



Full wwPDB NMR Structure Validation Report ⓘ

May 29, 2020 – 09:06 am BST

PDB ID : 5YJ4
Title : structure for the protective mutant G127V of Human prion protein
Authors : Zheng, Z.; Lin, D.
Deposited on : 2017-10-07

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 ⓘ symbol.

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

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
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 : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

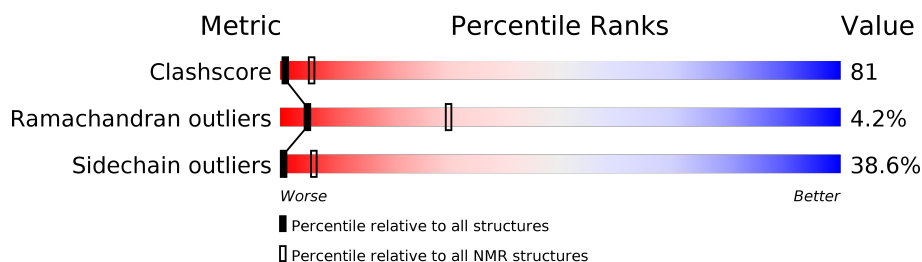
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 82%.

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	142	

2 Ensemble composition and analysis

This entry contains 20 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:128-A:164, A:174-A:192, A:199-A:221 (79)	0.20	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 4 clusters and 3 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2216 atoms, of which 1079 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major prion protein.

Mol	Chain	Residues	Atoms						Trace
1	A	142	Total	C	H	N	O	S	0
			2216	701	1079	204	220	12	

There are 2 discrepancies between the modelled and reference sequences:

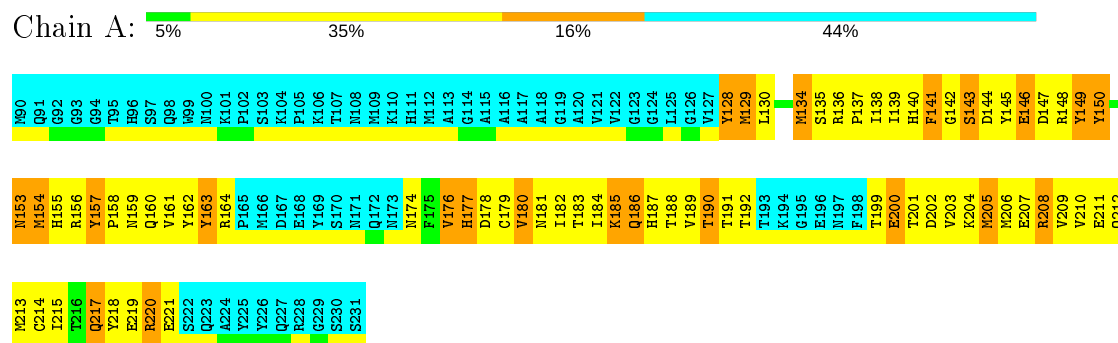
Chain	Residue	Modelled	Actual	Comment	Reference
A	90	MET	-	initiating methionine	UNP P04156
A	127	VAL	GLY	variant	UNP P04156

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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: Major prion protein

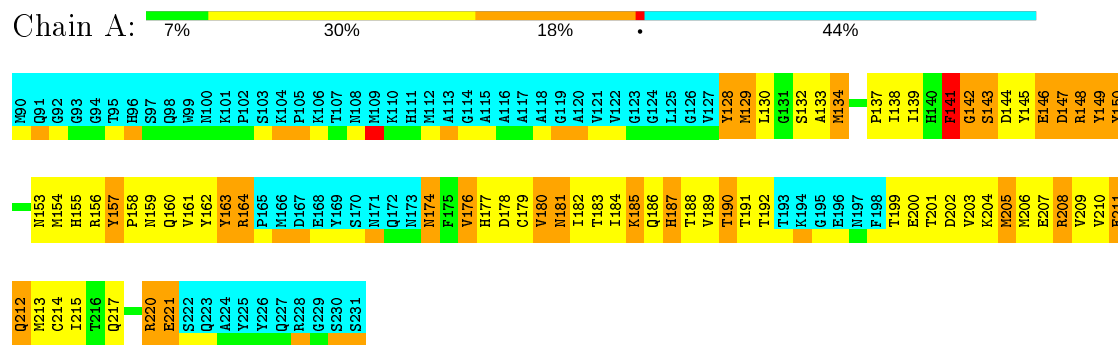


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

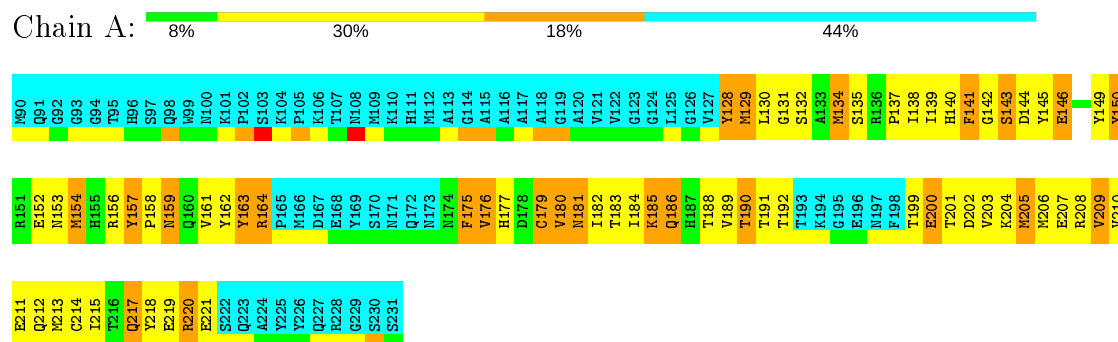
4.2.1 Score per residue for model 1 (medoid)

