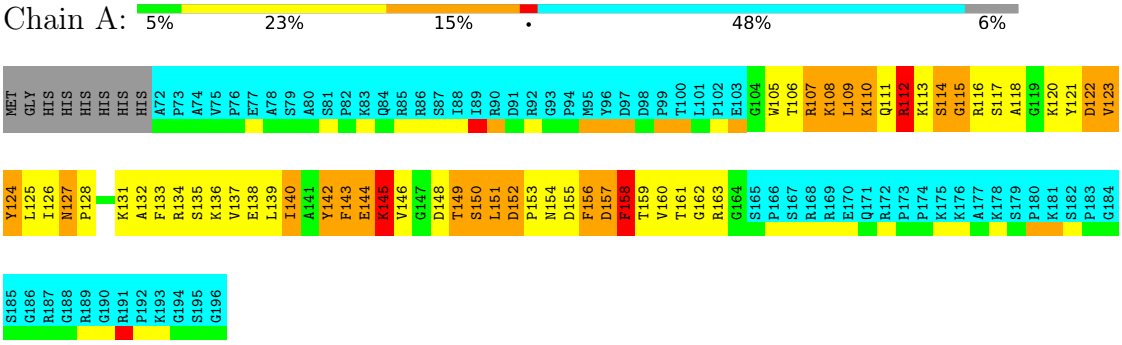
Chain A:



4.2.7 Score per residue for model 7

• Molecule 1: attachment region binding protein

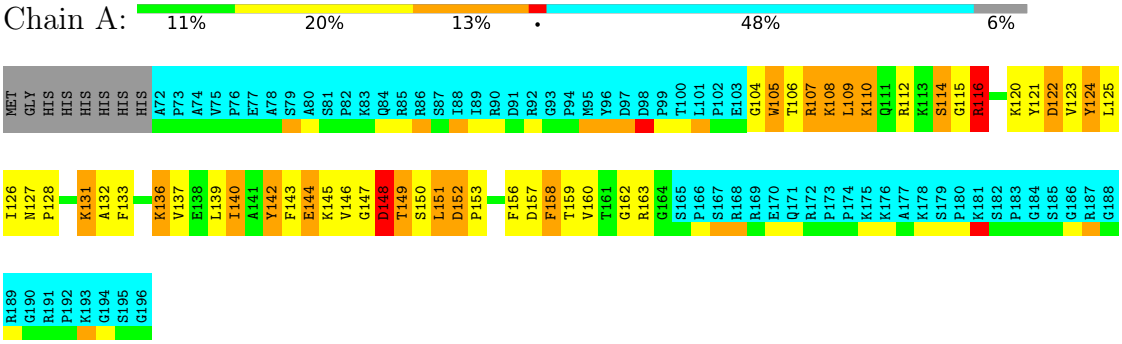
Chain A:



4.2.8 Score per residue for model 8

• Molecule 1: attachment region binding protein

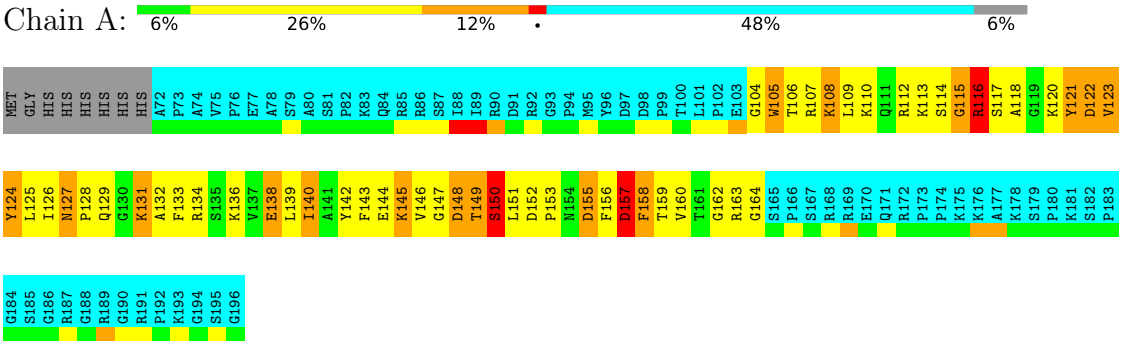
Chain A:



4.2.9 Score per residue for model 9

• Molecule 1: attachment region binding protein

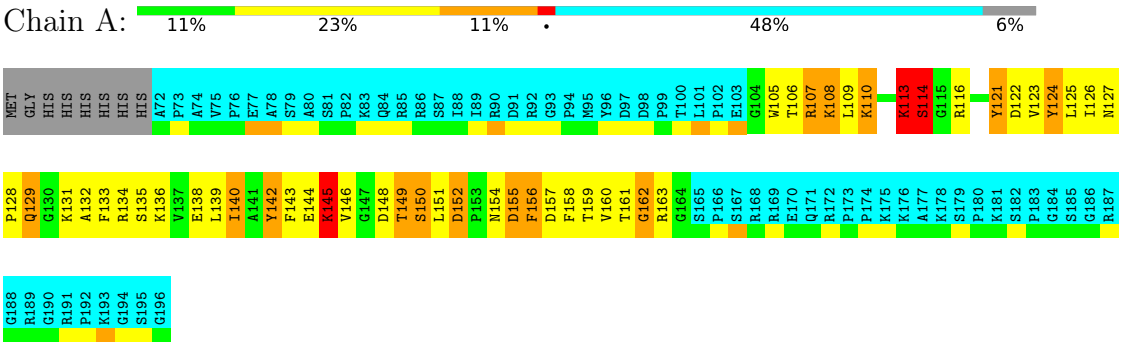
Chain A:



4.2.10 Score per residue for model 10

• Molecule 1: attachment region binding protein

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 240 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
DYANA	refinement	1.5

