



Full wwPDB NMR Structure Validation Report ⓘ

Mar 6, 2026 – 09:00 AM UTC

PDB ID : 2JOM / pdb_00002jom
Title : NMR structure of rabbit prion protein mutation I214V
Authors : Li, J.; Lin, D.
Deposited on : 2007-03-14

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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
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)	:	2.49

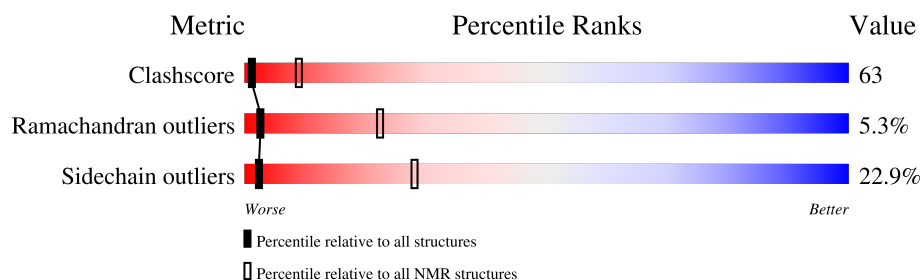
1 Overall quality at a glance

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	148	18% 41% 13% 29%

2 Ensemble composition and analysis

This entry contains 15 models. Model 6 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *closest to the average*.

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:124-A:228 (105)	0.76	6

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 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1692 atoms, of which 819 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
			1692	543	819	152	171	7	

There are 11 discrepancies between the modelled and reference sequences:

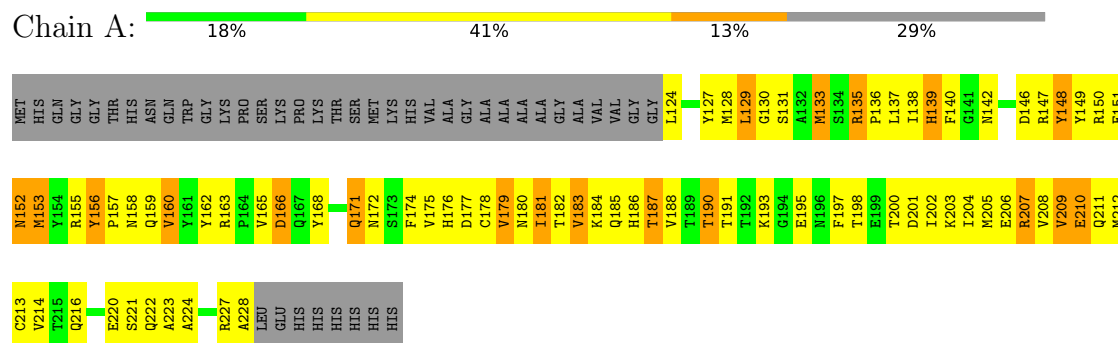
Chain	Residue	Modelled	Actual	Comment	Reference
A	89	MET	-	initiating methionine	UNP Q95211
A	90	HIS	-	expression tag	UNP Q95211
A	214	VAL	ILE	engineered mutation	UNP Q95211
A	229	LEU	-	expression tag	UNP Q95211
A	230	GLU	-	expression tag	UNP Q95211
A	231	HIS	-	expression tag	UNP Q95211
A	232	HIS	-	expression tag	UNP Q95211
A	233	HIS	-	expression tag	UNP Q95211
A	234	HIS	-	expression tag	UNP Q95211
A	235	HIS	-	expression tag	UNP Q95211
A	236	HIS	-	expression tag	UNP Q95211