- Molecule 1: Major prion protein



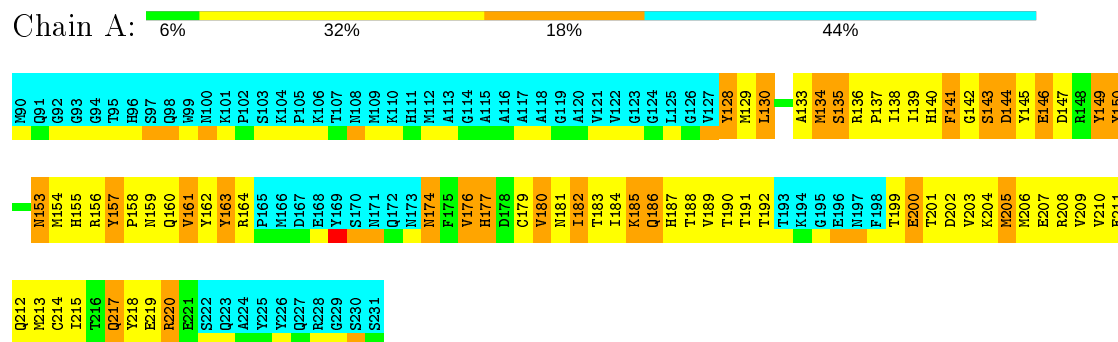
4.2.2 Score per residue for model 2

- Molecule 1: Major prion protein



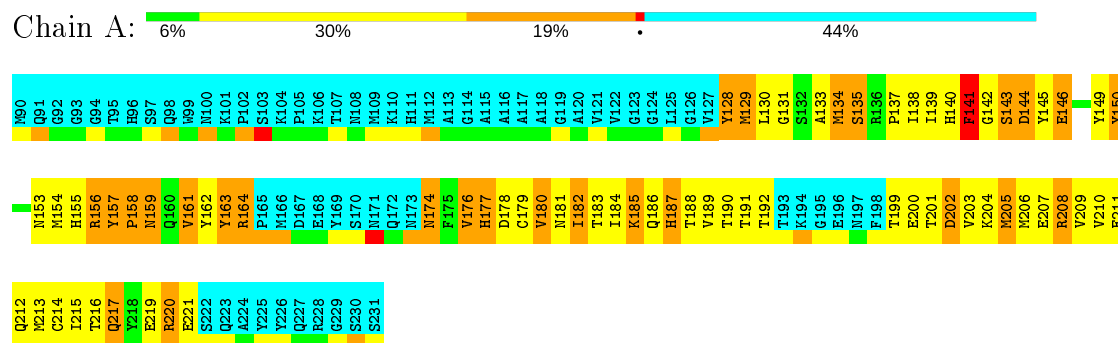
4.2.3 Score per residue for model 3

- Molecule 1: Major prion protein



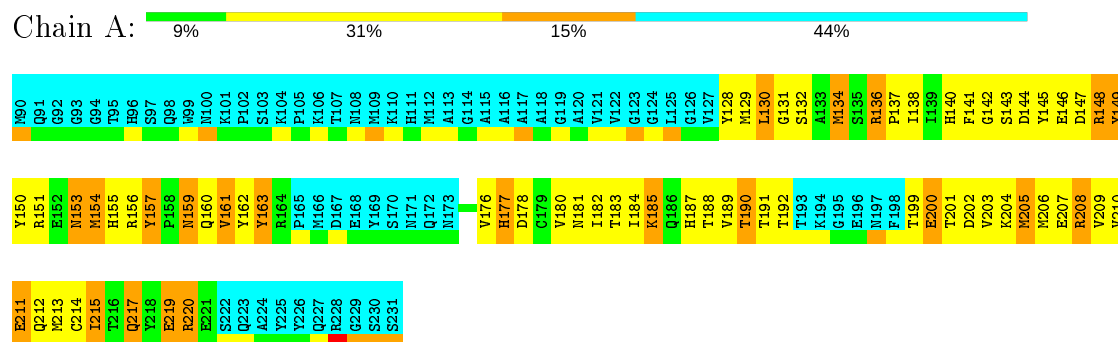
4.2.4 Score per residue for model 4

- Molecule 1: Major prion protein



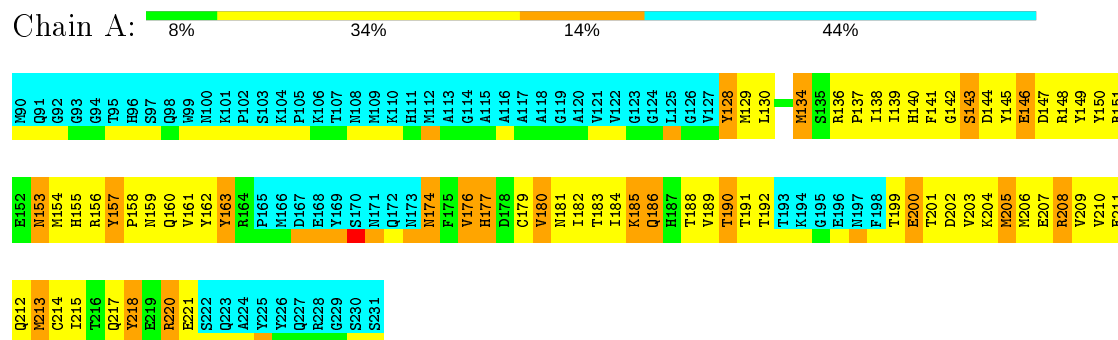
4.2.5 Score per residue for model 5

- Molecule 1: Major prion protein



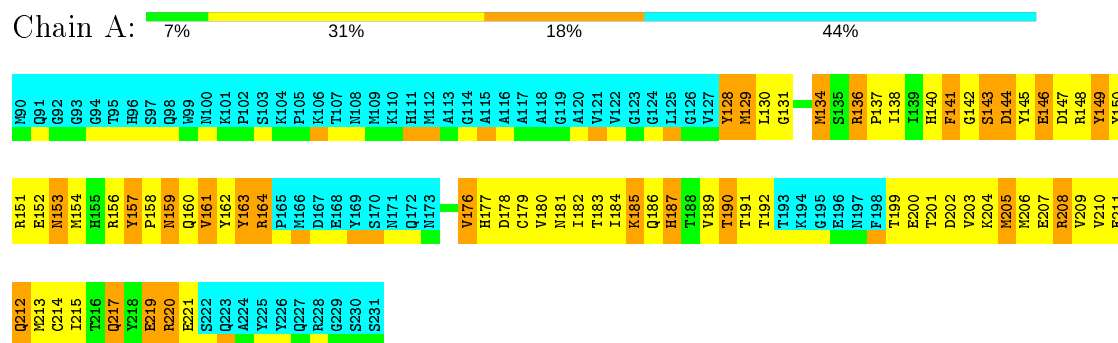
4.2.6 Score per residue for model 6

- Molecule 1: Major prion protein



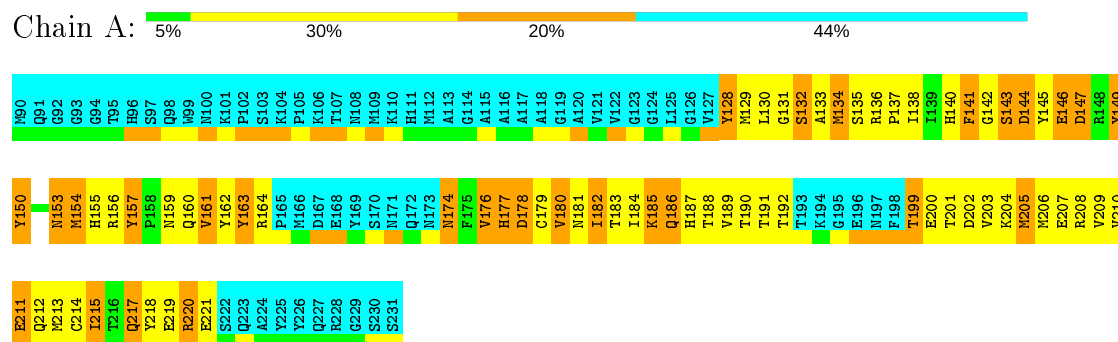
4.2.7 Score per residue for model 7

- Molecule 1: Major prion protein



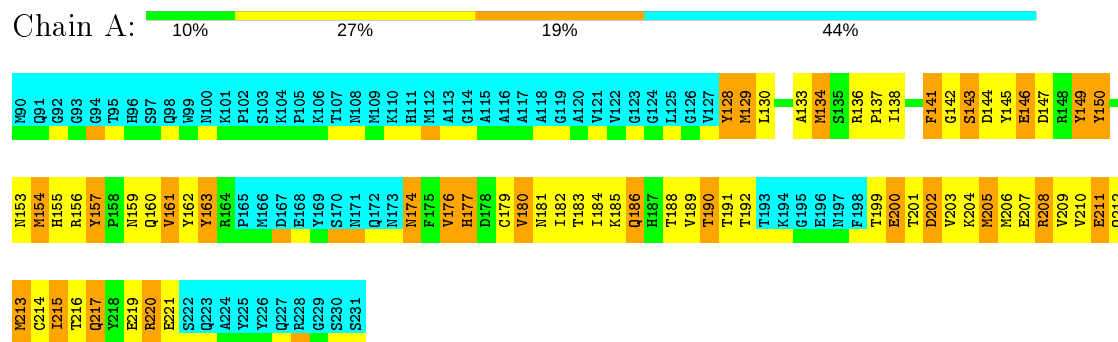
4.2.8 Score per residue for model 8

- Molecule 1: Major prion protein



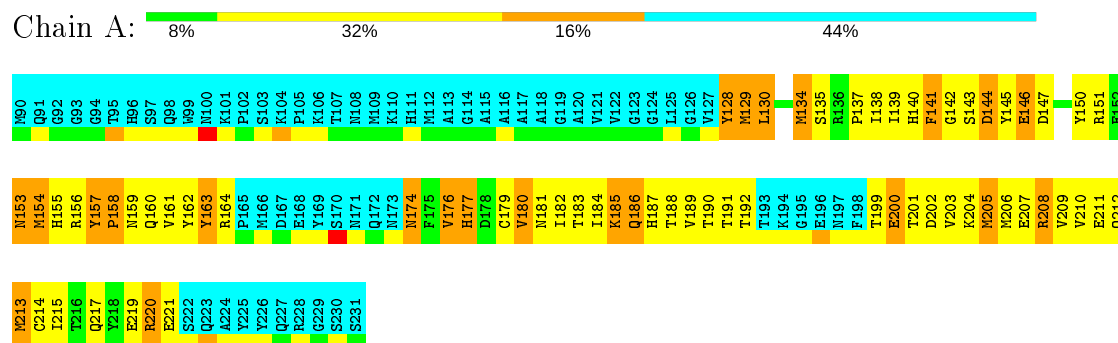
4.2.9 Score per residue for model 9

- Molecule 1: Major prion protein



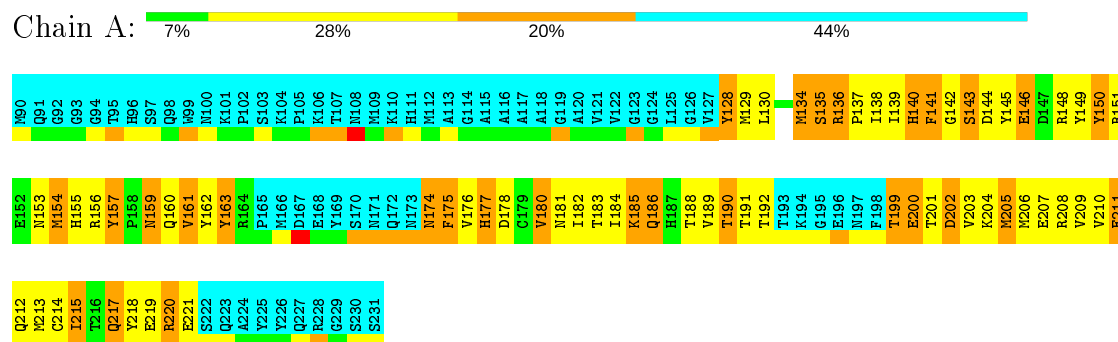
4.2.10 Score per residue for model 10

- Molecule 1: Major prion protein



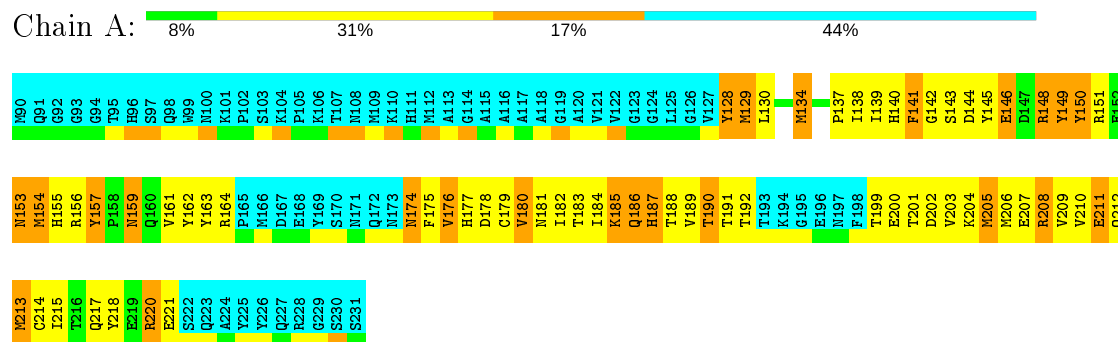
4.2.11 Score per residue for model 11

- Molecule 1: Major prion protein



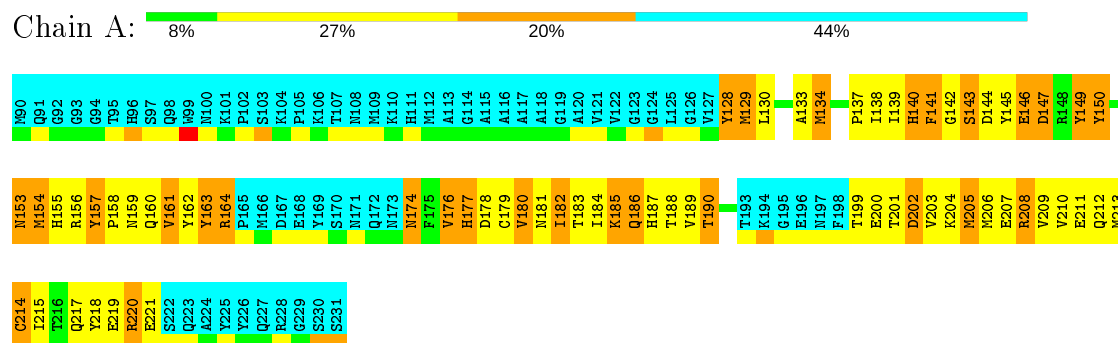
4.2.12 Score per residue for model 12

- Molecule 1: Major prion protein