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	489	496	489	86±7
All	All	4890	4960	4890	860

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:123:VAL:HG23	1:A:160:VAL:HG12	1.08	1.19	5	10
1:A:123:VAL:HG21	1:A:159:THR:OG1	0.98	1.58	6	9
1:A:158:PHE:CD1	1:A:158:PHE:O	0.94	2.20	9	3
1:A:139:LEU:HD11	1:A:151:LEU:HD11	0.90	1.43	6	3
1:A:125:LEU:HD11	1:A:157:ASP:O	0.89	1.68	7	2
1:A:135:SER:OG	1:A:137:VAL:HG12	0.87	1.69	7	2
1:A:133:PHE:CE1	1:A:142:TYR:CD2	0.87	2.62	4	2
1:A:121:TYR:HB2	1:A:160:VAL:HG21	0.86	1.46	5	7
1:A:142:TYR:CD2	1:A:146:VAL:HG11	0.86	2.06	10	3
1:A:142:TYR:O	1:A:146:VAL:HG12	0.86	1.71	10	8
1:A:109:LEU:HD21	1:A:121:TYR:CB	0.84	2.00	1	9
1:A:156:PHE:CE1	1:A:158:PHE:CE1	0.83	2.65	6	2
1:A:133:PHE:CZ	1:A:142:TYR:CD2	0.83	2.67	4	1
1:A:105:TRP:CH2	1:A:151:LEU:HD21	0.82	2.09	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:PHE:CD1	1:A:142:TYR:CD2	0.82	2.68	9	1
1:A:139:LEU:HD11	1:A:143:PHE:CZ	0.81	2.11	1	2
1:A:109:LEU:HD11	1:A:160:VAL:HB	0.81	1.52	7	10
1:A:133:PHE:CE1	1:A:142:TYR:CE2	0.80	2.69	4	1
1:A:133:PHE:CD1	1:A:142:TYR:CE2	0.80	2.69	4	2
1:A:140:ILE:O	1:A:144:GLU:N	0.79	2.15	6	10
1:A:109:LEU:HD23	1:A:110:LYS:N	0.78	1.94	1	6
1:A:108:LYS:O	1:A:124:TYR:N	0.78	2.17	1	10
1:A:124:TYR:CD1	1:A:132:ALA:HB1	0.77	2.14	8	9
1:A:151:LEU:HD11	1:A:157:ASP:OD1	0.77	1.79	10	1
1:A:128:PRO:O	1:A:129:GLN:CB	0.77	2.33	10	1
1:A:139:LEU:HD11	1:A:151:LEU:HD21	0.76	1.57	2	1
1:A:143:PHE:O	1:A:147:GLY:N	0.74	2.21	9	3
1:A:109:LEU:HD21	1:A:121:TYR:HB2	0.74	1.59	6	9
1:A:125:LEU:HD13	1:A:157:ASP:OD2	0.74	1.83	9	1
1:A:123:VAL:CG2	1:A:160:VAL:HG12	0.73	2.08	5	8
1:A:127:ASN:OD1	1:A:151:LEU:HD23	0.73	1.82	6	1
1:A:127:ASN:OD1	1:A:127:ASN:C	0.72	2.27	10	5
1:A:125:LEU:HD21	1:A:157:ASP:O	0.72	1.83	3	2
1:A:105:TRP:O	1:A:105:TRP:CG	0.72	2.42	6	1
1:A:128:PRO:O	1:A:129:GLN:CG	0.72	2.37	10	1
1:A:159:THR:OG1	1:A:160:VAL:N	0.72	2.17	8	3
1:A:105:TRP:CE3	1:A:126:ILE:O	0.72	2.43	7	1
1:A:127:ASN:CB	1:A:128:PRO:CD	0.71	2.67	10	10
1:A:142:TYR:O	1:A:146:VAL:CG1	0.71	2.39	1	8
1:A:109:LEU:HD21	1:A:121:TYR:HB3	0.71	1.61	1	4
1:A:156:PHE:CZ	1:A:158:PHE:CZ	0.71	2.79	6	1
1:A:105:TRP:O	1:A:106:THR:HG23	0.70	1.86	6	3
1:A:108:LYS:N	1:A:124:TYR:O	0.70	2.23	3	10
1:A:151:LEU:HD21	1:A:157:ASP:OD2	0.70	1.87	10	1
1:A:127:ASN:HB2	1:A:128:PRO:CD	0.69	2.16	10	4
1:A:149:THR:HG22	1:A:150:SER:N	0.69	2.03	6	2
1:A:139:LEU:CD1	1:A:143:PHE:CZ	0.69	2.76	1	2
1:A:127:ASN:HB2	1:A:128:PRO:HD2	0.69	1.64	4	4
1:A:109:LEU:HG	1:A:160:VAL:HG11	0.69	1.63	1	10
1:A:158:PHE:O	1:A:158:PHE:CG	0.68	2.46	4	4
1:A:133:PHE:CZ	1:A:142:TYR:CG	0.67	2.82	4	1
1:A:106:THR:O	1:A:126:ILE:HD12	0.67	1.90	3	3
1:A:136:LYS:CD	1:A:156:PHE:CE2	0.67	2.78	8	2
1:A:126:ILE:HA	1:A:131:LYS:O	0.66	1.90	10	10
1:A:143:PHE:O	1:A:147:GLY:HA2	0.66	1.90	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:127:ASN:ND2	1:A:142:TYR:CE2	0.66	2.63	10	1
1:A:124:TYR:CE2	1:A:132:ALA:HB3	0.66	2.26	7	1
1:A:123:VAL:HG21	1:A:159:THR:H	0.66	1.50	7	2
1:A:131:LYS:CD	1:A:142:TYR:CE1	0.65	2.79	8	1
1:A:136:LYS:CE	1:A:156:PHE:CZ	0.65	2.80	3	1
1:A:158:PHE:CD2	1:A:162:GLY:CA	0.65	2.79	7	3
1:A:122:ASP:C	1:A:160:VAL:CG1	0.65	2.66	1	10
1:A:138:GLU:O	1:A:142:TYR:CD2	0.64	2.50	4	2
