



Full wwPDB NMR Structure Validation Report ⓘ

Oct 11, 2021 – 03:34 PM EDT

PDB ID : 2JOH
Title : NMR structure of rabbit prion protein mutation S173N
Authors : Li, J.; Lin, D.
Deposited on : 2007-03-13

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:

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

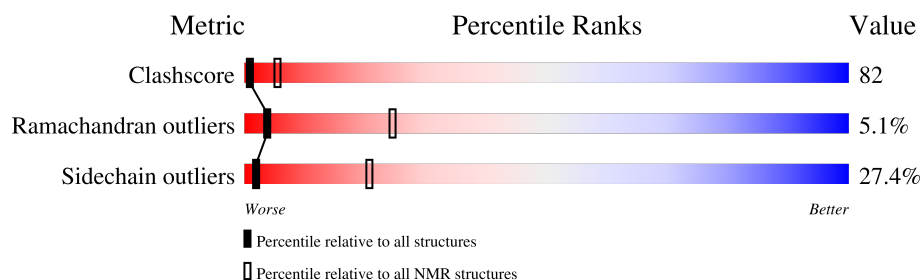
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	NMR archive (#Entries)
Clashscore	158937	12864
Ramachandran outliers	154571	11451
Sidechain outliers	154315	11428

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	148	

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: *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:127-A:166, A:170-A:190, A:194-A:226 (94)	0.31	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 2 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1698 atoms, of which 822 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
			1698	545	822	153	171	7	

There are 11 discrepancies between the modelled and reference sequences:

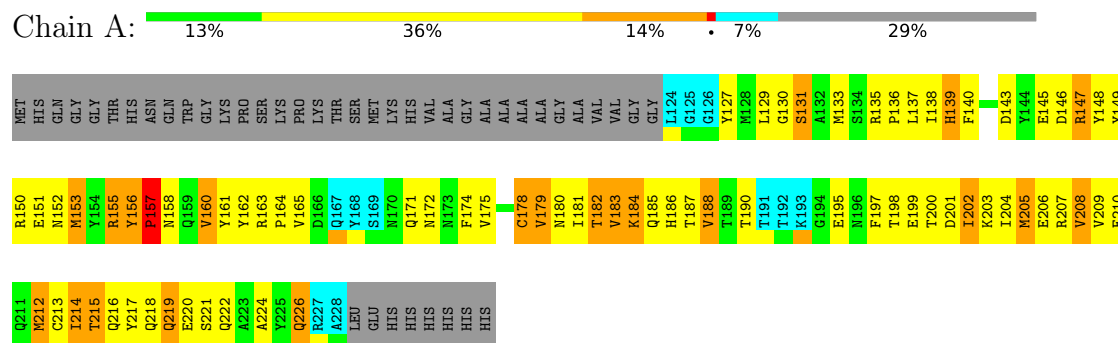
Chain	Residue	Modelled	Actual	Comment	Reference
A	89	MET	-	initiating methionine	UNP Q95211
A	90	HIS	-	expression tag	UNP Q95211
A	173	ASN	SER	engineered mutation	UNP Q95211
A	229	LEU	-	expression tag	UNP Q95211
A	230	GLU	-	expression tag	UNP Q95211
A	231	HIS	-	expression tag	UNP Q95211
A	232	HIS	-	expression 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