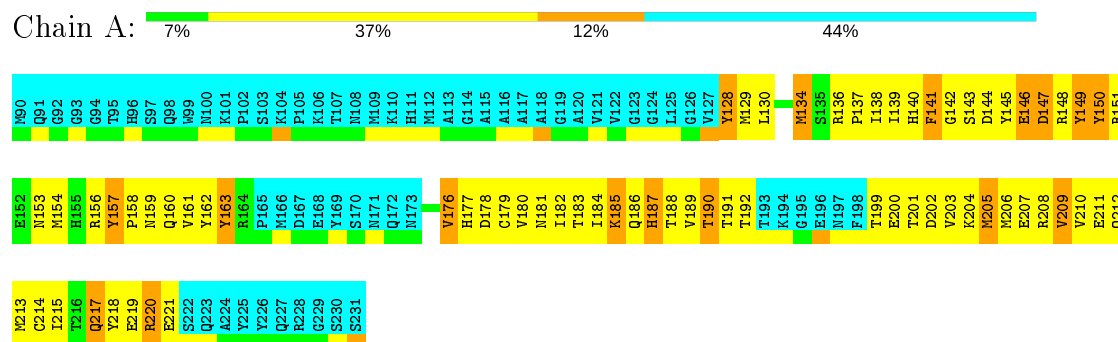
4.2.13 Score per residue for model 13

- Molecule 1: Major prion protein



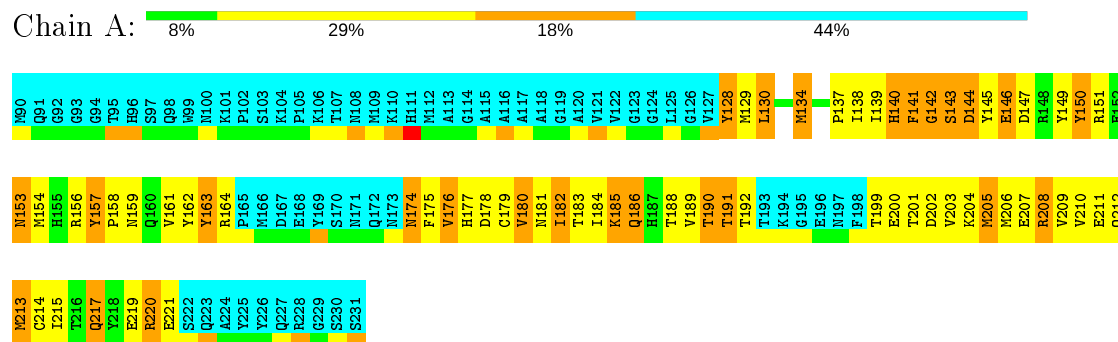
4.2.14 Score per residue for model 14

- Molecule 1: Major prion protein



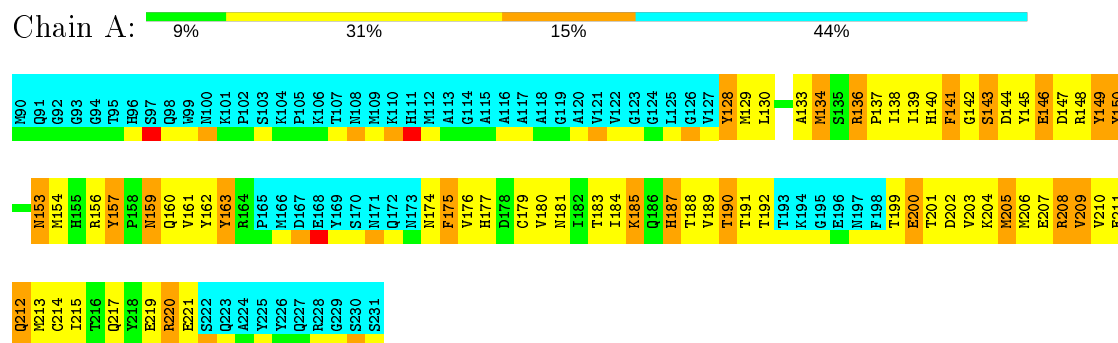
4.2.15 Score per residue for model 15

- Molecule 1: Major prion protein



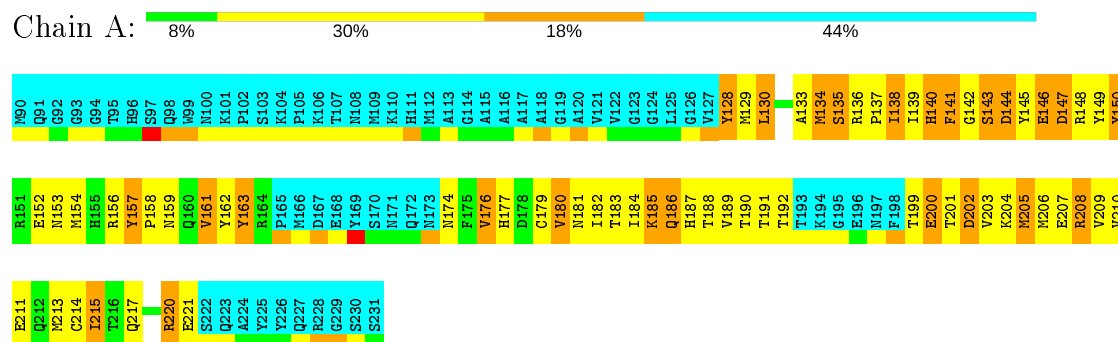
4.2.16 Score per residue for model 16

- Molecule 1: Major prion protein



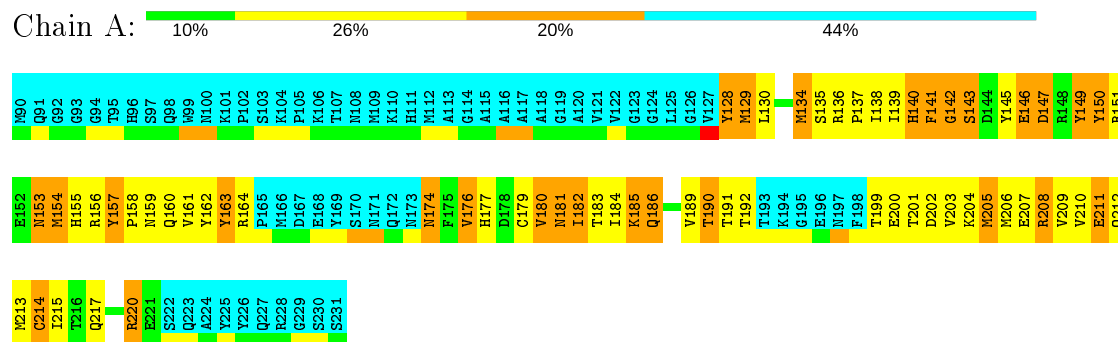
4.2.17 Score per residue for model 17

- Molecule 1: Major prion protein



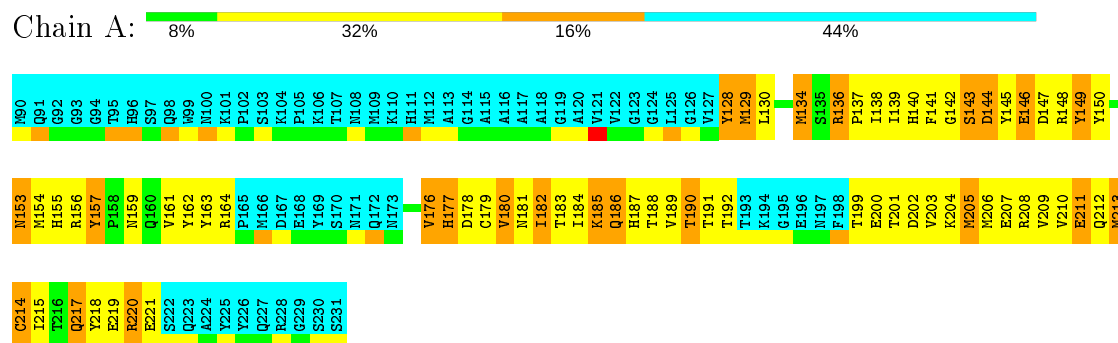
4.2.18 Score per residue for model 18

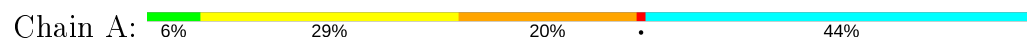
- Molecule 1: Major prion protein



4.2.19 Score per residue for model 19

- Molecule 1: Major prion protein





5 Refinement protocol and experimental data overview

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

Of the 500 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
X-PLOR NIH	structure calculation	
X-PLOR NIH	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1579
Number of shifts mapped to atoms	1579
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	82%

No validations of the models with respect to experimental NMR restraints is performed at this time.