1:A:158:PHE:CD1	1:A:158:PHE:N	0.64	2.65	3	3
1:A:153:PRO:O	1:A:156:PHE:CE2	0.64	2.50	4	2
1:A:127:ASN:ND2	1:A:133:PHE:CE2	0.64	2.65	7	1
1:A:128:PRO:O	1:A:129:GLN:HB2	0.64	1.92	10	1
1:A:105:TRP:CE2	1:A:151:LEU:HD12	0.64	2.28	10	1
1:A:157:ASP:O	1:A:158:PHE:C	0.64	2.36	4	1
1:A:123:VAL:N	1:A:160:VAL:CG1	0.64	2.60	1	8
1:A:127:ASN:OD1	1:A:133:PHE:CE2	0.64	2.51	3	1
1:A:108:LYS:NZ	1:A:126:ILE:HD12	0.64	2.08	2	1
1:A:139:LEU:HD11	1:A:151:LEU:CD1	0.64	2.20	6	3
1:A:125:LEU:HD12	1:A:158:PHE:CE2	0.63	2.28	10	1
1:A:149:THR:HG22	1:A:149:THR:O	0.63	1.94	3	6
1:A:123:VAL:HB	1:A:161:THR:HG22	0.63	1.69	5	2
1:A:127:ASN:CB	1:A:128:PRO:HD2	0.63	2.22	10	6
1:A:143:PHE:C	1:A:143:PHE:CD1	0.62	2.72	3	2
1:A:139:LEU:HD23	1:A:153:PRO:HA	0.62	1.71	9	3
1:A:158:PHE:CE2	1:A:163:ARG:CD	0.62	2.83	4	1
1:A:121:TYR:CB	1:A:160:VAL:HG21	0.62	2.24	5	1
1:A:153:PRO:O	1:A:156:PHE:CD1	0.62	2.53	2	1
1:A:105:TRP:CD1	1:A:105:TRP:N	0.62	2.68	3	1
1:A:142:TYR:O	1:A:146:VAL:HB	0.61	1.95	4	2
1:A:105:TRP:CH2	1:A:157:ASP:CG	0.61	2.73	9	1
1:A:145:LYS:O	1:A:145:LYS:CG	0.61	2.49	2	4
1:A:105:TRP:C	1:A:105:TRP:CD1	0.61	2.73	2	2
1:A:105:TRP:HE1	1:A:151:LEU:HD22	0.61	1.56	8	1
1:A:156:PHE:CZ	1:A:158:PHE:HB3	0.61	2.30	9	1
1:A:157:ASP:O	1:A:159:THR:HG23	0.60	1.96	10	3
1:A:143:PHE:CE1	1:A:152:ASP:OD1	0.60	2.54	4	2
1:A:143:PHE:CE1	1:A:151:LEU:O	0.60	2.55	5	1
1:A:109:LEU:CD2	1:A:121:TYR:CB	0.60	2.79	6	5
1:A:124:TYR:CZ	1:A:132:ALA:HB3	0.60	2.32	7	1
1:A:109:LEU:HG	1:A:122:ASP:O	0.60	1.96	5	2
1:A:105:TRP:CZ2	1:A:151:LEU:HD21	0.59	2.32	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:VAL:HB	1:A:160:VAL:HG12	0.59	1.74	9	2
1:A:105:TRP:CD1	1:A:126:ILE:O	0.59	2.55	2	1
1:A:105:TRP:CZ2	1:A:157:ASP:OD1	0.59	2.56	9	1
1:A:149:THR:O	1:A:150:SER:CB	0.59	2.50	3	5
1:A:123:VAL:HG11	1:A:158:PHE:HA	0.59	1.75	5	5
1:A:109:LEU:CD2	1:A:121:TYR:HB3	0.59	2.27	6	10
1:A:124:TYR:CE2	1:A:132:ALA:CB	0.59	2.86	7	1
1:A:123:VAL:CG2	1:A:159:THR:OG1	0.58	2.50	3	5
1:A:143:PHE:O	1:A:147:GLY:CA	0.58	2.51	3	3
1:A:158:PHE:CD2	1:A:162:GLY:HA3	0.58	2.32	7	3
1:A:133:PHE:CD2	1:A:139:LEU:HD12	0.58	2.33	9	2
1:A:125:LEU:HD21	1:A:157:ASP:HB3	0.58	1.74	4	1
1:A:156:PHE:N	1:A:156:PHE:CD1	0.58	2.66	6	2
1:A:143:PHE:CZ	1:A:152:ASP:OD1	0.58	2.56	6	1
1:A:108:LYS:O	1:A:124:TYR:CB	0.58	2.51	7	5
1:A:139:LEU:CD1	1:A:151:LEU:HD11	0.58	2.26	6	1
1:A:105:TRP:CE2	1:A:151:LEU:HD22	0.58	2.34	7	1
1:A:125:LEU:HD22	1:A:157:ASP:OD1	0.57	1.99	3	1
1:A:144:GLU:O	1:A:145:LYS:HB3	0.57	2.00	7	4
1:A:158:PHE:CD2	1:A:161:THR:HG23	0.57	2.34	2	1
1:A:127:ASN:OD1	1:A:128:PRO:N	0.57	2.38	10	1
1:A:142:TYR:CG	1:A:146:VAL:HG11	0.57	2.34	10	3
1:A:142:TYR:O	1:A:146:VAL:CB	0.57	2.53	4	3
1:A:123:VAL:CB	1:A:160:VAL:HG12	0.56	2.30	9	6
1:A:138:GLU:CG	1:A:142:TYR:CE2	0.56	2.88	9	2
1:A:139:LEU:O	1:A:143:PHE:CB	0.56	2.54	5	8
1:A:136:LYS:HD2	1:A:156:PHE:CE2	0.56	2.36	2	3
1:A:136:LYS:HD3	1:A:156:PHE:CE2	0.56	2.35	8	2
1:A:143:PHE:CD1	1:A:143:PHE:O	0.55	2.59	4	1
1:A:156:PHE:CZ	1:A:158:PHE:CB	0.55	2.90	9	1
1:A:136:LYS:HA	1:A:158:PHE:CE2	0.55	2.37	5	3
1:A:122:ASP:C	1:A:160:VAL:HG11	0.55	2.22	3	8
1:A:131:LYS:HD3	1:A:142:TYR:CE1	0.55	2.35	8	1
1:A:131:LYS:HD2	1:A:142:TYR:CE1	0.55	2.36	8	2
