



# Full wwPDB NMR Structure Validation Report ⓘ

Oct 13, 2024 – 10:16 AM EDT

PDB ID : 2FJ3  
BMRB ID : 7142  
Title : NMR solution of rabbit Prion Protein (91-228)  
Authors : Li, J.; Lin, D.H.  
Deposited on : 2005-12-31

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
wwPDB-RCI : v\_1n\_11\_5\_13\_A (Berjanski et al., 2005)  
PANAV : Wang et al. (2010)  
wwPDB-ShiftChecker : v1.2  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

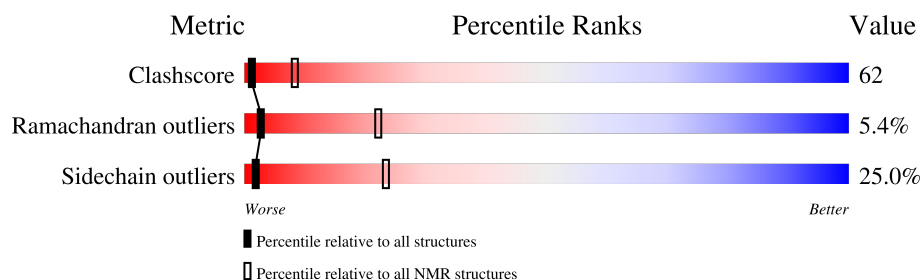
# 1 Overall quality at a glance

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	210492	14027
Ramachandran outliers	207382	12486
Sidechain outliers	206894	12463

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  $\geq 3$ , 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	138	

## 2 Ensemble composition and analysis

This entry contains 15 models. Model 11 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:127-A:228 (102)	0.67	11

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 and 5 single-model clusters were found.

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

### 3 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 1694 atoms, of which 821 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Major prion protein.

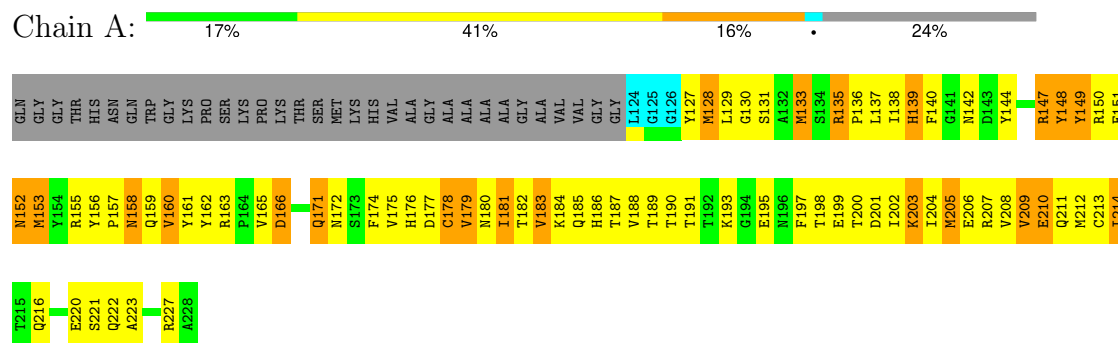
Mol	Chain	Residues	Atoms						Trace
1	A	105	Total	C	H	N	O	S	0
			1694	544	821	152	170	7	

## 4 Residue-property plots

### 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: Major prion protein

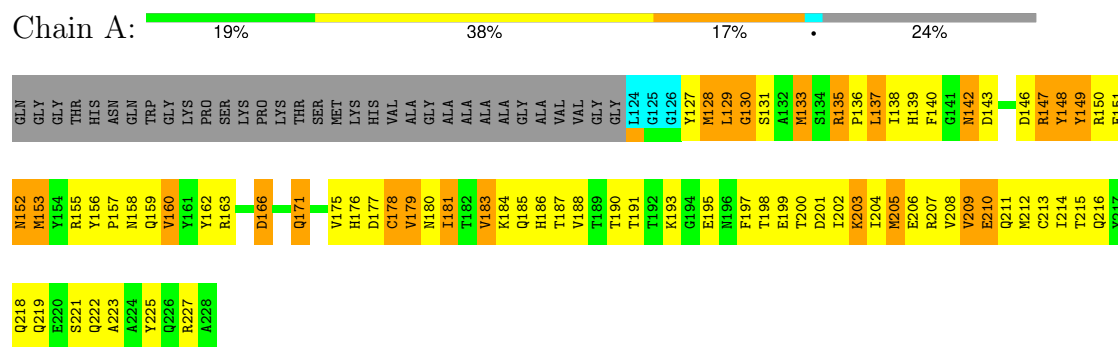


### 4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

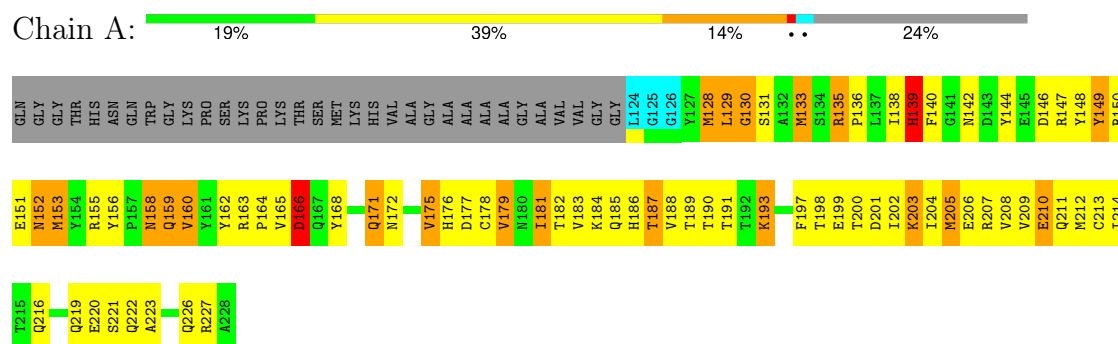
#### 4.2.1 Score per residue for model 1