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

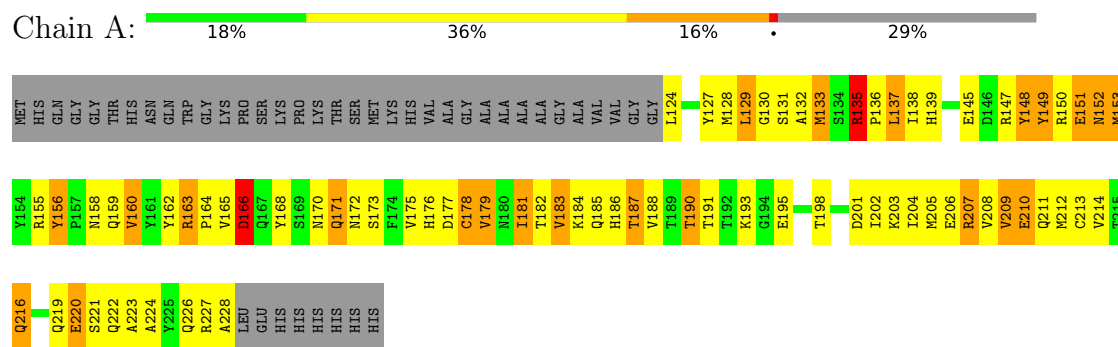


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

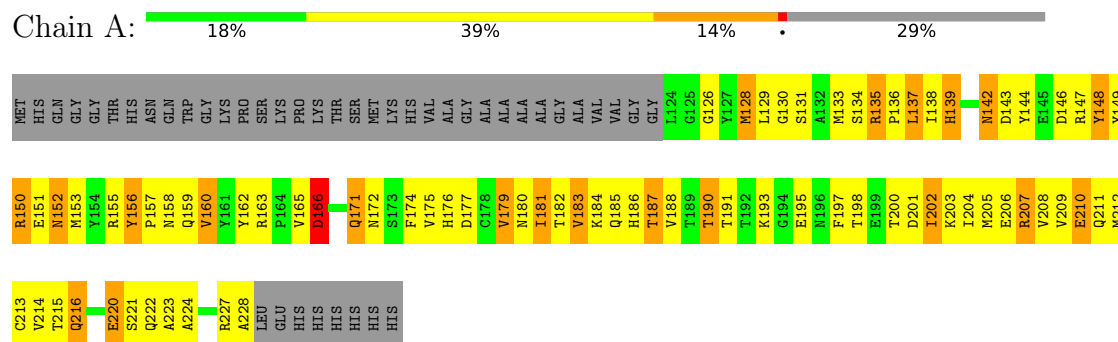
4.2.1 Score per residue for model 1

- Molecule 1: Major prion protein



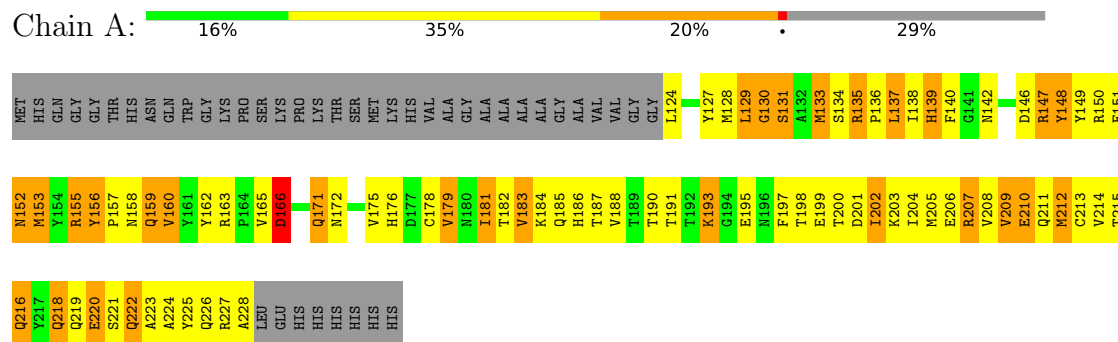
4.2.2 Score per residue for model 2

- Molecule 1: Major prion protein



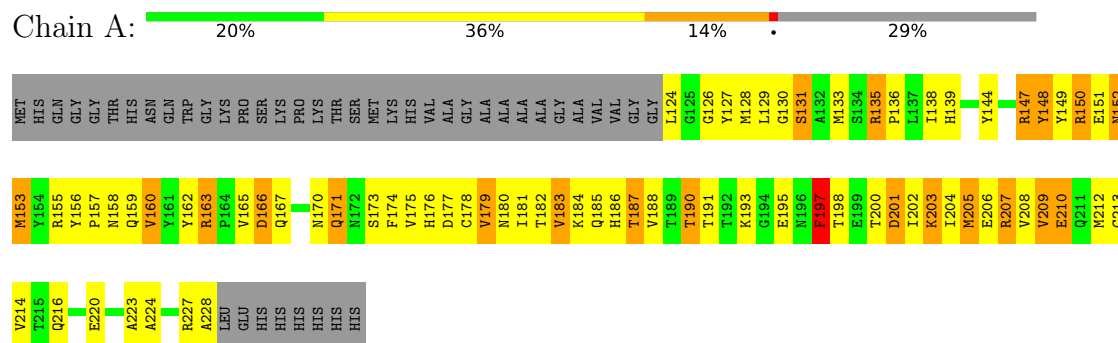
4.2.3 Score per residue for model 3

- Molecule 1: Major prion protein



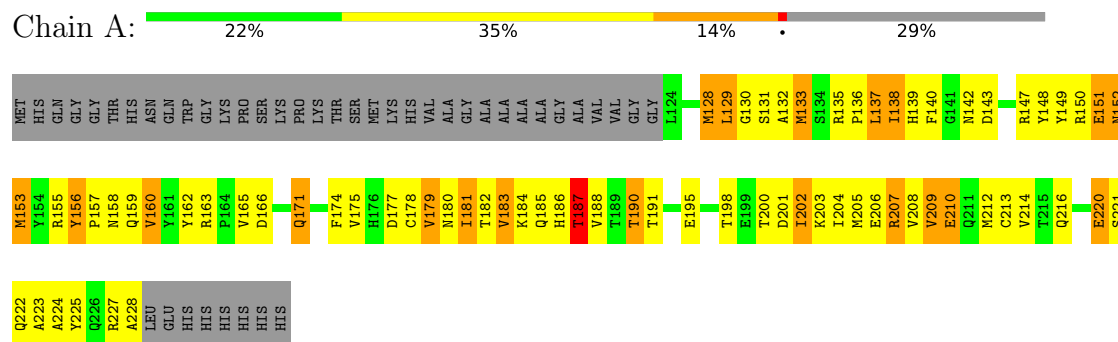
4.2.4 Score per residue for model 4

- Molecule 1: Major prion protein



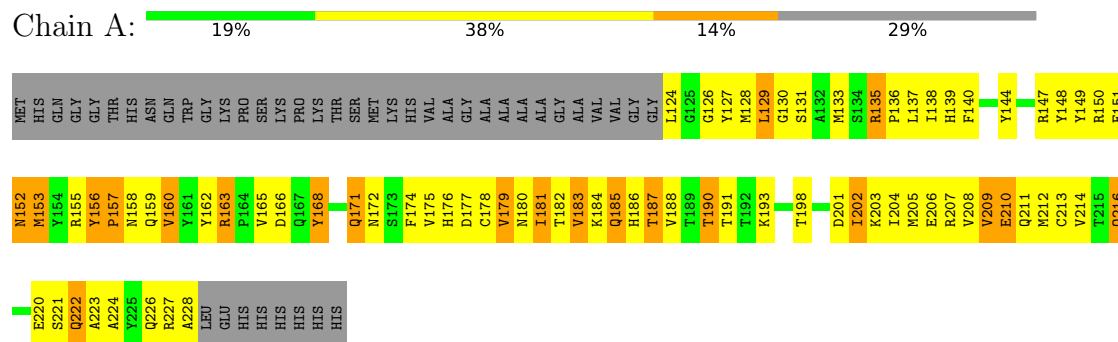
4.2.5 Score per residue for model 5

- Molecule 1: Major prion protein



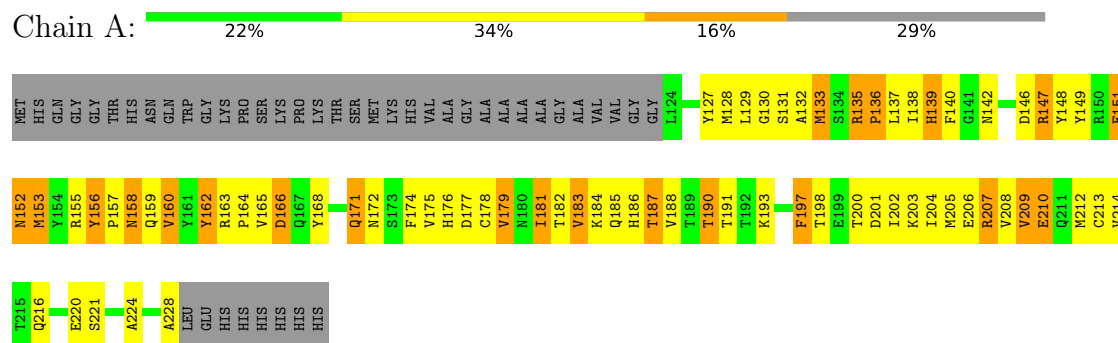
4.2.6 Score per residue for model 6 (medoid)