1:A:139:LEU:HG	1:A:143:PHE:CE2	0.55	2.36	8	3
1:A:108:LYS:HZ1	1:A:126:ILE:HD12	0.55	1.62	2	1
1:A:156:PHE:CE2	1:A:158:PHE:CD1	0.55	2.95	3	1
1:A:127:ASN:N	1:A:131:LYS:O	0.55	2.38	10	1
1:A:108:LYS:O	1:A:124:TYR:HB2	0.54	2.02	8	8
1:A:140:ILE:HD12	1:A:153:PRO:HG3	0.54	1.77	3	1
1:A:105:TRP:O	1:A:106:THR:CG2	0.54	2.55	10	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:105:TRP:CE3	1:A:106:THR:N	0.54	2.76	7	2
1:A:122:ASP:CA	1:A:160:VAL:HG13	0.54	2.32	1	2
1:A:105:TRP:CH2	1:A:157:ASP:OD1	0.54	2.60	9	1
1:A:109:LEU:HA	1:A:122:ASP:O	0.54	2.02	5	7
1:A:133:PHE:CE1	1:A:138:GLU:CG	0.54	2.91	6	1
1:A:112:ARG:HH11	1:A:118:ALA:HB1	0.54	1.63	6	1
1:A:156:PHE:CE2	1:A:158:PHE:HB3	0.53	2.38	9	1
1:A:107:ARG:HA	1:A:124:TYR:O	0.53	2.03	6	7
1:A:107:ARG:CB	1:A:125:LEU:HD23	0.53	2.33	3	1
1:A:131:LYS:HG2	1:A:142:TYR:CE2	0.53	2.38	1	1
1:A:139:LEU:O	1:A:143:PHE:HB2	0.53	2.04	1	3
1:A:136:LYS:HE2	1:A:156:PHE:CZ	0.53	2.38	3	1
1:A:149:THR:CG2	1:A:150:SER:N	0.53	2.69	6	2
1:A:136:LYS:HG3	1:A:156:PHE:CD2	0.53	2.38	8	3
1:A:157:ASP:O	1:A:158:PHE:O	0.53	2.25	2	1
1:A:146:VAL:O	1:A:148:ASP:N	0.53	2.41	3	2
1:A:110:LYS:O	1:A:122:ASP:N	0.53	2.41	3	7
1:A:127:ASN:HA	1:A:151:LEU:HD23	0.53	1.81	4	1
1:A:121:TYR:O	1:A:160:VAL:HG22	0.53	2.04	7	1
1:A:125:LEU:O	1:A:133:PHE:N	0.53	2.36	7	10
1:A:124:TYR:CD1	1:A:132:ALA:CB	0.53	2.92	8	3
1:A:126:ILE:HG23	1:A:131:LYS:O	0.53	2.03	3	2
1:A:143:PHE:CD1	1:A:151:LEU:O	0.53	2.61	5	1
1:A:112:ARG:O	1:A:113:LYS:CB	0.53	2.57	5	1
1:A:139:LEU:O	1:A:143:PHE:CG	0.53	2.61	8	2
1:A:124:TYR:CE1	1:A:132:ALA:C	0.53	2.83	8	8
1:A:136:LYS:CD	1:A:156:PHE:CD2	0.52	2.93	8	2
1:A:136:LYS:HD2	1:A:156:PHE:CD2	0.52	2.39	2	2
1:A:144:GLU:O	1:A:145:LYS:CB	0.52	2.57	2	2
1:A:158:PHE:CD2	1:A:162:GLY:HA2	0.52	2.39	7	1
1:A:105:TRP:NE1	1:A:151:LEU:HD22	0.52	2.19	8	1
1:A:152:ASP:CB	1:A:153:PRO:CD	0.52	2.88	2	4
1:A:133:PHE:CD1	1:A:138:GLU:HB3	0.52	2.39	6	2
1:A:143:PHE:CD2	1:A:153:PRO:HD3	0.52	2.39	6	1
1:A:105:TRP:CE3	1:A:128:PRO:HD3	0.52	2.40	1	1
1:A:123:VAL:CG1	1:A:161:THR:HG22	0.52	2.35	3	2
1:A:124:TYR:CE1	1:A:134:ARG:HG3	0.52	2.40	4	3
1:A:124:TYR:CG	1:A:132:ALA:HB1	0.52	2.40	8	3
1:A:107:ARG:CG	1:A:125:LEU:CD2	0.52	2.87	2	1
1:A:149:THR:O	1:A:149:THR:CG2	0.52	2.58	3	4
1:A:125:LEU:HD12	1:A:158:PHE:CZ	0.52	2.40	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:156:PHE:CE1	1:A:158:PHE:CZ	0.52	2.97	6	1
1:A:105:TRP:CE3	1:A:105:TRP:C	0.52	2.83	9	1
1:A:125:LEU:HD21	1:A:157:ASP:OD1	0.52	2.05	2	1
1:A:133:PHE:CE1	1:A:142:TYR:CG	0.52	2.98	9	2
1:A:151:LEU:HD13	1:A:157:ASP:OD1	0.52	2.04	1	1
1:A:139:LEU:O	1:A:143:PHE:HB3	0.52	2.05	4	6
1:A:139:LEU:O	1:A:143:PHE:N	0.51	2.39	1	7
1:A:140:ILE:HA	1:A:143:PHE:HB3	0.51	1.81	10	4
1:A:140:ILE:HA	1:A:143:PHE:HB2	0.51	1.82	8	2
1:A:139:LEU:HD23	1:A:153:PRO:CA	0.51	2.36	9	2
1:A:131:LYS:HD2	1:A:133:PHE:CE1	0.51	2.40	6	2
1:A:143:PHE:HA	1:A:147:GLY:CA	0.51	2.36	3	1
1:A:149:THR:O	1:A:149:THR:HG22	0.51	2.05	5	1
1:A:136:LYS:CE	1:A:153:PRO:O	0.51	2.58	9	1
1:A:136:LYS:HD2	1:A:156:PHE:CE1	0.51	2.40	7	1
1:A:152:ASP:OD1	1:A:154:ASN:CB	0.51	2.59	1	1
1:A:158:PHE:CG	1:A:162:GLY:HA3	0.51	2.40	7	2
1:A:125:LEU:CD2	1:A:157:ASP:OD1	0.51	2.59	2	1
1:A:146:VAL:HG12	1:A:148:ASP:OD2	0.51	2.06	10	1