- Molecule 1: Major prion protein



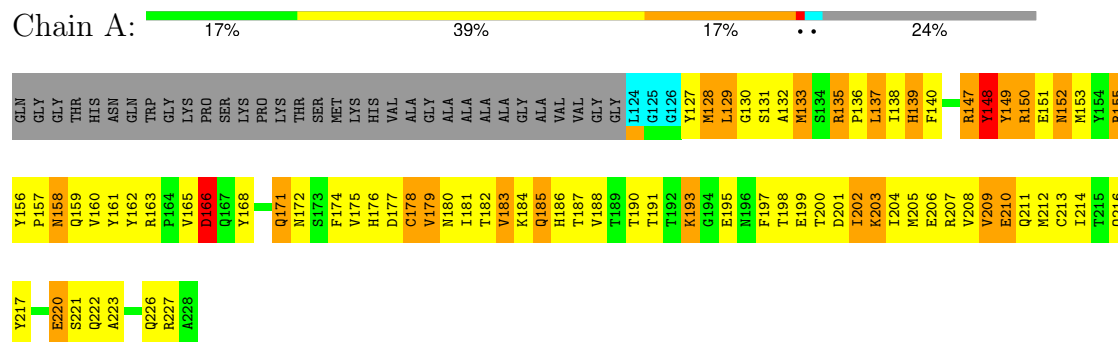
## 4.2.2 Score per residue for model 2

- Molecule 1: Major prion protein



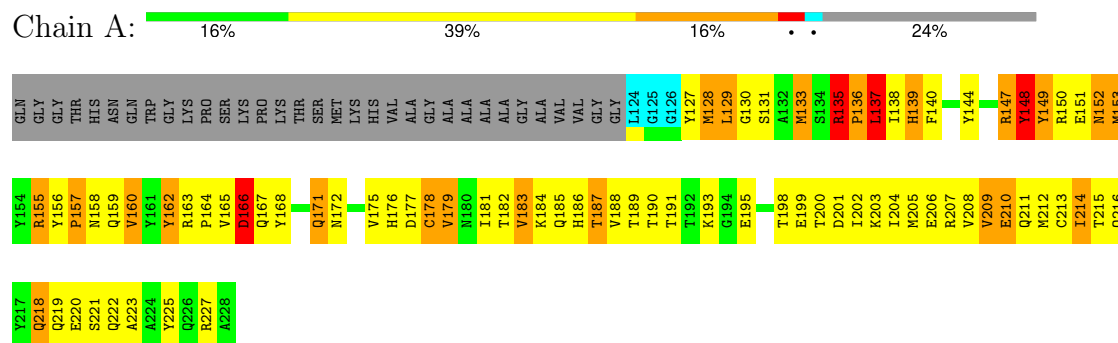
## 4.2.3 Score per residue for model 3

- Molecule 1: Major prion protein



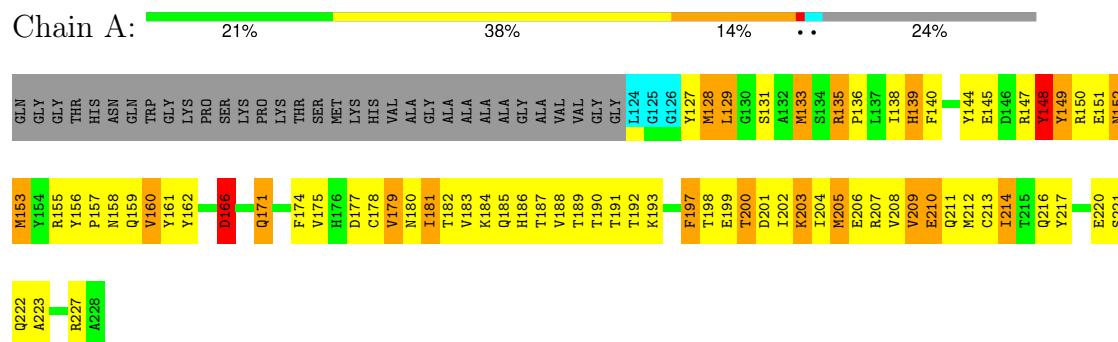
## 4.2.4 Score per residue for model 4

- Molecule 1: Major prion protein



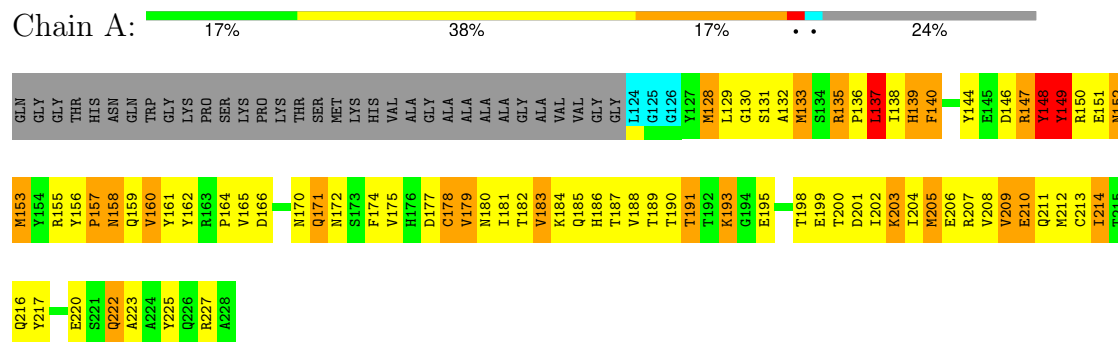
### 4.2.5 Score per residue for model 5

- Molecule 1: Major prion protein



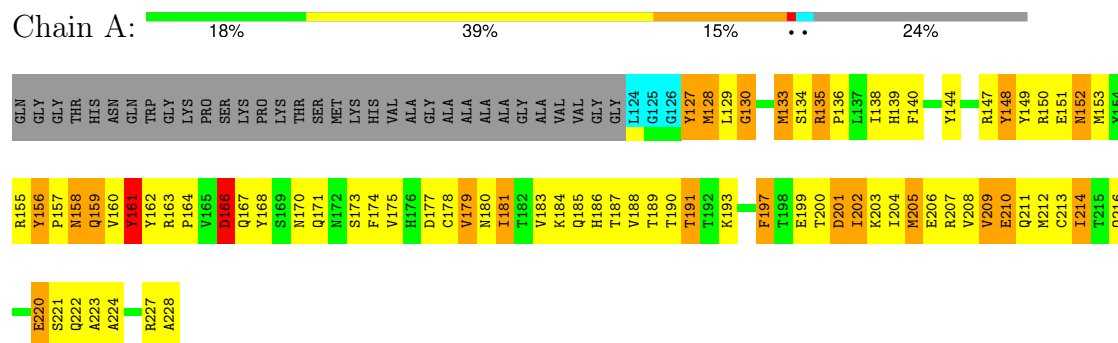
### 4.2.6 Score per residue for model 6

- Molecule 1: Major prion protein



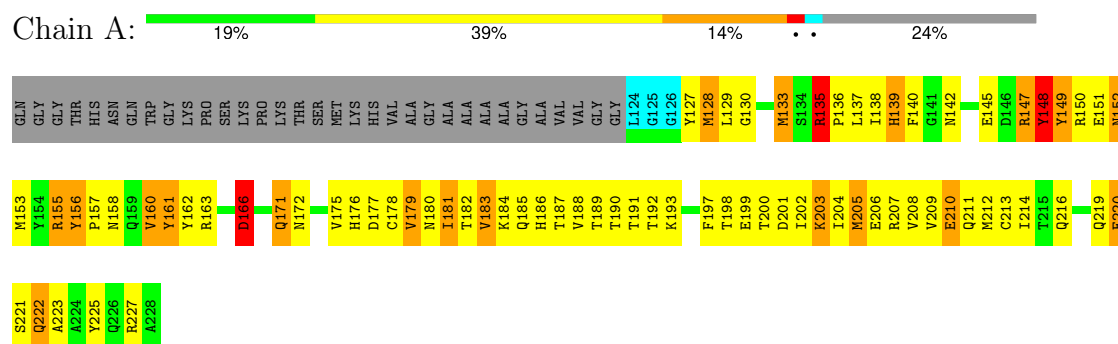
### 4.2.7 Score per residue for model 7

- Molecule 1: Major prion protein



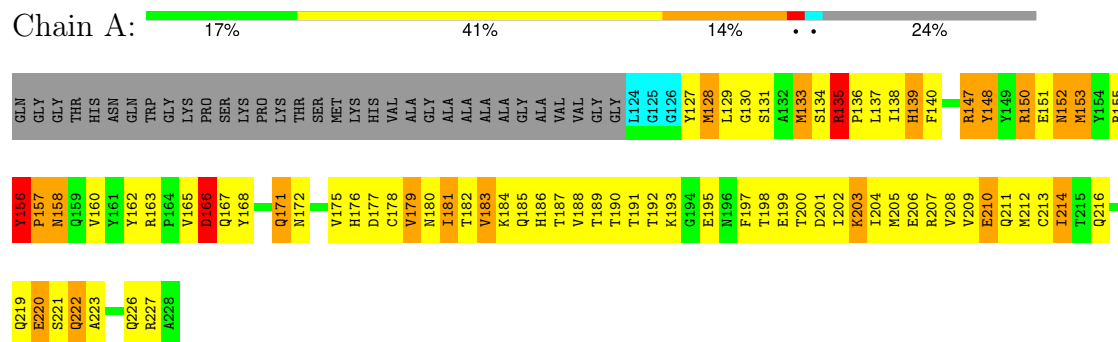
#### 4.2.8 Score per residue for model 8

- Molecule 1: Major prion protein



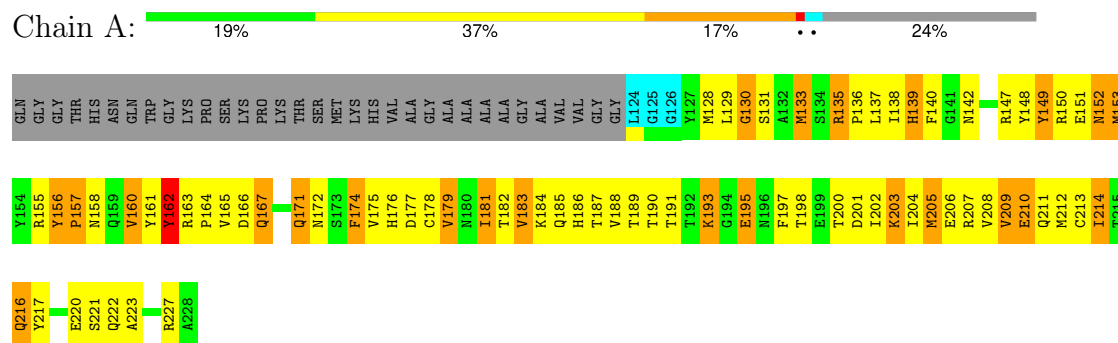
#### 4.2.9 Score per residue for model 9