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	674	640	636	106±10
All	All	13480	12800	12720	2115

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 81.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:LEU:HD11	1:A:162:TYR:CE2	1.01	1.89	10	1
1:A:130:LEU:HD21	1:A:162:TYR:CD1	1.00	1.92	12	7
1:A:130:LEU:HD11	1:A:162:TYR:CZ	0.99	1.92	12	17
1:A:130:LEU:HD22	1:A:162:TYR:CZ	0.99	1.92	5	2
1:A:130:LEU:HD11	1:A:162:TYR:CE1	0.99	1.91	15	2
1:A:130:LEU:HD21	1:A:162:TYR:CD2	0.98	1.94	18	10
1:A:137:PRO:O	1:A:138:ILE:HD13	0.96	1.61	2	13
1:A:206:MET:O	1:A:210:VAL:HG23	0.93	1.64	4	20
1:A:130:LEU:HD13	1:A:162:TYR:CD1	0.91	2.00	3	1
1:A:130:LEU:HD13	1:A:162:TYR:CD2	0.91	2.01	5	1
1:A:181:ASN:HD22	1:A:182:ILE:N	0.89	1.65	1	2
1:A:137:PRO:C	1:A:138:ILE:HD12	0.88	1.89	3	7
1:A:137:PRO:C	1:A:138:ILE:HD13	0.88	1.89	17	12
1:A:161:VAL:HG21	1:A:214:CYS:SG	0.86	2.10	11	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:205:MET:O	1:A:209:VAL:HG12	0.86	1.68	4	20
1:A:130:LEU:HD23	1:A:161:VAL:O	0.85	1.70	15	2
1:A:130:LEU:HD23	1:A:161:VAL:C	0.83	1.93	10	2
1:A:176:VAL:O	1:A:180:VAL:HG12	0.80	1.77	20	20
1:A:130:LEU:HD21	1:A:162:TYR:CG	0.80	2.12	16	16
1:A:153:ASN:ND2	1:A:154:MET:N	0.80	2.30	10	5
1:A:153:ASN:ND2	1:A:157:TYR:CZ	0.79	2.51	15	2
1:A:134:MET:SD	1:A:134:MET:N	0.79	2.56	8	14
1:A:134:MET:N	1:A:134:MET:SD	0.78	2.56	12	6
1:A:136:ARG:NH2	1:A:154:MET:SD	0.78	2.55	17	2
1:A:154:MET:SD	1:A:155:HIS:N	0.78	2.56	13	4
1:A:163:TYR:CE2	1:A:217:GLN:NE2	0.78	2.51	4	3
1:A:129:MET:SD	1:A:163:TYR:O	0.77	2.43	10	5
1:A:175:PHE:CD2	1:A:176:VAL:N	0.77	2.53	16	2
1:A:136:ARG:NH2	1:A:213:MET:SD	0.77	2.58	20	2
1:A:153:ASN:HD22	1:A:154:MET:N	0.76	1.78	16	5
1:A:150:TYR:N	1:A:205:MET:SD	0.76	2.58	5	11
1:A:184:ILE:HG23	1:A:206:MET:SD	0.76	2.21	20	20
1:A:153:ASN:ND2	1:A:157:TYR:CE2	0.75	2.54	6	2
1:A:128:TYR:N	1:A:128:TYR:CD1	0.75	2.53	7	3
1:A:186:GLN:NE2	1:A:186:GLN:N	0.74	2.34	11	5
1:A:138:ILE:HD12	1:A:138:ILE:N	0.74	1.96	11	6
1:A:136:ARG:NE	1:A:154:MET:SD	0.74	2.61	20	1
1:A:136:ARG:NH2	1:A:157:TYR:O	0.74	2.18	20	1
1:A:203:VAL:HG23	1:A:204:LYS:N	0.74	1.98	11	20
1:A:128:TYR:N	1:A:128:TYR:CD2	0.73	2.56	13	3
1:A:136:ARG:NH1	1:A:157:TYR:O	0.73	2.22	20	1
1:A:153:ASN:OD1	1:A:154:MET:N	0.73	2.21	5	8
1:A:130:LEU:CD2	1:A:130:LEU:N	0.73	2.52	17	1
1:A:217:GLN:NE2	1:A:218:TYR:N	0.72	2.36	8	2
1:A:129:MET:O	1:A:129:MET:SD	0.72	2.47	3	3
1:A:162:TYR:N	1:A:183:THR:OG1	0.72	2.22	5	20
1:A:130:LEU:HD22	1:A:162:TYR:CE2	0.72	2.20	17	2
1:A:161:VAL:O	1:A:163:TYR:CE1	0.72	2.43	11	7
1:A:136:ARG:CD	1:A:154:MET:SD	0.72	2.77	20	1
1:A:175:PHE:CG	1:A:176:VAL:N	0.71	2.58	16	3
1:A:186:GLN:N	1:A:186:GLN:HE21	0.71	1.84	19	5
1:A:161:VAL:O	1:A:163:TYR:CE2	0.71	2.44	3	9
1:A:129:MET:SD	1:A:129:MET:O	0.71	2.48	17	2
1:A:136:ARG:NH1	1:A:150:TYR:OH	0.71	2.23	11	1
1:A:137:PRO:O	1:A:154:MET:SD	0.71	2.49	7	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:159:ASN:N	1:A:159:ASN:OD1	0.71	2.23	12	10
1:A:185:LYS:O	1:A:189:VAL:HG23	0.71	1.85	10	15
1:A:136:ARG:O	1:A:136:ARG:NE	0.71	2.24	19	1
1:A:159:ASN:OD1	1:A:159:ASN:N	0.70	2.24	11	7
1:A:208:ARG:O	1:A:212:GLN:NE2	0.70	2.24	10	4
1:A:153:ASN:O	1:A:157:TYR:CZ	0.70	2.45	18	4
1:A:130:LEU:CD2	1:A:162:TYR:CD1	0.70	2.75	9	6
1:A:181:ASN:ND2	1:A:182:ILE:N	0.70	2.39	1	1
1:A:130:LEU:CD2	1:A:162:TYR:CD2	0.70	2.75	2	9
1:A:181:ASN:OD1	1:A:182:ILE:N	0.70	2.25	11	9
1:A:153:ASN:ND2	1:A:157:TYR:OH	0.70	2.25	2	7
1:A:186:GLN:N	1:A:186:GLN:NE2	0.69	2.40	13	10
1:A:145:TYR:CD2	1:A:146:GLU:OE2	0.69	2.46	5	1
1:A:156:ARG:NH1	1:A:187:HIS:O	0.69	2.25	8	1
1:A:143:SER:N	1:A:146:GLU:OE2	0.69	2.26	18	7
1:A:178:ASP:O	1:A:181:ASN:OD1	0.69	2.11	13	9
1:A:186:GLN:HE21	1:A:186:GLN:N	0.69	1.85	11	2
1:A:150:TYR:CE2	1:A:154:MET:SD	0.69	2.86	17	2
1:A:149:TYR:O	1:A:153:ASN:ND2	0.69	2.26	3	5
1:A:184:ILE:HD12	1:A:206:MET:SD	0.69	2.28	7	18
1:A:150:TYR:C	1:A:150:TYR:CD1	0.68	2.67	5	8
1:A:150:TYR:O	1:A:153:ASN:ND2	0.68	2.26	20	1
1:A:178:ASP:O	1:A:181:ASN:ND2	0.68	2.26	1	1
1:A:143:SER:N	1:A:146:GLU:OE1	0.68	2.26	19	7
1:A:150:TYR:CA	1:A:205:MET:SD	0.68	2.81	5	2
1:A:163:TYR:OH	1:A:217:GLN:NE2	0.68	2.27	1	4
1:A:133:ALA:HB1	1:A:159:ASN:HB3	0.68	1.65	4	2
1:A:150:TYR:CZ	1:A:154:MET:SD	0.68	2.87	17	4
1:A:134:MET:SD	1:A:159:ASN:O	0.67	2.53	1	8
1:A:130:LEU:HD21	1:A:162:TYR:CE1	0.67	2.24	10	7
1:A:218:TYR:O	1:A:218:TYR:CD2	0.67	2.47	13	2
1:A:136:ARG:HH22	1:A:209:VAL:CG2	0.67	2.02	11	1
1:A:150:TYR:CD1	1:A:150:TYR:C	0.67	2.68	9	3
1:A:136:ARG:NH2	1:A:209:VAL:HG23	0.67	2.04	17	2
1:A:150:TYR:O	1:A:150:TYR:CD2	0.67	2.47	1	2
1:A:214:CYS:O	1:A:217:GLN:N	0.67	2.28	20	15
1:A:130:LEU:CD1	1:A:162:TYR:CE1	0.67	2.77	15	1
1:A:150:TYR:C	1:A:150:TYR:CD2	0.67	2.67	11	5
1:A:136:ARG:HE	1:A:154:MET:CG	0.67	2.03	20	1
1:A:163:TYR:CZ	1:A:217:GLN:NE2	0.67	2.63	13	3
1:A:150:TYR:OH	1:A:154:MET:SD	0.67	2.53	17	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:LEU:HD13	1:A:162:TYR:CE1	0.67	2.25	3	1
1:A:156:ARG:NH1	1:A:191:THR:OG1	0.66	2.28	18	2
1:A:217:GLN:CD	1:A:218:TYR:N	0.66	2.49	2	2
1:A:139:ILE:O	1:A:141:PHE:N	0.66	2.28	17	3
1:A:155:HIS:CD2	1:A:155:HIS:O	0.66	2.48	10	4
1:A:181:ASN:HD21	1:A:185:LYS:NZ	0.66	1.86	17	1
1:A:144:ASP:CG	1:A:145:TYR:N	0.66	2.48	5	2
1:A:130:LEU:CD2	1:A:162:TYR:CE2	0.66	2.78	17	10
1:A:142:GLY:N	1:A:146:GLU:OE2	0.65	2.29	18	3
1:A:176:VAL:HG21	1:A:215:ILE:HD13	0.65	1.68	17	5