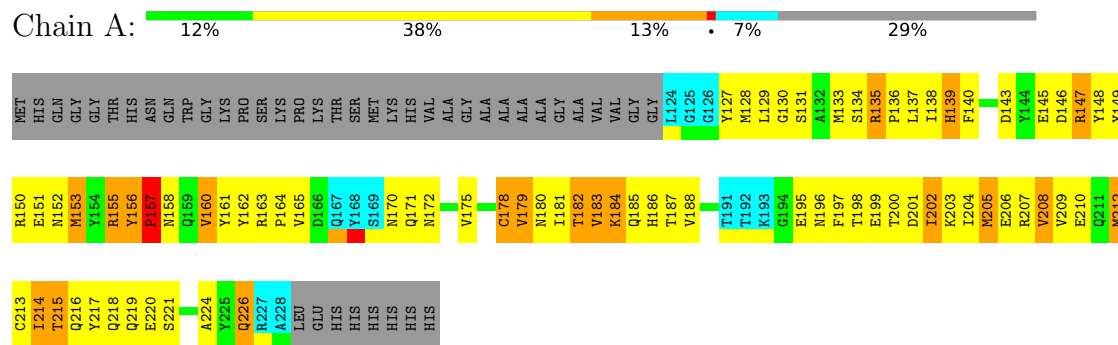


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

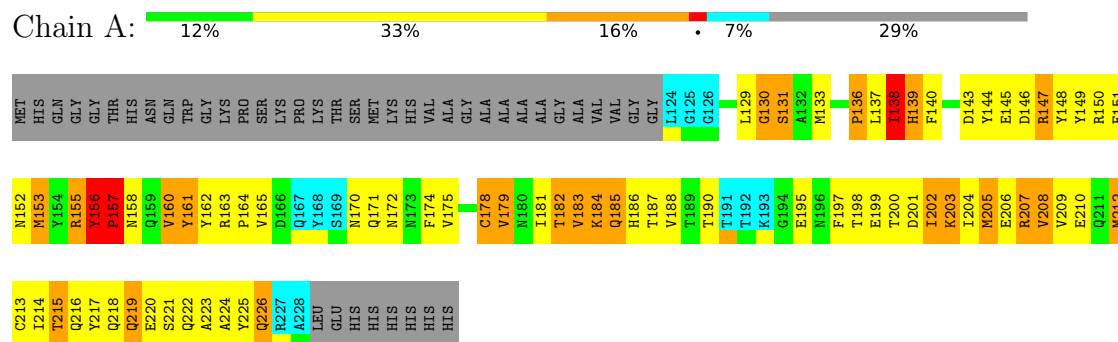
4.2.1 Score per residue for model 1

- Molecule 1: Major prion protein



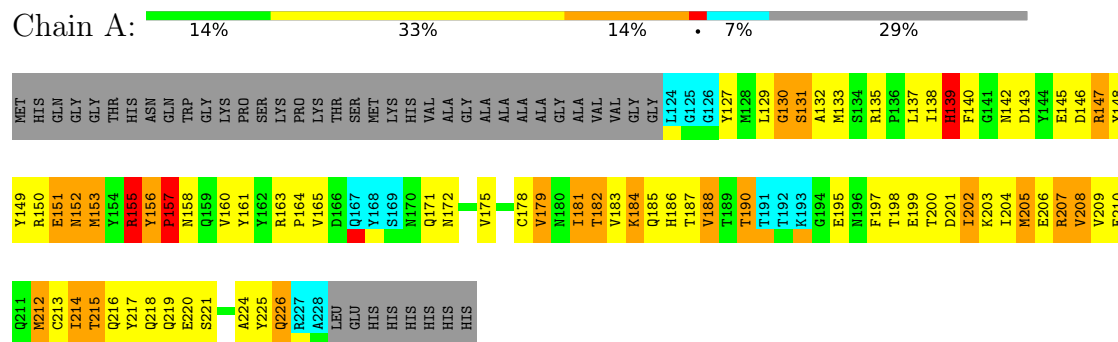
4.2.2 Score per residue for model 2

- Molecule 1: Major prion protein



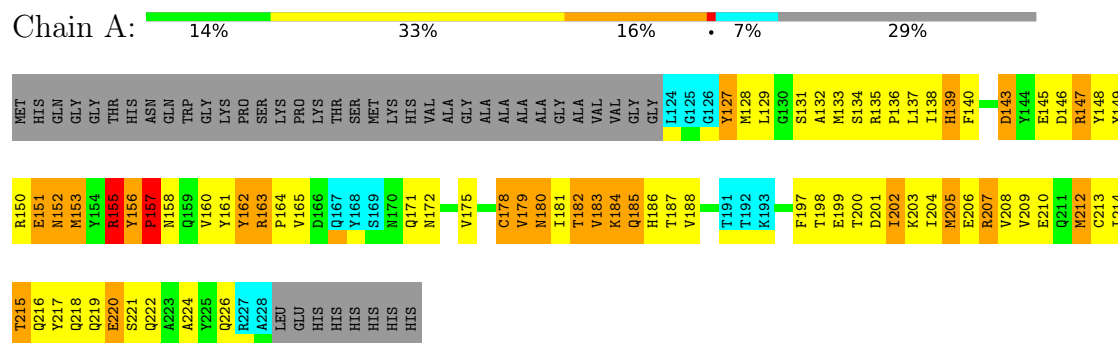
4.2.3 Score per residue for model 3

- Molecule 1: Major prion protein



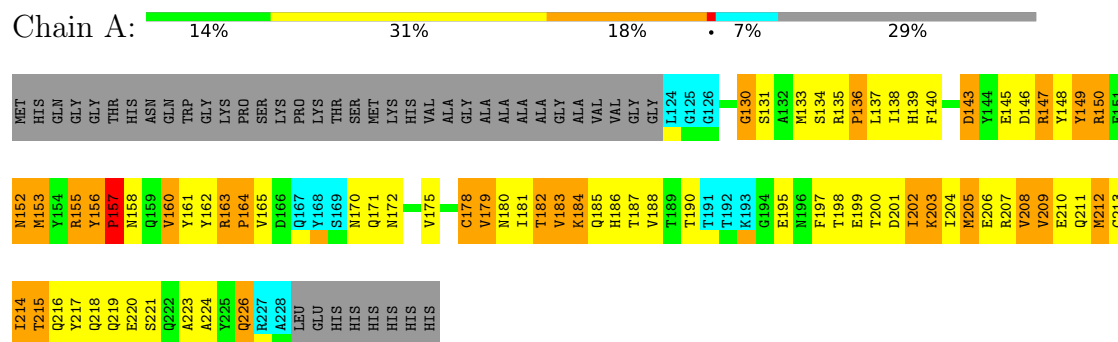
4.2.4 Score per residue for model 4

- Molecule 1: Major prion protein



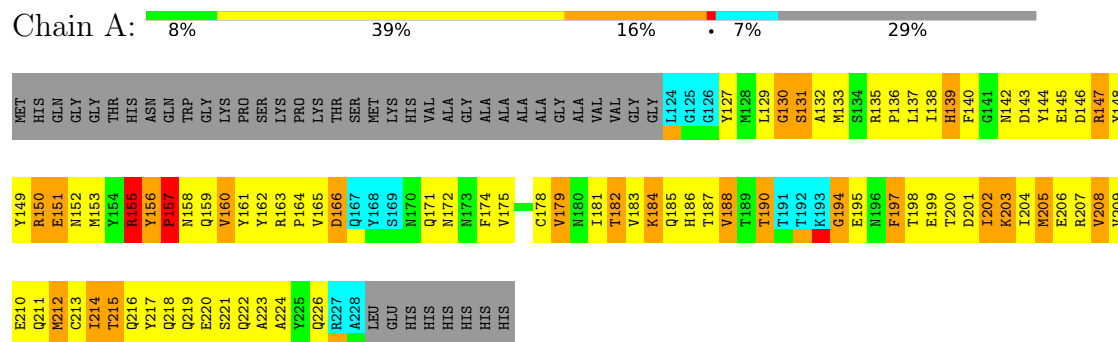
4.2.5 Score per residue for model 5

- Molecule 1: Major prion protein



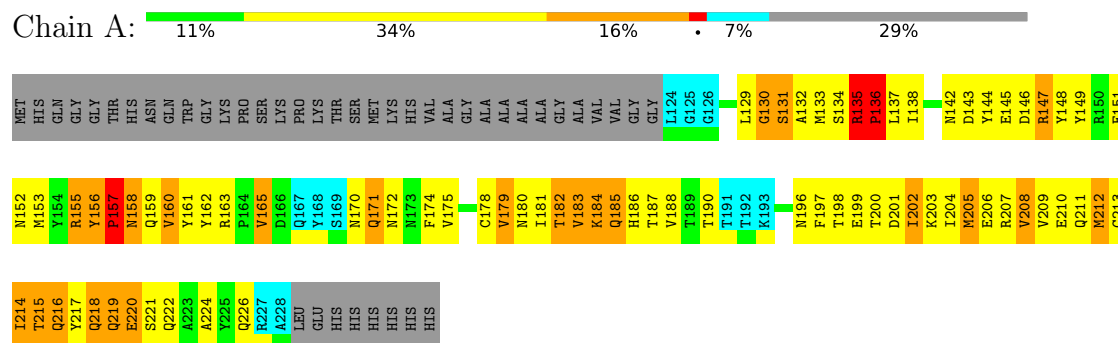
4.2.6 Score per residue for model 6

- Molecule 1: Major prion protein



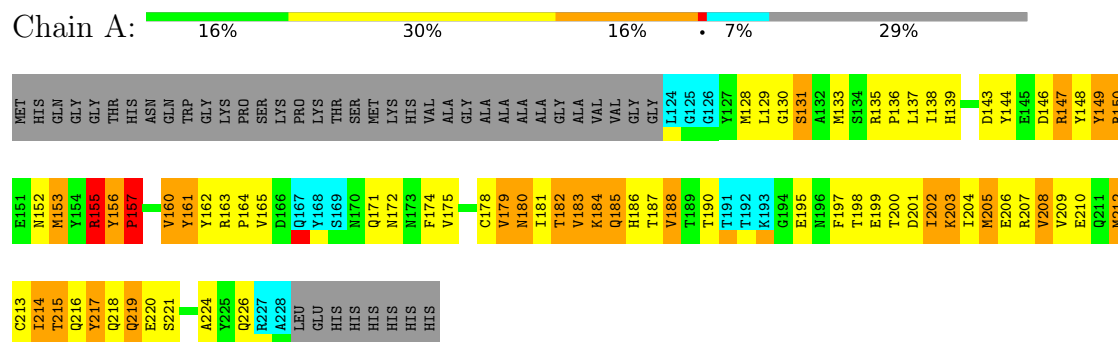
4.2.7 Score per residue for model 7

- Molecule 1: Major prion protein



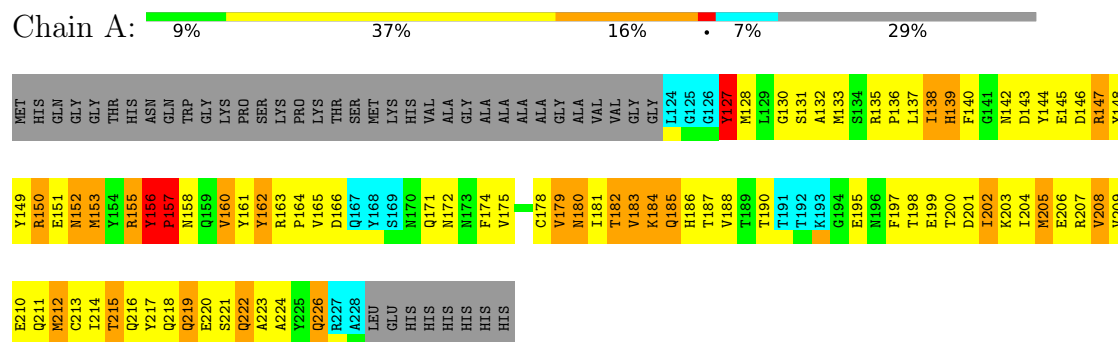
4.2.8 Score per residue for model 8

- Molecule 1: Major prion protein



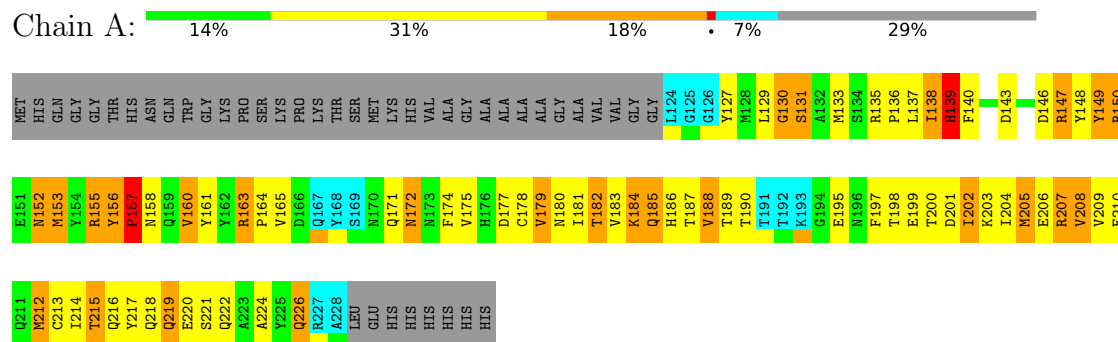
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: Major prion protein



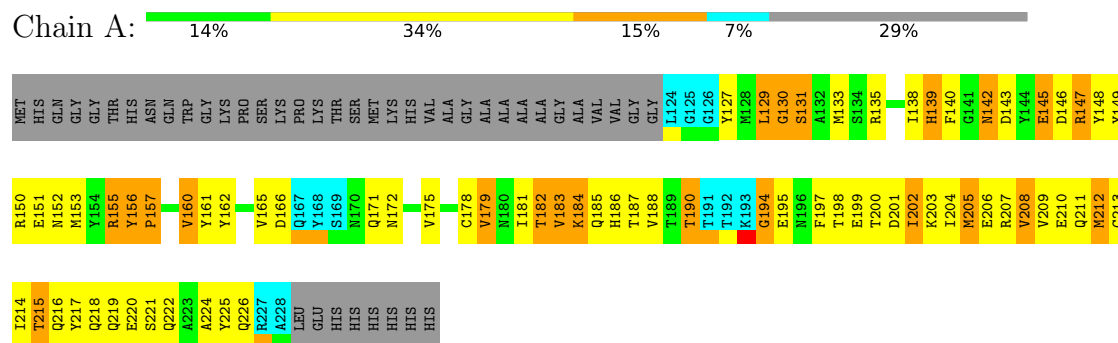
4.2.12 Score per residue for model 12

- Molecule 1: Major prion protein



4.2.13 Score per residue for model 13

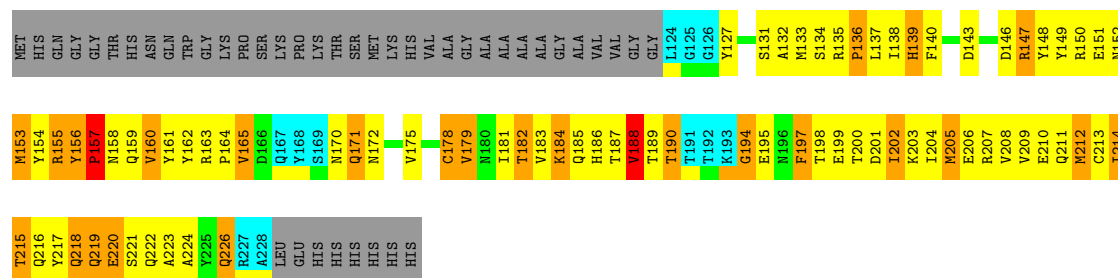
- Molecule 1: Major prion protein



4.2.14 Score per residue for model 14

- Molecule 1: Major prion protein

Chain A: 



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

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	0.74±0.06	1±1/813 (0.1± 0.2%)	0.75±0.02	0±0/1103 (0.0± 0.0%)
All	All	0.75	14/12195 (0.1%)	0.75	6/16545 (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	1.3±0.6
All	All	0	19

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	156	TYR	CE1-CZ	10.99	1.52	1.38	2	1
1	A	156	TYR	CE2-CZ	-10.84	1.24	1.38	2	2
1	A	161	TYR	CE1-CZ	-7.96	1.28	1.38	2	2
1	A	161	TYR	CE2-CZ	7.59	1.48	1.38	2	2
1	A	127	TYR	CE2-CZ	-7.29	1.29	1.38	4	1
1	A	197	PHE	CE1-CZ	6.90	1.50	1.37	15	1
1	A	127	TYR	CE1-CZ	6.42	1.46	1.38	4	2
1	A	197	PHE	CE2-CZ	-5.85	1.26	1.37	15	1
1	A	217	TYR	CE2-CZ	-5.27	1.31	1.38	9	1
1	A	217	TYR	CE1-CZ	5.14	1.45	1.38	9	1

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	157	PRO	N-CA-CB	-5.78	96.25	102.60	6	6

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	15
1	A	127	TYR	Sidechain	1
1	A	154	TYR	Sidechain	1
1	A	189	THR	Peptide	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	794	738	735	125±7
All	All	11910	11070	11025	1879

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 82.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:165:VAL:HG13	1:A:220:GLU:HG3	1.08	1.13	7	4
1:A:165:VAL:HG13	1:A:220:GLU:HG2	0.98	1.31	10	5
1:A:179:VAL:HG13	1:A:209:VAL:HG22	0.96	1.34	5	2
1:A:216:GLN:HA	1:A:219:GLN:HG2	0.96	1.32	14	11
1:A:161:TYR:HB3	1:A:181:ILE:HD13	0.94	1.35	13	1
1:A:186:HIS:HA	1:A:190:THR:HB	0.91	1.37	9	8
1:A:175:VAL:HG21	1:A:214:ILE:HD12	0.91	1.39	4	15
1:A:175:VAL:HG22	1:A:213:CYS:HB3	0.91	1.42	14	10
1:A:175:VAL:HG13	1:A:213:CYS:HB2	0.89	1.42	10	13
1:A:139:HIS:HA	1:A:149:TYR:HE2	0.89	1.28	12	1
1:A:181:ILE:HD12	1:A:182:THR:N	0.89	1.80	13	13
1:A:198:THR:H	1:A:201:ASP:HB2	0.87	1.29	15	8
1:A:133:MET:HE2	1:A:212:MET:HG3	0.87	1.47	14	7
1:A:171:GLN:HB3	1:A:217:TYR:HA	0.86	1.48	12	13
1:A:205:MET:O	1:A:209:VAL:HB	0.85	1.71	1	13
1:A:143:ASP:HA	1:A:146:ASP:HB2	0.85	1.49	7	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:202:ILE:HD13	1:A:205:MET:HE3	0.84	1.46	10	4
1:A:200:THR:O	1:A:204:ILE:HG13	0.84	1.72	12	14
1:A:208:VAL:O	1:A:212:MET:HB2	0.84	1.71	10	8
1:A:181:ILE:HD13	1:A:182:THR:N	0.84	1.88	3	1
1:A:204:ILE:O	1:A:208:VAL:HG23	0.83	1.74	7	10
1:A:206:GLU:O	1:A:210:GLU:HB3	0.82	1.74	1	14
1:A:206:GLU:O	1:A:210:GLU:HB2	0.82	1.73	4	1
1:A:175:VAL:HG22	1:A:213:CYS:HB2	0.82	1.52	11	4
1:A:160:VAL:HG21	1:A:212:MET:SD	0.81	2.14	6	7
1:A:179:VAL:HG13	1:A:209:VAL:HG12	0.81	1.53	9	11
1:A:135:ARG:HA	1:A:158:ASN:OD1	0.80	1.77	10	1
1:A:135:ARG:O	1:A:137:LEU:HG	0.79	1.76	5	6
1:A:186:HIS:HB3	1:A:197:PHE:HZ	0.78	1.39	8	5
1:A:149:TYR:HE1	1:A:204:ILE:HG12	0.77	1.39	2	8
1:A:205:MET:O	1:A:209:VAL:HG13	0.77	1.79	5	2
1:A:171:GLN:O	1:A:175:VAL:HG23	0.77	1.80	13	15
1:A:175:VAL:HA	1:A:178:CYS:HB3	0.77	1.54	15	8
1:A:201:ASP:O	1:A:204:ILE:HB	0.77	1.80	9	15
1:A:165:VAL:CG1	1:A:220:GLU:HG3	0.77	2.05	4	2
1:A:202:ILE:O	1:A:206:GLU:HG3	0.76	1.80	9	12
1:A:163:ARG:HG2	1:A:164:PRO:CD	0.76	2.09	1	2
1:A:171:GLN:CD	1:A:217:TYR:HB2	0.76	2.00	10	4
1:A:149:TYR:HA	1:A:152:ASN:ND2	0.76	1.95	11	9
1:A:163:ARG:HG2	1:A:164:PRO:HD3	0.76	1.57	1	2
1:A:180:ASN:HA	1:A:184:LYS:HE2	0.76	1.57	8	3
1:A:149:TYR:HA	1:A:152:ASN:HB2	0.76	1.55	13	5
1:A:165:VAL:CG1	1:A:220:GLU:HG2	0.76	2.11	2	6
1:A:182:THR:HA	1:A:185:GLN:HG2	0.76	1.58	13	1
1:A:143:ASP:HA	1:A:146:ASP:HB3	0.75	1.57	4	14
1:A:199:GLU:O	1:A:203:LYS:HB3	0.75	1.82	12	15
1:A:184:LYS:HA	1:A:187:THR:HG22	0.75	1.58	8	12
1:A:155:ARG:HB2	1:A:156:TYR:CD1	0.75	2.17	2	1
1:A:156:TYR:HD1	1:A:156:TYR:N	0.74	1.80	2	1
1:A:165:VAL:HG13	1:A:220:GLU:CG	0.74	2.04	7	5
1:A:153:MET:HA	1:A:157:PRO:HA	0.74	1.57	15	15
1:A:161:TYR:HB2	1:A:181:ILE:HD13	0.74	1.59	11	12
1:A:184:LYS:HA	1:A:188:VAL:HG13	0.74	1.57	10	2
1:A:214:ILE:O	1:A:217:TYR:HB3	0.74	1.81	9	11
1:A:215:THR:O	1:A:218:GLN:HG3	0.74	1.82	14	15
1:A:160:VAL:HG11	1:A:209:VAL:HG13	0.74	1.58	12	13
1:A:160:VAL:HA	1:A:182:THR:OG1	0.73	1.81	11	14

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:216:GLN:HE21	1:A:220:GLU:HB2	0.73	1.43	6	2
1:A:163:ARG:HG3	1:A:164:PRO:CD	0.73	2.14	11	10
1:A:208:VAL:O	1:A:212:MET:HB3	0.73	1.82	6	7
1:A:139:HIS:HA	1:A:149:TYR:CE2	0.73	2.18	12	1
1:A:156:TYR:CD1	1:A:156:TYR:N	0.73	2.56	2	2
1:A:186:HIS:CA	1:A:190:THR:HB	0.73	2.14	9	6
1:A:216:GLN:HA	1:A:219:GLN:HB3	0.72	1.61	3	1
1:A:179:VAL:O	1:A:183:VAL:HG13	0.72	1.84	13	15
1:A:179:VAL:HG12	1:A:183:VAL:HG11	0.72	1.60	10	14
1:A:140:PHE:HZ	1:A:204:ILE:HG12	0.72	1.42	12	1
1:A:152:ASN:ND2	1:A:204:ILE:HD13	0.72	1.99	1	14
1:A:179:VAL:HG23	1:A:209:VAL:HG12	0.72	1.58	6	1
1:A:171:GLN:NE2	1:A:217:TYR:HB2	0.72	1.99	10	1
1:A:179:VAL:HG13	1:A:209:VAL:CG1	0.71	2.15	4	12
1:A:183:VAL:O	1:A:187:THR:HG22	0.71	1.84	10	15
1:A:130:GLY:HA2	1:A:162:TYR:HE1	0.71	1.44	11	5
1:A:171:GLN:CG	1:A:217:TYR:HA	0.71	2.14	9	1
1:A:200:THR:O	1:A:203:LYS:HG2	0.71	1.85	7	15
1:A:183:VAL:HB	1:A:205:MET:SD	0.71	2.25	10	6
1:A:139:HIS:HA	1:A:146:ASP:HA	0.71	1.60	1	5
1:A:175:VAL:HG22	1:A:213:CYS:CB	0.71	2.15	3	14
1:A:149:TYR:CE1	1:A:204:ILE:HG12	0.71	2.21	15	12
1:A:146:ASP:HA	1:A:149:TYR:CE2	0.71	2.21	5	2
1:A:157:PRO:HG3	1:A:186:HIS:CE1	0.70	2.20	6	12
1:A:163:ARG:H	1:A:174:PHE:HE2	0.70	1.26	2	2
1:A:148:TYR:O	1:A:152:ASN:HB3	0.70	1.86	12	7
1:A:147:ARG:HA	1:A:150:ARG:HD2	0.70	1.64	5	3
1:A:179:VAL:HG23	1:A:209:VAL:CG1	0.70	2.16	6	1
1:A:152:ASN:HB3	1:A:156:TYR:HB2	0.70	1.63	6	4
1:A:204:ILE:O	1:A:207:ARG:HG2	0.70	1.87	13	10
1:A:216:GLN:CA	1:A:219:GLN:HG2	0.70	2.14	14	5
1:A:161:TYR:HB2	1:A:181:ILE:HD11	0.70	1.63	3	1
1:A:160:VAL:HG12	1:A:182:THR:HG21	0.69	1.64	10	15
1:A:149:TYR:HA	1:A:152:ASN:CG	0.69	2.07	5	9
1:A:175:VAL:HG21	1:A:214:ILE:CD1	0.69	2.17	9	8
1:A:155:ARG:HG2	1:A:156:TYR:CD1	0.69	2.23	6	2
1:A:171:GLN:NE2	1:A:171:GLN:H	0.69	1.86	7	2
1:A:209:VAL:HA	1:A:212:MET:HB3	0.69	1.65	9	3
1:A:152:ASN:HA	1:A:155:ARG:CD	0.68	2.17	4	15
1:A:165:VAL:HG12	1:A:220:GLU:HG2	0.68	1.64	12	4
1:A:207:ARG:HB2	1:A:207:ARG:NH1	0.68	2.04	12	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:128:MET:HG3	1:A:162:TYR:O	0.68	1.87	8	3
1:A:137:LEU:HD22	1:A:149:TYR:HE1	0.68	1.48	5	1
1:A:186:HIS:HA	1:A:190:THR:HG22	0.68	1.66	6	1
1:A:171:GLN:NE2	1:A:172:ASN:H	0.68	1.87	15	1
1:A:171:GLN:HB3	1:A:217:TYR:CA	0.67	2.19	3	10
1:A:178:CYS:HA	1:A:181:ILE:HG13	0.67	1.63	1	8
1:A:216:GLN:HA	1:A:219:GLN:CG	0.67	2.20	9	8
1:A:171:GLN:HG3	1:A:217:TYR:N	0.67	2.04	14	4
1:A:183:VAL:HA	1:A:205:MET:SD	0.67	2.30	15	13
1:A:140:PHE:CZ	1:A:204:ILE:HG12	0.66	2.25	12	1
1:A:165:VAL:HG11	1:A:171:GLN:HB2	0.65	1.68	6	2
1:A:171:GLN:HG2	1:A:217:TYR:HA	0.65	1.69	9	1
1:A:187:THR:HB	1:A:197:PHE:CE2	0.65	2.27	11	5
1:A:216:GLN:HB3	1:A:220:GLU:HB2	0.65	1.68	12	3
1:A:161:TYR:HB2	1:A:181:ILE:CD1	0.65	2.22	5	11
1:A:197:PHE:CE2	1:A:202:ILE:HG12	0.65	2.26	10	3
1:A:186:HIS:HB3	1:A:197:PHE:CZ	0.64	2.24	8	2
1:A:171:GLN:N	1:A:171:GLN:HE21	0.64	1.89	15	1
1:A:222:GLN:O	1:A:226:GLN:HG2	0.64	1.92	6	2
1:A:216:GLN:O	1:A:220:GLU:HB3	0.64	1.92	4	4
1:A:153:MET:HA	1:A:153:MET:CE	0.64	2.23	12	15
1:A:136:PRO:HB2	1:A:208:VAL:HG12	0.64	1.70	12	2
1:A:138:ILE:HG13	1:A:207:ARG:HG3	0.63	1.68	1	6
1:A:197:PHE:CE1	1:A:202:ILE:HG12	0.63	2.28	1	2
1:A:149:TYR:O	1:A:153:MET:HE2	0.63	1.92	7	1
1:A:172:ASN:HA	1:A:214:ILE:HD12	0.63	1.70	9	11
1:A:202:ILE:CD1	1:A:205:MET:HE3	0.63	2.22	10	4
1:A:163:ARG:HG3	1:A:164:PRO:HD3	0.63	1.69	4	5
1:A:155:ARG:HG2	1:A:156:TYR:N	0.63	2.07	10	12
1:A:177:ASP:O	1:A:181:ILE:HD13	0.63	1.93	10	1
1:A:152:ASN:HA	1:A:155:ARG:HD2	0.62	1.71	11	13
1:A:204:ILE:O	1:A:207:ARG:HG3	0.62	1.94	9	5
1:A:198:THR:HG22	1:A:201:ASP:OD2	0.62	1.94	4	14
1:A:179:VAL:HG13	1:A:209:VAL:CG2	0.62	2.20	5	1
1:A:171:GLN:HG3	1:A:220:GLU:OE1	0.62	1.94	9	1
1:A:130:GLY:CA	1:A:162:TYR:HE1	0.62	2.08	1	6
1:A:152:ASN:HD21	1:A:204:ILE:HD13	0.62	1.53	5	7
1:A:152:ASN:HA	1:A:155:ARG:HD3	0.62	1.71	14	5
1:A:136:PRO:HG2	1:A:208:VAL:HG12	0.62	1.72	6	6
1:A:179:VAL:HG12	1:A:183:VAL:CG1	0.62	2.25	2	13
1:A:187:THR:HB	1:A:197:PHE:CD2	0.62	2.30	2	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:156:TYR:HA	1:A:205:MET:SD	0.61	2.36	13	10
1:A:186:HIS:HA	1:A:190:THR:CB	0.61	2.19	9	6
1:A:213:CYS:HA	1:A:216:GLN:HG2	0.61	1.73	10	3
1:A:155:ARG:HB3	1:A:195:GLU:OE1	0.60	1.96	2	1
1:A:143:ASP:O	1:A:147:ARG:HB3	0.60	1.96	7	2
1:A:204:ILE:HA	1:A:207:ARG:HG2	0.60	1.72	10	9
1:A:179:VAL:HG21	1:A:210:GLU:HG2	0.60	1.72	4	1
1:A:147:ARG:O	1:A:150:ARG:HG3	0.60	1.97	6	3
1:A:147:ARG:HA	1:A:150:ARG:HG2	0.60	1.72	11	3
1:A:204:ILE:HA	1:A:207:ARG:HG3	0.60	1.72	3	5
1:A:171:GLN:HG3	1:A:217:TYR:H	0.60	1.57	7	2
1:A:172:ASN:HD22	1:A:214:ILE:HD11	0.59	1.56	9	8
1:A:147:ARG:HA	1:A:150:ARG:CD	0.59	2.27	9	3
1:A:165:VAL:O	1:A:220:GLU:HG3	0.59	1.98	14	5
1:A:175:VAL:HG22	1:A:213:CYS:C	0.59	2.17	9	11
1:A:186:HIS:O	1:A:190:THR:HG22	0.59	1.98	3	1
1:A:184:LYS:HG3	1:A:188:VAL:HG11	0.59	1.75	6	7
1:A:204:ILE:HG22	1:A:205:MET:N	0.59	2.10	14	1
1:A:212:MET:O	1:A:215:THR:HG22	0.59	1.98	14	11
1:A:135:ARG:HH11	1:A:137:LEU:HD21	0.59	1.57	12	1
1:A:152:ASN:O	1:A:155:ARG:HD2	0.59	1.97	5	10
1:A:171:GLN:HE21	1:A:171:GLN:H	0.59	1.41	15	1
1:A:153:MET:HA	1:A:153:MET:HE3	0.58	1.75	8	8
1:A:218:GLN:O	1:A:222:GLN:HG3	0.58	1.98	10	2
1:A:143:ASP:HA	1:A:146:ASP:CB	0.58	2.28	3	12
1:A:200:THR:HG23	1:A:203:LYS:HE3	0.58	1.75	1	2
1:A:140:PHE:HA	1:A:207:ARG:HH21	0.58	1.58	12	1
1:A:135:ARG:HA	1:A:158:ASN:HB2	0.58	1.74	5	2
1:A:149:TYR:O	1:A:153:MET:HG2	0.58	1.98	13	3
1:A:149:TYR:HD1	1:A:152:ASN:HD21	0.58	1.41	2	4
1:A:138:ILE:HB	1:A:207:ARG:CZ	0.58	2.28	12	2
1:A:175:VAL:CG1	1:A:213:CYS:HB2	0.58	2.24	6	2
1:A:172:ASN:ND2	1:A:214:ILE:HD11	0.58	2.14	9	3
1:A:222:GLN:HG3	1:A:223:ALA:N	0.58	2.13	11	1
1:A:153:MET:HG3	1:A:158:ASN:HB3	0.57	1.75	14	2
1:A:164:PRO:HA	1:A:220:GLU:OE2	0.57	1.98	10	1
1:A:220:GLU:OE2	1:A:224:ALA:HB2	0.57	1.99	12	3
1:A:148:TYR:O	1:A:151:GLU:HG2	0.57	1.99	15	4
1:A:145:GLU:HB3	1:A:149:TYR:CZ	0.57	2.35	15	1
1:A:155:ARG:HB2	1:A:156:TYR:HD1	0.57	1.57	2	1
1:A:171:GLN:OE1	1:A:217:TYR:HB2	0.57	1.98	15	2

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:201:ASP:HA	1:A:204:ILE:HD12	0.57	1.75	1	11
1:A:149:TYR:HA	1:A:152:ASN:OD1	0.57	2.00	14	1
1:A:204:ILE:O	1:A:208:VAL:HG22	0.57	2.00	5	3
1:A:165:VAL:CG1	1:A:171:GLN:HB2	0.57	2.29	6	1
1:A:175:VAL:HG11	1:A:214:ILE:HD13	0.57	1.75	15	1
1:A:140:PHE:HD2	1:A:142:ASN:HB2	0.56	1.60	13	2
1:A:139:HIS:HB3	1:A:146:ASP:HB2	0.56	1.77	8	1
1:A:198:THR:N	1:A:201:ASP:HB2	0.56	2.10	15	8
1:A:219:GLN:O	1:A:222:GLN:HG2	0.56	1.99	11	1
1:A:155:ARG:HB2	1:A:195:GLU:OE2	0.56	2.00	12	2
1:A:221:SER:O	1:A:225:TYR:HB2	0.56	2.01	13	4
1:A:178:CYS:O	1:A:182:THR:HB	0.56	2.00	7	8
1:A:171:GLN:CD	1:A:217:TYR:HA	0.56	2.21	9	1
1:A:171:GLN:H	1:A:217:TYR:HD1	0.56	1.44	1	3
1:A:204:ILE:HA	1:A:207:ARG:CG	0.56	2.30	4	7
1:A:152:ASN:OD1	1:A:153:MET:HE3	0.56	2.01	8	4
1:A:178:CYS:HA	1:A:181:ILE:HD11	0.56	1.78	10	1
1:A:175:VAL:O	1:A:179:VAL:HG23	0.56	2.01	15	13
1:A:132:ALA:HA	1:A:158:ASN:O	0.56	1.99	9	7
1:A:146:ASP:O	1:A:150:ARG:HB3	0.56	2.01	5	2
1:A:139:HIS:HA	1:A:146:ASP:HB2	0.56	1.76	10	6
1:A:135:ARG:NH1	1:A:137:LEU:HD21	0.56	2.16	12	1
1:A:160:VAL:CG1	1:A:209:VAL:HG13	0.56	2.30	7	9
1:A:145:GLU:HA	1:A:148:TYR:CB	0.56	2.31	4	5
1:A:175:VAL:HG13	1:A:213:CYS:CB	0.55	2.26	10	5
1:A:181:ILE:O	1:A:185:GLN:HB3	0.55	2.01	4	3
1:A:139:HIS:HA	1:A:146:ASP:CB	0.55	2.32	10	7
1:A:197:PHE:CD2	1:A:202:ILE:HG12	0.55	2.36	13	2
1:A:138:ILE:HD11	1:A:208:VAL:HA	0.55	1.78	5	5
1:A:183:VAL:CG1	1:A:205:MET:HB3	0.55	2.32	8	8
1:A:153:MET:HA	1:A:153:MET:HE2	0.55	1.78	12	1
1:A:133:MET:CG	1:A:160:VAL:HG22	0.55	2.32	5	6
1:A:133:MET:HG2	1:A:212:MET:HE2	0.55	1.77	15	3
1:A:155:ARG:HB2	1:A:156:TYR:CE1	0.55	2.36	2	1
1:A:147:ARG:NH1	1:A:148:TYR:HA	0.54	2.17	10	1
1:A:140:PHE:HD1	1:A:207:ARG:HH12	0.54	1.43	3	1
1:A:175:VAL:CG2	1:A:213:CYS:HB2	0.54	2.31	11	3
1:A:185:GLN:O	1:A:190:THR:HB	0.54	2.02	3	3
1:A:171:GLN:HG2	1:A:217:TYR:CA	0.54	2.32	9	1
1:A:127:TYR:HB2	1:A:161:TYR:CZ	0.54	2.37	13	1
1:A:134:SER:O	1:A:135:ARG:HD2	0.54	2.03	4	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:139:HIS:HB3	1:A:146:ASP:OD1	0.54	2.03	12	4
1:A:140:PHE:HB2	1:A:149:TYR:HE2	0.54	1.62	2	1
1:A:186:HIS:O	1:A:195:GLU:HG2	0.54	2.03	3	2
1:A:204:ILE:CA	1:A:207:ARG:HG3	0.54	2.33	3	4
1:A:207:ARG:HD3	1:A:208:VAL:HG22	0.54	1.77	4	1
1:A:138:ILE:HG13	1:A:207:ARG:HD3	0.54	1.80	9	1
1:A:152:ASN:HB2	1:A:156:TYR:CD2	0.53	2.38	4	5
1:A:153:MET:HB3	1:A:158:ASN:OD1	0.53	2.03	6	1
1:A:163:ARG:HD3	1:A:174:PHE:CE1	0.53	2.38	6	1
1:A:216:GLN:HA	1:A:219:GLN:HG3	0.53	1.78	15	1
1:A:198:THR:HG23	1:A:200:THR:H	0.53	1.63	9	4
1:A:152:ASN:CA	1:A:155:ARG:HD2	0.53	2.33	5	10
1:A:175:VAL:CG2	1:A:214:ILE:HD12	0.53	2.28	12	1
1:A:137:LEU:HD21	1:A:153:MET:SD	0.53	2.43	8	1
1:A:180:ASN:HA	1:A:184:LYS:HE3	0.53	1.81	7	4
1:A:133:MET:HG2	1:A:160:VAL:HG22	0.53	1.81	8	1
1:A:165:VAL:HG11	1:A:171:GLN:NE2	0.53	2.18	11	1
1:A:184:LYS:O	1:A:188:VAL:HG13	0.53	2.04	15	2
1:A:156:TYR:CE1	1:A:197:PHE:HE1	0.53	2.22	2	1
1:A:165:VAL:HB	1:A:174:PHE:CE2	0.53	2.39	7	1
1:A:215:THR:O	1:A:219:GLN:N	0.53	2.41	11	13
1:A:147:ARG:O	1:A:150:ARG:HG2	0.52	2.04	15	5
1:A:127:TYR:HD2	1:A:162:TYR:HA	0.52	1.64	11	1
1:A:175:VAL:CG1	1:A:210:GLU:HA	0.52	2.34	3	8
1:A:213:CYS:HA	1:A:216:GLN:CD	0.52	2.25	1	2
1:A:212:MET:SD	1:A:212:MET:C	0.52	2.88	13	7
1:A:153:MET:HE3	1:A:153:MET:CA	0.52	2.34	1	6
1:A:220:GLU:HG3	1:A:224:ALA:CB	0.52	2.35	3	6
1:A:161:TYR:HB3	1:A:181:ILE:CD1	0.52	2.22	13	1
1:A:135:ARG:HD3	1:A:158:ASN:OD1	0.52	2.04	10	1
1:A:135:ARG:O	1:A:135:ARG:HD3	0.52	2.05	5	5
1:A:204:ILE:CA	1:A:207:ARG:HG2	0.52	2.34	10	4
1:A:205:MET:HA	1:A:208:VAL:HG23	0.52	1.81	5	3
1:A:181:ILE:HD12	1:A:182:THR:CA	0.52	2.34	6	7
1:A:133:MET:SD	1:A:212:MET:HE2	0.52	2.45	10	1
1:A:149:TYR:C	1:A:149:TYR:CD1	0.52	2.83	12	2
1:A:138:ILE:HG21	1:A:207:ARG:HE	0.52	1.64	9	1
1:A:186:HIS:C	1:A:190:THR:HB	0.52	2.24	11	2
1:A:207:ARG:O	1:A:211:GLN:HB3	0.52	2.05	10	7
1:A:153:MET:HE1	1:A:156:TYR:O	0.52	2.05	13	2
1:A:199:GLU:O	1:A:202:ILE:HG22	0.51	2.05	10	4

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:166:ASP:HB2	1:A:221:SER:HA	0.51	1.82	6	1
1:A:155:ARG:HB2	1:A:195:GLU:CD	0.51	2.25	15	2
1:A:136:PRO:HG3	1:A:212:MET:CG	0.51	2.35	12	1
1:A:153:MET:CG	1:A:158:ASN:HB3	0.51	2.36	12	4
1:A:171:GLN:CB	1:A:217:TYR:HA	0.51	2.34	3	1
1:A:133:MET:SD	1:A:158:ASN:HA	0.51	2.45	6	5
1:A:200:THR:HA	1:A:203:LYS:HG2	0.51	1.81	11	4
1:A:185:GLN:HG3	1:A:186:HIS:N	0.51	2.20	12	6
1:A:139:HIS:HA	1:A:146:ASP:OD1	0.51	2.06	15	1
1:A:144:TYR:O	1:A:147:ARG:HD3	0.51	2.05	2	3
1:A:147:ARG:O	1:A:151:GLU:HB3	0.51	2.06	3	3
1:A:171:GLN:HG2	1:A:216:GLN:HB2	0.51	1.83	6	3
1:A:160:VAL:HB	1:A:178:CYS:SG	0.50	2.46	6	1
1:A:172:ASN:O	1:A:175:VAL:HB	0.50	2.06	13	3
1:A:190:THR:HG22	1:A:195:GLU:HB3	0.50	1.83	15	1
1:A:147:ARG:HD3	1:A:148:TYR:N	0.50	2.21	13	8
1:A:138:ILE:HD12	1:A:138:ILE:H	0.50	1.66	8	1
1:A:171:GLN:NE2	1:A:217:TYR:HA	0.50	2.22	9	1
1:A:153:MET:CA	1:A:157:PRO:HA	0.50	2.36	14	2
1:A:152:ASN:C	1:A:155:ARG:HD2	0.50	2.27	1	8
1:A:187:THR:HG21	1:A:197:PHE:CE2	0.50	2.41	1	3
1:A:149:TYR:CD1	1:A:153:MET:HE1	0.50	2.42	8	1
1:A:152:ASN:CA	1:A:155:ARG:HD3	0.50	2.37	14	2
1:A:184:LYS:O	1:A:188:VAL:HG22	0.49	2.07	7	8
1:A:187:THR:HG23	1:A:188:VAL:HG12	0.49	1.83	6	1
1:A:147:ARG:HA	1:A:150:ARG:HB3	0.49	1.83	13	1
1:A:202:ILE:C	1:A:204:ILE:N	0.49	2.65	4	14
1:A:149:TYR:HD1	1:A:153:MET:HE1	0.49	1.67	8	1
1:A:137:LEU:CD2	1:A:137:LEU:N	0.49	2.75	11	1
1:A:147:ARG:HD2	1:A:148:TYR:N	0.49	2.21	4	5
1:A:140:PHE:HB2	1:A:149:TYR:CE2	0.49	2.42	2	2
1:A:165:VAL:CG1	1:A:220:GLU:HB3	0.49	2.36	6	1
1:A:184:LYS:HD2	1:A:184:LYS:C	0.49	2.26	15	1
1:A:129:LEU:HD23	1:A:131:SER:N	0.49	2.23	8	2
1:A:212:MET:SD	1:A:215:THR:HG21	0.49	2.47	4	5
1:A:175:VAL:CG2	1:A:213:CYS:HB3	0.49	2.25	15	1
1:A:182:THR:O	1:A:185:GLN:HG2	0.49	2.06	11	3
1:A:204:ILE:HA	1:A:207:ARG:CD	0.49	2.38	8	2
1:A:138:ILE:HD12	1:A:138:ILE:N	0.49	2.22	8	1
1:A:149:TYR:HD1	1:A:152:ASN:ND2	0.49	2.05	11	4
1:A:172:ASN:HA	1:A:214:ILE:CD1	0.49	2.38	11	10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:155:ARG:N	1:A:157:PRO:HB3	0.49	2.22	6	4
1:A:136:PRO:HG2	1:A:208:VAL:CG1	0.49	2.38	4	4
1:A:182:THR:HA	1:A:185:GLN:HB2	0.49	1.84	3	3
1:A:160:VAL:HG12	1:A:182:THR:CG2	0.49	2.37	12	5
1:A:137:LEU:HD22	1:A:149:TYR:CE1	0.48	2.36	5	1
1:A:147:ARG:HH11	1:A:148:TYR:HA	0.48	1.68	10	1
1:A:161:TYR:H	1:A:181:ILE:HD11	0.48	1.67	7	6
1:A:147:ARG:HA	1:A:150:ARG:CG	0.48	2.38	12	1
1:A:138:ILE:HD12	1:A:207:ARG:O	0.48	2.08	12	2
1:A:186:HIS:HA	1:A:190:THR:CG2	0.48	2.36	6	2
1:A:148:TYR:CD2	1:A:204:ILE:HD11	0.48	2.43	3	1
1:A:181:ILE:HD12	1:A:182:THR:CB	0.48	2.38	13	5
1:A:222:GLN:O	1:A:225:TYR:HB3	0.48	2.08	2	1
1:A:137:LEU:HD23	1:A:153:MET:SD	0.48	2.49	3	2
1:A:172:ASN:HA	1:A:175:VAL:CG2	0.48	2.38	7	4
1:A:153:MET:HG3	1:A:158:ASN:N	0.48	2.23	1	2
1:A:163:ARG:N	1:A:174:PHE:HE2	0.48	2.06	11	2
1:A:197:PHE:CD1	1:A:197:PHE:N	0.48	2.82	6	4
1:A:139:HIS:O	1:A:140:PHE:HB3	0.48	2.08	11	1
1:A:165:VAL:HG11	1:A:171:GLN:OE1	0.48	2.08	1	3
1:A:219:GLN:O	1:A:222:GLN:HB2	0.48	2.09	4	5
1:A:220:GLU:C	1:A:222:GLN:N	0.48	2.67	14	4
1:A:165:VAL:O	1:A:224:ALA:HB3	0.48	2.09	12	2
1:A:197:PHE:H	1:A:197:PHE:HD1	0.48	1.51	14	1
1:A:133:MET:SD	1:A:159:GLN:N	0.48	2.87	7	2
1:A:171:GLN:OE1	1:A:171:GLN:N	0.48	2.47	9	1
1:A:145:GLU:HA	1:A:148:TYR:HB3	0.47	1.85	11	5
1:A:136:PRO:CG	1:A:212:MET:HG3	0.47	2.39	12	1
1:A:198:THR:HG23	1:A:200:THR:HB	0.47	1.86	3	2
1:A:212:MET:CE	1:A:216:GLN:HE21	0.47	2.22	4	1
1:A:165:VAL:HB	1:A:174:PHE:CD2	0.47	2.44	7	1
1:A:133:MET:CE	1:A:136:PRO:HG2	0.47	2.40	2	1
1:A:213:CYS:HA	1:A:216:GLN:HG3	0.47	1.86	7	3
1:A:171:GLN:HE22	1:A:217:TYR:HD1	0.47	1.52	14	1
1:A:220:GLU:HG3	1:A:224:ALA:HB2	0.47	1.86	8	4
1:A:195:GLU:HG3	1:A:197:PHE:CE1	0.47	2.45	5	2
1:A:135:ARG:HD2	1:A:137:LEU:HD21	0.47	1.85	11	1
1:A:149:TYR:HA	1:A:152:ASN:CB	0.47	2.35	10	3
1:A:153:MET:CE	1:A:153:MET:CA	0.47	2.92	14	4
1:A:182:THR:HA	1:A:185:GLN:HB3	0.47	1.85	12	2
1:A:138:ILE:C	1:A:140:PHE:H	0.47	2.13	1	6