1:A:123:VAL:O	1:A:161:THR:HG21	0.50	2.06	10	1
1:A:113:LYS:O	1:A:114:SER:CB	0.50	2.58	1	2
1:A:139:LEU:HD22	1:A:156:PHE:CB	0.50	2.36	9	1
1:A:156:PHE:CE2	1:A:158:PHE:CB	0.50	2.95	9	1
1:A:136:LYS:HG3	1:A:156:PHE:CD1	0.50	2.41	9	1
1:A:136:LYS:HE3	1:A:156:PHE:CZ	0.50	2.42	3	1
1:A:143:PHE:CD2	1:A:153:PRO:HG3	0.50	2.41	4	1
1:A:140:ILE:O	1:A:144:GLU:HB2	0.50	2.07	5	6
1:A:145:LYS:CG	1:A:146:VAL:N	0.50	2.74	9	1
1:A:153:PRO:O	1:A:156:PHE:CD2	0.50	2.65	5	3
1:A:143:PHE:CD2	1:A:148:ASP:HB2	0.50	2.42	9	2
1:A:125:LEU:O	1:A:133:PHE:CD2	0.50	2.65	5	2
1:A:105:TRP:C	1:A:105:TRP:CD2	0.50	2.86	9	1
1:A:109:LEU:CG	1:A:160:VAL:HG11	0.49	2.37	4	8
1:A:143:PHE:HA	1:A:146:VAL:HG12	0.49	1.83	8	1
1:A:122:ASP:HA	1:A:160:VAL:HG13	0.49	1.84	1	2
1:A:147:GLY:O	1:A:148:ASP:C	0.49	2.50	3	2
1:A:123:VAL:N	1:A:160:VAL:HG13	0.49	2.22	3	5
1:A:124:TYR:CD2	1:A:132:ALA:HB1	0.49	2.42	7	1
1:A:110:LYS:N	1:A:122:ASP:O	0.49	2.40	4	2
1:A:105:TRP:CD1	1:A:128:PRO:HB3	0.49	2.43	4	1
1:A:144:GLU:OE1	1:A:145:LYS:CE	0.49	2.60	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:124:TYR:CZ	1:A:134:ARG:HG3	0.49	2.43	1	5
1:A:131:LYS:HG2	1:A:133:PHE:CE1	0.49	2.43	2	1
1:A:105:TRP:NE1	1:A:149:THR:CG2	0.49	2.76	4	1
1:A:136:LYS:HD2	1:A:156:PHE:CD1	0.49	2.43	7	1
1:A:139:LEU:HG	1:A:143:PHE:CD2	0.49	2.43	1	1
1:A:131:LYS:HD3	1:A:133:PHE:CE1	0.49	2.43	3	3
1:A:111:GLN:HB2	1:A:121:TYR:CE2	0.49	2.43	7	1
1:A:127:ASN:ND2	1:A:133:PHE:CZ	0.49	2.80	7	1
1:A:125:LEU:CD1	1:A:157:ASP:OD2	0.48	2.58	9	1
1:A:127:ASN:OD1	1:A:130:GLY:N	0.48	2.47	4	1
1:A:156:PHE:O	1:A:158:PHE:N	0.48	2.46	9	1
1:A:104:GLY:O	1:A:105:TRP:C	0.48	2.50	4	1
1:A:129:GLN:NE2	1:A:142:TYR:OH	0.48	2.47	2	1
1:A:131:LYS:CE	1:A:133:PHE:CE1	0.48	2.96	6	1
1:A:158:PHE:CE2	1:A:163:ARG:HD3	0.48	2.43	4	1
1:A:128:PRO:CG	1:A:148:ASP:OD1	0.48	2.62	5	1
1:A:124:TYR:CE1	1:A:132:ALA:CB	0.48	2.97	1	5
1:A:146:VAL:C	1:A:148:ASP:N	0.48	2.66	3	1
1:A:139:LEU:O	1:A:143:PHE:CD1	0.48	2.66	1	1
1:A:131:LYS:HD2	1:A:142:TYR:CZ	0.48	2.43	8	3
1:A:143:PHE:CZ	1:A:152:ASP:HB3	0.48	2.44	2	2
1:A:123:VAL:CB	1:A:161:THR:HG22	0.48	2.39	5	2
1:A:105:TRP:CE3	1:A:127:ASN:HA	0.48	2.43	10	1
1:A:127:ASN:OD1	1:A:131:LYS:O	0.47	2.32	7	1
1:A:143:PHE:CE2	1:A:153:PRO:CD	0.47	2.97	6	1
1:A:115:GLY:O	1:A:117:SER:N	0.47	2.47	7	3
1:A:139:LEU:CD1	1:A:143:PHE:CE1	0.47	2.97	1	1
1:A:127:ASN:OD1	1:A:127:ASN:N	0.47	2.46	3	1
1:A:140:ILE:HG13	1:A:143:PHE:CD1	0.47	2.44	3	1
1:A:109:LEU:HD11	1:A:160:VAL:CB	0.47	2.34	7	4
1:A:112:ARG:NE	1:A:120:LYS:O	0.47	2.47	6	1
1:A:135:SER:CB	1:A:137:VAL:HG12	0.47	2.39	7	1
1:A:156:PHE:CD1	1:A:158:PHE:HB2	0.47	2.44	1	2
1:A:143:PHE:CA	1:A:147:GLY:HA2	0.47	2.40	3	1
1:A:136:LYS:HA	1:A:158:PHE:CZ	0.47	2.44	8	2
1:A:136:LYS:HB2	1:A:156:PHE:CZ	0.47	2.45	9	1
1:A:127:ASN:ND2	1:A:131:LYS:CG	0.47	2.78	10	1
1:A:127:ASN:CG	1:A:128:PRO:HD2	0.47	2.30	9	3
1:A:109:LEU:HD23	1:A:121:TYR:HB3	0.47	1.87	7	1
1:A:149:THR:CG2	1:A:149:THR:O	0.47	2.63	4	1
1:A:152:ASP:OD2	1:A:155:ASP:N	0.46	2.48	9	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:143:PHE:CG	1:A:147:GLY:HA2	0.46	2.45	3	1
1:A:105:TRP:C	1:A:106:THR:HG23	0.46	2.31	10	1
1:A:104:GLY:O	1:A:105:TRP:CB	0.46	2.63	2	1
1:A:147:GLY:O	1:A:148:ASP:O	0.46	2.33	3	1