1:A:136:ARG:NE	1:A:154:MET:CG	0.65	2.59	20	1
1:A:150:TYR:CD2	1:A:150:TYR:C	0.65	2.69	17	3
1:A:138:ILE:N	1:A:138:ILE:HD13	0.65	2.04	20	1
1:A:137:PRO:O	1:A:154:MET:CE	0.65	2.44	15	7
1:A:211:GLU:O	1:A:215:ILE:CD1	0.65	2.44	8	4
1:A:199:THR:HG23	1:A:201:THR:H	0.65	1.51	17	10
1:A:214:CYS:SG	1:A:217:GLN:OE1	0.65	2.55	2	2
1:A:186:GLN:H	1:A:186:GLN:HE21	0.65	1.35	9	2
1:A:182:ILE:HG22	1:A:186:GLN:OE1	0.65	1.90	7	1
1:A:163:TYR:CE2	1:A:217:GLN:OE1	0.65	2.49	13	1
1:A:156:ARG:CZ	1:A:190:THR:HG21	0.65	2.21	4	1
1:A:175:PHE:CD2	1:A:175:PHE:C	0.65	2.71	16	1
1:A:176:VAL:HG21	1:A:215:ILE:CD1	0.65	2.22	1	20
1:A:185:LYS:O	1:A:189:VAL:CG2	0.65	2.45	10	14
1:A:132:SER:OG	1:A:220:ARG:NH2	0.65	2.30	8	2
1:A:147:ASP:OD2	1:A:151:ARG:NH1	0.65	2.30	14	2
1:A:130:LEU:HD23	1:A:130:LEU:N	0.64	2.06	17	1
1:A:130:LEU:HD21	1:A:162:TYR:CE2	0.64	2.28	15	10
1:A:146:GLU:O	1:A:205:MET:SD	0.64	2.55	9	19
1:A:155:HIS:O	1:A:155:HIS:CD2	0.64	2.50	4	1
1:A:164:ARG:NH2	1:A:178:ASP:OD1	0.64	2.31	4	1
1:A:200:GLU:OE2	1:A:201:THR:N	0.64	2.29	6	1
1:A:217:GLN:HE22	1:A:220:ARG:HH21	0.64	1.35	6	1
1:A:150:TYR:CD1	1:A:150:TYR:O	0.64	2.51	6	1
1:A:163:TYR:CD2	1:A:163:TYR:N	0.64	2.65	13	4
1:A:217:GLN:C	1:A:217:GLN:NE2	0.64	2.51	8	2
1:A:157:TYR:CE1	1:A:209:VAL:HG11	0.63	2.28	6	10
1:A:186:GLN:CD	1:A:186:GLN:N	0.63	2.52	14	1
1:A:152:GLU:O	1:A:156:ARG:NH2	0.63	2.31	17	3
1:A:130:LEU:HD13	1:A:162:TYR:CE2	0.63	2.29	5	1
1:A:176:VAL:CG1	1:A:177:HIS:N	0.62	2.62	16	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:150:TYR:O	1:A:153:ASN:OD1	0.62	2.16	5	7
1:A:136:ARG:HH22	1:A:209:VAL:HG23	0.62	1.52	11	1
1:A:177:HIS:O	1:A:181:ASN:OD1	0.62	2.17	1	7
1:A:181:ASN:ND2	1:A:185:LYS:NZ	0.62	2.47	17	1
1:A:148:ARG:NE	1:A:151:ARG:NH1	0.62	2.47	11	1
1:A:139:ILE:HD11	1:A:212:GLN:NE2	0.62	2.10	16	7
1:A:154:MET:O	1:A:157:TYR:N	0.62	2.32	11	20
1:A:211:GLU:O	1:A:215:ILE:HD13	0.62	1.93	16	12
1:A:203:VAL:CG2	1:A:204:LYS:N	0.61	2.63	5	20
1:A:153:ASN:ND2	1:A:206:MET:N	0.61	2.49	5	2
1:A:136:ARG:NH1	1:A:209:VAL:HG21	0.61	2.09	20	1
1:A:209:VAL:HG13	1:A:210:VAL:H	0.61	1.54	4	18
1:A:188:THR:O	1:A:192:THR:OG1	0.61	2.18	4	13
1:A:150:TYR:CD2	1:A:150:TYR:O	0.61	2.54	4	3
1:A:136:ARG:NH2	1:A:209:VAL:CG2	0.60	2.64	17	2
1:A:153:ASN:CG	1:A:157:TYR:HH	0.60	2.00	4	2
1:A:150:TYR:O	1:A:150:TYR:CD1	0.60	2.54	15	2
1:A:129:MET:SD	1:A:129:MET:C	0.60	2.79	13	5
1:A:200:GLU:OE2	1:A:201:THR:CA	0.60	2.49	6	1
1:A:164:ARG:CZ	1:A:178:ASP:OD1	0.60	2.49	1	1
1:A:187:HIS:C	1:A:187:HIS:CD2	0.60	2.75	10	3
1:A:187:HIS:CD2	1:A:187:HIS:C	0.60	2.75	19	1
1:A:137:PRO:O	1:A:150:TYR:OH	0.60	2.19	20	13
1:A:163:TYR:CE1	1:A:217:GLN:NE2	0.60	2.70	3	2
1:A:136:ARG:CZ	1:A:157:TYR:O	0.60	2.50	20	1
1:A:128:TYR:CD1	1:A:128:TYR:N	0.60	2.68	14	2
1:A:200:GLU:CD	1:A:201:THR:N	0.60	2.55	4	5
1:A:149:TYR:O	1:A:153:ASN:OD1	0.60	2.20	16	2
1:A:133:ALA:HB1	1:A:159:ASN:O	0.60	1.96	13	4
1:A:149:TYR:C	1:A:153:ASN:ND2	0.59	2.56	3	4
1:A:202:ASP:OD2	1:A:206:MET:HE2	0.59	1.96	7	1
1:A:161:VAL:HG23	1:A:183:THR:OG1	0.59	1.96	11	6
1:A:147:ASP:OD2	1:A:151:ARG:CZ	0.59	2.51	10	3
1:A:136:ARG:CZ	1:A:150:TYR:OH	0.59	2.49	11	1
1:A:157:TYR:HH	1:A:187:HIS:CE1	0.59	2.15	17	1
1:A:163:TYR:CD1	1:A:163:TYR:N	0.59	2.71	2	1
1:A:215:ILE:O	1:A:219:GLU:CB	0.58	2.52	2	4
1:A:153:ASN:CG	1:A:157:TYR:OH	0.58	2.42	6	5
1:A:134:MET:O	1:A:135:SER:O	0.58	2.21	11	2
1:A:187:HIS:CG	1:A:188:THR:N	0.58	2.70	12	2
1:A:208:ARG:HH21	1:A:208:ARG:CG	0.58	2.11	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:144:ASP:OD2	1:A:145:TYR:N	0.58	2.36	1	2
1:A:210:VAL:O	1:A:211:GLU:C	0.58	2.42	11	15
1:A:147:ASP:OD2	1:A:151:ARG:NE	0.58	2.36	15	2
1:A:129:MET:C	1:A:129:MET:SD	0.58	2.82	3	3
1:A:153:ASN:HD22	1:A:153:ASN:C	0.58	2.01	10	3
1:A:175:PHE:CD1	1:A:176:VAL:N	0.58	2.72	11	1
1:A:220:ARG:C	1:A:220:ARG:HH21	0.57	2.01	17	1
1:A:177:HIS:O	1:A:181:ASN:CG	0.57	2.43	1	3
1:A:130:LEU:HD11	1:A:161:VAL:O	0.57	1.99	5	2
1:A:157:TYR:CE2	1:A:209:VAL:HG11	0.57	2.35	1	9
1:A:177:HIS:O	1:A:181:ASN:CB	0.57	2.53	10	11
1:A:149:TYR:O	1:A:153:ASN:CG	0.57	2.43	3	5
1:A:208:ARG:NH2	1:A:212:GLN:NE2	0.57	2.52	4	1
1:A:188:THR:OG1	1:A:206:MET:SD	0.57	2.63	6	5
1:A:208:ARG:NH2	1:A:212:GLN:OE1	0.57	2.38	5	1
1:A:211:GLU:O	1:A:215:ILE:HD11	0.56	2.00	8	1
1:A:144:ASP:CG	1:A:145:TYR:H	0.56	2.02	5	2
1:A:214:CYS:O	1:A:215:ILE:C	0.56	2.44	17	17
1:A:139:ILE:N	1:A:150:TYR:CE2	0.56	2.73	15	2
1:A:156:ARG:NH1	1:A:187:HIS:C	0.56	2.59	8	1
1:A:149:TYR:C	1:A:153:ASN:HD21	0.56	2.04	3	3
1:A:153:ASN:CB	1:A:157:TYR:OH	0.56	2.53	8	5
1:A:208:ARG:CG	1:A:208:ARG:NH2	0.56	2.67	12	2
1:A:148:ARG:HE	1:A:151:ARG:NH1	0.56	1.98	11	1
1:A:136:ARG:CZ	1:A:154:MET:SD	0.56	2.94	18	1
1:A:139:ILE:N	1:A:150:TYR:CE1	0.56	2.74	4	3
1:A:184:ILE:O	1:A:185:LYS:C	0.56	2.43	10	18
1:A:163:TYR:N	1:A:163:TYR:CD2	0.56	2.74	12	3
1:A:153:ASN:O	1:A:156:ARG:N	0.55	2.27	15	6
1:A:218:TYR:C	1:A:218:TYR:CD2	0.55	2.79	20	3
1:A:138:ILE:HD13	1:A:138:ILE:N	0.55	2.16	17	1
1:A:140:HIS:O	1:A:141:PHE:C	0.55	2.45	16	16
1:A:182:ILE:O	1:A:186:GLN:NE2	0.55	2.40	1	3
1:A:218:TYR:CD1	1:A:218:TYR:C	0.55	2.80	3	2
1:A:175:PHE:CZ	1:A:218:TYR:CB	0.55	2.89	11	1
1:A:143:SER:OG	1:A:146:GLU:CD	0.55	2.44	8	2
1:A:176:VAL:HG13	1:A:177:HIS:N	0.55	2.15	16	4
1:A:220:ARG:CD	1:A:220:ARG:C	0.55	2.74	19	11
1:A:177:HIS:C	1:A:181:ASN:OD1	0.55	2.46	1	1
1:A:217:GLN:C	1:A:217:GLN:OE1	0.55	2.45	5	2
1:A:190:THR:CG2	1:A:191:THR:N	0.55	2.70	17	19