- Molecule 1: Major prion protein



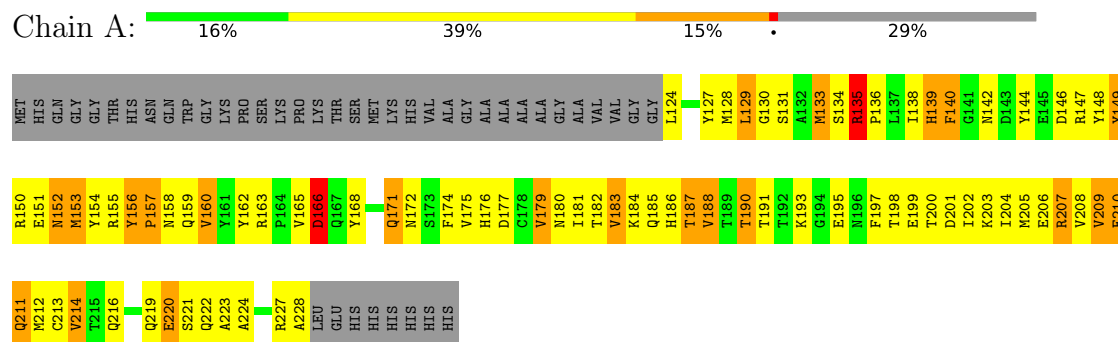
4.2.7 Score per residue for model 7

- Molecule 1: Major prion protein



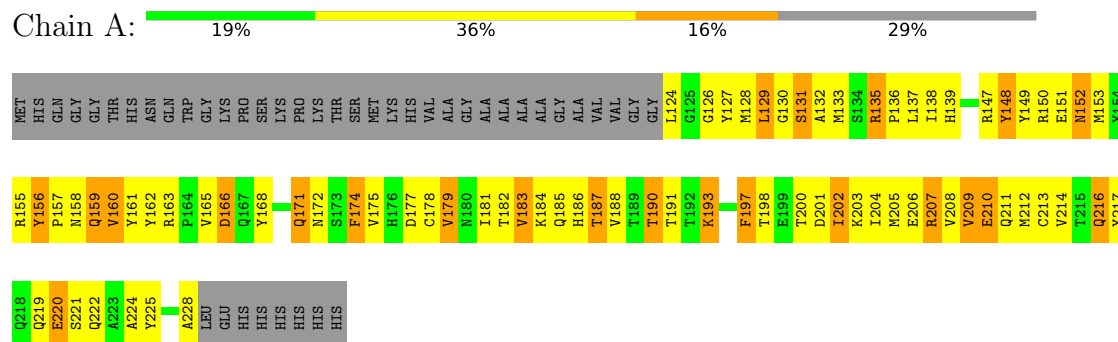
4.2.8 Score per residue for model 8

- Molecule 1: Major prion protein



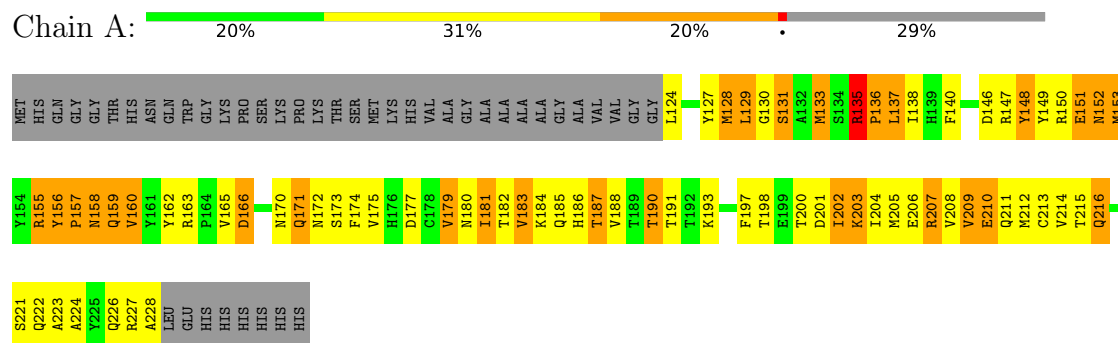
4.2.9 Score per residue for model 9

- Molecule 1: Major prion protein



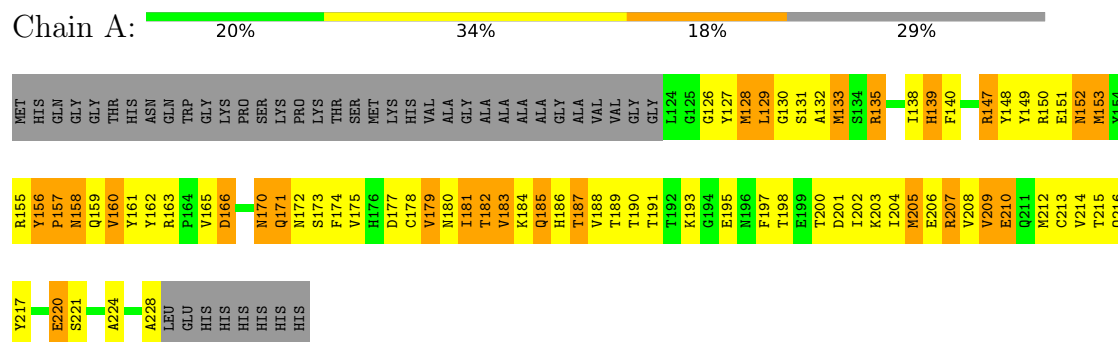
4.2.10 Score per residue for model 10

- Molecule 1: Major prion protein



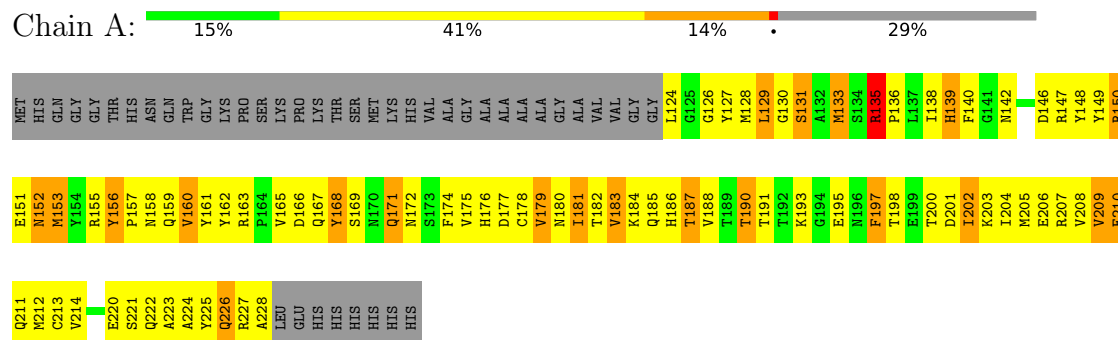
4.2.11 Score per residue for model 11

- Molecule 1: Major prion protein



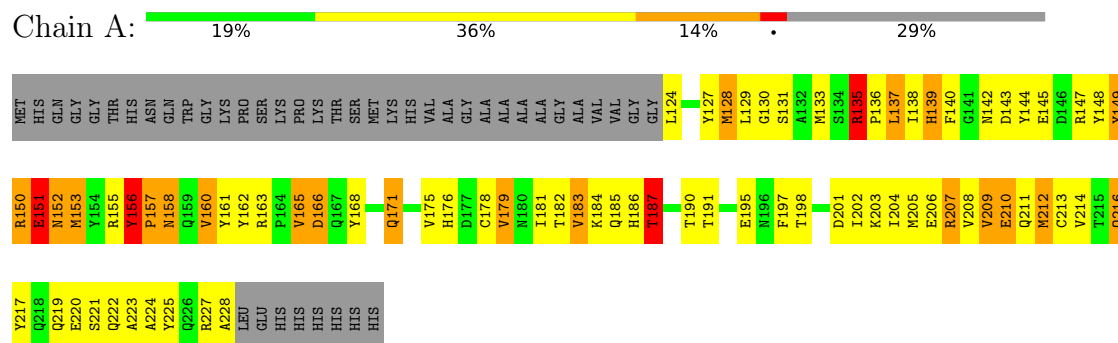
4.2.12 Score per residue for model 12

- Molecule 1: Major prion protein



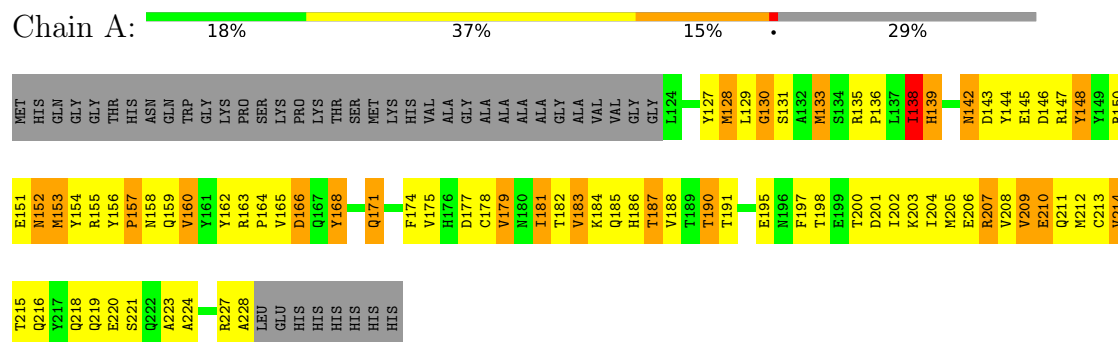
4.2.13 Score per residue for model 13

- Molecule 1: Major prion protein



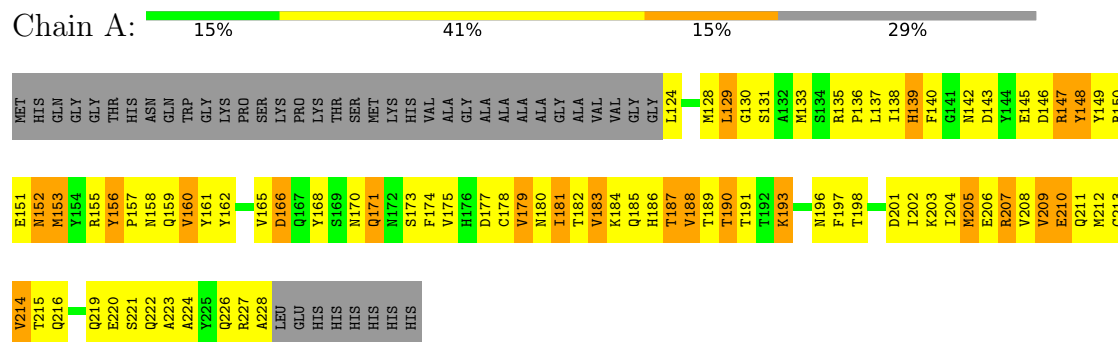
4.2.14 Score per residue for model 14

- Molecule 1: Major prion protein



4.2.15 Score per residue for model 15

- Molecule 1: Major prion protein



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	
ARIA	refinement	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

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	0.78±0.03	0±0/892 (0.0± 0.0%)	0.96±0.03	1±1/1207 (0.1± 0.1%)
All	All	0.78	1/13380 (0.0%)	0.97	15/18105 (0.1%)

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	0.1±0.3
All	All	0	2

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
1	A	182	THR	C-N	-5.13	1.29	1.34	11	1

All unique angle 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(°)	Ideal(°)	Models	
								Worst	Total
1	A	156	TYR	N-CA-C	-6.97	102.11	110.13	8	9
1	A	151	GLU	N-CA-C	-5.47	106.77	113.50	13	4
1	A	197	PHE	CA-CB-CG	5.38	119.18	113.80	4	1
1	A	189	THR	N-CA-C	-5.28	108.60	114.62	11	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	156	TYR	Peptide	2

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	873	819	815	106±9
All	All	13095	12285	12225	1593

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 63.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:133:MET:HE2	1:A:212:MET:HG2	0.98	1.31	12	8
1:A:133:MET:HG2	1:A:212:MET:HE3	0.95	1.37	7	9
1:A:160:VAL:HG13	1:A:209:VAL:HG22	0.95	1.38	13	14
1:A:149:TYR:HA	1:A:152:ASN:HD22	0.92	1.20	12	2
1:A:166:ASP:HB2	1:A:221:SER:HA	0.92	1.36	12	13
1:A:179:VAL:HG11	1:A:210:GLU:HA	0.89	1.42	15	15
1:A:175:VAL:HG11	1:A:214:VAL:HG12	0.87	1.44	15	2
1:A:175:VAL:HG13	1:A:213:CYS:HB3	0.86	1.47	3	12
1:A:170:ASN:HB3	1:A:173:SER:HB2	0.86	1.47	1	1
1:A:206:GLU:O	1:A:210:GLU:HB3	0.85	1.72	11	15
1:A:175:VAL:HG11	1:A:214:VAL:HG23	0.84	1.49	4	8
1:A:201:ASP:HA	1:A:204:ILE:HD11	0.83	1.47	2	12
1:A:128:MET:HG3	1:A:162:TYR:O	0.82	1.75	11	14
1:A:138:ILE:HB	1:A:149:TYR:CZ	0.81	2.10	10	3
1:A:149:TYR:HA	1:A:152:ASN:ND2	0.80	1.90	12	2
1:A:207:ARG:HG3	1:A:208:VAL:N	0.80	1.92	4	2
1:A:128:MET:HE3	1:A:130:GLY:HA2	0.80	1.54	10	8
1:A:133:MET:HB3	1:A:216:GLN:HE22	0.80	1.34	3	1
1:A:187:THR:HA	1:A:191:THR:OG1	0.79	1.77	7	7
1:A:138:ILE:HG13	1:A:208:VAL:HG22	0.79	1.53	1	10
1:A:152:ASN:HA	1:A:155:ARG:HE	0.78	1.38	4	4
1:A:142:ASN:HB3	1:A:146:ASP:H	0.78	1.38	14	3
1:A:127:TYR:HD1	1:A:162:TYR:HA	0.78	1.36	11	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:182:THR:HG21	1:A:209:VAL:HG21	0.77	1.56	9	13
1:A:152:ASN:HB2	1:A:156:TYR:HD2	0.77	1.40	14	7
1:A:174:PHE:HE2	1:A:217:TYR:HB3	0.77	1.39	9	1
1:A:204:ILE:O	1:A:208:VAL:HG23	0.77	1.78	10	15
1:A:187:THR:HA	1:A:191:THR:HG23	0.76	1.55	9	5
1:A:128:MET:HG2	1:A:163:ARG:HA	0.76	1.56	7	3
1:A:193:LYS:HE3	1:A:195:GLU:HG2	0.76	1.57	8	2
1:A:135:ARG:HH21	1:A:137:LEU:HD23	0.75	1.40	6	3
1:A:152:ASN:HA	1:A:155:ARG:CG	0.75	2.12	14	13
1:A:181:ILE:O	1:A:185:GLN:HG2	0.75	1.80	14	13
1:A:148:TYR:CD1	1:A:204:ILE:HD13	0.75	2.17	14	2
1:A:208:VAL:O	1:A:212:MET:HG3	0.73	1.82	4	10
1:A:198:THR:H	1:A:201:ASP:HB3	0.73	1.43	4	2
1:A:133:MET:SD	1:A:212:MET:HG3	0.73	2.22	1	3
1:A:129:LEU:HD21	1:A:159:GLN:HB2	0.72	1.61	1	6
1:A:165:VAL:HG21	1:A:174:PHE:CZ	0.72	2.19	2	4
1:A:147:ARG:HD3	1:A:147:ARG:C	0.72	2.09	11	9
1:A:152:ASN:HA	1:A:155:ARG:CD	0.72	2.14	5	5
1:A:133:MET:CE	1:A:212:MET:HG2	0.72	2.13	14	11
1:A:149:TYR:HA	1:A:152:ASN:HB3	0.71	1.62	13	3
1:A:216:GLN:HG3	1:A:220:GLU:HG2	0.71	1.62	7	1
1:A:133:MET:HG2	1:A:212:MET:HE2	0.71	1.61	5	2
1:A:204:ILE:O	1:A:207:ARG:HG2	0.71	1.86	6	2
1:A:150:ARG:HG3	1:A:151:GLU:HG2	0.70	1.63	12	2
1:A:152:ASN:O	1:A:156:TYR:HB2	0.70	1.85	11	9
1:A:198:THR:H	1:A:201:ASP:HB2	0.70	1.46	3	3
1:A:177:ASP:O	1:A:181:ILE:HG12	0.70	1.86	8	13
1:A:179:VAL:O	1:A:183:VAL:HG13	0.70	1.87	9	15
1:A:183:VAL:O	1:A:187:THR:HB	0.70	1.87	2	10
1:A:216:GLN:O	1:A:220:GLU:HB2	0.69	1.87	11	11
1:A:133:MET:HE2	1:A:212:MET:CG	0.69	2.18	9	6
1:A:179:VAL:HB	1:A:209:VAL:CG1	0.68	2.17	13	13
1:A:156:TYR:CD1	1:A:205:MET:HG3	0.68	2.23	13	1
1:A:129:LEU:HA	1:A:160:VAL:O	0.68	1.89	14	1
1:A:200:THR:O	1:A:204:ILE:HG12	0.67	1.90	3	10
1:A:157:PRO:HB2	1:A:159:GLN:HG2	0.67	1.64	8	7
1:A:127:TYR:CD1	1:A:162:TYR:HA	0.67	2.24	9	6
1:A:151:GLU:O	1:A:155:ARG:HG2	0.67	1.88	9	12
1:A:156:TYR:HD2	1:A:205:MET:HG3	0.67	1.49	10	1
1:A:152:ASN:HB2	1:A:156:TYR:CD2	0.67	2.24	12	7
1:A:171:GLN:HG2	1:A:172:ASN:N	0.67	2.05	6	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:166:ASP:CB	1:A:221:SER:HA	0.66	2.19	12	3
1:A:170:ASN:HB3	1:A:173:SER:HB3	0.66	1.67	15	3
1:A:171:GLN:O	1:A:175:VAL:HB	0.66	1.90	1	2
1:A:202:ILE:O	1:A:206:GLU:HG3	0.66	1.90	11	15
1:A:195:GLU:HG2	1:A:197:PHE:CE1	0.66	2.26	11	1
1:A:130:GLY:HA3	1:A:162:TYR:CE2	0.65	2.26	13	10
1:A:133:MET:SD	1:A:136:PRO:HD3	0.65	2.31	9	13
1:A:186:HIS:C	1:A:190:THR:HB	0.65	2.17	3	12
1:A:179:VAL:HB	1:A:209:VAL:CG2	0.65	2.21	2	1
1:A:133:MET:HG3	1:A:158:ASN:O	0.65	1.92	9	5
1:A:156:TYR:HE1	1:A:187:THR:HB	0.65	1.52	11	2
1:A:171:GLN:N	1:A:171:GLN:HE21	0.65	1.89	14	9
1:A:171:GLN:HG2	1:A:172:ASN:H	0.65	1.51	6	2
1:A:160:VAL:HA	1:A:182:THR:OG1	0.64	1.92	5	11
1:A:135:ARG:HH11	1:A:135:ARG:HG3	0.64	1.51	12	1
1:A:157:PRO:HB2	1:A:159:GLN:NE2	0.64	2.08	10	1
1:A:147:ARG:O	1:A:150:ARG:HG2	0.64	1.92	11	12
1:A:204:ILE:O	1:A:207:ARG:HG3	0.64	1.92	13	11
1:A:124:LEU:HG	1:A:127:TYR:HB2	0.64	1.69	8	7
1:A:160:VAL:HB	1:A:178:CYS:SG	0.64	2.33	14	8
1:A:152:ASN:HA	1:A:155:ARG:NE	0.64	2.07	4	6
1:A:183:VAL:O	1:A:187:THR:HG22	0.64	1.92	15	3
1:A:162:TYR:HB3	1:A:178:CYS:HB2	0.64	1.70	1	7
1:A:152:ASN:CA	1:A:155:ARG:HE	0.63	2.05	13	4
1:A:207:ARG:O	1:A:211:GLN:HG2	0.63	1.94	14	2
1:A:165:VAL:HG11	1:A:174:PHE:CZ	0.63	2.27	4	1
1:A:187:THR:HA	1:A:191:THR:CG2	0.63	2.22	9	3
1:A:186:HIS:O	1:A:190:THR:HB	0.63	1.94	10	15
1:A:135:ARG:HD2	1:A:153:MET:HB2	0.63	1.71	12	1
1:A:146:ASP:O	1:A:149:TYR:HB3	0.62	1.94	10	4
1:A:174:PHE:CE2	1:A:217:TYR:HB3	0.62	2.27	9	1
1:A:186:HIS:HA	1:A:190:THR:HB	0.62	1.69	8	3
1:A:127:TYR:CE2	1:A:181:ILE:HG13	0.62	2.29	1	1
1:A:224:ALA:O	1:A:228:ALA:HB3	0.62	1.93	4	13
1:A:133:MET:SD	1:A:135:ARG:HA	0.62	2.35	12	3
1:A:186:HIS:CA	1:A:190:THR:HB	0.62	2.24	8	6
1:A:203:LYS:O	1:A:207:ARG:HB3	0.62	1.95	4	3
1:A:135:ARG:HG3	1:A:135:ARG:NH1	0.62	2.09	12	1
1:A:165:VAL:HG23	1:A:168:TYR:HB2	0.62	1.71	14	6
1:A:179:VAL:HB	1:A:209:VAL:HG23	0.62	1.70	2	1
1:A:179:VAL:HG11	1:A:210:GLU:CA	0.61	2.25	4	13

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:193:LYS:HE3	1:A:195:GLU:HB2	0.61	1.70	12	3
1:A:175:VAL:HA	1:A:213:CYS:SG	0.61	2.34	9	8
1:A:156:TYR:CD2	1:A:205:MET:HG3	0.61	2.30	10	1
1:A:216:GLN:HA	1:A:219:GLN:HB3	0.61	1.73	3	3
1:A:133:MET:HE3	1:A:158:ASN:HA	0.61	1.71	3	9
1:A:201:ASP:HA	1:A:204:ILE:CD1	0.61	2.26	9	8
1:A:182:THR:HA	1:A:185:GLN:HG2	0.61	1.71	12	1
1:A:190:THR:O	1:A:193:LYS:HG3	0.61	1.96	6	11
1:A:152:ASN:O	1:A:155:ARG:HG2	0.61	1.96	5	2
1:A:133:MET:HG2	1:A:212:MET:CE	0.60	2.26	5	2
1:A:162:TYR:OH	1:A:216:GLN:HB3	0.60	1.96	13	3
1:A:163:ARG:HD2	1:A:163:ARG:H	0.60	1.56	4	2
1:A:138:ILE:HD12	1:A:207:ARG:HH11	0.60	1.56	8	1
1:A:156:TYR:HE2	1:A:209:VAL:HB	0.60	1.56	10	1
1:A:162:TYR:HD2	1:A:174:PHE:HE1	0.60	1.40	15	1
1:A:155:ARG:HG3	1:A:156:TYR:H	0.60	1.55	10	8
1:A:133:MET:HG3	1:A:158:ASN:HB2	0.60	1.73	2	5
1:A:155:ARG:O	1:A:190:THR:HG21	0.60	1.97	6	4
1:A:127:TYR:HE2	1:A:181:ILE:HG13	0.60	1.55	1	1
1:A:135:ARG:CD	1:A:153:MET:HB2	0.60	2.27	12	1
1:A:147:ARG:HD2	1:A:147:ARG:C	0.59	2.22	4	3
1:A:175:VAL:HG11	1:A:214:VAL:CG2	0.59	2.27	11	5
1:A:126:GLY:O	1:A:163:ARG:HB3	0.59	1.97	9	5
1:A:156:TYR:HB3	1:A:205:MET:HB2	0.59	1.73	1	2
1:A:183:VAL:HB	1:A:205:MET:SD	0.59	2.37	5	4
1:A:193:LYS:CE	1:A:195:GLU:HG2	0.59	2.27	8	2
1:A:226:GLN:HE21	1:A:226:GLN:HA	0.59	1.58	12	1
1:A:160:VAL:HG11	1:A:179:VAL:HG12	0.59	1.74	3	8
1:A:160:VAL:HG22	1:A:212:MET:SD	0.59	2.37	12	4
1:A:153:MET:HA	1:A:156:TYR:CD2	0.58	2.33	5	1
1:A:158:ASN:HD22	1:A:158:ASN:N	0.58	1.95	11	1
1:A:124:LEU:HA	1:A:127:TYR:HB2	0.58	1.75	1	1
1:A:151:GLU:HG3	1:A:155:ARG:HE	0.58	1.58	14	1
1:A:129:LEU:CD2	1:A:159:GLN:HB2	0.58	2.28	11	6
1:A:132:ALA:HA	1:A:159:GLN:HB3	0.58	1.75	5	5
1:A:135:ARG:HB2	1:A:153:MET:HG3	0.58	1.76	1	3
1:A:187:THR:O	1:A:191:THR:HB	0.58	1.98	1	5
1:A:223:ALA:O	1:A:227:ARG:HG2	0.58	1.99	14	12
1:A:133:MET:O	1:A:158:ASN:HB2	0.58	1.98	5	4
1:A:156:TYR:HE1	1:A:209:VAL:CG2	0.58	2.12	13	1
1:A:124:LEU:HG	1:A:127:TYR:HD2	0.58	1.59	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:LEU:HD23	1:A:159:GLN:HG3	0.58	1.76	9	1
1:A:156:TYR:CE1	1:A:197:PHE:CZ	0.58	2.92	8	1
1:A:191:THR:HA	1:A:197:PHE:CE1	0.58	2.33	8	1
1:A:204:ILE:HG13	1:A:205:MET:N	0.57	2.14	9	12
1:A:222:GLN:HA	1:A:225:TYR:CD2	0.57	2.34	5	4
1:A:148:TYR:O	1:A:152:ASN:HB3	0.57	2.00	9	14
1:A:147:ARG:HA	1:A:150:ARG:HB3	0.57	1.75	2	2
1:A:140:PHE:HZ	1:A:207:ARG:HD3	0.57	1.59	12	2
1:A:204:ILE:HG13	1:A:205:MET:H	0.57	1.58	9	12
1:A:136:PRO:HG3	1:A:212:MET:HB3	0.57	1.77	14	1
1:A:198:THR:O	1:A:202:ILE:HG12	0.56	2.00	3	10
1:A:142:ASN:HB2	1:A:146:ASP:HB2	0.56	1.76	12	1
1:A:128:MET:HG3	1:A:128:MET:O	0.56	2.00	14	1
1:A:157:PRO:HB2	1:A:159:GLN:HE21	0.56	1.60	9	1
1:A:191:THR:HA	1:A:195:GLU:HB3	0.56	1.78	12	1
1:A:131:SER:HB2	1:A:216:GLN:HG2	0.56	1.76	4	2
1:A:156:TYR:OH	1:A:201:ASP:HB3	0.56	1.99	8	2
1:A:155:ARG:HG3	1:A:156:TYR:N	0.56	2.14	14	2
1:A:197:PHE:HA	1:A:201:ASP:CB	0.56	2.30	9	5
1:A:160:VAL:HG23	1:A:162:TYR:CE2	0.56	2.36	3	5
1:A:138:ILE:HB	1:A:149:TYR:CE2	0.56	2.36	10	2
1:A:197:PHE:HB2	1:A:201:ASP:OD2	0.56	2.01	4	1
1:A:149:TYR:CA	1:A:152:ASN:HB3	0.56	2.30	13	3
1:A:203:LYS:HG3	1:A:204:ILE:H	0.56	1.61	15	12
1:A:133:MET:HE1	1:A:208:VAL:HG12	0.56	1.78	12	7
1:A:215:THR:O	1:A:219:GLN:HG3	0.56	2.00	14	1
1:A:191:THR:O	1:A:195:GLU:HB2	0.56	2.01	5	2
1:A:124:LEU:HG	1:A:127:TYR:CD2	0.56	2.36	4	2
1:A:147:ARG:O	1:A:151:GLU:HG2	0.55	2.00	14	8
1:A:149:TYR:CE1	1:A:208:VAL:HG21	0.55	2.36	5	6
1:A:133:MET:HE2	1:A:212:MET:SD	0.55	2.42	3	1
1:A:133:MET:HG2	1:A:212:MET:SD	0.55	2.41	3	1
1:A:215:THR:O	1:A:218:GLN:HG3	0.55	2.00	3	1
1:A:145:GLU:HG2	1:A:148:TYR:CE2	0.55	2.36	15	2
1:A:142:ASN:CB	1:A:145:GLU:HG2	0.55	2.31	13	1
1:A:198:THR:HG22	1:A:201:ASP:OD2	0.55	2.02	3	9
1:A:156:TYR:CD2	1:A:205:MET:HB2	0.54	2.36	3	4
1:A:217:TYR:O	1:A:221:SER:HB2	0.54	2.01	9	1
1:A:175:VAL:HG11	1:A:214:VAL:HB	0.54	1.77	3	2
1:A:148:TYR:CE1	1:A:204:ILE:HG21	0.54	2.37	15	1
1:A:124:LEU:HD12	1:A:127:TYR:CB	0.54	2.32	1	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:153:MET:O	1:A:153:MET:HG2	0.54	2.02	5	1
1:A:162:TYR:HD1	1:A:163:ARG:O	0.54	1.86	2	12
1:A:144:TYR:O	1:A:148:TYR:HB2	0.54	2.02	2	4
1:A:124:LEU:HD21	1:A:161:TYR:CE1	0.54	2.37	12	1
1:A:149:TYR:CA	1:A:152:ASN:HD22	0.54	2.04	12	1
1:A:175:VAL:HG13	1:A:213:CYS:CB	0.54	2.28	3	3
1:A:197:PHE:H	1:A:197:PHE:HD1	0.54	1.45	4	1
1:A:133:MET:HE2	1:A:212:MET:HE2	0.54	1.78	13	1
1:A:144:TYR:C	1:A:147:ARG:HB3	0.54	2.28	14	1
1:A:184:LYS:O	1:A:188:VAL:HG13	0.54	2.03	2	10
1:A:128:MET:O	1:A:129:LEU:C	0.54	2.50	15	3
1:A:224:ALA:O	1:A:228:ALA:HB2	0.54	2.03	12	2
1:A:156:TYR:CB	1:A:205:MET:HB2	0.53	2.33	1	1
1:A:210:GLU:HG3	1:A:211:GLN:N	0.53	2.17	3	1
1:A:140:PHE:CZ	1:A:207:ARG:HD3	0.53	2.37	6	2
1:A:147:ARG:HA	1:A:150:ARG:HG2	0.53	1.79	14	3
1:A:207:ARG:C	1:A:207:ARG:HD3	0.53	2.29	2	6
1:A:143:ASP:O	1:A:147:ARG:HB3	0.53	2.03	2	1
1:A:135:ARG:HB2	1:A:153:MET:HG2	0.53	1.80	3	1
1:A:128:MET:HG2	1:A:163:ARG:CA	0.53	2.33	9	2
1:A:214:VAL:HG13	1:A:217:TYR:CE2	0.53	2.39	9	1
1:A:124:LEU:HA	1:A:127:TYR:CD1	0.53	2.38	10	1
1:A:151:GLU:HB3	1:A:155:ARG:HE	0.53	1.63	12	1
1:A:198:THR:N	1:A:201:ASP:HB2	0.53	2.17	15	8
1:A:133:MET:SD	1:A:158:ASN:HB3	0.53	2.44	5	1
1:A:160:VAL:HG23	1:A:162:TYR:HE2	0.53	1.62	3	3
1:A:172:ASN:HA	1:A:175:VAL:HG22	0.53	1.79	6	2
1:A:156:TYR:N	1:A:156:TYR:CD1	0.53	2.72	8	1
1:A:212:MET:O	1:A:216:GLN:HB2	0.53	2.04	10	4
1:A:135:ARG:HG3	1:A:153:MET:SD	0.53	2.44	7	1
1:A:139:HIS:O	1:A:140:PHE:HB2	0.53	2.03	8	2
1:A:138:ILE:HB	1:A:149:TYR:CE1	0.53	2.39	1	1
1:A:138:ILE:HG22	1:A:139:HIS:N	0.53	2.18	5	1
1:A:135:ARG:CZ	1:A:153:MET:HB2	0.53	2.34	12	1
1:A:149:TYR:CD1	1:A:208:VAL:HG21	0.52	2.39	9	6
1:A:223:ALA:HA	1:A:226:GLN:CG	0.52	2.34	3	1
1:A:133:MET:HE2	1:A:212:MET:HG3	0.52	1.81	5	1
1:A:187:THR:HB	1:A:197:PHE:CZ	0.52	2.39	3	1
1:A:140:PHE:CE2	1:A:207:ARG:HD2	0.52	2.39	5	1
1:A:133:MET:SD	1:A:212:MET:HG2	0.52	2.44	2	3
1:A:165:VAL:HG11	1:A:174:PHE:CE2	0.52	2.39	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:182:THR:HG21	1:A:209:VAL:CG2	0.52	2.33	11	4
1:A:187:THR:HG23	1:A:191:THR:HG21	0.52	1.81	2	1
1:A:133:MET:HG2	1:A:158:ASN:O	0.52	2.04	11	2
1:A:143:ASP:O	1:A:147:ARG:HB2	0.52	2.03	14	4
1:A:135:ARG:HG3	1:A:153:MET:HE3	0.52	1.81	10	1
1:A:136:PRO:C	1:A:137:LEU:HG	0.52	2.30	13	1
1:A:152:ASN:O	1:A:156:TYR:N	0.52	2.42	2	5
1:A:139:HIS:CD2	1:A:140:PHE:H	0.52	2.23	15	4
1:A:161:TYR:CE2	1:A:185:GLN:HG3	0.52	2.39	15	1
1:A:133:MET:CE	1:A:212:MET:HG3	0.52	2.35	5	3
1:A:142:ASN:HD22	1:A:145:GLU:HB2	0.52	1.64	15	1
1:A:184:LYS:N	1:A:184:LYS:HD2	0.52	2.20	4	1
1:A:180:ASN:O	1:A:184:LYS:HG2	0.52	2.04	8	7
1:A:175:VAL:HG23	1:A:176:HIS:H	0.51	1.64	12	3
1:A:175:VAL:HG23	1:A:176:HIS:N	0.51	2.20	12	3
1:A:152:ASN:OD1	1:A:205:MET:HA	0.51	2.04	14	4
1:A:128:MET:HE3	1:A:131:SER:H	0.51	1.65	9	1
1:A:179:VAL:HB	1:A:209:VAL:HG13	0.51	1.81	13	8
1:A:145:GLU:HA	1:A:148:TYR:HB2	0.51	1.82	1	1
1:A:148:TYR:O	1:A:151:GLU:HG3	0.51	2.05	13	4
1:A:155:ARG:CG	1:A:156:TYR:H	0.51	2.18	5	6
1:A:162:TYR:CD2	1:A:174:PHE:CE2	0.51	2.98	7	1
1:A:153:MET:HE1	1:A:154:TYR:CE2	0.51	2.40	8	2
1:A:152:ASN:OD1	1:A:156:TYR:HB2	0.51	2.06	4	3
1:A:153:MET:HG2	1:A:158:ASN:OD1	0.51	2.06	6	1
1:A:150:ARG:CG	1:A:151:GLU:HG2	0.51	2.34	12	1
1:A:124:LEU:HD21	1:A:161:TYR:CD1	0.51	2.41	15	1
1:A:170:ASN:HB3	1:A:173:SER:CB	0.51	2.31	1	1
1:A:182:THR:O	1:A:185:GLN:HG3	0.51	2.05	11	2
1:A:135:ARG:HG2	1:A:149:TYR:OH	0.51	2.05	5	3
1:A:150:ARG:O	1:A:153:MET:HE2	0.51	2.06	5	2
1:A:128:MET:HE3	1:A:131:SER:N	0.51	2.20	9	1
1:A:207:ARG:CG	1:A:208:VAL:N	0.51	2.74	6	2
1:A:216:GLN:O	1:A:220:GLU:N	0.51	2.42	7	1
1:A:181:ILE:O	1:A:184:LYS:HB2	0.50	2.06	14	8
1:A:155:ARG:HG2	1:A:156:TYR:H	0.50	1.66	5	2
1:A:151:GLU:HB2	1:A:155:ARG:NH2	0.50	2.21	2	1
1:A:197:PHE:CZ	1:A:205:MET:HE1	0.50	2.41	3	1
1:A:172:ASN:O	1:A:176:HIS:HB3	0.50	2.05	8	2
1:A:223:ALA:HA	1:A:226:GLN:HG2	0.50	1.84	3	1
1:A:140:PHE:HE2	1:A:149:TYR:HB2	0.50	1.66	15	3

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:138:ILE:HD12	1:A:207:ARG:NH1	0.50	2.21	8	1
1:A:152:ASN:HA	1:A:155:ARG:HG2	0.50	1.83	6	3
1:A:215:THR:O	1:A:218:GLN:HG2	0.50	2.07	14	1
1:A:171:GLN:O	1:A:175:VAL:HG22	0.50	2.07	12	3
1:A:219:GLN:HA	1:A:222:GLN:HB3	0.50	1.83	8	1
1:A:184:LYS:O	1:A:188:VAL:HG22	0.50	2.06	7	7
1:A:204:ILE:HA	1:A:207:ARG:HG2	0.50	1.84	14	1
1:A:187:THR:CG2	1:A:205:MET:SD	0.50	3.00	3	1
1:A:135:ARG:HD2	1:A:135:ARG:C	0.50	2.32	13	1
1:A:191:THR:HA	1:A:195:GLU:HB2	0.49	1.83	3	1
1:A:198:THR:O	1:A:201:ASP:N	0.49	2.46	10	14
1:A:157:PRO:HD3	1:A:186:HIS:CG	0.49	2.41	3	5
1:A:153:MET:SD	1:A:156:TYR:HE1	0.49	2.29	10	1
1:A:197:PHE:HA	1:A:201:ASP:HB2	0.49	1.83	9	4
1:A:211:GLN:O	1:A:214:VAL:HG12	0.49	2.08	3	1
1:A:175:VAL:O	1:A:179:VAL:HG13	0.49	2.07	12	1
1:A:128:MET:CG	1:A:163:ARG:HA	0.49	2.38	11	2
1:A:179:VAL:CB	1:A:209:VAL:HG23	0.49	2.37	2	1
1:A:148:TYR:O	1:A:152:ASN:N	0.49	2.45	13	4
1:A:156:TYR:CG	1:A:205:MET:HB2	0.49	2.42	14	2
1:A:135:ARG:HD2	1:A:137:LEU:H	0.49	1.67	13	2
1:A:152:ASN:CB	1:A:156:TYR:HD2	0.49	2.20	7	1
1:A:165:VAL:O	1:A:220:GLU:HB3	0.49	2.07	12	2
1:A:208:VAL:O	1:A:212:MET:HB2	0.49	2.08	13	1
1:A:179:VAL:C	1:A:181:ILE:N	0.49	2.68	13	15
1:A:135:ARG:HG3	1:A:158:ASN:OD1	0.49	2.08	5	1
1:A:199:GLU:HG3	1:A:200:THR:N	0.49	2.23	8	1
1:A:222:GLN:O	1:A:225:TYR:HB2	0.49	2.08	12	3
1:A:133:MET:HG3	1:A:158:ASN:CB	0.49	2.38	11	1
1:A:130:GLY:N	1:A:160:VAL:O	0.48	2.45	14	1
1:A:186:HIS:O	1:A:188:VAL:N	0.48	2.46	4	6
1:A:156:TYR:OH	1:A:197:PHE:HB3	0.48	2.08	12	3
1:A:170:ASN:CG	1:A:173:SER:HB3	0.48	2.34	11	1
1:A:148:TYR:HB3	1:A:204:ILE:HD13	0.48	1.84	7	2
1:A:156:TYR:CD1	1:A:205:MET:SD	0.48	3.06	15	2
1:A:158:ASN:N	1:A:158:ASN:ND2	0.48	2.62	11	1
1:A:135:ARG:NE	1:A:153:MET:HB2	0.48	2.24	12	1
1:A:138:ILE:HG21	1:A:207:ARG:HD3	0.48	1.85	4	1
1:A:140:PHE:CZ	1:A:204:ILE:HG22	0.48	2.43	5	2
1:A:138:ILE:HG13	1:A:208:VAL:HG13	0.48	1.85	10	1
1:A:171:GLN:C	1:A:175:VAL:HG22	0.48	2.33	12	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:ASN:HA	1:A:155:ARG:HG3	0.48	1.85	1	9
1:A:129:LEU:O	1:A:161:TYR:HA	0.48	2.09	15	1
1:A:191:THR:HA	1:A:197:PHE:CE2	0.48	2.42	15	1
1:A:222:GLN:O	1:A:226:GLN:HG3	0.48	2.08	15	1
1:A:171:GLN:NE2	1:A:171:GLN:H	0.48	2.06	3	1
1:A:142:ASN:HB2	1:A:146:ASP:H	0.48	1.69	7	3
1:A:183:VAL:HG12	1:A:209:VAL:HG11	0.48	1.86	4	4
1:A:124:LEU:HD21	1:A:161:TYR:HD2	0.48	1.69	9	1
1:A:191:THR:HG23	1:A:197:PHE:HB2	0.48	1.86	11	1
1:A:138:ILE:HG22	1:A:139:HIS:H	0.48	1.68	14	1
1:A:211:GLN:HA	1:A:214:VAL:HG13	0.48	1.86	15	1
1:A:129:LEU:O	1:A:131:SER:N	0.47	2.47	9	4
1:A:184:LYS:HD3	1:A:184:LYS:N	0.47	2.24	3	3
1:A:150:ARG:O	1:A:153:MET:HE3	0.47	2.08	13	1
1:A:138:ILE:HD12	1:A:208:VAL:HG22	0.47	1.84	15	1
1:A:179:VAL:CG1	1:A:209:VAL:HG23	0.47	2.39	2	1
1:A:135:ARG:HH21	1:A:152:ASN:ND2	0.47	2.07	12	1
1:A:130:GLY:HA3	1:A:160:VAL:HG23	0.47	1.87	15	1
1:A:145:GLU:HA	1:A:148:TYR:CG	0.47	2.44	15	1
1:A:209:VAL:HA	1:A:212:MET:SD	0.47	2.50	10	2
1:A:135:ARG:HG2	1:A:137:LEU:H	0.47	1.68	2	2
1:A:157:PRO:HB2	1:A:159:GLN:HG3	0.47	1.84	3	1
1:A:162:TYR:CD2	1:A:163:ARG:O	0.47	2.67	9	1
1:A:128:MET:CE	1:A:130:GLY:HA2	0.47	2.40	1	4
1:A:155:ARG:CG	1:A:156:TYR:N	0.47	2.78	5	2
1:A:162:TYR:HB3	1:A:178:CYS:CB	0.47	2.40	7	2
1:A:156:TYR:CE1	1:A:187:THR:HB	0.47	2.40	11	2
1:A:152:ASN:O	1:A:156:TYR:HB3	0.47	2.10	13	1
1:A:144:TYR:O	1:A:147:ARG:HB3	0.47	2.10	14	1
1:A:155:ARG:HG3	1:A:156:TYR:CD2	0.47	2.45	2	4
1:A:162:TYR:HB2	1:A:174:PHE:CZ	0.47	2.44	11	1
1:A:136:PRO:HG3	1:A:212:MET:CG	0.47	2.39	1	1
1:A:203:LYS:HG3	1:A:204:ILE:N	0.47	2.24	5	10
1:A:135:ARG:HD3	1:A:149:TYR:HE1	0.47	1.69	1	2
1:A:161:TYR:O	1:A:178:CYS:HB2	0.47	2.09	15	2
1:A:182:THR:C	1:A:184:LYS:N	0.46	2.73	6	13
1:A:140:PHE:CE2	1:A:149:TYR:HB2	0.46	2.44	7	1
1:A:133:MET:HE2	1:A:212:MET:HE3	0.46	1.86	10	1
1:A:167:GLN:HG3	1:A:221:SER:HB2	0.46	1.85	12	1
1:A:179:VAL:CG1	1:A:210:GLU:HA	0.46	2.36	11	4
1:A:165:VAL:HB	1:A:174:PHE:CE2	0.46	2.45	7	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:219:GLN:O	1:A:222:GLN:HB3	0.46	2.11	8	1
1:A:190:THR:O	1:A:193:LYS:HB3	0.46	2.10	15	1
1:A:162:TYR:OH	1:A:165:VAL:HB	0.46	2.10	9	1
1:A:191:THR:HA	1:A:197:PHE:CD2	0.46	2.45	11	1
1:A:186:HIS:HA	1:A:190:THR:CB	0.46	2.40	3	1
1:A:133:MET:CG	1:A:212:MET:HE3	0.46	2.40	2	1
1:A:190:THR:HG22	1:A:197:PHE:CZ	0.46	2.45	11	1
1:A:140:PHE:CB	1:A:142:ASN:HD22	0.46	2.23	5	1
1:A:171:GLN:HB2	1:A:217:TYR:CD2	0.46	2.45	9	1
1:A:183:VAL:HG22	1:A:184:LYS:HD3	0.46	1.88	8	2
1:A:129:LEU:HD23	1:A:159:GLN:CG	0.46	2.41	9	1
1:A:153:MET:HG2	1:A:158:ASN:HD22	0.46	1.70	15	1
1:A:147:ARG:C	1:A:147:ARG:CD	0.46	2.88	12	6
1:A:203:LYS:O	1:A:207:ARG:N	0.46	2.49	5	5
1:A:165:VAL:HG11	1:A:174:PHE:CE1	0.46	2.45	14	4
1:A:140:PHE:HE1	1:A:207:ARG:HE	0.46	1.54	13	1
1:A:138:ILE:O	1:A:139:HIS:CD2	0.45	2.69	2	3
1:A:156:TYR:HE2	1:A:204:ILE:HD11	0.45	1.71	8	1
1:A:135:ARG:NE	1:A:149:TYR:CE1	0.45	2.84	12	1
1:A:155:ARG:O	1:A:190:THR:HG22	0.45	2.11	13	1
1:A:172:ASN:OD1	1:A:176:HIS:HB2	0.45	2.11	2	1
1:A:177:ASP:O	1:A:180:ASN:HB3	0.45	2.11	2	1
1:A:186:HIS:O	1:A:190:THR:N	0.45	2.50	8	3
1:A:129:LEU:HD21	1:A:159:GLN:CD	0.45	2.36	15	2
1:A:156:TYR:CE2	1:A:209:VAL:HB	0.45	2.43	10	1
1:A:172:ASN:HB3	1:A:176:HIS:CD2	0.45	2.46	7	1
1:A:134:SER:HA	1:A:158:ASN:ND2	0.45	2.26	8	1
1:A:136:PRO:HD2	1:A:149:TYR:OH	0.45	2.12	10	1
1:A:129:LEU:O	1:A:162:TYR:N	0.45	2.47	15	1
1:A:145:GLU:HG2	1:A:148:TYR:CZ	0.45	2.46	14	1
1:A:149:TYR:HA	1:A:152:ASN:CB	0.45	2.39	13	1
1:A:165:VAL:HG23	1:A:168:TYR:CD1	0.45	2.46	13	1
1:A:151:GLU:C	1:A:153:MET:H	0.45	2.19	14	1
1:A:135:ARG:HD3	1:A:149:TYR:CE1	0.45	2.47	1	1
1:A:133:MET:HG3	1:A:158:ASN:HB3	0.45	1.88	11	1
1:A:197:PHE:HA	1:A:201:ASP:OD2	0.45	2.11	12	1
1:A:203:LYS:HE2	1:A:204:ILE:HG23	0.45	1.87	15	3
1:A:176:HIS:O	1:A:179:VAL:HG22	0.45	2.11	1	3
1:A:187:THR:O	1:A:187:THR:HG22	0.45	2.12	12	3
1:A:204:ILE:HA	1:A:207:ARG:CG	0.45	2.42	11	3
1:A:140:PHE:CZ	1:A:207:ARG:HD2	0.45	2.47	11	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:MET:HG2	1:A:162:TYR:O	0.45	2.12	9	1
1:A:162:TYR:CD2	1:A:174:PHE:CE1	0.45	3.04	9	1
1:A:135:ARG:HD2	1:A:153:MET:CB	0.45	2.40	12	1
1:A:142:ASN:HB3	1:A:145:GLU:HG2	0.45	1.87	13	1
1:A:134:SER:O	1:A:135:ARG:HB3	0.45	2.12	2	2
1:A:212:MET:HA	1:A:215:THR:HB	0.45	1.89	11	4
1:A:150:ARG:HG3	1:A:151:GLU:N	0.45	2.26	5	3
1:A:198:THR:H	1:A:201:ASP:CG	0.45	2.20	8	1
1:A:156:TYR:HE2	1:A:209:VAL:CB	0.45	2.24	10	1
1:A:198:THR:N	1:A:201:ASP:HB3	0.45	2.27	12	1
1:A:200:THR:O	1:A:203:LYS:HG3	0.45	2.12	12	1
1:A:165:VAL:HA	1:A:168:TYR:CD2	0.45	2.47	15	1
1:A:198:THR:HG22	1:A:201:ASP:OD1	0.45	2.11	5	1
1:A:165:VAL:CG2	1:A:168:TYR:HB2	0.45	2.41	6	1
1:A:222:GLN:O	1:A:226:GLN:HG2	0.44	2.12	10	3
1:A:124:LEU:HD12	1:A:127:TYR:HB3	0.44	1.89	1	1
1:A:174:PHE:CD1	1:A:174:PHE:C	0.44	2.95	9	1
1:A:124:LEU:HG	1:A:124:LEU:O	0.44	2.12	1	1
1:A:160:VAL:CG1	1:A:179:VAL:HG12	0.44	2.42	12	3
1:A:133:MET:SD	1:A:135:ARG:CA	0.44	3.05	12	1
1:A:165:VAL:HG21	1:A:174:PHE:CE2	0.44	2.47	2	1
1:A:155:ARG:HB2	1:A:195:GLU:CD	0.44	2.38	3	1
1:A:153:MET:HE2	1:A:153:MET:HB2	0.44	1.63	7	1
1:A:216:GLN:NE2	1:A:216:GLN:HA	0.44	2.26	9	1
1:A:175:VAL:O	1:A:178:CYS:SG	0.44	2.75	13	2
1:A:153:MET:HG2	1:A:153:MET:O	0.44	2.12	15	1
1:A:155:ARG:HD2	1:A:197:PHE:HE1	0.44	1.72	15	1
1:A:211:GLN:O	1:A:214:VAL:HB	0.44	2.12	6	1
1:A:193:LYS:CE	1:A:195:GLU:HB2	0.44	2.43	12	1
1:A:129:LEU:C	1:A:160:VAL:O	0.44	2.60	15	1
1:A:156:TYR:HB2	1:A:205:MET:CG	0.44	2.43	5	1
1:A:180:ASN:C	1:A:184:LYS:HD3	0.44	2.38	4	1
1:A:219:GLN:C	1:A:222:GLN:HB3	0.44	2.38	8	1
1:A:160:VAL:HG11	1:A:178:CYS:SG	0.44	2.53	9	1
1:A:198:THR:HG23	1:A:200:THR:H	0.44	1.72	14	1
1:A:183:VAL:HG22	1:A:184:LYS:HD2	0.44	1.90	4	1
1:A:186:HIS:ND1	1:A:190:THR:HG21	0.44	2.27	7	1
1:A:191:THR:O	1:A:195:GLU:HB3	0.44	2.12	13	1
1:A:163:ARG:O	1:A:165:VAL:HG13	0.43	2.13	2	1
1:A:186:HIS:C	1:A:188:VAL:H	0.43	2.20	12	2
1:A:172:ASN:HA	1:A:175:VAL:CG2	0.43	2.42	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:124:LEU:HD21	1:A:161:TYR:CD2	0.43	2.48	13	2
1:A:212:MET:SD	1:A:212:MET:C	0.43	3.01	12	1
1:A:148:TYR:CD1	1:A:204:ILE:HG21	0.43	2.48	15	1
1:A:156:TYR:CD1	1:A:157:PRO:HD2	0.43	2.47	13	1
1:A:156:TYR:CE1	1:A:205:MET:SD	0.43	3.11	15	1
1:A:183:VAL:O	1:A:187:THR:CB	0.43	2.66	4	1
1:A:142:ASN:HB2	1:A:146:ASP:N	0.43	2.29	7	1
1:A:151:GLU:C	1:A:153:MET:N	0.43	2.75	14	1
1:A:165:VAL:HB	1:A:174:PHE:CZ	0.43	2.48	11	2
1:A:152:ASN:OD1	1:A:205:MET:HB2	0.43	2.14	4	1
1:A:205:MET:O	1:A:209:VAL:HB	0.43	2.14	8	1
1:A:152:ASN:O	1:A:156:TYR:HD1	0.43	1.96	10	1
1:A:163:ARG:HB2	1:A:164:PRO:CD	0.43	2.43	14	3
1:A:142:ASN:CB	1:A:146:ASP:HB2	0.43	2.43	2	1
1:A:198:THR:HG22	1:A:201:ASP:CG	0.43	2.39	8	1
1:A:147:ARG:HD3	1:A:147:ARG:O	0.43	2.13	7	4
1:A:156:TYR:CE2	1:A:201:ASP:HB3	0.43	2.49	2	1
1:A:133:MET:HE3	1:A:158:ASN:CA	0.43	2.43	3	1
1:A:155:ARG:HH21	1:A:204:ILE:HD11	0.43	1.73	3	1
1:A:187:THR:HB	1:A:197:PHE:CE1	0.43	2.49	3	1
1:A:152:ASN:CB	1:A:204:ILE:HD12	0.43	2.44	2	1
1:A:182:THR:C	1:A:184:LYS:H	0.43	2.21	6	2
1:A:197:PHE:HA	1:A:201:ASP:HB3	0.43	1.90	12	1
1:A:160:VAL:CG1	1:A:209:VAL:HB	0.42	2.44	2	1
1:A:166:ASP:H	1:A:168:TYR:HD1	0.42	1.56	12	1
1:A:179:VAL:C	1:A:181:ILE:H	0.42	2.22	3	3
1:A:175:VAL:HG12	1:A:176:HIS:N	0.42	2.30	4	1
1:A:135:ARG:HG2	1:A:136:PRO:CD	0.42	2.43	7	1
1:A:162:TYR:CE2	1:A:163:ARG:O	0.42	2.73	9	1
1:A:149:TYR:CE1	1:A:153:MET:HE1	0.42	2.49	10	1
1:A:144:TYR:HA	1:A:147:ARG:HB3	0.42	1.90	14	1
1:A:214:VAL:O	1:A:217:TYR:HB3	0.42	2.14	13	1
1:A:140:PHE:HZ	1:A:207:ARG:HD2	0.42	1.74	11	2
1:A:162:TYR:CE2	1:A:165:VAL:HB	0.42	2.49	9	1
1:A:219:GLN:O	1:A:222:GLN:HG2	0.42	2.14	9	1
1:A:138:ILE:CG2	1:A:139:HIS:N	0.42	2.82	5	1
1:A:138:ILE:HG23	1:A:207:ARG:NH1	0.42	2.30	8	1
1:A:135:ARG:NH2	1:A:137:LEU:HD23	0.42	2.30	9	1
1:A:161:TYR:HB2	1:A:181:ILE:HB	0.42	1.91	12	2
1:A:162:TYR:CG	1:A:163:ARG:N	0.42	2.87	9	1
1:A:198:THR:H	1:A:201:ASP:CB	0.42	2.23	3	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:MET:HG3	1:A:129:LEU:N	0.42	2.29	9	1
1:A:165:VAL:HG12	1:A:168:TYR:CE1	0.42	2.50	8	1
1:A:153:MET:HA	1:A:156:TYR:CD1	0.42	2.50	10	1
1:A:175:VAL:CG2	1:A:176:HIS:H	0.42	2.28	12	1
1:A:219:GLN:O	1:A:223:ALA:N	0.42	2.53	15	1
1:A:205:MET:HE2	1:A:205:MET:HB3	0.42	1.75	2	3
1:A:211:GLN:HA	1:A:214:VAL:HG12	0.42	1.92	13	1
1:A:175:VAL:HG21	1:A:214:VAL:CG2	0.41	2.45	6	2
1:A:171:GLN:CG	1:A:172:ASN:N	0.41	2.83	7	1
1:A:190:THR:HG22	1:A:197:PHE:CE2	0.41	2.50	11	1
1:A:155:ARG:CZ	1:A:156:TYR:HE2	0.41	2.28	1	1
1:A:153:MET:HG3	1:A:158:ASN:HB3	0.41	1.92	3	1
1:A:205:MET:HG2	1:A:206:GLU:N	0.41	2.27	11	1
1:A:211:GLN:O	1:A:214:VAL:HG13	0.41	2.16	8	1
1:A:142:ASN:H	1:A:146:ASP:HB2	0.41	1.75	14	1
1:A:175:VAL:HG11	1:A:214:VAL:HA	0.41	1.91	12	1
1:A:156:TYR:CE1	1:A:209:VAL:HB	0.41	2.51	13	1
1:A:152:ASN:HB2	1:A:204:ILE:HD12	0.41	1.91	1	1
1:A:187:THR:O	1:A:187:THR:CG2	0.41	2.69	2	2
1:A:222:GLN:O	1:A:225:TYR:HB3	0.41	2.16	3	1
1:A:151:GLU:C	1:A:155:ARG:HE	0.41	2.23	6	1
1:A:128:MET:O	1:A:162:TYR:O	0.41	2.38	2	1
1:A:135:ARG:HD2	1:A:153:MET:HE3	0.41	1.92	3	1
1:A:131:SER:HB2	1:A:216:GLN:CD	0.41	2.40	9	1
1:A:133:MET:HE3	1:A:158:ASN:HB3	0.41	1.92	11	1
1:A:130:GLY:HA2	1:A:162:TYR:CD1	0.41	2.50	15	1
1:A:130:GLY:HA3	1:A:162:TYR:CZ	0.41	2.50	3	1
1:A:140:PHE:CE2	1:A:204:ILE:HG22	0.41	2.50	5	1
1:A:129:LEU:O	1:A:129:LEU:HD12	0.41	2.15	14	1
1:A:142:ASN:CB	1:A:146:ASP:H	0.41	2.20	14	1
1:A:156:TYR:OH	1:A:191:THR:HG22	0.41	2.16	4	1
1:A:180:ASN:O	1:A:184:LYS:HD3	0.41	2.15	4	1
1:A:217:TYR:CD1	1:A:217:TYR:C	0.41	2.99	9	1
1:A:153:MET:HG2	1:A:158:ASN:ND2	0.41	2.31	11	1
1:A:128:MET:O	1:A:128:MET:CG	0.41	2.68	14	1
1:A:127:TYR:CD2	1:A:181:ILE:HG21	0.41	2.50	14	1
1:A:151:GLU:CD	1:A:155:ARG:HH21	0.41	2.24	14	1
1:A:175:VAL:HG21	1:A:214:VAL:HG22	0.40	1.92	6	1
1:A:175:VAL:HB	1:A:213:CYS:HB3	0.40	1.93	13	1
1:A:124:LEU:HD12	1:A:127:TYR:HB2	0.40	1.93	1	1
1:A:222:GLN:C	1:A:225:TYR:H	0.40	2.24	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:144:TYR:CA	1:A:147:ARG:HB3	0.40	2.46	14	1
1:A:145:GLU:HA	1:A:148:TYR:CD1	0.40	2.51	15	1
1:A:162:TYR:CD1	1:A:163:ARG:O	0.40	2.74	1	1
1:A:204:ILE:O	1:A:208:VAL:CG2	0.40	2.69	15	1
1:A:155:ARG:HG2	1:A:155:ARG:H	0.40	1.49	4	1
1:A:145:GLU:HA	1:A:148:TYR:CD2	0.40	2.51	15	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	103/148 (70%)	80±2 (78±2%)	18±2 (17±2%)	5±1 (5±1%)	2	22
All	All	1545/2220 (70%)	1200 (78%)	263 (17%)	82 (5%)	2	22

All 14 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
1	A	131	SER	15
1	A	135	ARG	14
1	A	139	HIS	13
1	A	166	ASP	12
1	A	187	THR	12
1	A	157	PRO	4
1	A	130	GLY	3
1	A	137	LEU	2
1	A	136	PRO	2
1	A	140	PHE	1
1	A	126	GLY	1
1	A	169	SER	1
1	A	138	ILE	1
1	A	129	LEU	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	96/126 (76%)	74±3 (77±3%)	22±3 (23±3%)	2	28
All	All	1440/1890 (76%)	1110 (77%)	330 (23%)	2	28

All 61 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	152	ASN	15
1	A	153	MET	15
1	A	160	VAL	15
1	A	171	GLN	15
1	A	179	VAL	15
1	A	183	VAL	15
1	A	210	GLU	15
1	A	209	VAL	14
1	A	207	ARG	13
1	A	190	THR	12
1	A	129	LEU	11
1	A	181	ILE	11
1	A	133	MET	9
1	A	148	TYR	9
1	A	216	GLN	8
1	A	220	GLU	8
1	A	137	LEU	7
1	A	202	ILE	7
1	A	135	ARG	6
1	A	166	ASP	6
1	A	211	GLN	6
1	A	128	MET	6
1	A	147	ARG	6
1	A	150	ARG	5
1	A	158	ASN	5
1	A	197	PHE	5
1	A	157	PRO	5
1	A	159	GLN	4
1	A	187	THR	4

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Mol	Chain	Res	Type	Models (Total)
1	A	149	TYR	3
1	A	163	ARG	3
1	A	222	GLN	3
1	A	193	LYS	3
1	A	205	MET	3
1	A	138	ILE	3
1	A	156	TYR	3
1	A	168	TYR	3
1	A	214	VAL	3
1	A	142	ASN	2
1	A	155	ARG	2
1	A	165	VAL	2
1	A	212	MET	2
1	A	203	LYS	2
1	A	185	GLN	2
1	A	188	VAL	2
1	A	151	GLU	2
1	A	178	CYS	1
1	A	195	GLU	1
1	A	199	GLU	1
1	A	218	GLN	1
1	A	167	GLN	1
1	A	201	ASP	1
1	A	162	TYR	1
1	A	174	PHE	1
1	A	170	ASN	1
1	A	172	ASN	1
1	A	217	TYR	1
1	A	226	GLN	1
1	A	144	TYR	1
1	A	189	THR	1
1	A	196	ASN	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 [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