1:A:139:LEU:HD21	1:A:151:LEU:HD11	0.46	1.88	5	1
1:A:128:PRO:HG3	1:A:149:THR:HG21	0.46	1.88	6	1
1:A:136:LYS:HG3	1:A:156:PHE:CG	0.46	2.45	9	3
1:A:127:ASN:HB3	1:A:133:PHE:CZ	0.46	2.45	4	1
1:A:156:PHE:CD1	1:A:158:PHE:CE1	0.46	3.04	4	2
1:A:131:LYS:HE3	1:A:142:TYR:CE1	0.46	2.46	5	1
1:A:148:ASP:CG	1:A:149:THR:N	0.46	2.68	6	1
1:A:131:LYS:HG2	1:A:142:TYR:CZ	0.46	2.46	5	1
1:A:143:PHE:CE1	1:A:152:ASP:CG	0.46	2.89	6	1
1:A:107:ARG:HG2	1:A:125:LEU:CD2	0.46	2.41	10	2
1:A:109:LEU:HG	1:A:160:VAL:CG1	0.46	2.40	3	5
1:A:125:LEU:CD2	1:A:157:ASP:O	0.46	2.61	3	1
1:A:110:LYS:O	1:A:122:ASP:CB	0.46	2.64	3	2
1:A:107:ARG:O	1:A:107:ARG:NE	0.46	2.48	8	1
1:A:107:ARG:HB2	1:A:125:LEU:HD23	0.46	1.86	3	1
1:A:138:GLU:HG3	1:A:142:TYR:CE2	0.46	2.46	4	2
1:A:117:SER:O	1:A:118:ALA:O	0.46	2.34	5	1
1:A:120:LYS:O	1:A:121:TYR:O	0.46	2.34	2	1
1:A:127:ASN:ND2	1:A:148:ASP:OD1	0.46	2.49	2	1
1:A:139:LEU:CD1	1:A:151:LEU:HD21	0.46	2.38	2	1
1:A:152:ASP:C	1:A:152:ASP:OD2	0.45	2.55	1	1
1:A:139:LEU:HD21	1:A:143:PHE:CE2	0.45	2.47	1	1
1:A:124:TYR:CE1	1:A:134:ARG:CG	0.45	3.00	4	1
1:A:133:PHE:CD2	1:A:139:LEU:CD1	0.45	3.00	9	1
1:A:158:PHE:CZ	1:A:163:ARG:HD3	0.45	2.47	4	1
1:A:136:LYS:HD2	1:A:156:PHE:CZ	0.45	2.46	2	1
1:A:159:THR:O	1:A:164:GLY:N	0.45	2.48	4	1
1:A:127:ASN:CG	1:A:128:PRO:CD	0.45	2.85	9	1
1:A:146:VAL:CG1	1:A:148:ASP:OD2	0.45	2.64	10	1
1:A:125:LEU:CD1	1:A:157:ASP:O	0.45	2.58	3	1
1:A:135:SER:OG	1:A:137:VAL:CG1	0.45	2.64	5	1
1:A:111:GLN:O	1:A:112:ARG:CB	0.45	2.65	7	1
1:A:109:LEU:HD12	1:A:123:VAL:HG23	0.45	1.88	9	1
1:A:139:LEU:HD11	1:A:151:LEU:CD2	0.45	2.35	2	1
1:A:122:ASP:CA	1:A:160:VAL:CG1	0.44	2.95	10	2
1:A:113:LYS:O	1:A:115:GLY:N	0.44	2.50	2	1
1:A:113:LYS:C	1:A:115:GLY:N	0.44	2.70	2	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:156:PHE:CD1	1:A:156:PHE:O	0.44	2.71	2	1
1:A:155:ASP:O	1:A:156:PHE:O	0.44	2.35	1	1
1:A:152:ASP:O	1:A:156:PHE:N	0.44	2.50	9	1
1:A:124:TYR:CE1	1:A:132:ALA:HB1	0.44	2.48	1	2
1:A:135:SER:HB3	1:A:137:VAL:CG1	0.44	2.43	1	2
1:A:117:SER:O	1:A:118:ALA:C	0.44	2.55	2	3
1:A:152:ASP:CB	1:A:153:PRO:HD2	0.44	2.43	2	2
1:A:136:LYS:HE2	1:A:156:PHE:CE2	0.44	2.48	6	1
1:A:121:TYR:N	1:A:121:TYR:CD1	0.44	2.81	5	1
1:A:136:LYS:HB2	1:A:156:PHE:CE2	0.44	2.47	9	1
1:A:124:TYR:CD1	1:A:133:PHE:C	0.44	2.91	6	2
1:A:133:PHE:CE2	1:A:139:LEU:HD12	0.44	2.48	7	1
1:A:123:VAL:N	1:A:160:VAL:HG12	0.43	2.27	1	1
1:A:161:THR:HG23	1:A:161:THR:O	0.43	2.13	3	2
1:A:127:ASN:OD1	1:A:151:LEU:CD2	0.43	2.60	6	1
1:A:139:LEU:CG	1:A:143:PHE:CE2	0.43	3.02	1	1
1:A:159:THR:C	1:A:161:THR:N	0.43	2.70	2	4
1:A:107:ARG:O	1:A:107:ARG:CG	0.43	2.67	3	3
1:A:110:LYS:O	1:A:121:TYR:CD2	0.43	2.71	7	1
1:A:131:LYS:HD3	1:A:142:TYR:CD1	0.43	2.49	8	1
1:A:124:TYR:HA	1:A:133:PHE:O	0.43	2.14	3	1
1:A:143:PHE:CA	1:A:147:GLY:CA	0.43	2.97	3	1
1:A:158:PHE:CE2	1:A:163:ARG:HD2	0.43	2.48	4	1
1:A:139:LEU:O	1:A:148:ASP:OD2	0.43	2.37	3	1
1:A:143:PHE:CE2	1:A:153:PRO:HD3	0.43	2.48	5	1
1:A:124:TYR:CE1	1:A:133:PHE:N	0.43	2.87	10	1
1:A:158:PHE:N	1:A:158:PHE:HD1	0.43	2.11	3	2
1:A:133:PHE:CE1	1:A:138:GLU:HG3	0.43	2.48	6	2
1:A:148:ASP:OD1	1:A:149:THR:N	0.43	2.52	8	1
1:A:136:LYS:CD	1:A:153:PRO:O	0.43	2.67	9	1
1:A:160:VAL:O	1:A:164:GLY:O	0.43	2.37	9	1