- Molecule 1: Major prion protein



#### 4.2.10 Score per residue for model 10

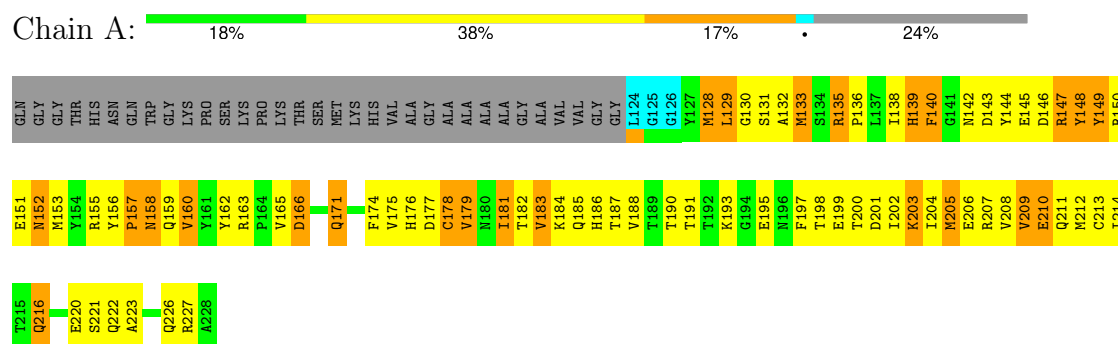
- Molecule 1: Major prion protein





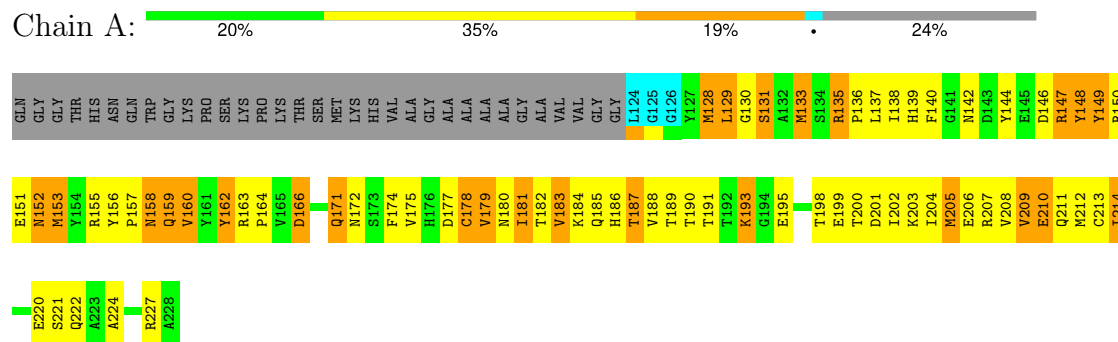
### 4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Major prion protein



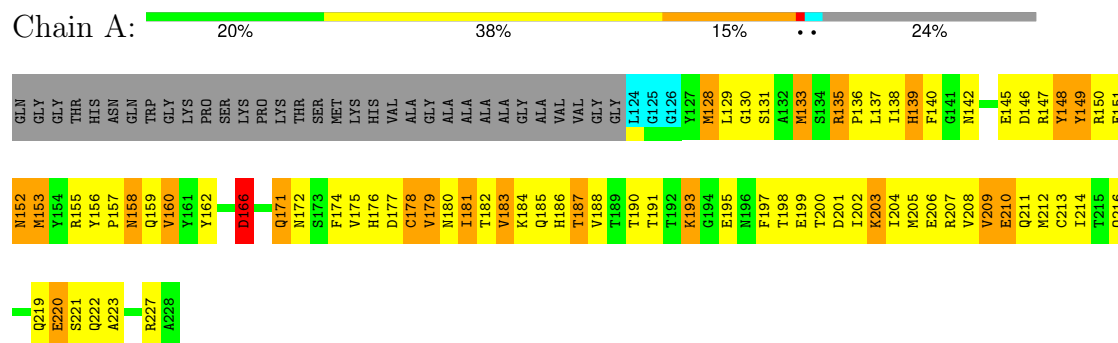
### 4.2.12 Score per residue for model 12

- Molecule 1: Major prion protein



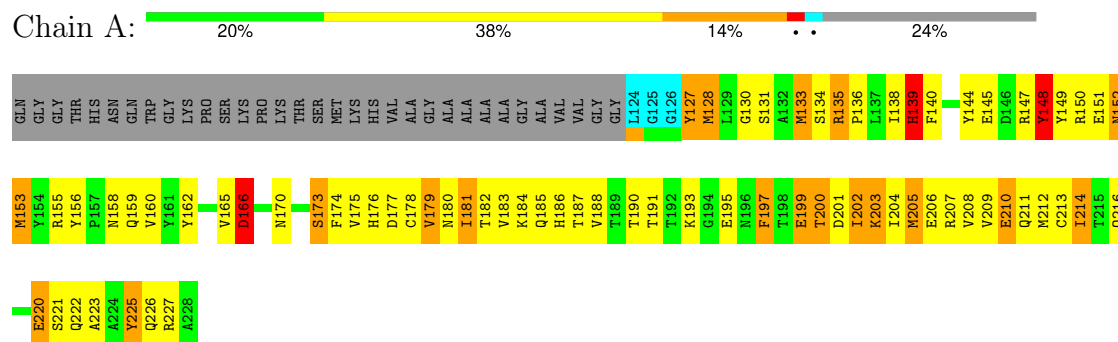
### 4.2.13 Score per residue for model 13

- Molecule 1: Major prion protein



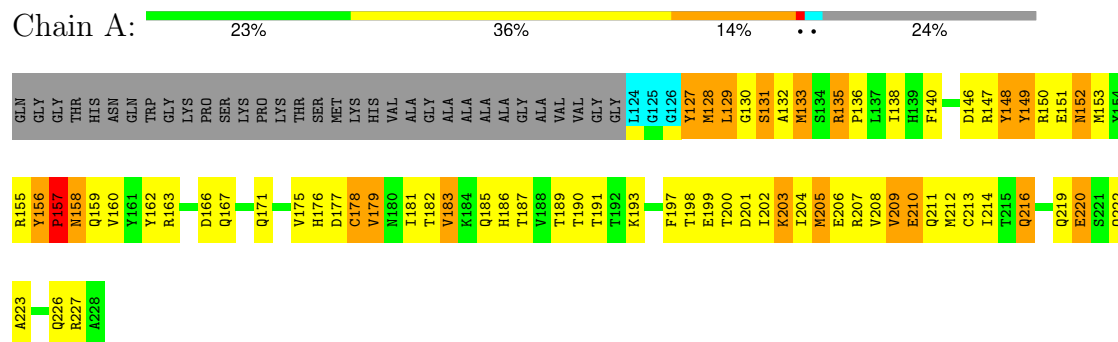
#### 4.2.14 Score per residue for model 14

- Molecule 1: Major prion protein



#### 4.2.15 Score per residue for model 15

- Molecule 1: Major prion protein



## 5 Refinement protocol and experimental data overview

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

Of the 200 calculated structures, 15 were deposited, based on the following criterion: *structures with the lowest energy*.

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

Software name	Classification	Version
ARIA	structure solution	1.2
ARIA	refinement	1.2

No chemical shift data was provided.

## 6 Model quality

### 6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.68±0.10	2±1/876 ( 0.2± 0.2%)	0.67±0.03	0±0/1186 ( 0.0± 0.0%)
All	All	0.69	23/13140 ( 0.2%)	0.67	0/17790 ( 0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	0.7±0.7
All	All	0	11

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	148	TYR	CE2-CZ	-10.55	1.24	1.38	3	6
1	A	148	TYR	CE1-CZ	10.33	1.51	1.38	14	4
1	A	162	TYR	CE1-CZ	6.62	1.47	1.38	10	3
1	A	197	PHE	CE1-CZ	6.20	1.49	1.37	7	3
1	A	162	TYR	CE2-CZ	-6.19	1.30	1.38	12	1
1	A	161	TYR	CE1-CZ	5.39	1.45	1.38	6	1
1	A	161	TYR	CE2-CZ	-5.36	1.31	1.38	6	2
1	A	217	TYR	CE2-CZ	-5.27	1.31	1.38	5	1
1	A	127	TYR	CE1-CZ	-5.24	1.31	1.38	7	1
1	A	156	TYR	CE2-CZ	-5.09	1.31	1.38	9	1

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	156	TYR	Peptide,Sidechain	5
1	A	148	TYR	Sidechain	2
1	A	217	TYR	Sidechain	1
1	A	149	TYR	Sidechain	1
1	A	161	TYR	Sidechain	1
1	A	162	TYR	Sidechain	1