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:TYR:HB2	1:A:162:TYR:CD2	0.55	2.37	11	11
1:A:145:TYR:CZ	1:A:201:THR:HG21	0.55	2.37	2	19
1:A:133:ALA:CB	1:A:159:ASN:O	0.55	2.55	8	3
1:A:156:ARG:CZ	1:A:191:THR:OG1	0.55	2.55	15	2
1:A:153:ASN:ND2	1:A:153:ASN:C	0.55	2.61	10	3
1:A:156:ARG:CG	1:A:156:ARG:HH21	0.54	2.14	4	1
1:A:130:LEU:H	1:A:130:LEU:HD23	0.54	1.61	17	1
1:A:203:VAL:HG23	1:A:204:LYS:H	0.54	1.63	13	13
1:A:133:ALA:C	1:A:134:MET:SD	0.54	2.86	17	4
1:A:164:ARG:CZ	1:A:178:ASP:OD2	0.54	2.54	8	1
1:A:206:MET:O	1:A:209:VAL:HG13	0.54	2.03	2	20
1:A:191:THR:CG2	1:A:192:THR:N	0.54	2.71	12	19
1:A:188:THR:O	1:A:192:THR:CB	0.54	2.56	4	12
1:A:139:ILE:HD11	1:A:212:GLN:HE22	0.54	1.63	16	1
1:A:200:GLU:OE1	1:A:200:GLU:C	0.54	2.46	5	1
1:A:138:ILE:CD1	1:A:138:ILE:N	0.54	2.65	20	2
1:A:187:HIS:C	1:A:187:HIS:ND1	0.54	2.61	12	1
1:A:208:ARG:NH2	1:A:212:GLN:CD	0.54	2.61	4	1
1:A:153:ASN:OD1	1:A:157:TYR:OH	0.54	2.22	20	2
1:A:186:GLN:NE2	1:A:186:GLN:CA	0.54	2.71	19	3
1:A:130:LEU:HD22	1:A:162:TYR:CD2	0.54	2.38	17	1
1:A:181:ASN:ND2	1:A:181:ASN:C	0.54	2.62	20	1
1:A:150:TYR:O	1:A:154:MET:CB	0.53	2.56	17	6
1:A:138:ILE:N	1:A:138:ILE:CD1	0.53	2.68	11	3
1:A:153:ASN:ND2	1:A:154:MET:H	0.53	2.01	16	2
1:A:130:LEU:CD1	1:A:162:TYR:CE2	0.53	2.79	10	1
1:A:163:TYR:CD2	1:A:217:GLN:OE1	0.53	2.61	13	1
1:A:220:ARG:O	1:A:220:ARG:NH2	0.53	2.41	17	1
1:A:153:ASN:O	1:A:157:TYR:CE2	0.53	2.61	8	1
1:A:131:GLY:N	1:A:163:TYR:OH	0.53	2.42	8	1
1:A:128:TYR:CE2	1:A:186:GLN:OE1	0.53	2.61	10	3
1:A:191:THR:HG23	1:A:192:THR:N	0.53	2.18	10	5
1:A:208:ARG:HH21	1:A:212:GLN:NE2	0.53	2.02	4	1
1:A:219:GLU:O	1:A:219:GLU:OE2	0.53	2.27	4	1
1:A:217:GLN:O	1:A:217:GLN:OE1	0.53	2.27	5	3
1:A:130:LEU:CD1	1:A:162:TYR:CZ	0.53	2.85	13	15
1:A:186:GLN:HE21	1:A:186:GLN:H	0.52	1.45	15	2
1:A:129:MET:O	1:A:130:LEU:HD23	0.52	2.05	9	13
1:A:156:ARG:NH2	1:A:156:ARG:CG	0.52	2.71	4	1
1:A:147:ASP:C	1:A:147:ASP:OD2	0.52	2.47	10	2
1:A:153:ASN:HD22	1:A:154:MET:H	0.52	1.45	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:181:ASN:HD22	1:A:182:ILE:HD12	0.52	1.65	2	3
1:A:128:TYR:HB2	1:A:162:TYR:CD1	0.52	2.40	15	8
1:A:217:GLN:O	1:A:217:GLN:NE2	0.52	2.43	9	1
1:A:153:ASN:O	1:A:157:TYR:CE1	0.52	2.62	20	2
1:A:136:ARG:NE	1:A:154:MET:HG3	0.52	2.19	20	1
1:A:136:ARG:HH22	1:A:155:HIS:CD2	0.52	2.21	3	1
1:A:186:GLN:CA	1:A:186:GLN:HE21	0.52	2.17	20	2
1:A:139:ILE:CD1	1:A:212:GLN:HE22	0.52	2.17	14	2
1:A:200:GLU:OE1	1:A:201:THR:N	0.52	2.43	9	3
1:A:136:ARG:CG	1:A:154:MET:SD	0.52	2.98	20	5
1:A:128:TYR:CD2	1:A:128:TYR:N	0.52	2.78	10	1
1:A:200:GLU:OE2	1:A:201:THR:OG1	0.51	2.23	6	3
1:A:184:ILE:CD1	1:A:206:MET:SD	0.51	2.98	7	13
1:A:145:TYR:CE1	1:A:201:THR:HG21	0.51	2.39	9	2
1:A:130:LEU:CG	1:A:162:TYR:CE2	0.51	2.94	6	9
1:A:180:VAL:HG11	1:A:211:GLU:HG3	0.51	1.81	16	2
1:A:136:ARG:HG3	1:A:154:MET:SD	0.51	2.45	9	3
1:A:153:ASN:OD1	1:A:153:ASN:C	0.51	2.48	4	1
1:A:181:ASN:CG	1:A:182:ILE:N	0.51	2.63	14	9
1:A:161:VAL:HG12	1:A:213:MET:CE	0.51	2.35	8	6
1:A:217:GLN:NE2	1:A:220:ARG:HH21	0.51	2.02	6	1
1:A:157:TYR:HH	1:A:206:MET:HB3	0.51	1.66	17	1
1:A:164:ARG:CD	1:A:164:ARG:N	0.51	2.74	1	1
1:A:176:VAL:O	1:A:180:VAL:CG1	0.51	2.59	2	12
1:A:220:ARG:C	1:A:220:ARG:CD	0.51	2.78	1	2
1:A:202:ASP:O	1:A:203:VAL:C	0.51	2.49	15	20
1:A:206:MET:HG3	1:A:207:GLU:N	0.50	2.21	3	20
1:A:174:ASN:ND2	1:A:174:ASN:C	0.50	2.65	18	1
1:A:153:ASN:O	1:A:154:MET:C	0.50	2.49	15	13
1:A:128:TYR:CB	1:A:162:TYR:CD2	0.50	2.94	8	6
1:A:137:PRO:O	1:A:154:MET:HE1	0.50	2.05	15	2
1:A:145:TYR:CE2	1:A:201:THR:HG21	0.50	2.42	18	3
1:A:153:ASN:C	1:A:153:ASN:HD22	0.50	2.08	6	1
1:A:164:ARG:NE	1:A:178:ASP:OD2	0.50	2.44	8	1
1:A:199:THR:O	1:A:203:VAL:HG22	0.50	2.06	8	1
1:A:208:ARG:CZ	1:A:212:GLN:OE1	0.50	2.59	18	2
1:A:138:ILE:HG23	1:A:150:TYR:CE2	0.50	2.41	11	1
1:A:130:LEU:CG	1:A:162:TYR:CE1	0.50	2.95	20	6
1:A:209:VAL:CG2	1:A:213:MET:SD	0.50	2.99	3	4
1:A:136:ARG:CZ	1:A:213:MET:SD	0.50	2.99	9	1
1:A:144:ASP:O	1:A:147:ASP:OD1	0.50	2.29	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:200:GLU:OE2	1:A:200:GLU:C	0.50	2.50	14	2
1:A:212:GLN:O	1:A:213:MET:C	0.50	2.49	6	14
1:A:180:VAL:O	1:A:181:ASN:C	0.50	2.49	4	20
1:A:156:ARG:CZ	1:A:190:THR:CG2	0.50	2.90	4	1
1:A:217:GLN:C	1:A:217:GLN:HE21	0.50	2.08	8	1
1:A:219:GLU:OE2	1:A:219:GLU:CA	0.50	2.60	7	1
1:A:209:VAL:HG13	1:A:210:VAL:N	0.49	2.22	4	15
1:A:200:GLU:CG	1:A:201:THR:N	0.49	2.75	8	10
1:A:156:ARG:CB	1:A:156:ARG:HH21	0.49	2.20	4	1
1:A:143:SER:OG	1:A:146:GLU:OE1	0.49	2.21	3	1
1:A:154:MET:HA	1:A:157:TYR:CE1	0.49	2.42	6	7
1:A:130:LEU:HD21	1:A:162:TYR:CZ	0.49	2.43	15	2
1:A:161:VAL:HG22	1:A:217:GLN:OE1	0.49	2.07	13	1
1:A:178:ASP:OD1	1:A:178:ASP:C	0.49	2.51	19	1
1:A:181:ASN:ND2	1:A:182:ILE:HD13	0.49	2.23	8	9
1:A:164:ARG:NH1	1:A:178:ASP:OD2	0.49	2.45	8	1
1:A:186:GLN:HE21	1:A:186:GLN:CA	0.49	2.20	11	1
1:A:176:VAL:O	1:A:177:HIS:C	0.49	2.51	1	19
1:A:146:GLU:OE2	1:A:146:GLU:CA	0.49	2.61	5	1
1:A:147:ASP:C	1:A:147:ASP:OD1	0.49	2.50	8	2
1:A:176:VAL:HG23	1:A:214:CYS:CB	0.49	2.37	11	1
1:A:187:HIS:C	1:A:189:VAL:N	0.49	2.66	14	7
1:A:175:PHE:CZ	1:A:218:TYR:HB2	0.49	2.43	11	1
1:A:200:GLU:C	1:A:200:GLU:CD	0.49	2.71	4	2
1:A:164:ARG:NH1	1:A:178:ASP:OD1	0.49	2.46	1	1
1:A:153:ASN:ND2	1:A:206:MET:CA	0.49	2.76	11	2
1:A:184:ILE:O	1:A:187:HIS:N	0.49	2.46	19	2
1:A:203:VAL:CG2	1:A:204:LYS:H	0.48	2.20	5	18
1:A:149:TYR:CD1	1:A:201:THR:HG22	0.48	2.43	9	2
1:A:130:LEU:CD2	1:A:162:TYR:CE1	0.48	2.95	13	6
1:A:181:ASN:O	1:A:185:LYS:CE	0.48	2.61	13	1
1:A:201:THR:O	1:A:205:MET:CG	0.48	2.60	4	10
1:A:156:ARG:CD	1:A:187:HIS:CE1	0.48	2.96	14	3
1:A:215:ILE:O	1:A:219:GLU:OE2	0.48	2.30	5	1
1:A:130:LEU:HB3	1:A:161:VAL:O	0.48	2.08	17	1
1:A:134:MET:O	1:A:135:SER:C	0.48	2.50	11	5
1:A:136:ARG:NE	1:A:138:ILE:HD11	0.48	2.24	5	1
1:A:208:ARG:CG	1:A:208:ARG:HH21	0.48	2.22	13	1
1:A:202:ASP:O	1:A:206:MET:HG2	0.48	2.09	2	20
1:A:163:TYR:CZ	1:A:217:GLN:CD	0.48	2.87	13	2
1:A:136:ARG:HH11	1:A:154:MET:CA	0.48	2.20	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:186:GLN:H	1:A:186:GLN:NE2	0.48	2.07	13	2
1:A:136:ARG:NH1	1:A:137:PRO:HD2	0.48	2.23	9	1
1:A:163:TYR:CE2	1:A:217:GLN:CD	0.48	2.87	13	1
1:A:139:ILE:CD1	1:A:212:GLN:NE2	0.48	2.76	14	3
1:A:157:TYR:OH	1:A:187:HIS:CE1	0.48	2.66	17	1
1:A:136:ARG:HD2	1:A:154:MET:SD	0.48	2.49	20	1
1:A:174:ASN:C	1:A:174:ASN:HD22	0.48	2.13	18	2
1:A:144:ASP:O	1:A:145:TYR:C	0.47	2.51	19	17
1:A:156:ARG:HB2	1:A:157:TYR:CE2	0.47	2.44	20	8
1:A:150:TYR:C	1:A:153:ASN:OD1	0.47	2.52	17	3
1:A:186:GLN:OE1	1:A:186:GLN:N	0.47	2.46	14	1
1:A:217:GLN:CD	1:A:218:TYR:H	0.47	2.13	2	1
1:A:176:VAL:HG12	1:A:177:HIS:N	0.47	2.24	8	3
1:A:181:ASN:HD22	1:A:181:ASN:C	0.47	2.12	20	1
1:A:176:VAL:HG21	1:A:215:ILE:HD12	0.47	1.85	10	2
1:A:151:ARG:O	1:A:154:MET:SD	0.47	2.72	5	1
1:A:174:ASN:HD22	1:A:174:ASN:C	0.47	2.13	10	1
1:A:137:PRO:O	1:A:138:ILE:HD12	0.47	2.08	16	1
1:A:182:ILE:O	1:A:183:THR:C	0.47	2.53	1	11
1:A:130:LEU:HD11	1:A:162:TYR:OH	0.47	2.09	4	14
1:A:157:TYR:HE2	1:A:209:VAL:HG11	0.47	1.70	10	9
1:A:177:HIS:ND1	1:A:181:ASN:OD1	0.47	2.47	1	1
1:A:136:ARG:NH2	1:A:213:MET:CG	0.47	2.77	9	1
1:A:129:MET:C	1:A:130:LEU:HD23	0.47	2.30	12	6