1:A:131:LYS:CG	1:A:142:TYR:CZ	0.42	3.02	1	1
1:A:157:ASP:CG	1:A:158:PHE:N	0.42	2.73	8	1
1:A:139:LEU:CG	1:A:143:PHE:CZ	0.42	3.02	1	1
1:A:139:LEU:HD11	1:A:151:LEU:HD12	0.42	1.90	3	1
1:A:156:PHE:CE2	1:A:158:PHE:CG	0.42	3.07	3	1
1:A:105:TRP:CD2	1:A:105:TRP:N	0.42	2.87	4	1
1:A:105:TRP:CD2	1:A:126:ILE:O	0.42	2.72	7	1
1:A:105:TRP:CD1	1:A:150:SER:OG	0.42	2.72	7	1
1:A:146:VAL:HG22	1:A:146:VAL:O	0.42	2.14	9	1
1:A:125:LEU:HD22	1:A:157:ASP:OD2	0.42	2.14	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:151:LEU:HD11	1:A:157:ASP:CG	0.42	2.35	10	1
1:A:154:ASN:O	1:A:155:ASP:OD1	0.42	2.38	10	1
1:A:149:THR:HG22	1:A:150:SER:H	0.42	1.74	6	1
1:A:144:GLU:OE1	1:A:145:LYS:CD	0.42	2.68	10	1
1:A:158:PHE:CB	1:A:162:GLY:HA3	0.42	2.44	9	1
1:A:135:SER:HB3	1:A:137:VAL:HG12	0.42	1.91	1	1
1:A:158:PHE:O	1:A:162:GLY:HA3	0.42	2.15	8	4
1:A:143:PHE:HA	1:A:147:GLY:N	0.42	2.29	3	1
1:A:149:THR:O	1:A:150:SER:HB2	0.42	2.12	3	1
1:A:123:VAL:HG23	1:A:160:VAL:CG1	0.42	2.14	5	1
1:A:123:VAL:HB	1:A:160:VAL:CG1	0.42	2.44	9	1
1:A:108:LYS:NZ	1:A:126:ILE:CD1	0.41	2.81	2	1
1:A:157:ASP:C	1:A:158:PHE:CD1	0.41	2.93	4	1
1:A:156:PHE:CZ	1:A:158:PHE:CE1	0.41	3.05	6	1
1:A:134:ARG:CZ	1:A:134:ARG:HB3	0.41	2.45	10	2
1:A:104:GLY:O	1:A:105:TRP:HB3	0.41	2.15	2	1
1:A:143:PHE:CE1	1:A:152:ASP:HA	0.41	2.50	10	1
1:A:107:ARG:CG	1:A:125:LEU:HD22	0.41	2.44	2	1
1:A:131:LYS:HB3	1:A:142:TYR:CE2	0.41	2.51	1	1
1:A:133:PHE:CD1	1:A:138:GLU:CG	0.41	3.03	6	1
1:A:105:TRP:HB2	1:A:126:ILE:O	0.41	2.16	7	1
1:A:131:LYS:CD	1:A:142:TYR:CZ	0.41	3.03	8	1
1:A:158:PHE:HB3	1:A:162:GLY:CA	0.41	2.45	8	1
1:A:107:ARG:O	1:A:107:ARG:HG2	0.41	2.15	6	1
1:A:112:ARG:CD	1:A:120:LYS:O	0.41	2.68	6	1
1:A:136:LYS:CA	1:A:158:PHE:CZ	0.41	3.04	8	1
1:A:124:TYR:CD1	1:A:133:PHE:N	0.41	2.89	1	1
1:A:114:SER:O	1:A:115:GLY:C	0.41	2.59	5	1
1:A:136:LYS:HD2	1:A:156:PHE:CG	0.41	2.51	2	1
1:A:114:SER:O	1:A:115:GLY:O	0.41	2.39	7	2
1:A:123:VAL:CG1	1:A:161:THR:CG2	0.41	2.99	7	1
1:A:115:GLY:O	1:A:116:ARG:C	0.41	2.59	8	2
1:A:157:ASP:O	1:A:158:PHE:HB3	0.41	2.16	7	1
1:A:107:ARG:HB2	1:A:125:LEU:CD2	0.41	2.45	8	1
1:A:125:LEU:CD2	1:A:157:ASP:HB2	0.40	2.46	3	1
1:A:123:VAL:HB	1:A:161:THR:CG2	0.40	2.47	7	1
1:A:107:ARG:CZ	1:A:107:ARG:HB3	0.40	2.45	1	1
1:A:104:GLY:O	1:A:106:THR:N	0.40	2.53	4	1
1:A:157:ASP:OD1	1:A:157:ASP:N	0.40	2.53	6	1
1:A:139:LEU:CD1	1:A:151:LEU:CD1	0.40	2.99	7	1
1:A:156:PHE:C	1:A:157:ASP:OD1	0.40	2.60	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:146:VAL:O	1:A:147:GLY:C	0.40	2.60	9	1
1:A:113:LYS:O	1:A:114:SER:C	0.40	2.60	2	1
1:A:143:PHE:CD1	1:A:152:ASP:HA	0.40	2.50	2	1
1:A:136:LYS:CG	1:A:156:PHE:CD2	0.40	3.04	8	1
1:A:148:ASP:OD1	1:A:151:LEU:O	0.40	2.38	8	1
1:A:109:LEU:CD1	1:A:123:VAL:HG23	0.40	2.46	9	1
1:A:139:LEU:HD22	1:A:156:PHE:HB3	0.40	1.94	9	1
1:A:128:PRO:O	1:A:129:GLN:HG3	0.40	2.12	10	1
1:A:107:ARG:CD	1:A:157:ASP:OD2	0.40	2.70	2	1
1:A:144:GLU:OE2	1:A:145:LYS:CE	0.40	2.70	7	1
1:A:108:LYS:HE3	1:A:126:ILE:CD1	0.40	2.45	8	1
1:A:111:GLN:HG3	1:A:121:TYR:CD1	0.40	2.51	2	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	61/133 (46%)	43±1 (70±2%)	11±2 (18±4%)	8±2 (12±3%)	1	6
All	All	610/1330 (46%)	427 (70%)	108 (18%)	75 (12%)	1	6