## 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	857	804	801	103±5
All	All	12855	12060	12015	1544

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 62.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:ILE:HG13	1:A:208:VAL:HG22	0.99	1.35	14	14
1:A:133:MET:HE1	1:A:212:MET:HG2	0.96	1.37	13	1
1:A:166:ASP:HB2	1:A:221:SER:HA	0.92	1.37	13	12
1:A:175:VAL:HG11	1:A:214:ILE:HG13	0.92	1.38	10	15
1:A:201:ASP:HA	1:A:204:ILE:HD11	0.91	1.39	1	15
1:A:175:VAL:HG13	1:A:213:CYS:HB3	0.88	1.41	15	15
1:A:161:TYR:HB2	1:A:181:ILE:HD13	0.88	1.41	3	1
1:A:191:THR:HG21	1:A:197:PHE:HB3	0.87	1.42	9	4
1:A:137:LEU:HA	1:A:149:TYR:OH	0.86	1.69	6	2
1:A:129:LEU:HD21	1:A:159:GLN:HB2	0.85	1.46	11	1
1:A:148:TYR:CE1	1:A:204:ILE:HG21	0.85	2.07	11	4
1:A:161:TYR:HB2	1:A:181:ILE:CD1	0.83	2.03	3	1
1:A:128:MET:HG3	1:A:162:TYR:O	0.82	1.74	15	12
1:A:149:TYR:HA	1:A:152:ASN:HB3	0.82	1.50	12	9
1:A:181:ILE:O	1:A:185:GLN:HG2	0.82	1.75	13	13
1:A:148:TYR:HE1	1:A:204:ILE:HG21	0.82	1.34	11	2
1:A:133:MET:HE3	1:A:212:MET:HG2	0.81	1.49	15	5
1:A:133:MET:CE	1:A:212:MET:HG2	0.80	2.05	11	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:183:VAL:HB	1:A:205:MET:SD	0.80	2.16	8	9
1:A:152:ASN:HA	1:A:155:ARG:CD	0.79	2.07	9	2
1:A:204:ILE:O	1:A:208:VAL:HG23	0.78	1.79	9	15
1:A:175:VAL:HG22	1:A:213:CYS:SG	0.78	2.19	2	2
1:A:129:LEU:HA	1:A:160:VAL:O	0.77	1.78	8	2
1:A:133:MET:HE2	1:A:212:MET:HG2	0.77	1.56	11	4
1:A:201:ASP:HA	1:A:204:ILE:CD1	0.76	2.11	12	12
1:A:133:MET:SD	1:A:136:PRO:HD3	0.76	2.20	1	14
1:A:186:HIS:O	1:A:190:THR:HB	0.76	1.79	15	5
1:A:145:GLU:HG2	1:A:148:TYR:CE2	0.75	2.16	14	3
1:A:200:THR:O	1:A:204:ILE:HG12	0.75	1.82	9	15
1:A:183:VAL:O	1:A:187:THR:HB	0.74	1.82	7	6
1:A:179:VAL:HG11	1:A:210:GLU:HA	0.74	1.58	13	13
1:A:208:VAL:O	1:A:212:MET:HG3	0.74	1.81	11	6
1:A:162:TYR:HB3	1:A:178:CYS:HB2	0.73	1.59	1	10
1:A:203:LYS:HE2	1:A:204:ILE:HG23	0.73	1.59	6	10
1:A:206:GLU:O	1:A:210:GLU:HB3	0.73	1.83	7	15
1:A:151:GLU:O	1:A:155:ARG:HG2	0.73	1.83	5	9
1:A:152:ASN:O	1:A:156:TYR:HB2	0.72	1.84	14	11
1:A:180:ASN:HA	1:A:184:LYS:HE2	0.71	1.62	8	1
1:A:175:VAL:HG21	1:A:214:ILE:HA	0.71	1.63	12	14
1:A:187:THR:HA	1:A:191:THR:OG1	0.70	1.86	11	7
1:A:207:ARG:O	1:A:211:GLN:HG2	0.70	1.86	15	10
1:A:133:MET:HG2	1:A:212:MET:SD	0.70	2.25	3	6
1:A:175:VAL:HA	1:A:178:CYS:SG	0.70	2.26	5	2
1:A:135:ARG:HB2	1:A:153:MET:HG3	0.70	1.62	12	3
1:A:179:VAL:HB	1:A:209:VAL:CG1	0.70	2.16	11	11
1:A:210:GLU:HG3	1:A:211:GLN:N	0.70	2.01	1	3
1:A:133:MET:SD	1:A:158:ASN:HB2	0.69	2.27	11	4
1:A:223:ALA:HA	1:A:226:GLN:HG2	0.69	1.64	15	1
1:A:203:LYS:HB2	1:A:207:ARG:NH1	0.69	2.02	6	3
1:A:140:PHE:HE2	1:A:204:ILE:HG22	0.69	1.46	6	1
1:A:133:MET:HG3	1:A:158:ASN:O	0.69	1.88	9	10
1:A:181:ILE:HD12	1:A:182:THR:N	0.69	2.02	3	1
1:A:149:TYR:HA	1:A:152:ASN:HD22	0.69	1.47	15	9
1:A:186:HIS:HA	1:A:190:THR:HB	0.69	1.63	1	9
1:A:203:LYS:HB2	1:A:207:ARG:HH11	0.69	1.48	4	2
1:A:152:ASN:HA	1:A:155:ARG:CG	0.68	2.18	13	7
1:A:165:VAL:HG23	1:A:168:TYR:HD2	0.68	1.48	2	2
1:A:203:LYS:O	1:A:207:ARG:HB3	0.68	1.88	2	12
1:A:187:THR:HA	1:A:191:THR:HG23	0.68	1.64	7	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:179:VAL:HB	1:A:209:VAL:CG2	0.68	2.18	2	4
1:A:152:ASN:HA	1:A:155:ARG:HE	0.68	1.49	7	1
1:A:127:TYR:CD1	1:A:162:TYR:HA	0.67	2.24	8	2
1:A:148:TYR:CD1	1:A:204:ILE:HD13	0.67	2.23	14	4
1:A:135:ARG:HD2	1:A:137:LEU:H	0.67	1.48	13	5
1:A:135:ARG:N	1:A:135:ARG:HD3	0.67	2.05	9	1
1:A:204:ILE:HG13	1:A:205:MET:N	0.67	2.05	10	14
1:A:183:VAL:O	1:A:187:THR:HG22	0.66	1.90	15	7
1:A:193:LYS:HE3	1:A:195:GLU:HB2	0.66	1.66	13	4
1:A:177:ASP:O	1:A:181:ILE:HG12	0.66	1.91	8	14
1:A:162:TYR:OH	1:A:216:GLN:HB3	0.66	1.91	15	5
1:A:160:VAL:HB	1:A:178:CYS:SG	0.66	2.31	10	11
1:A:128:MET:CE	1:A:130:GLY:HA2	0.65	2.22	15	9
1:A:150:ARG:HA	1:A:153:MET:HE3	0.65	1.69	9	2
1:A:127:TYR:CD2	1:A:162:TYR:HA	0.65	2.27	15	3
1:A:198:THR:O	1:A:202:ILE:HG12	0.64	1.93	15	10
1:A:152:ASN:HB2	1:A:156:TYR:HD2	0.64	1.52	3	9
1:A:182:THR:HG21	1:A:209:VAL:HG21	0.64	1.68	15	8
1:A:186:HIS:C	1:A:190:THR:HB	0.64	2.11	13	13
1:A:165:VAL:HG11	1:A:174:PHE:CZ	0.64	2.27	14	2
1:A:135:ARG:HD3	1:A:149:TYR:CE1	0.64	2.27	12	4
1:A:156:TYR:OH	1:A:208:VAL:HG11	0.64	1.93	9	1
1:A:133:MET:HG3	1:A:158:ASN:HB2	0.64	1.69	13	2
1:A:202:ILE:O	1:A:206:GLU:HG3	0.64	1.93	11	12
1:A:133:MET:HG2	1:A:212:MET:CE	0.64	2.23	6	9
1:A:135:ARG:HD3	1:A:149:TYR:HE1	0.64	1.52	12	4
1:A:127:TYR:HD2	1:A:162:TYR:HA	0.64	1.51	15	1
1:A:155:ARG:HD2	1:A:195:GLU:OE2	0.63	1.93	10	1
1:A:133:MET:SD	1:A:135:ARG:HA	0.63	2.33	8	12
1:A:129:LEU:HD21	1:A:159:GLN:HE21	0.63	1.53	4	1
1:A:179:VAL:O	1:A:183:VAL:HG13	0.63	1.92	15	13
1:A:200:THR:O	1:A:203:LYS:HG3	0.63	1.93	9	14
1:A:147:ARG:HD3	1:A:147:ARG:C	0.63	2.14	8	9
1:A:179:VAL:HB	1:A:209:VAL:HG23	0.63	1.69	2	4
1:A:152:ASN:OD1	1:A:205:MET:HA	0.63	1.94	10	6
1:A:160:VAL:HG21	1:A:213:CYS:HB2	0.63	1.69	7	2
1:A:171:GLN:O	1:A:175:VAL:HB	0.62	1.94	2	4
1:A:216:GLN:O	1:A:220:GLU:HB2	0.62	1.95	5	12
1:A:165:VAL:HG21	1:A:174:PHE:CE2	0.62	2.29	3	2
1:A:162:TYR:CE2	1:A:174:PHE:CE1	0.62	2.87	10	1
1:A:147:ARG:HA	1:A:150:ARG:HG2	0.62	1.71	1	12

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:180:ASN:O	1:A:184:LYS:HG2	0.62	1.93	13	9
1:A:208:VAL:O	1:A:212:MET:HB2	0.62	1.95	7	7
1:A:129:LEU:HD11	1:A:159:GLN:NE2	0.62	2.10	11	1
1:A:147:ARG:O	1:A:150:ARG:HG2	0.62	1.95	10	11
1:A:152:ASN:HA	1:A:155:ARG:HG3	0.61	1.71	15	8
1:A:152:ASN:OD1	1:A:205:MET:HB2	0.61	1.96	9	2
1:A:199:GLU:HA	1:A:202:ILE:HG13	0.61	1.72	11	9
1:A:135:ARG:HH21	1:A:152:ASN:ND2	0.61	1.94	2	4
1:A:156:TYR:CE2	1:A:201:ASP:HB2	0.61	2.31	7	1
1:A:140:PHE:HZ	1:A:207:ARG:HD3	0.61	1.53	6	8
1:A:184:LYS:O	1:A:188:VAL:HG13	0.60	1.95	6	14
1:A:140:PHE:HB2	1:A:146:ASP:OD1	0.60	1.95	6	2
1:A:149:TYR:CA	1:A:152:ASN:HB3	0.60	2.24	12	3
1:A:152:ASN:HB2	1:A:156:TYR:CD2	0.60	2.31	3	5
1:A:197:PHE:HB2	1:A:201:ASP:OD1	0.60	1.96	7	1
1:A:138:ILE:HB	1:A:149:TYR:CE1	0.60	2.31	14	7
1:A:133:MET:SD	1:A:212:MET:HG3	0.60	2.36	12	3
1:A:140:PHE:HB3	1:A:142:ASN:HD22	0.60	1.55	11	1
1:A:145:GLU:HG2	1:A:148:TYR:HE2	0.60	1.56	14	1
1:A:204:ILE:O	1:A:207:ARG:HG2	0.60	1.96	9	11
1:A:179:VAL:HG11	1:A:210:GLU:CA	0.60	2.26	11	11
1:A:156:TYR:OH	1:A:208:VAL:CG1	0.59	2.50	9	1
1:A:182:THR:O	1:A:185:GLN:HG3	0.59	1.96	3	1
1:A:150:ARG:O	1:A:153:MET:HE3	0.59	1.97	10	3
1:A:181:ILE:O	1:A:184:LYS:HB2	0.59	1.97	3	10
1:A:152:ASN:HA	1:A:155:ARG:HG2	0.59	1.74	12	5
1:A:149:TYR:HA	1:A:152:ASN:CB	0.59	2.24	12	2
1:A:148:TYR:O	1:A:152:ASN:HB3	0.59	1.97	5	12
1:A:150:ARG:HA	1:A:153:MET:CE	0.59	2.28	9	3
1:A:160:VAL:HA	1:A:182:THR:OG1	0.59	1.98	9	10
1:A:174:PHE:C	1:A:174:PHE:CD1	0.59	2.76	10	1
1:A:129:LEU:HD23	1:A:160:VAL:O	0.59	1.98	11	1
1:A:138:ILE:HG13	1:A:208:VAL:CG2	0.59	2.24	1	10
1:A:184:LYS:HD3	1:A:184:LYS:N	0.59	2.11	1	7
1:A:175:VAL:CG1	1:A:214:ILE:HG13	0.59	2.27	8	15
1:A:199:GLU:HA	1:A:202:ILE:CG1	0.58	2.29	6	11
1:A:223:ALA:O	1:A:227:ARG:HG2	0.58	1.99	3	13
1:A:163:ARG:HG3	1:A:164:PRO:CD	0.58	2.28	4	2
1:A:186:HIS:HA	1:A:190:THR:CB	0.58	2.28	1	9
1:A:155:ARG:HG3	1:A:156:TYR:CD2	0.58	2.34	13	1
1:A:222:GLN:HA	1:A:225:TYR:HB3	0.58	1.76	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:140:PHE:CE2	1:A:204:ILE:HG22	0.58	2.32	6	6
1:A:128:MET:O	1:A:128:MET:HE3	0.58	1.98	11	1
1:A:157:PRO:HB2	1:A:159:GLN:HG2	0.57	1.75	11	7
1:A:171:GLN:N	1:A:171:GLN:HE21	0.57	1.96	1	1
1:A:183:VAL:HG22	1:A:184:LYS:HD3	0.57	1.75	5	3
1:A:160:VAL:CG1	1:A:209:VAL:HB	0.57	2.29	8	4
1:A:162:TYR:CE2	1:A:174:PHE:CD1	0.57	2.92	10	1
1:A:135:ARG:HD3	1:A:136:PRO:CD	0.57	2.29	1	1
1:A:128:MET:N	1:A:162:TYR:O	0.57	2.37	10	2
1:A:216:GLN:HA	1:A:219:GLN:HB3	0.57	1.75	2	7
1:A:133:MET:SD	1:A:158:ASN:HB3	0.57	2.39	2	2
1:A:160:VAL:HG23	1:A:162:TYR:HE1	0.57	1.59	6	1
1:A:146:ASP:O	1:A:150:ARG:HG3	0.57	1.99	13	1
1:A:149:TYR:HA	1:A:152:ASN:ND2	0.57	2.15	3	5
1:A:145:GLU:HA	1:A:148:TYR:CD2	0.57	2.35	13	2
1:A:142:ASN:HB2	1:A:146:ASP:HB2	0.56	1.76	1	1
1:A:133:MET:SD	1:A:212:MET:CE	0.56	2.93	15	1
1:A:156:TYR:HH	1:A:197:PHE:CB	0.56	2.12	15	1
1:A:207:ARG:CG	1:A:208:VAL:N	0.56	2.69	12	13
1:A:162:TYR:HD2	1:A:174:PHE:CE2	0.56	2.19	5	1
1:A:176:HIS:O	1:A:179:VAL:HG22	0.56	2.01	2	11
1:A:197:PHE:HA	1:A:201:ASP:OD2	0.56	2.01	2	1
1:A:130:GLY:HA3	1:A:162:TYR:CE2	0.56	2.36	11	2
1:A:198:THR:HG22	1:A:200:THR:H	0.56	1.61	9	1
1:A:180:ASN:HA	1:A:184:LYS:HE3	0.55	1.76	1	1
1:A:207:ARG:HG2	1:A:208:VAL:N	0.55	2.16	12	5
1:A:133:MET:HG2	1:A:212:MET:HE1	0.55	1.78	6	6
1:A:203:LYS:CE	1:A:204:ILE:HG23	0.55	2.31	11	1
1:A:147:ARG:O	1:A:151:GLU:HG2	0.55	2.01	9	11
1:A:153:MET:HA	1:A:156:TYR:CD2	0.55	2.36	9	1
1:A:157:PRO:HB2	1:A:159:GLN:HG3	0.55	1.78	12	1
1:A:187:THR:HA	1:A:191:THR:CB	0.55	2.32	3	5
1:A:205:MET:HG2	1:A:206:GLU:N	0.55	2.15	7	5
1:A:152:ASN:O	1:A:156:TYR:N	0.55	2.39	12	4
1:A:145:GLU:HA	1:A:148:TYR:CG	0.55	2.37	13	3
1:A:152:ASN:OD1	1:A:156:TYR:HB2	0.54	2.02	7	2
1:A:133:MET:HG2	1:A:212:MET:HE2	0.54	1.78	11	4
1:A:202:ILE:HA	1:A:205:MET:CE	0.54	2.32	11	8
1:A:175:VAL:O	1:A:179:VAL:HG13	0.54	2.02	11	2
1:A:133:MET:SD	1:A:135:ARG:CA	0.54	2.96	8	2
1:A:179:VAL:HB	1:A:209:VAL:HG21	0.54	1.78	9	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:135:ARG:HG3	1:A:153:MET:HE2	0.54	1.80	2	3
1:A:191:THR:HA	1:A:197:PHE:CE2	0.54	2.37	15	2
1:A:152:ASN:HA	1:A:155:ARG:HD2	0.54	1.77	9	2
1:A:133:MET:SD	1:A:158:ASN:C	0.54	2.86	15	1
1:A:144:TYR:O	1:A:148:TYR:HB2	0.53	2.02	12	4
1:A:151:GLU:HB3	1:A:155:ARG:HD3	0.53	1.78	10	1
1:A:132:ALA:HA	1:A:159:GLN:HB3	0.53	1.79	15	4
1:A:133:MET:O	1:A:158:ASN:HB2	0.53	2.04	2	3
1:A:136:PRO:O	1:A:137:LEU:HD22	0.53	2.03	4	2
1:A:156:TYR:OH	1:A:197:PHE:HB3	0.53	2.04	15	1
1:A:200:THR:HG23	1:A:203:LYS:HE2	0.53	1.81	2	1
1:A:162:TYR:HD1	1:A:163:ARG:O	0.53	1.86	11	2
1:A:135:ARG:HG2	1:A:153:MET:HE2	0.53	1.80	9	1
1:A:138:ILE:O	1:A:139:HIS:CD2	0.52	2.62	9	2
1:A:180:ASN:O	1:A:184:LYS:HG3	0.52	2.03	9	1
1:A:162:TYR:CD2	1:A:174:PHE:HE2	0.52	2.23	14	2
1:A:135:ARG:HH12	1:A:152:ASN:ND2	0.52	2.03	1	2
1:A:175:VAL:HG13	1:A:213:CYS:CB	0.52	2.32	12	9
1:A:165:VAL:HG11	1:A:174:PHE:CE1	0.52	2.40	3	1
1:A:179:VAL:HB	1:A:209:VAL:HG12	0.52	1.82	5	4
1:A:162:TYR:CD2	1:A:174:PHE:HE1	0.52	2.23	13	3
1:A:152:ASN:CA	1:A:155:ARG:HE	0.52	2.16	7	2
1:A:186:HIS:CA	1:A:190:THR:HB	0.52	2.35	8	8
1:A:220:GLU:HA	1:A:223:ALA:HB3	0.52	1.80	10	3
1:A:162:TYR:HB2	1:A:174:PHE:CZ	0.52	2.40	14	1
1:A:183:VAL:HG11	1:A:206:GLU:HG2	0.52	1.82	8	1
1:A:156:TYR:HE2	1:A:201:ASP:HB2	0.51	1.65	7	1
1:A:186:HIS:ND1	1:A:190:THR:HG21	0.51	2.20	3	1
1:A:175:VAL:HA	1:A:213:CYS:SG	0.51	2.46	10	1
1:A:223:ALA:O	1:A:227:ARG:HG3	0.51	2.06	14	1
1:A:201:ASP:O	1:A:205:MET:HB3	0.51	2.05	7	6
1:A:156:TYR:CD2	1:A:205:MET:HB2	0.51	2.40	11	4
1:A:204:ILE:HA	1:A:207:ARG:CD	0.51	2.34	15	2
1:A:129:LEU:HD21	1:A:159:GLN:HG3	0.51	1.82	2	1
1:A:133:MET:HE2	1:A:212:MET:HG3	0.51	1.83	7	4
1:A:148:TYR:HD1	1:A:149:TYR:N	0.51	2.04	5	3
1:A:140:PHE:CZ	1:A:204:ILE:HG22	0.51	2.41	11	2
1:A:165:VAL:HG23	1:A:167:GLN:HE21	0.51	1.66	10	1
1:A:171:GLN:NE2	1:A:172:ASN:H	0.50	2.04	4	3
1:A:135:ARG:HD2	1:A:135:ARG:C	0.50	2.27	4	2
1:A:152:ASN:HA	1:A:155:ARG:NE	0.50	2.18	7	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:201:ASP:CA	1:A:204:ILE:HD11	0.50	2.26	12	2
1:A:133:MET:CE	1:A:212:MET:HG3	0.50	2.36	12	1
1:A:133:MET:HE1	1:A:212:MET:HG3	0.50	1.82	12	1
1:A:187:THR:HA	1:A:191:THR:CG2	0.50	2.36	4	3
1:A:202:ILE:HA	1:A:205:MET:HE2	0.50	1.83	8	1
1:A:165:VAL:HG23	1:A:168:TYR:CD2	0.50	2.35	2	1
1:A:129:LEU:HD23	1:A:161:TYR:CE2	0.50	2.42	7	1
1:A:147:ARG:HA	1:A:150:ARG:HG3	0.50	1.83	13	1
1:A:133:MET:SD	1:A:136:PRO:CD	0.50	2.99	13	4
1:A:128:MET:HG3	1:A:128:MET:O	0.49	2.06	5	3
1:A:175:VAL:HG12	1:A:176:HIS:N	0.49	2.20	8	8
1:A:165:VAL:HB	1:A:174:PHE:CZ	0.49	2.42	6	1
1:A:127:TYR:HD1	1:A:162:TYR:HA	0.49	1.67	5	1
1:A:129:LEU:CD2	1:A:159:GLN:HB2	0.49	2.29	11	1
1:A:160:VAL:HG11	1:A:213:CYS:HB2	0.49	1.84	11	1
1:A:155:ARG:HG2	1:A:156:TYR:H	0.49	1.66	9	2
1:A:130:GLY:HA3	1:A:162:TYR:CE1	0.49	2.42	6	4
1:A:174:PHE:O	1:A:177:ASP:HB3	0.49	2.06	5	3
1:A:204:ILE:HG13	1:A:205:MET:H	0.49	1.68	5	4
1:A:198:THR:HG23	1:A:200:THR:HB	0.49	1.84	13	1
1:A:171:GLN:HE21	1:A:172:ASN:N	0.49	2.05	9	6
1:A:175:VAL:HG11	1:A:214:ILE:CG1	0.49	2.26	10	4
1:A:178:CYS:SG	1:A:179:VAL:N	0.49	2.86	2	1
1:A:165:VAL:HG21	1:A:217:TYR:CE2	0.49	2.42	6	1
1:A:145:GLU:HA	1:A:148:TYR:CD1	0.49	2.43	5	2
1:A:178:CYS:O	1:A:181:ILE:HD11	0.48	2.07	3	1
1:A:129:LEU:HD11	1:A:159:GLN:HE21	0.48	1.68	5	1
1:A:160:VAL:HG23	1:A:162:TYR:CE1	0.48	2.42	6	1
1:A:179:VAL:CG1	1:A:210:GLU:HA	0.48	2.36	11	5
1:A:163:ARG:HB2	1:A:164:PRO:HD3	0.48	1.85	7	1
1:A:139:HIS:CD2	1:A:140:PHE:H	0.48	2.25	11	5
1:A:144:TYR:HA	1:A:147:ARG:HB3	0.48	1.85	14	4
1:A:156:TYR:CE1	1:A:205:MET:SD	0.48	3.06	2	2
1:A:179:VAL:CG1	1:A:209:VAL:HG23	0.48	2.38	2	3
1:A:189:THR:HA	1:A:192:THR:OG1	0.48	2.08	9	3
1:A:133:MET:SD	1:A:135:ARG:N	0.48	2.87	8	2
1:A:152:ASN:CB	1:A:156:TYR:HD2	0.48	2.22	14	5
1:A:179:VAL:CB	1:A:209:VAL:HG23	0.48	2.36	2	2
1:A:135:ARG:CD	1:A:208:VAL:HG11	0.48	2.39	7	1
1:A:156:TYR:OH	1:A:197:PHE:HB2	0.48	2.08	14	1
1:A:135:ARG:HD3	1:A:136:PRO:HD2	0.48	1.85	1	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:191:THR:O	1:A:195:GLU:HB3	0.48	2.09	11	6
1:A:134:SER:O	1:A:135:ARG:HB2	0.48	2.09	14	3
1:A:140:PHE:HB3	1:A:142:ASN:ND2	0.48	2.24	11	1
1:A:198:THR:O	1:A:201:ASP:N	0.48	2.47	15	10
1:A:210:GLU:CG	1:A:211:GLN:N	0.48	2.77	4	3
1:A:222:GLN:O	1:A:225:TYR:HB2	0.48	2.09	8	2
1:A:183:VAL:HG12	1:A:209:VAL:HG11	0.47	1.85	11	4
1:A:184:LYS:N	1:A:184:LYS:CD	0.47	2.77	5	7
1:A:152:ASN:CA	1:A:156:TYR:HB2	0.47	2.38	10	1
1:A:160:VAL:HG13	1:A:209:VAL:HG22	0.47	1.86	1	8
1:A:162:TYR:CD2	1:A:174:PHE:CE2	0.47	3.02	14	2
1:A:145:GLU:HA	1:A:148:TYR:CE2	0.47	2.45	14	1
1:A:190:THR:O	1:A:193:LYS:HG3	0.47	2.10	2	2
1:A:216:GLN:O	1:A:220:GLU:N	0.47	2.46	6	1
1:A:183:VAL:HG12	1:A:209:VAL:HG21	0.47	1.87	8	2
1:A:142:ASN:HB3	1:A:146:ASP:H	0.47	1.70	13	2
1:A:128:MET:CG	1:A:163:ARG:HA	0.47	2.40	15	1
1:A:160:VAL:CG2	1:A:162:TYR:HE1	0.46	2.24	6	1
1:A:148:TYR:HE1	1:A:204:ILE:CG2	0.46	2.23	13	1
1:A:135:ARG:NE	1:A:208:VAL:HG11	0.46	2.25	2	6
1:A:164:PRO:HB2	1:A:227:ARG:NH2	0.46	2.25	2	1
1:A:182:THR:HG21	1:A:209:VAL:CG2	0.46	2.38	15	4
1:A:212:MET:SD	1:A:213:CYS:N	0.46	2.88	15	3
1:A:172:ASN:O	1:A:176:HIS:N	0.46	2.49	3	1
1:A:128:MET:HE3	1:A:130:GLY:HA2	0.46	1.87	15	1
1:A:143:ASP:O	1:A:147:ARG:HB2	0.46	2.10	11	2
1:A:215:THR:O	1:A:218:GLN:HG3	0.46	2.09	4	1
1:A:149:TYR:CA	1:A:152:ASN:HD22	0.46	2.23	1	3
1:A:203:LYS:HG3	1:A:204:ILE:H	0.46	1.70	12	2
1:A:135:ARG:HB2	1:A:158:ASN:OD1	0.46	2.09	10	1
1:A:160:VAL:CB	1:A:178:CYS:SG	0.46	3.03	10	1
1:A:133:MET:SD	1:A:212:MET:HE1	0.46	2.50	15	1
1:A:157:PRO:HD3	1:A:186:HIS:CG	0.46	2.46	10	3
1:A:148:TYR:O	1:A:151:GLU:HG3	0.46	2.11	7	1
1:A:165:VAL:HG11	1:A:174:PHE:CE2	0.46	2.45	14	1
1:A:148:TYR:HB3	1:A:204:ILE:HD13	0.46	1.88	3	2
1:A:135:ARG:HD2	1:A:149:TYR:HE1	0.46	1.69	3	2
1:A:135:ARG:C	1:A:137:LEU:H	0.46	2.13	6	2
1:A:223:ALA:O	1:A:226:GLN:HG3	0.46	2.10	11	1
1:A:197:PHE:HA	1:A:201:ASP:CG	0.46	2.31	1	2
1:A:165:VAL:HG23	1:A:168:TYR:CD1	0.46	2.46	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:172:ASN:O	1:A:176:HIS:HB2	0.46	2.11	4	1
1:A:199:GLU:CA	1:A:202:ILE:HG12	0.46	2.41	4	2
1:A:201:ASP:HA	1:A:204:ILE:CG1	0.45	2.41	8	2
1:A:145:GLU:HA	1:A:148:TYR:CE1	0.45	2.46	5	1
1:A:214:ILE:O	1:A:217:TYR:HB3	0.45	2.11	10	1
1:A:198:THR:N	1:A:201:ASP:HB2	0.45	2.27	15	1
1:A:156:TYR:CD1	1:A:205:MET:SD	0.45	3.09	10	4
1:A:138:ILE:O	1:A:140:PHE:N	0.45	2.49	5	2
1:A:160:VAL:HA	1:A:182:THR:HG1	0.45	1.71	10	1
1:A:135:ARG:CZ	1:A:208:VAL:HG11	0.45	2.41	5	3
1:A:199:GLU:HA	1:A:202:ILE:HG12	0.45	1.87	6	2
1:A:191:THR:HB	1:A:197:PHE:CD1	0.45	2.46	13	2
1:A:137:LEU:N	1:A:137:LEU:HD13	0.45	2.26	4	1
1:A:160:VAL:HG21	1:A:213:CYS:CB	0.45	2.42	11	3
1:A:135:ARG:NH1	1:A:158:ASN:HA	0.45	2.26	15	1
1:A:138:ILE:HG13	1:A:208:VAL:HG13	0.45	1.88	15	1
1:A:155:ARG:HG3	1:A:156:TYR:H	0.45	1.70	1	1
1:A:202:ILE:HG22	1:A:206:GLU:OE2	0.45	2.12	2	1
1:A:198:THR:HG22	1:A:201:ASP:OD1	0.45	2.10	11	2
1:A:156:TYR:CG	1:A:205:MET:HB2	0.45	2.46	14	2
1:A:187:THR:HA	1:A:191:THR:HG1	0.45	1.72	14	1
1:A:190:THR:O	1:A:193:LYS:HE2	0.45	2.11	10	1
1:A:187:THR:HG23	1:A:197:PHE:HD2	0.44	1.72	2	1
1:A:147:ARG:HD3	1:A:147:ARG:O	0.44	2.11	6	2
1:A:207:ARG:HG2	1:A:208:VAL:H	0.44	1.72	12	3
1:A:171:GLN:HE21	1:A:172:ASN:H	0.44	1.55	6	4
1:A:209:VAL:O	1:A:213:CYS:HB2	0.44	2.12	2	1
1:A:198:THR:HG23	1:A:200:THR:H	0.44	1.72	10	1
1:A:152:ASN:N	1:A:155:ARG:HE	0.44	2.10	15	1
1:A:129:LEU:O	1:A:131:SER:N	0.44	2.51	1	5
1:A:128:MET:HG3	1:A:164:PRO:HG3	0.44	1.88	10	1
1:A:145:GLU:CG	1:A:148:TYR:CE2	0.44	2.97	14	1
1:A:207:ARG:HG3	1:A:208:VAL:N	0.44	2.28	11	2
1:A:129:LEU:HA	1:A:161:TYR:HA	0.44	1.88	8	1
1:A:162:TYR:HB3	1:A:178:CYS:CB	0.44	2.42	13	2
1:A:174:PHE:CE2	1:A:217:TYR:HD2	0.44	2.31	10	1
1:A:148:TYR:CE1	1:A:204:ILE:CG2	0.44	3.01	14	3
1:A:152:ASN:OD1	1:A:156:TYR:HB3	0.44	2.12	9	1
1:A:155:ARG:O	1:A:190:THR:HG21	0.44	2.13	2	1
1:A:183:VAL:CG2	1:A:184:LYS:HD3	0.44	2.43	5	2
1:A:186:HIS:O	1:A:190:THR:N	0.44	2.51	13	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:130:GLY:N	1:A:160:VAL:O	0.44	2.49	7	2
1:A:171:GLN:HE21	1:A:171:GLN:H	0.43	1.56	1	1
1:A:136:PRO:HG3	1:A:212:MET:HG3	0.43	1.90	4	1
1:A:179:VAL:HG11	1:A:210:GLU:CB	0.43	2.43	5	1
1:A:168:TYR:CE2	1:A:170:ASN:HB2	0.43	2.49	7	1
1:A:224:ALA:HA	1:A:227:ARG:HG2	0.43	1.89	12	1
1:A:135:ARG:HH12	1:A:158:ASN:HA	0.43	1.73	14	1
1:A:178:CYS:O	1:A:181:ILE:CD1	0.43	2.66	3	1
1:A:184:LYS:N	1:A:184:LYS:HD3	0.43	2.27	3	2
1:A:204:ILE:HA	1:A:207:ARG:HD2	0.43	1.88	11	1
1:A:222:GLN:O	1:A:225:TYR:HB3	0.43	2.13	14	1
1:A:139:HIS:HD2	1:A:140:PHE:H	0.43	1.56	2	2
1:A:136:PRO:C	1:A:137:LEU:HD13	0.43	2.34	6	1
1:A:145:GLU:OE1	1:A:148:TYR:OH	0.43	2.36	14	1
1:A:187:THR:HG23	1:A:191:THR:HG21	0.43	1.90	6	1
1:A:222:GLN:O	1:A:226:GLN:HG2	0.43	2.14	9	1
1:A:162:TYR:OH	1:A:174:PHE:CG	0.43	2.70	10	1
1:A:142:ASN:HB2	1:A:146:ASP:H	0.43	1.74	12	1
1:A:222:GLN:HA	1:A:225:TYR:CD1	0.43	2.49	8	1
1:A:170:ASN:HB3	1:A:173:SER:HB3	0.43	1.89	7	1
1:A:160:VAL:HG13	1:A:209:VAL:HB	0.43	1.90	14	1
1:A:148:TYR:CD1	1:A:204:ILE:HG21	0.43	2.48	13	1
1:A:162:TYR:CD2	1:A:174:PHE:CE1	0.43	3.07	7	2
1:A:128:MET:HG2	1:A:163:ARG:HA	0.43	1.91	8	1
1:A:217:TYR:O	1:A:221:SER:HB2	0.43	2.13	10	1
1:A:155:ARG:HG3	1:A:156:TYR:CE2	0.43	2.49	12	1
1:A:186:HIS:O	1:A:188:VAL:N	0.42	2.52	12	3
1:A:129:LEU:CA	1:A:160:VAL:O	0.42	2.66	10	1
1:A:135:ARG:NH2	1:A:153:MET:HA	0.42	2.30	1	1
1:A:162:TYR:HD2	1:A:163:ARG:O	0.42	1.98	2	4
1:A:156:TYR:CD1	1:A:157:PRO:HD2	0.42	2.49	9	1
1:A:129:LEU:O	1:A:129:LEU:HD12	0.42	2.14	10	1
1:A:147:ARG:O	1:A:147:ARG:HD3	0.42	2.14	9	2
1:A:133:MET:HE1	1:A:135:ARG:NH1	0.42	2.29	2	1
1:A:152:ASN:HA	1:A:156:TYR:HB2	0.42	1.91	10	1
1:A:129:LEU:HD12	1:A:161:TYR:CE2	0.42	2.50	3	1
1:A:135:ARG:CD	1:A:149:TYR:HE1	0.42	2.28	15	3
1:A:156:TYR:OH	1:A:197:PHE:CB	0.42	2.66	15	1
1:A:162:TYR:HD2	1:A:174:PHE:CE1	0.42	2.32	7	1
1:A:135:ARG:HB2	1:A:153:MET:CG	0.42	2.44	1	1
1:A:162:TYR:CD2	1:A:163:ARG:O	0.42	2.73	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:MET:O	1:A:129:LEU:C	0.42	2.58	5	1
1:A:222:GLN:O	1:A:226:GLN:HG3	0.42	2.15	14	1
1:A:160:VAL:CG1	1:A:209:VAL:HG22	0.42	2.45	15	1
1:A:147:ARG:HA	1:A:150:ARG:CG	0.42	2.44	13	2
1:A:187:THR:HG21	1:A:205:MET:SD	0.42	2.55	4	1
1:A:224:ALA:O	1:A:228:ALA:HB2	0.42	2.14	7	1
1:A:156:TYR:HE1	1:A:187:THR:HB	0.42	1.75	15	1
1:A:160:VAL:HG21	1:A:213:CYS:SG	0.42	2.55	2	1
1:A:179:VAL:C	1:A:181:ILE:N	0.42	2.73	13	4
1:A:175:VAL:O	1:A:178:CYS:SG	0.42	2.78	14	3
1:A:137:LEU:HD22	1:A:137:LEU:N	0.41	2.31	3	1
1:A:191:THR:HG21	1:A:197:PHE:CD1	0.41	2.50	8	2
1:A:145:GLU:N	1:A:145:GLU:CD	0.41	2.73	8	1
1:A:170:ASN:HD22	1:A:173:SER:HB3	0.41	1.75	14	1
1:A:140:PHE:CZ	1:A:207:ARG:HD3	0.41	2.46	8	1
1:A:162:TYR:HE2	1:A:165:VAL:CG1	0.41	2.28	10	1
1:A:162:TYR:CZ	1:A:174:PHE:CD1	0.41	3.08	10	1
1:A:147:ARG:HD2	1:A:147:ARG:C	0.41	2.35	13	1
1:A:216:GLN:NE2	1:A:219:GLN:HG2	0.41	2.30	13	1
1:A:133:MET:HG3	1:A:136:PRO:HD3	0.41	1.91	15	1
1:A:156:TYR:OH	1:A:197:PHE:CG	0.41	2.51	15	1
1:A:184:LYS:O	1:A:188:VAL:HG22	0.41	2.15	1	1
1:A:161:TYR:CE1	1:A:182:THR:HA	0.41	2.50	8	2
1:A:198:THR:HG22	1:A:201:ASP:OD2	0.41	2.16	15	2
1:A:179:VAL:HA	1:A:182:THR:HB	0.41	1.93	14	2
1:A:161:TYR:HE1	1:A:185:GLN:OE1	0.41	1.98	3	1
1:A:153:MET:HE3	1:A:153:MET:HB3	0.41	1.67	4	1
1:A:129:LEU:HA	1:A:160:VAL:C	0.41	2.35	8	1
1:A:202:ILE:HG22	1:A:206:GLU:OE1	0.41	2.14	10	1
1:A:145:GLU:O	1:A:149:TYR:HB3	0.41	2.15	14	1
1:A:131:SER:HB2	1:A:216:GLN:HG2	0.41	1.92	15	1
1:A:155:ARG:NH2	1:A:201:ASP:OD2	0.41	2.50	8	1
1:A:155:ARG:CG	1:A:156:TYR:N	0.41	2.84	11	2
1:A:147:ARG:O	1:A:150:ARG:HB2	0.41	2.16	13	1
1:A:162:TYR:OH	1:A:216:GLN:HG3	0.41	2.15	13	1
1:A:163:ARG:O	1:A:165:VAL:HG13	0.41	2.16	3	1
1:A:164:PRO:HA	1:A:220:GLU:OE2	0.41	2.15	6	1
1:A:151:GLU:C	1:A:153:MET:N	0.41	2.74	10	1
1:A:191:THR:HG23	1:A:197:PHE:CD2	0.41	2.50	15	1
1:A:147:ARG:CA	1:A:150:ARG:HG2	0.41	2.45	1	1
1:A:182:THR:CG2	1:A:209:VAL:HG21	0.41	2.45	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:191:THR:O	1:A:195:GLU:HB2	0.41	2.16	4	1
1:A:128:MET:O	1:A:128:MET:CG	0.41	2.69	7	1
1:A:157:PRO:HB2	1:A:159:GLN:OE1	0.41	2.15	7	1
1:A:152:ASN:O	1:A:155:ARG:HG2	0.41	2.16	9	1
1:A:153:MET:HB2	1:A:158:ASN:HD21	0.41	1.75	10	1
1:A:164:PRO:HB3	1:A:220:GLU:OE1	0.41	2.15	12	1
1:A:171:GLN:HB3	1:A:214:ILE:HG12	0.41	1.92	5	1
1:A:135:ARG:HA	1:A:136:PRO:HD3	0.41	1.81	8	1
1:A:158:ASN:C	1:A:158:ASN:HD22	0.41	2.20	11	1
1:A:215:THR:O	1:A:218:GLN:HG2	0.40	2.15	1	1
1:A:162:TYR:CG	1:A:163:ARG:N	0.40	2.89	10	1
1:A:142:ASN:N	1:A:146:ASP:OD1	0.40	2.47	11	1
1:A:203:LYS:O	1:A:207:ARG:CB	0.40	2.69	3	1
1:A:182:THR:C	1:A:184:LYS:N	0.40	2.74	12	1
1:A:219:GLN:O	1:A:223:ALA:N	0.40	2.53	4	1
1:A:151:GLU:C	1:A:153:MET:H	0.40	2.20	5	2
1:A:138:ILE:HG22	1:A:139:HIS:N	0.40	2.32	7	1
1:A:128:MET:O	1:A:162:TYR:O	0.40	2.40	11	2

## 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	101/138 (73%)	78±3 (77±3%)	17±3 (17±3%)	5±1 (5±1%)	<b>3</b>	<b>22</b>
All	All	1515/2070 (73%)	1174 (77%)	259 (17%)	82 (5%)	<b>3</b>	<b>22</b>

All 13 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	135	ARG	15
1	A	166	ASP	15
1	A	139	HIS	13
1	A	131	SER	10

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Mol	Chain	Res	Type	Models (Total)
1	A	189	THR	7
1	A	130	GLY	5
1	A	127	TYR	4
1	A	137	LEU	3
1	A	187	THR	3
1	A	157	PRO	3
1	A	140	PHE	2
1	A	136	PRO	1
1	A	158	ASN	1

### 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	95/116 (82%)	71±2 (75±2%)	24±2 (25±2%)	2	23
All	All	1425/1740 (82%)	1069 (75%)	356 (25%)	2	23

All 56 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	133	MET	15
1	A	152	ASN	15
1	A	153	MET	15
1	A	179	VAL	15
1	A	193	LYS	15
1	A	210	GLU	15
1	A	128	MET	14
1	A	148	TYR	14
1	A	171	GLN	14
1	A	222	GLN	14
1	A	149	TYR	12
1	A	203	LYS	12
1	A	129	LEU	11
1	A	181	ILE	11
1	A	183	VAL	11
1	A	205	MET	11

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Mol	Chain	Res	Type	Models (Total)
1	A	209	VAL	11
1	A	160	VAL	10
1	A	166	ASP	9
1	A	147	ARG	8
1	A	178	CYS	8
1	A	158	ASN	8
1	A	214	ILE	8
1	A	220	GLU	7
1	A	139	HIS	6
1	A	157	PRO	6
1	A	167	GLN	5
1	A	159	GLN	4
1	A	142	ASN	3
1	A	225	TYR	3
1	A	199	GLU	3
1	A	137	LEU	3
1	A	155	ARG	3
1	A	202	ILE	3
1	A	135	ARG	3
1	A	216	GLN	3
1	A	211	GLN	3
1	A	195	GLU	2
1	A	226	GLN	2
1	A	150	ARG	2
1	A	185	GLN	2
1	A	200	THR	2
1	A	191	THR	2
1	A	175	VAL	1
1	A	168	TYR	1
1	A	177	ASP	1
1	A	187	THR	1
1	A	218	GLN	1
1	A	170	ASN	1
1	A	201	ASP	1
1	A	161	TYR	1
1	A	156	TYR	1
1	A	174	PHE	1
1	A	163	ARG	1
1	A	173	SER	1
1	A	146	ASP	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 oligosaccharides in this entry.

### 6.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 6.7 Other polymers [i](#)

There are no such molecules in this entry.

### 6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 7 Chemical shift validation

No chemical shift data were provided