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:149:TYR:C	1:A:152:ASN:H	0.47	2.13	12	2
1:A:152:ASN:HD21	1:A:204:ILE:HG21	0.47	1.69	12	2
1:A:209:VAL:HA	1:A:212:MET:CG	0.47	2.39	6	1
1:A:133:MET:HE2	1:A:212:MET:HB2	0.47	1.86	9	2
1:A:200:THR:HA	1:A:203:LYS:CD	0.47	2.40	14	1
1:A:206:GLU:O	1:A:210:GLU:CB	0.47	2.61	9	1
1:A:183:VAL:HG12	1:A:205:MET:HB3	0.47	1.86	12	1
1:A:127:TYR:HB2	1:A:161:TYR:CE2	0.47	2.45	13	1
1:A:152:ASN:HA	1:A:155:ARG:NE	0.46	2.24	3	1
1:A:171:GLN:HG3	1:A:217:TYR:CA	0.46	2.40	7	1
1:A:135:ARG:CD	1:A:135:ARG:O	0.46	2.63	8	1
1:A:177:ASP:HA	1:A:180:ASN:HB2	0.46	1.87	12	1
1:A:133:MET:HG2	1:A:212:MET:CE	0.46	2.40	6	3
1:A:171:GLN:HG3	1:A:213:CYS:O	0.46	2.10	3	6
1:A:161:TYR:O	1:A:181:ILE:HG12	0.46	2.10	7	2
1:A:185:GLN:HG3	1:A:186:HIS:CD2	0.46	2.46	13	1
1:A:129:LEU:O	1:A:131:SER:N	0.46	2.49	9	7
1:A:145:GLU:HA	1:A:148:TYR:HB2	0.46	1.85	4	2
1:A:208:VAL:O	1:A:212:MET:N	0.46	2.49	8	2
1:A:137:LEU:CD2	1:A:149:TYR:HE1	0.46	2.21	5	1
1:A:175:VAL:CA	1:A:178:CYS:HB3	0.46	2.34	15	1
1:A:207:ARG:HG2	1:A:207:ARG:HH11	0.46	1.70	4	2
1:A:142:ASN:ND2	1:A:144:TYR:HB3	0.46	2.26	6	2
1:A:216:GLN:OE1	1:A:219:GLN:HG2	0.46	2.11	15	1
1:A:165:VAL:HG13	1:A:220:GLU:HB3	0.46	1.88	3	1
1:A:184:LYS:HD3	1:A:184:LYS:N	0.46	2.25	10	1
1:A:171:GLN:OE1	1:A:214:ILE:HA	0.46	2.11	15	1
1:A:187:THR:HG21	1:A:197:PHE:HE2	0.46	1.68	1	2
1:A:181:ILE:HD12	1:A:182:THR:HB	0.46	1.88	8	3
1:A:198:THR:O	1:A:202:ILE:N	0.46	2.48	13	5
1:A:129:LEU:HD12	1:A:160:VAL:O	0.46	2.11	4	1
1:A:147:ARG:HD2	1:A:147:ARG:C	0.46	2.31	11	2
1:A:156:TYR:CD1	1:A:205:MET:HE1	0.46	2.46	12	6
1:A:129:LEU:HD22	1:A:160:VAL:O	0.46	2.10	12	1
1:A:213:CYS:HA	1:A:216:GLN:CG	0.45	2.41	8	3
1:A:199:GLU:HA	1:A:202:ILE:CG2	0.45	2.41	13	2
1:A:181:ILE:HD13	1:A:181:ILE:C	0.45	2.30	3	1
1:A:130:GLY:CA	1:A:162:TYR:CE1	0.45	2.99	6	3
1:A:185:GLN:O	1:A:190:THR:HG22	0.45	2.10	6	1
1:A:183:VAL:HG21	1:A:202:ILE:HD11	0.45	1.87	15	1
1:A:177:ASP:O	1:A:180:ASN:HB2	0.45	2.11	10	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:129:LEU:HD23	1:A:131:SER:HA	0.45	1.87	13	1
1:A:171:GLN:NE2	1:A:172:ASN:N	0.45	2.62	15	1
1:A:135:ARG:O	1:A:135:ARG:CD	0.45	2.65	4	5
1:A:171:GLN:C	1:A:175:VAL:HG23	0.45	2.30	10	3
1:A:213:CYS:O	1:A:216:GLN:HB2	0.45	2.12	7	1
1:A:184:LYS:HA	1:A:187:THR:CG2	0.45	2.36	8	2
1:A:140:PHE:HD1	1:A:207:ARG:NH1	0.45	2.09	10	1
1:A:130:GLY:N	1:A:160:VAL:O	0.45	2.49	12	7
1:A:152:ASN:OD1	1:A:156:TYR:HB2	0.45	2.11	11	3
1:A:165:VAL:HG13	1:A:165:VAL:O	0.45	2.12	3	1
1:A:166:ASP:CB	1:A:221:SER:HA	0.45	2.42	6	1
1:A:135:ARG:O	1:A:135:ARG:HD2	0.45	2.12	8	1
1:A:165:VAL:HG13	1:A:220:GLU:CD	0.45	2.32	9	1
1:A:155:ARG:O	1:A:186:HIS:HB3	0.45	2.12	10	1
1:A:165:VAL:O	1:A:165:VAL:HG13	0.45	2.12	1	3
1:A:181:ILE:HD13	1:A:182:THR:CA	0.45	2.42	3	1
1:A:133:MET:CE	1:A:212:MET:HG3	0.45	2.41	10	1
1:A:149:TYR:OH	1:A:207:ARG:HG3	0.44	2.12	8	1
1:A:139:HIS:HA	1:A:146:ASP:CG	0.44	2.33	15	1
1:A:156:TYR:HD2	1:A:204:ILE:HD12	0.44	1.72	2	1
1:A:163:ARG:HB2	1:A:164:PRO:HD3	0.44	1.88	6	1
1:A:153:MET:HG2	1:A:158:ASN:HB3	0.44	1.89	12	1
1:A:197:PHE:CD2	1:A:202:ILE:HD13	0.44	2.47	12	1
1:A:149:TYR:CE2	1:A:207:ARG:CZ	0.44	3.00	15	1
1:A:149:TYR:CA	1:A:152:ASN:HB2	0.44	2.36	13	2
1:A:220:GLU:O	1:A:224:ALA:N	0.44	2.47	2	6
1:A:178:CYS:SG	1:A:179:VAL:N	0.44	2.90	10	3
1:A:166:ASP:O	1:A:221:SER:HA	0.44	2.12	13	1
1:A:163:ARG:CG	1:A:164:PRO:HD3	0.44	2.38	1	1
1:A:156:TYR:N	1:A:156:TYR:CD1	0.44	2.82	3	3
1:A:152:ASN:O	1:A:156:TYR:N	0.44	2.50	6	2
1:A:220:GLU:CG	1:A:224:ALA:HB3	0.44	2.43	9	1
1:A:175:VAL:HG11	1:A:210:GLU:O	0.44	2.13	6	1
1:A:212:MET:SD	1:A:213:CYS:N	0.44	2.91	6	1
1:A:144:TYR:O	1:A:148:TYR:HB2	0.44	2.13	7	1
1:A:129:LEU:HD23	1:A:129:LEU:C	0.44	2.33	8	2
1:A:157:PRO:HG3	1:A:186:HIS:ND1	0.44	2.28	14	1
1:A:161:TYR:O	1:A:181:ILE:HD11	0.44	2.13	8	2
1:A:133:MET:HE2	1:A:212:MET:CG	0.44	2.34	7	2
1:A:195:GLU:HG3	1:A:197:PHE:HE1	0.44	1.73	12	2
1:A:135:ARG:HB3	1:A:158:ASN:HB3	0.44	1.90	15	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:156:TYR:CE1	1:A:197:PHE:CE1	0.43	3.05	3	2
1:A:152:ASN:CA	1:A:155:ARG:CD	0.43	2.96	4	2
1:A:156:TYR:HE1	1:A:197:PHE:CE1	0.43	2.31	7	1
1:A:130:GLY:HA3	1:A:162:TYR:HE1	0.43	1.72	1	2
1:A:140:PHE:HB2	1:A:149:TYR:OH	0.43	2.13	6	1
1:A:183:VAL:HG22	1:A:184:LYS:HD3	0.43	1.91	10	1
1:A:202:ILE:HD12	1:A:202:ILE:HA	0.43	1.60	7	1
1:A:181:ILE:HG12	1:A:182:THR:N	0.43	2.29	10	1
1:A:182:THR:CA	1:A:185:GLN:HG2	0.43	2.38	13	1
1:A:198:THR:CG2	1:A:200:THR:HB	0.43	2.43	3	1
1:A:156:TYR:HB3	1:A:205:MET:HE2	0.43	1.89	11	1
1:A:147:ARG:HA	1:A:150:ARG:HG3	0.43	1.89	12	1
1:A:212:MET:O	1:A:212:MET:HE3	0.43	2.13	1	2
1:A:155:ARG:HD3	1:A:156:TYR:CE1	0.43	2.48	2	1
1:A:162:TYR:CD1	1:A:162:TYR:N	0.43	2.86	4	1
1:A:210:GLU:O	1:A:214:ILE:HB	0.43	2.14	10	3
1:A:161:TYR:CB	1:A:181:ILE:HD11	0.43	2.40	3	1
1:A:135:ARG:CD	1:A:135:ARG:C	0.43	2.86	7	1
1:A:183:VAL:CB	1:A:205:MET:SD	0.43	3.04	13	1
1:A:156:TYR:CB	1:A:204:ILE:HG21	0.43	2.44	14	1
1:A:136:PRO:O	1:A:137:LEU:HB2	0.43	2.14	2	1
1:A:162:TYR:HB2	1:A:171:GLN:HE22	0.43	1.73	6	1
1:A:171:GLN:CG	1:A:172:ASN:N	0.43	2.82	10	1
1:A:205:MET:HG2	1:A:209:VAL:HG11	0.42	1.91	5	1
1:A:153:MET:HA	1:A:153:MET:HE1	0.42	1.91	7	1
1:A:204:ILE:O	1:A:208:VAL:N	0.42	2.51	15	1
1:A:198:THR:HG22	1:A:201:ASP:CG	0.42	2.35	2	1
1:A:204:ILE:HG12	1:A:207:ARG:CZ	0.42	2.44	5	1
1:A:155:ARG:HB2	1:A:195:GLU:OE1	0.42	2.14	8	1
1:A:160:VAL:CG1	1:A:182:THR:HG21	0.42	2.43	12	1
1:A:198:THR:HG23	1:A:201:ASP:H	0.42	1.73	4	2
1:A:202:ILE:CG2	1:A:203:LYS:N	0.42	2.82	4	2
1:A:204:ILE:C	1:A:208:VAL:HG23	0.42	2.31	15	1
1:A:138:ILE:O	1:A:140:PHE:N	0.42	2.52	11	2
1:A:137:LEU:CD2	1:A:149:TYR:CE1	0.42	3.03	5	1
1:A:171:GLN:CD	1:A:172:ASN:N	0.42	2.73	7	1
1:A:184:LYS:N	1:A:184:LYS:HD3	0.42	2.30	6	2
1:A:187:THR:HA	1:A:197:PHE:CE1	0.42	2.50	9	1
1:A:136:PRO:HD2	1:A:158:ASN:OD1	0.42	2.14	10	1
1:A:171:GLN:HB2	1:A:220:GLU:OE2	0.42	2.14	4	1
1:A:135:ARG:HD2	1:A:137:LEU:CD2	0.42	2.43	11	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:197:PHE:C	1:A:197:PHE:CD1	0.42	2.92	4	1
1:A:201:ASP:HA	1:A:204:ILE:CD1	0.42	2.45	15	1
1:A:204:ILE:O	1:A:208:VAL:CG2	0.42	2.68	10	4
1:A:220:GLU:O	1:A:224:ALA:HB3	0.42	2.14	3	1
1:A:175:VAL:O	1:A:178:CYS:N	0.42	2.52	9	3
1:A:171:GLN:CD	1:A:172:ASN:H	0.42	2.18	7	1
1:A:212:MET:HB3	1:A:212:MET:HE2	0.42	1.51	7	1
1:A:213:CYS:HA	1:A:216:GLN:HE21	0.42	1.74	14	1
1:A:156:TYR:CD2	1:A:204:ILE:HD12	0.41	2.50	2	1
1:A:165:VAL:CB	1:A:171:GLN:HB2	0.41	2.45	6	1
1:A:174:PHE:O	1:A:178:CYS:HB3	0.41	2.14	10	1
1:A:179:VAL:O	1:A:183:VAL:HG22	0.41	2.15	10	1
1:A:180:ASN:O	1:A:184:LYS:HB2	0.41	2.15	11	3
1:A:202:ILE:HG22	1:A:203:LYS:N	0.41	2.29	14	2
1:A:215:THR:HG22	1:A:216:GLN:N	0.41	2.30	9	1
1:A:178:CYS:HA	1:A:181:ILE:CD1	0.41	2.44	10	1
1:A:137:LEU:HD22	1:A:153:MET:SD	0.41	2.56	11	1
1:A:207:ARG:HB2	1:A:207:ARG:HH11	0.41	1.73	12	1
1:A:216:GLN:O	1:A:217:TYR:C	0.41	2.57	7	1
1:A:137:LEU:HD22	1:A:137:LEU:H	0.41	1.74	11	1
1:A:139:HIS:CA	1:A:149:TYR:HE2	0.41	2.14	12	1
1:A:149:TYR:CD1	1:A:150:ARG:N	0.41	2.89	12	1
1:A:138:ILE:CB	1:A:207:ARG:HE	0.41	2.29	4	1
1:A:142:ASN:O	1:A:145:GLU:N	0.41	2.54	7	1
1:A:139:HIS:HA	1:A:146:ASP:CA	0.41	2.45	11	1
1:A:216:GLN:CA	1:A:219:GLN:HB3	0.41	2.41	3	1
1:A:152:ASN:OD1	1:A:152:ASN:C	0.41	2.58	12	1
1:A:133:MET:HG3	1:A:160:VAL:HG22	0.41	1.92	5	1
1:A:220:GLU:O	1:A:220:GLU:HG3	0.41	2.14	10	1
1:A:220:GLU:CD	1:A:224:ALA:HB2	0.41	2.36	10	1
1:A:172:ASN:HB2	1:A:214:ILE:HD11	0.41	1.93	14	1
1:A:174:PHE:O	1:A:178:CYS:N	0.41	2.53	8	2
1:A:149:TYR:CZ	1:A:207:ARG:HD3	0.41	2.51	13	1
1:A:130:GLY:O	1:A:132:ALA:N	0.41	2.53	6	1
1:A:212:MET:CG	1:A:213:CYS:N	0.41	2.83	6	2
1:A:153:MET:N	1:A:153:MET:HE3	0.41	2.31	10	1
1:A:139:HIS:O	1:A:140:PHE:HB2	0.41	2.15	12	1
1:A:153:MET:CA	1:A:153:MET:HE3	0.41	2.45	14	1
1:A:127:TYR:HB2	1:A:161:TYR:CE1	0.41	2.50	13	1
1:A:155:ARG:O	1:A:157:PRO:HD3	0.41	2.16	15	1
1:A:163:ARG:HG3	1:A:164:PRO:HD2	0.40	1.93	2	1

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:152:ASN:O	1:A:155:ARG:HD3	0.40	2.16	3	1
1:A:152:ASN:CG	1:A:156:TYR:HD2	0.40	2.18	7	1
1:A:135:ARG:HD3	1:A:137:LEU:HD12	0.40	1.92	8	1
1:A:181:ILE:O	1:A:185:GLN:HG2	0.40	2.16	10	1
1:A:157:PRO:HG3	1:A:186:HIS:CD2	0.40	2.51	13	1
1:A:211:GLN:O	1:A:215:THR:N	0.40	2.52	14	1
1:A:212:MET:HE2	1:A:212:MET:HB3	0.40	1.68	1	1
1:A:219:GLN:HG3	1:A:220:GLU:N	0.40	2.28	9	1
1:A:129:LEU:HD23	1:A:130:GLY:C	0.40	2.37	1	1
1:A:153:MET:CA	1:A:153:MET:HE2	0.40	2.47	13	1
1:A:138:ILE:HB	1:A:207:ARG:NH2	0.40	2.31	15	1
1:A:220:GLU:HG3	1:A:220:GLU:O	0.40	2.16	15	1
1:A:178:CYS:HA	1:A:181:ILE:CG1	0.40	2.45	4	1
1:A:137:LEU:N	1:A:137:LEU:HD22	0.40	2.32	11	1
1:A:199:GLU:O	1:A:203:LYS:N	0.40	2.55	13	1
1:A:155:ARG:HG2	1:A:156:TYR:H	0.40	1.77	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	94/148 (64%)	72±3 (76±3%)	17±2 (19±2%)	5±1 (5±1%)	4	24
All	All	1410/2220 (64%)	1077 (76%)	261 (19%)	72 (5%)	4	24

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	131	SER	15
1	A	157	PRO	14
1	A	139	HIS	11
1	A	130	GLY	9
1	A	155	ARG	4
1	A	188	VAL	4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	170	ASN	3
1	A	136	PRO	3
1	A	190	THR	3
1	A	194	GLY	3
1	A	138	ILE	1
1	A	166	ASP	1
1	A	135	ARG	1

6.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all NMR entries. The Analysed column shows the number of residues for which the sidechain conformation was analysed and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/126 (70%)	64±3 (73±4%)	24±3 (27±4%)	2	21
All	All	1320/1890 (70%)	958 (73%)	362 (27%)	2	21

All 58 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	147	ARG	15
1	A	155	ARG	15
1	A	157	PRO	15
1	A	179	VAL	15
1	A	184	LYS	15
1	A	202	ILE	15
1	A	212	MET	15
1	A	215	THR	15
1	A	182	THR	14
1	A	205	MET	14
1	A	153	MET	12
1	A	160	VAL	12
1	A	208	VAL	12
1	A	151	GLU	10
1	A	183	VAL	10
1	A	226	GLN	10
1	A	178	CYS	9
1	A	185	GLN	9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Models (Total)
1	A	214	ILE	9
1	A	219	GLN	9
1	A	188	VAL	7
1	A	162	TYR	7
1	A	152	ASN	6
1	A	145	GLU	6
1	A	135	ARG	5
1	A	203	LYS	5
1	A	207	ARG	5
1	A	150	ARG	5
1	A	218	GLN	5
1	A	138	ILE	4
1	A	163	ARG	4
1	A	180	ASN	4
1	A	220	GLU	4
1	A	165	VAL	4
1	A	196	ASN	3
1	A	139	HIS	3
1	A	149	TYR	3
1	A	197	PHE	3
1	A	158	ASN	3
1	A	171	GLN	3
1	A	156	TYR	2
1	A	181	ILE	2
1	A	143	ASP	2
1	A	136	PRO	2
1	A	142	ASN	2
1	A	190	THR	1
1	A	128	MET	1
1	A	164	PRO	1
1	A	209	VAL	1
1	A	159	GLN	1
1	A	216	GLN	1
1	A	217	TYR	1
1	A	195	GLU	1
1	A	222	GLN	1
1	A	172	ASN	1
1	A	174	PHE	1
1	A	189	THR	1
1	A	129	LEU	1

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.6 Ligand geometry [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