All 18 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	150	SER	8
1	A	116	ARG	8
1	A	145	LYS	7
1	A	156	PHE	6
1	A	113	LYS	5
1	A	114	SER	5
1	A	118	ALA	5
1	A	121	TYR	5
1	A	158	PHE	5
1	A	148	ASP	4

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Mol	Chain	Res	Type	Models (Total)
1	A	115	GLY	4
1	A	105	TRP	3
1	A	104	GLY	3
1	A	129	GLN	2
1	A	162	GLY	2
1	A	147	GLY	1
1	A	112	ARG	1
1	A	157	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	51/110 (46%)	30±4 (58±8%)	21±4 (42±8%)	0 4
All	All	510/1100 (46%)	296 (58%)	214 (42%)	0 4

All 42 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	108	LYS	10
1	A	124	TYR	10
1	A	140	ILE	10
1	A	149	THR	10
1	A	122	ASP	9
1	A	151	LEU	9
1	A	112	ARG	8
1	A	152	ASP	8
1	A	113	LYS	7
1	A	163	ARG	7
1	A	105	TRP	7
1	A	127	ASN	6
1	A	131	LYS	6
1	A	114	SER	6
1	A	120	LYS	6
1	A	138	GLU	6
1	A	145	LYS	6

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Mol	Chain	Res	Type	Models (Total)
1	A	107	ARG	5
1	A	135	SER	5
1	A	142	TYR	5
1	A	158	PHE	5
1	A	110	LYS	5
1	A	157	ASP	5
1	A	148	ASP	5
1	A	144	GLU	4
1	A	116	ARG	4
1	A	156	PHE	4
1	A	123	VAL	4
1	A	155	ASP	4
1	A	129	GLN	3
1	A	137	VAL	3
1	A	159	THR	3
1	A	136	LYS	3
1	A	143	PHE	3
1	A	109	LEU	3
1	A	146	VAL	2
1	A	150	SER	2
1	A	154	ASN	2
1	A	106	THR	1
1	A	126	ILE	1
1	A	134	ARG	1
1	A	121	TYR	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 (i)

No chemical shift data were provided