1:A:181:ASN:ND2	1:A:182:ILE:H	0.46	2.06	1	1
1:A:176:VAL:CG2	1:A:215:ILE:HD12	0.46	2.40	10	3
1:A:186:GLN:N	1:A:186:GLN:CD	0.46	2.69	4	1
1:A:136:ARG:HH22	1:A:213:MET:CG	0.46	2.23	9	1
1:A:136:ARG:NH2	1:A:158:PRO:HA	0.46	2.25	20	1
1:A:186:GLN:CA	1:A:186:GLN:NE2	0.46	2.78	20	1
1:A:200:GLU:HG3	1:A:201:THR:N	0.46	2.26	16	10
1:A:147:ASP:OD1	1:A:147:ASP:C	0.46	2.54	17	2
1:A:136:ARG:HG3	1:A:154:MET:CE	0.46	2.39	9	2
1:A:182:ILE:CD1	1:A:182:ILE:N	0.46	2.79	9	1
1:A:200:GLU:C	1:A:200:GLU:OE1	0.46	2.54	10	2
1:A:136:ARG:HE	1:A:137:PRO:HD2	0.46	1.70	11	2
1:A:205:MET:O	1:A:206:MET:C	0.46	2.53	18	10
1:A:187:HIS:O	1:A:190:THR:N	0.46	2.49	14	2
1:A:153:ASN:OD1	1:A:202:ASP:OD2	0.46	2.33	6	1
1:A:129:MET:SD	1:A:130:LEU:N	0.46	2.88	13	1
1:A:199:THR:O	1:A:203:VAL:HG13	0.46	2.11	8	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:202:ASP:O	1:A:205:MET:N	0.46	2.49	15	1
1:A:179:CYS:SG	1:A:180:VAL:N	0.45	2.88	2	1
1:A:148:ARG:CG	1:A:149:TYR:N	0.45	2.79	19	3
1:A:147:ASP:CG	1:A:148:ARG:N	0.45	2.69	1	1
1:A:130:LEU:HD22	1:A:162:TYR:OH	0.45	2.11	3	2
1:A:150:TYR:HA	1:A:153:ASN:ND2	0.45	2.27	8	3
1:A:138:ILE:N	1:A:138:ILE:HD12	0.45	2.26	10	1
1:A:207:GLU:O	1:A:208:ARG:C	0.45	2.54	15	12
1:A:175:PHE:CZ	1:A:218:TYR:HB3	0.45	2.47	11	1
1:A:199:THR:O	1:A:200:GLU:C	0.45	2.55	20	4
1:A:154:MET:HA	1:A:157:TYR:CE2	0.45	2.47	14	8
1:A:153:ASN:ND2	1:A:206:MET:HA	0.45	2.27	11	2
1:A:150:TYR:O	1:A:154:MET:HB3	0.45	2.11	17	3
1:A:130:LEU:HG	1:A:162:TYR:CE2	0.45	2.47	8	8
1:A:156:ARG:HG2	1:A:156:ARG:NH2	0.45	2.27	4	1
1:A:130:LEU:HG	1:A:162:TYR:CE1	0.44	2.47	20	4
1:A:180:VAL:HG13	1:A:181:ASN:H	0.44	1.72	5	4
1:A:136:ARG:NE	1:A:137:PRO:HD2	0.44	2.26	11	2
1:A:148:ARG:NE	1:A:151:ARG:HH11	0.44	2.07	11	1
1:A:156:ARG:HB2	1:A:157:TYR:CE1	0.44	2.47	8	9
1:A:187:HIS:O	1:A:188:THR:C	0.44	2.54	8	7
1:A:128:TYR:CB	1:A:162:TYR:CD1	0.44	3.01	20	4
1:A:174:ASN:C	1:A:174:ASN:ND2	0.44	2.71	1	1
1:A:163:TYR:OH	1:A:217:GLN:CD	0.44	2.56	1	1
1:A:157:TYR:CD1	1:A:157:TYR:N	0.44	2.84	4	1
1:A:128:TYR:HB3	1:A:162:TYR:HB3	0.44	1.89	8	1
1:A:154:MET:HG2	1:A:155:HIS:N	0.44	2.28	18	3
1:A:220:ARG:HD3	1:A:221:GLU:N	0.44	2.28	9	15
1:A:148:ARG:HG2	1:A:149:TYR:N	0.44	2.28	7	5
1:A:220:ARG:NH2	1:A:221:GLU:HG3	0.44	2.27	9	1
1:A:136:ARG:HG2	1:A:154:MET:SD	0.44	2.52	16	5
1:A:153:ASN:OD1	1:A:157:TYR:CE2	0.44	2.71	4	1
1:A:161:VAL:O	1:A:163:TYR:CD2	0.44	2.71	18	4
1:A:139:ILE:HD13	1:A:212:GLN:HE22	0.44	1.73	19	1
1:A:129:MET:SD	1:A:163:TYR:CD1	0.43	3.11	3	1
1:A:133:ALA:HB1	1:A:159:ASN:C	0.43	2.33	13	2
1:A:136:ARG:CZ	1:A:209:VAL:HG23	0.43	2.43	17	1
1:A:153:ASN:OD1	1:A:206:MET:N	0.43	2.51	20	1
1:A:181:ASN:ND2	1:A:185:LYS:HZ1	0.43	2.12	17	1
1:A:136:ARG:HH11	1:A:154:MET:HA	0.43	1.73	20	1
1:A:218:TYR:CD1	1:A:218:TYR:O	0.43	2.71	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:212:GLN:O	1:A:215:ILE:HG12	0.43	2.12	9	3
1:A:136:ARG:HE	1:A:154:MET:CB	0.43	2.26	20	1
1:A:199:THR:HG23	1:A:200:GLU:N	0.43	2.27	7	1
1:A:139:ILE:HD11	1:A:209:VAL:HA	0.43	1.89	18	1
1:A:181:ASN:C	1:A:181:ASN:ND2	0.43	2.72	2	1
1:A:164:ARG:CZ	1:A:178:ASP:CG	0.43	2.87	8	1
1:A:148:ARG:HG3	1:A:149:TYR:N	0.43	2.29	20	1
1:A:187:HIS:NE2	1:A:206:MET:CE	0.43	2.82	12	1
1:A:136:ARG:HH12	1:A:213:MET:HG3	0.43	1.74	9	1
1:A:150:TYR:CD2	1:A:151:ARG:N	0.43	2.87	20	1
1:A:157:TYR:HE1	1:A:209:VAL:HG11	0.43	1.73	12	8
1:A:136:ARG:HA	1:A:136:ARG:NE	0.43	2.29	9	1
1:A:210:VAL:HG12	1:A:214:CYS:SG	0.43	2.53	10	2
1:A:156:ARG:HD3	1:A:187:HIS:ND1	0.43	2.28	1	3
1:A:154:MET:C	1:A:156:ARG:N	0.43	2.71	15	1
1:A:150:TYR:HB2	1:A:205:MET:SD	0.43	2.54	15	6
1:A:156:ARG:HD3	1:A:187:HIS:CD2	0.43	2.48	10	2
1:A:177:HIS:O	1:A:178:ASP:C	0.42	2.56	1	1
1:A:130:LEU:HD22	1:A:161:VAL:O	0.42	2.14	9	8
1:A:130:LEU:CD2	1:A:162:TYR:HA	0.42	2.44	12	15
1:A:215:ILE:O	1:A:219:GLU:HB2	0.42	2.13	9	2
1:A:150:TYR:HA	1:A:205:MET:SD	0.42	2.51	5	1
1:A:177:HIS:O	1:A:181:ASN:HB3	0.42	2.14	10	1
1:A:149:TYR:O	1:A:150:TYR:C	0.42	2.57	5	2
1:A:178:ASP:C	1:A:181:ASN:OD1	0.42	2.57	14	3
1:A:217:GLN:O	1:A:220:ARG:N	0.42	2.53	14	1
1:A:145:TYR:OH	1:A:201:THR:OG1	0.42	2.34	12	1
1:A:187:HIS:O	1:A:189:VAL:N	0.42	2.52	14	4
1:A:154:MET:O	1:A:155:HIS:C	0.42	2.57	6	1
1:A:216:THR:O	1:A:220:ARG:HB3	0.42	2.15	9	1
1:A:217:GLN:HE22	1:A:221:GLU:CD	0.42	2.18	20	1
1:A:203:VAL:HA	1:A:206:MET:CG	0.42	2.44	19	8
1:A:182:ILE:C	1:A:184:ILE:N	0.42	2.72	19	2
1:A:145:TYR:OH	1:A:201:THR:HG21	0.42	2.15	16	2
1:A:133:ALA:HB2	1:A:160:GLN:HG2	0.42	1.91	1	1
1:A:141:PHE:CG	1:A:205:MET:CE	0.42	3.03	16	6
1:A:157:TYR:N	1:A:157:TYR:CD2	0.42	2.84	20	2
1:A:153:ASN:OD1	1:A:206:MET:CA	0.42	2.67	20	1
1:A:161:VAL:HG22	1:A:163:TYR:CD1	0.42	2.49	6	3
1:A:130:LEU:H	1:A:130:LEU:HD12	0.42	1.74	10	1
1:A:136:ARG:HE	1:A:137:PRO:CD	0.42	2.27	11	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:176:VAL:HG23	1:A:214:CYS:HB3	0.42	1.92	11	1
1:A:182:ILE:O	1:A:184:ILE:N	0.42	2.53	19	2
1:A:163:TYR:CZ	1:A:217:GLN:HG3	0.42	2.50	1	1
1:A:130:LEU:CD1	1:A:161:VAL:O	0.42	2.67	5	1
1:A:134:MET:CE	1:A:217:GLN:HG2	0.42	2.45	13	1
1:A:157:TYR:N	1:A:157:TYR:CD1	0.42	2.86	13	1
1:A:144:ASP:O	1:A:147:ASP:N	0.42	2.52	19	1
1:A:187:HIS:O	1:A:190:THR:HG22	0.41	2.14	13	2
1:A:130:LEU:HD12	1:A:130:LEU:N	0.41	2.30	10	1
1:A:185:LYS:O	1:A:189:VAL:CB	0.41	2.68	4	3
1:A:153:ASN:OD1	1:A:157:TYR:CZ	0.41	2.74	4	1
1:A:154:MET:HA	1:A:157:TYR:CD2	0.41	2.50	5	2
1:A:150:TYR:CB	1:A:205:MET:SD	0.41	3.08	5	1
1:A:175:PHE:CE2	1:A:218:TYR:HB2	0.41	2.50	11	1
1:A:220:ARG:NH2	1:A:220:ARG:HG2	0.41	2.31	17	1
1:A:129:MET:CG	1:A:163:TYR:O	0.41	2.69	5	1
1:A:130:LEU:HD13	1:A:162:TYR:CG	0.41	2.48	3	1
1:A:145:TYR:CE2	1:A:149:TYR:CD2	0.41	3.07	9	1
1:A:130:LEU:HG	1:A:162:TYR:CD1	0.41	2.51	15	1
1:A:217:GLN:HE22	1:A:220:ARG:NH2	0.41	2.09	6	1
1:A:186:GLN:OE1	1:A:186:GLN:CA	0.41	2.67	14	1
1:A:161:VAL:O	1:A:163:TYR:CD1	0.41	2.74	2	1
1:A:134:MET:CE	1:A:213:MET:O	0.41	2.68	8	1
1:A:181:ASN:O	1:A:184:ILE:HB	0.41	2.16	17	1
1:A:145:TYR:OH	1:A:201:THR:CB	0.41	2.69	12	1
1:A:182:ILE:N	1:A:182:ILE:CD1	0.41	2.84	2	1
1:A:141:PHE:CZ	1:A:208:ARG:HG3	0.41	2.50	16	2
1:A:161:VAL:CG2	1:A:214:CYS:SG	0.41	2.97	11	1
1:A:154:MET:HA	1:A:157:TYR:CD1	0.41	2.51	3	2
1:A:213:MET:O	1:A:214:CYS:C	0.41	2.59	6	2
1:A:187:HIS:ND1	1:A:206:MET:HB3	0.41	2.31	10	1
1:A:153:ASN:CG	1:A:154:MET:N	0.41	2.75	11	1
1:A:144:ASP:O	1:A:148:ARG:CG	0.41	2.69	12	1
1:A:156:ARG:HD2	1:A:187:HIS:CE1	0.40	2.50	1	1
1:A:182:ILE:HG22	1:A:183:THR:N	0.40	2.30	3	1
1:A:128:TYR:CD2	1:A:186:GLN:OE1	0.40	2.74	10	1
1:A:157:TYR:CD2	1:A:157:TYR:N	0.40	2.86	11	1
1:A:215:ILE:O	1:A:219:GLU:HB3	0.40	2.15	13	1
1:A:175:PHE:C	1:A:175:PHE:CD2	0.40	2.94	15	1
1:A:157:TYR:CZ	1:A:206:MET:HA	0.40	2.51	15	1
1:A:220:ARG:NE	1:A:220:ARG:C	0.40	2.75	19	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:176:VAL:CG2	1:A:215:ILE:CD1	0.40	2.98	2	1
1:A:129:MET:HE2	1:A:163:TYR:CE1	0.40	2.52	10	1
1:A:134:MET:C	1:A:135:SER:O	0.40	2.60	11	1
1:A:153:ASN:HB2	1:A:157:TYR:OH	0.40	2.16	18	1
1:A:201:THR:O	1:A:205:MET:HG3	0.40	2.15	18	1
1:A:153:ASN:O	1:A:156:ARG:HB2	0.40	2.16	20	1
1:A:150:TYR:CE2	1:A:154:MET:HB2	0.40	2.52	4	1
1:A:200:GLU:OE1	1:A:201:THR:CA	0.40	2.70	9	1

6.3 Torsion angles ⓘ

6.3.1 Protein backbone ⓘ

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	79/142 (56%)	61±2 (78±3%)	14±2 (18±3%)	3±1 (4±1%)	5	30
All	All	1580/2840 (56%)	1225 (78%)	289 (18%)	66 (4%)	5	30

All 7 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	142	GLY	20
1	A	179	CYS	18
1	A	158	PRO	12
1	A	141	PHE	5
1	A	131	GLY	4
1	A	135	SER	4
1	A	140	HIS	3

6.3.2 Protein sidechains ⓘ

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	76/122 (62%)	47±3 (61±4%)	29±3 (39±4%)	0	6
All	All	1520/2440 (62%)	934 (61%)	586 (39%)	0	6

All 59 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	157	TYR	20
1	A	134	MET	20
1	A	143	SER	20
1	A	220	ARG	20
1	A	185	LYS	20
1	A	205	MET	20
1	A	208	ARG	20
1	A	128	TYR	20
1	A	149	TYR	19
1	A	146	GLU	19
1	A	163	TYR	18
1	A	141	PHE	17
1	A	180	VAL	16
1	A	176	VAL	16
1	A	150	TYR	15
1	A	174	ASN	15
1	A	190	THR	14
1	A	186	GLN	14
1	A	153	ASN	13
1	A	160	GLN	13
1	A	217	GLN	12
1	A	177	HIS	11
1	A	129	MET	11
1	A	144	ASP	11
1	A	147	ASP	11
1	A	164	ARG	10
1	A	200	GLU	10
1	A	154	MET	10
1	A	219	GLU	9
1	A	199	THR	9
1	A	161	VAL	9
1	A	213	MET	9
1	A	211	GLU	9
1	A	182	ILE	9
1	A	136	ARG	8
1	A	187	HIS	7

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Mol	Chain	Res	Type	Models (Total)
1	A	159	ASN	7
1	A	148	ARG	6
1	A	135	SER	6
1	A	215	ILE	6
1	A	130	LEU	5
1	A	202	ASP	5
1	A	175	PHE	5
1	A	181	ASN	4
1	A	212	GLN	4
1	A	140	HIS	4
1	A	151	ARG	4
1	A	132	SER	4
1	A	214	CYS	4
1	A	209	VAL	3
1	A	218	TYR	3
1	A	178	ASP	2
1	A	155	HIS	2
1	A	158	PRO	2
1	A	138	ILE	2
1	A	191	THR	1
1	A	216	THR	1
1	A	156	ARG	1
1	A	221	GLU	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.6 Ligand geometry ⓘ

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 82% for the well-defined parts and 81% for the entire structure.

7.1 Chemical shift list 1

File name: input_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1579
Number of shifts mapped to atoms	1579
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	139	-0.07 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	125	0.38 ± 0.08	None needed (< 0.5 ppm)
$^{13}\text{C}'$	137	0.02 ± 0.08	None needed (< 0.5 ppm)
^{15}N	127	-0.22 ± 0.12	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 82%, i.e. 851 atoms were assigned a chemical shift out of a possible 1043. 8 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	376/391 (96%)	149/156 (96%)	155/158 (98%)	72/77 (94%)
Sidechain	437/538 (81%)	272/317 (86%)	152/190 (80%)	13/31 (42%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	38/114 (33%)	38/58 (66%)	0/48 (0%)	0/8 (0%)
Overall	851/1043 (82%)	459/531 (86%)	307/396 (78%)	85/116 (73%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 81%, i.e. 1425 atoms were assigned a chemical shift out of a possible 1750. 12 out of 12 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	668/700 (95%)	265/279 (95%)	276/284 (97%)	127/137 (93%)
Sidechain	708/875 (81%)	444/519 (86%)	245/307 (80%)	19/49 (39%)
Aromatic	49/175 (28%)	48/89 (54%)	0/73 (0%)	1/13 (8%)
Overall	1425/1750 (81%)	757/887 (85%)	521/664 (78%)	147/199 (74%)

7.1.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:

