Full wwPDB NMR Structure Validation Report (i)

Feb 23, 2022 – 01:02 PM EST

PDB ID	:	1XX3
Title	:	Solution Structure of Escherichia coli TonB-CTD
Authors	:	Peacock, R.S.; Weljie, A.M.; Howard, S.P.; Price, F.D.; Vogel, H.J.
Deposited on	:	2004-11-03

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/NMRValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

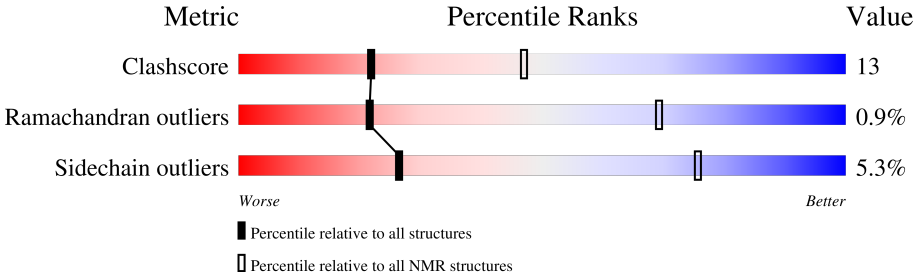
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.26
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	144	46% 13% • • 38%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 7 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:154-A:239 (86)	0.32	7

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

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

The models can be grouped into 3 clusters and 5 single-model clusters were found.

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

3 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 1427 atoms, of which 722 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called TonB protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	89	1427	441	722	135	127	2	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	96	MET	-	cloning artifact	UNP P02929
A	97	HIS	-	cloning artifact	UNP P02929
A	98	HIS	-	cloning artifact	UNP P02929
A	99	HIS	-	cloning artifact	UNP P02929
A	100	HIS	-	cloning artifact	UNP P02929
A	101	HIS	-	cloning artifact	UNP P02929
A	102	HIS	-	cloning artifact	UNP P02929

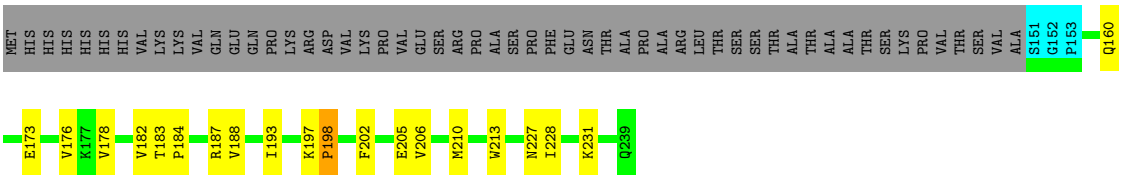
4 Residue-property plots (i)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

• Molecule 1: TonB protein

Chain A: 46% 13% • • 38%



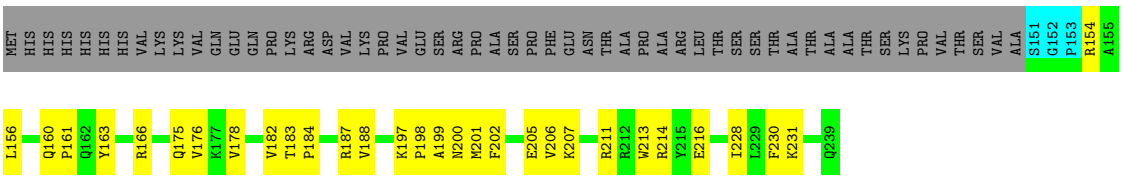
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: TonB protein

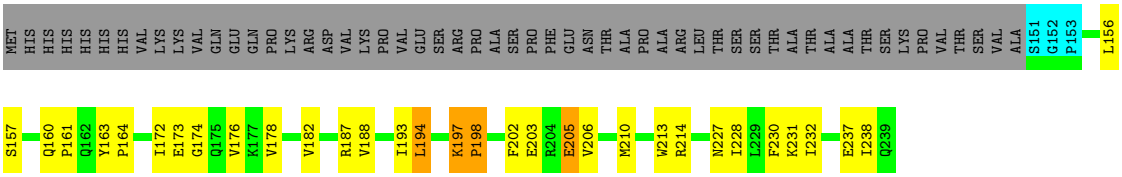
Chain A: 39% 21% • 38%



4.2.2 Score per residue for model 2

• Molecule 1: TonB protein

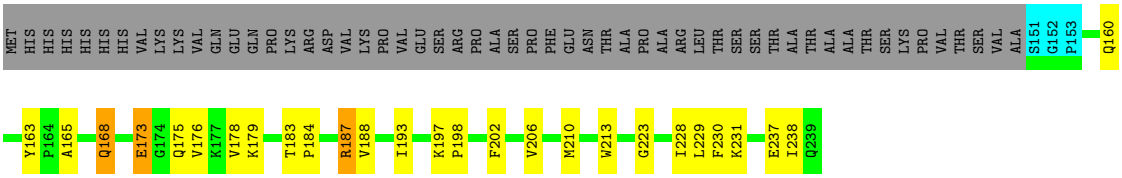
Chain A: 38% 19% • • 38%



4.2.3 Score per residue for model 3

- Molecule 1: TonB protein

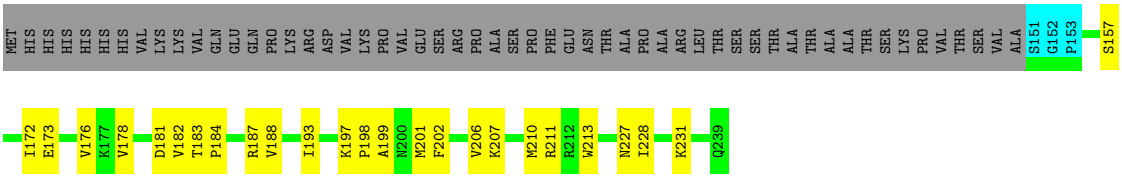
Chain A: 41% 17% • • 38%



4.2.4 Score per residue for model 4

- Molecule 1: TonB protein

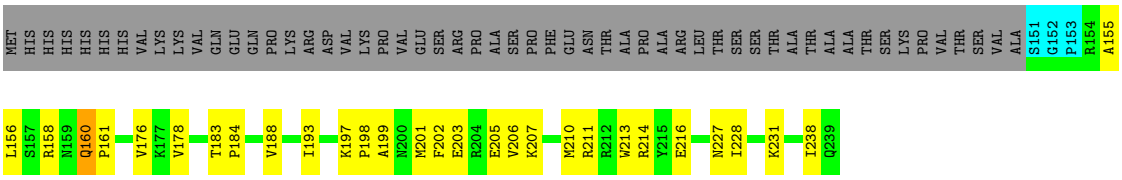
Chain A: 42% 17% • 38%



4.2.5 Score per residue for model 5

- Molecule 1: TonB protein

Chain A: 40% 19% • • 38%



4.2.6 Score per residue for model 6

- Molecule 1: TonB protein

Chain A: 42% 17% • • 38%

MET HIS HIS HIS HIS HIS HIS VAL LYS LYS VAL GLN GLU GLN PRO LYS ARG ASP VAL LYS PRO VAL GLU SER ARG PRO ALA SER PRO PHE GLU ASN THR ALA PRO ALA ARG LEU THR SER SER THR ALA THR ALA ALA THR SER LYS PRO VAL THR SER VAL ALA S151 G152 P153 L156

Q160 P161 A165 Q168 G174 Q175 V176 K177 V178 D181 V188 D189 N190 V191 Q192 I193 K197 P198 F202 E203 R204 E205 V206 M210 W213 N227 I228 L229 F230 K231 I238 Q239

4.2.7 Score per residue for model 7 (medoid)

- Molecule 1: TonB protein

Chain A: 43% 16% • • 38%

MET HIS HIS HIS HIS HIS HIS VAL LYS LYS VAL GLN GLU GLN PRO LYS ARG ASP VAL LYS PRO VAL GLU SER ARG PRO ALA SER PRO PHE GLU ASN THR ALA PRO ALA ARG LEU THR SER SER THR ALA THR ALA ALA THR SER LYS PRO VAL THR SER VAL ALA S151 G152 P153 Q160

P161 Q162 Y163 P164 E173 V176 K177 V178 K179 T183 P184 R187 I193 L194 K197 P198 F202 V206 K207 R211 V226 N227 I228 L229 F230 I238 Q239

4.2.8 Score per residue for model 8

- Molecule 1: TonB protein

Chain A: 44% 14% • • 38%

MET HIS HIS HIS HIS HIS HIS VAL LYS LYS VAL GLN GLU GLN PRO LYS ARG ASP VAL LYS PRO VAL GLU SER ARG PRO ALA SER PRO PHE GLU ASN THR ALA PRO ALA ARG LEU THR SER SER THR ALA THR ALA ALA THR SER LYS PRO VAL THR SER VAL ALA S151 G152 P153 R166

L170 E173 G174 Q175 V178 V188 I193 A196 K197 P198 A199 N200 M201 F202 E203 R204 E205 V206 M210 W213 V226 N227 I228 L229 F230 K231 Q239

4.2.9 Score per residue for model 9

- Molecule 1: TonB protein

Chain A: 44% 15% • • 38%

MET HIS HIS HIS HIS HIS HIS VAL LYS LYS VAL GLN GLU GLN PRO LYS ARG ASP VAL LYS PRO VAL GLU SER ARG PRO ALA SER PRO PHE GLU ASN THR ALA PRO ALA ARG LEU THR SER SER THR ALA THR ALA ALA THR SER LYS PRO VAL THR SER VAL ALA S151 G152 P153 L170

R171 I172 Q175 V176 V182 R187 V188 K197 P198 F202 E205 V206 K207 M210 R211 R212 W213 R214 N227 I228 L229 F230 K231 I232 E237 I238 Q239

4.2.10 Score per residue for model 10

- Molecule 1: TonB protein

Chain A: 44% 16% • 38%

MET HIS HIS HIS HIS HIS HIS VAL LYS LYS VAL GLN GLU GLN PRO LYS ARG ASP VAL LYS PRO VAL GLU SER ARG PRO ALA SER PRO PHE GLU ASN THR ALA PRO ALA ARG LEU THR SER SER THR ALA THR ALA ALA THR SER LYS PRO VAL THR SER VAL ALA S151 G152 P153 L170

R171 I172 V176 K177 V178 V182 V188 A196 K197 P198 F202 E203 V206 M210 W213 N227 I228 L229 F230 K231 I232 T235 T236 Q239

4.2.11 Score per residue for model 11

- Molecule 1: TonB protein

Chain A: 41% 18% • • 38%

MET HIS HIS HIS HIS HIS HIS VAL LYS LYS VAL GLN GLU GLN PRO LYS ARG ASP VAL LYS PRO VAL GLU SER ARG PRO ALA SER PRO PHE GLU ASN THR ALA PRO ALA ARG LEU THR SER SER THR ALA THR ALA ALA THR SER LYS PRO VAL THR SER VAL ALA S151 G152 P153 S157

Q162 A165 Q168 R171 Q175 V178 D181 V182 T183 P184 R187 V188 A196 K197 P198 F202 E205 V206 M210 W213 R214 Y215 K219 S222 I228 K231 I238 Q239

4.2.12 Score per residue for model 12

- Molecule 1: TonB protein

Chain A: 41% 17% • • 38%

MET HIS HIS HIS HIS HIS HIS VAL LYS LYS VAL GLN GLU GLN PRO LYS ARG ASP VAL LYS PRO VAL GLU SER ARG PRO ALA SER PRO PHE GLU ASN THR ALA PRO ALA ARG LEU THR SER SER THR ALA THR ALA ALA THR SER LYS PRO VAL THR SER VAL ALA S151 G152 P153 R154 A155

L156 S157 R158 N159 Q160 E173 G174 Q175 K179 F180 D181 V182 T183 P184 V188 A196 K197 P198 F202 V206 M210 W213 R214 Y215 E216 P217 S222 I228 L229 F230 K231 E237 I238 Q239

4.2.13 Score per residue for model 13

- Molecule 1: TonB protein

Chain A: 42% 17% • 38%

MET HIS HIS HIS HIS HIS HIS VAL LYS LYS VAL GLN GLU GLN PRO LYS ARG ASP VAL LYS PRO VAL GLU SER ARG PRO ALA SER PRO PHE GLU ASN THR ALA PRO ALA ARG LEU THR SER SER THR ALA THR ALA ALA THR SER LYS PRO VAL THR SER VAL ALA S151 G152 P153 R158

P161 Q168 E173 G174 Q175 V176 K177 V178 V182 T183 P184 D185 G186 R187 I193 K197 P198 F202 E203 V206 K207 R211 N227 I228 L229 F230 K231 I232 E237 I238 Q239

4.2.14 Score per residue for model 14

- Molecule 1: TonB protein

Chain A: 47% 11% • • 38%

MET HIS HIS HIS HIS HIS HIS VAL LYS LYS VAL GLN GLU GLN PRO LYS ARG ASP VAL LYS PRO VAL GLU SER ARG PRO ALA SER PRO PHE GLU ASN THR ALA PRO ALA ARG LEU THR SER SER THR ALA THR ALA ALA THR SER LYS PRO VAL THR SER VAL ALA S151 G152 P153 L156

V176 K177 V178 T183 P184 R187 V188 I193 A196 K197 P198 F202 V206 K207 R211 R212 W213 E216 K231 Q239

4.2.15 Score per residue for model 15

- Molecule 1: TonB protein

Chain A: 40% 19% • • 38%

MET HIS HIS HIS HIS HIS HIS VAL LYS LYS VAL GLN GLU GLN PRO LYS ARG ASP VAL LYS PRO VAL GLU SER ARG PRO ALA SER PRO PHE GLU ASN THR ALA PRO ALA ARG LEU THR SER SER THR ALA THR ALA ALA THR SER LYS PRO VAL THR SER VAL ALA S151 G152 P153 L156

P164 A165 R166 R171 G174 V178 D181 V182 T183 P184 R187 V188 D189 N190 I193 K197 P198 F202 E205 V206 M210 W213 E216 P217 G218 I228 L229 F230 K231 T236 E237 I238 Q239

4.2.16 Score per residue for model 16

- Molecule 1: TonB protein

Chain A: 40% 19% • • 38%

MET HIS HIS HIS HIS HIS HIS VAL LYS LYS VAL GLN GLU GLN PRO LYS ARG ASP VAL LYS PRO VAL GLU SER ARG PRO ALA SER PRO PHE GLU ASN THR ALA PRO ALA ARG LEU THR SER SER THR ALA THR ALA ALA THR SER LYS PRO VAL THR SER VAL ALA S151 G152 P153 L156

S157 Q160 P161 A165 Q168 A169 L170 R171 I172 E173 V176 R177 V178 V182 T183 P184 R187 V188 I193 K197 P198 M201 F202 E205 V206 M210 W213 E216 I228 L229 F230 K231 Q239

4.2.17 Score per residue for model 17

- Molecule 1: TonB protein

Chain A: 35% 24% • • 38%

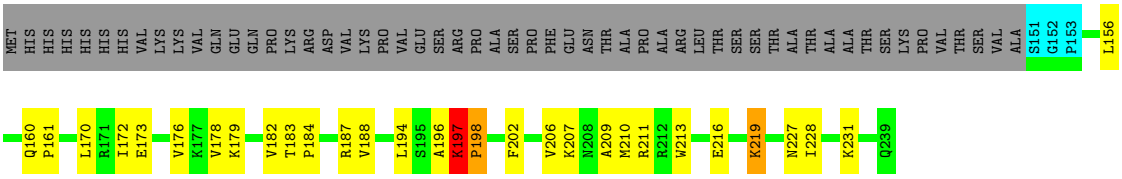
MET HIS HIS HIS HIS HIS HIS VAL LYS LYS VAL GLN GLU GLN PRO LYS ARG ASP VAL LYS PRO VAL GLU SER ARG PRO ALA SER PRO PHE GLU ASN THR ALA PRO ALA ARG LEU THR SER SER THR ALA THR ALA ALA THR SER LYS PRO VAL THR SER VAL ALA S151 G152 P153 L156

L170 R171 I172 E173 G174 Q175 V176 K177 V178 D181 V182 T183 P184 R187 V188 I193 L194 S195 A196 K197 P198 F202 E203 R204 E205 V206 K207 N208 R211 R212 W213 R214 Y215 K219 N227 F230 K231 I232 N233 T236 Q239

4.2.18 Score per residue for model 18

- Molecule 1: TonB protein

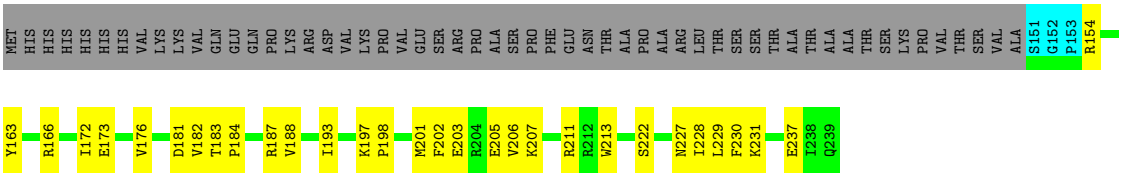
Chain A: 39% 19% • • • 38%



4.2.19 Score per residue for model 19

- Molecule 1: TonB protein

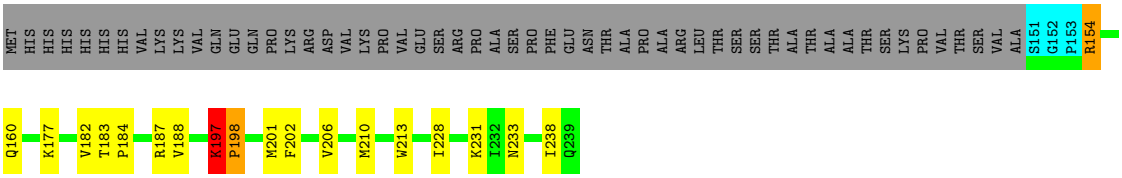
Chain A: 39% 21% • 38%



4.2.20 Score per residue for model 20

- Molecule 1: TonB protein

Chain A: 47% 11% • • • 38%



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *This structure was refined using standard Aria2.0 protocols (distance geometry,simulated annealing, torsion angle dynamics, water refinement).*

Of the 200 calculated structures, 20 were deposited, based on the following criterion: *structures with the lowest energy.*

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

Software name	Classification	Version
CNS	refinement	1.1

No chemical shift data was provided.

6 Model quality (i)

6.1 Standard geometry (i)

There are no covalent bond-length or bond-angle outliers.

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts (i)

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	688	707	707	18±3
All	All	13760	14140	14140	359

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 13.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:197:LYS:HB3	1:A:198:PRO:HD3	0.92	1.39	10	15
1:A:197:LYS:HB2	1:A:198:PRO:HD2	0.90	1.42	20	2
1:A:154:ARG:HE	1:A:154:ARG:HA	0.76	1.41	20	1
1:A:197:LYS:HD2	1:A:202:PHE:HB2	0.76	1.57	20	2
1:A:229:LEU:HB3	1:A:231:LYS:HE3	0.75	1.59	3	6
1:A:197:LYS:HB2	1:A:198:PRO:CD	0.72	2.15	20	2
1:A:197:LYS:HA	1:A:197:LYS:HE2	0.70	1.62	2	1
1:A:183:THR:HB	1:A:184:PRO:HD2	0.70	1.62	15	15
1:A:173:GLU:HG2	1:A:232:ILE:HB	0.67	1.65	2	2
1:A:163:TYR:CE1	1:A:230:PHE:HB3	0.66	2.26	7	4
1:A:229:LEU:HB2	1:A:237:GLU:HB3	0.65	1.68	3	1
1:A:197:LYS:HB2	1:A:198:PRO:HD3	0.63	1.69	12	2
1:A:187:ARG:HA	1:A:187:ARG:HE	0.63	1.51	3	1
1:A:202:PHE:O	1:A:206:VAL:HG23	0.62	1.95	18	20

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:197:LYS:CB	1:A:198:PRO:HD3	0.61	2.25	12	10
1:A:194:LEU:H	1:A:194:LEU:HD22	0.61	1.55	2	2
1:A:188:VAL:HG21	1:A:213:TRP:HB2	0.61	1.72	19	18
1:A:183:THR:HB	1:A:184:PRO:CD	0.60	2.26	19	4
1:A:183:THR:OG1	1:A:187:ARG:HG3	0.60	1.96	14	2
1:A:175:GLN:O	1:A:196:ALA:HA	0.60	1.97	8	4
1:A:206:VAL:O	1:A:210:MET:HG2	0.59	1.98	8	6
1:A:161:PRO:HG2	1:A:228:ILE:HD13	0.58	1.74	16	7
1:A:162:GLN:HB3	1:A:205:GLU:HG2	0.58	1.74	11	1
1:A:178:VAL:HG21	1:A:206:VAL:HG11	0.58	1.76	18	11
1:A:154:ARG:HA	1:A:154:ARG:NE	0.58	2.11	20	1
1:A:156:LEU:HD11	1:A:216:GLU:HG3	0.58	1.75	18	2
1:A:197:LYS:HB3	1:A:198:PRO:CD	0.58	2.26	14	8
1:A:207:LYS:O	1:A:211:ARG:HG3	0.57	1.99	7	10
1:A:178:VAL:HG22	1:A:193:ILE:HG13	0.57	1.75	14	10
1:A:229:LEU:HB3	1:A:231:LYS:HE2	0.56	1.77	9	1
1:A:176:VAL:HG22	1:A:228:ILE:HB	0.56	1.77	19	11
1:A:231:LYS:HA	1:A:231:LYS:HE2	0.56	1.78	11	12
1:A:179:LYS:HE2	1:A:223:GLY:HA2	0.55	1.76	3	1
1:A:182:VAL:HA	1:A:187:ARG:O	0.55	2.02	13	12
1:A:197:LYS:HE3	1:A:202:PHE:HD1	0.54	1.62	20	2
1:A:181:ASP:HB3	1:A:190:ASN:HB2	0.54	1.79	15	1
1:A:191:VAL:HG11	1:A:210:MET:HG3	0.53	1.79	6	1
1:A:156:LEU:HD11	1:A:216:GLU:CG	0.53	2.33	14	2
1:A:197:LYS:HE2	1:A:198:PRO:HD2	0.53	1.80	20	2
1:A:179:LYS:HB2	1:A:194:LEU:HD11	0.53	1.80	7	2
1:A:156:LEU:HD21	1:A:216:GLU:HG3	0.52	1.81	16	3
1:A:230:PHE:CD2	1:A:236:THR:HG22	0.52	2.39	17	2
1:A:229:LEU:HB2	1:A:237:GLU:HB2	0.52	1.81	12	1
1:A:156:LEU:HD23	1:A:216:GLU:HG3	0.52	1.80	15	1
1:A:161:PRO:HA	1:A:209:ALA:HB2	0.52	1.82	18	1
1:A:170:LEU:HB3	1:A:172:ILE:HG13	0.51	1.82	18	5
1:A:163:TYR:CD2	1:A:164:PRO:HD2	0.51	2.40	2	2
1:A:206:VAL:O	1:A:210:MET:HG3	0.51	2.05	11	7
1:A:198:PRO:HB2	1:A:201:MET:HB2	0.51	1.82	4	3
1:A:188:VAL:HG21	1:A:213:TRP:CB	0.51	2.36	19	6
1:A:172:ILE:HG21	1:A:198:PRO:HG3	0.51	1.82	10	1
1:A:215:TYR:HE1	1:A:219:LYS:HB2	0.50	1.67	11	2
1:A:201:MET:HG2	1:A:202:PHE:CD1	0.50	2.41	16	1
1:A:175:GLN:HG3	1:A:197:LYS:HB2	0.50	1.82	9	1
1:A:157:SER:O	1:A:213:TRP:HA	0.50	2.07	2	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:228:ILE:HG23	1:A:238:ILE:HG13	0.49	1.84	20	5
1:A:200:ASN:HA	1:A:203:GLU:HB2	0.49	1.84	8	1
1:A:193:ILE:CG1	1:A:203:GLU:HG2	0.49	2.38	6	5
1:A:229:LEU:O	1:A:236:THR:HA	0.49	2.08	15	1
1:A:197:LYS:HA	1:A:197:LYS:CE	0.49	2.35	2	1
1:A:163:TYR:HE1	1:A:230:PHE:HB3	0.49	1.64	7	1
1:A:163:TYR:HE2	1:A:168:GLN:HB3	0.49	1.68	3	1
1:A:215:TYR:CE1	1:A:219:LYS:HB2	0.49	2.42	11	2
1:A:166:ARG:HB2	1:A:201:MET:SD	0.49	2.48	19	1
1:A:181:ASP:OD1	1:A:222:SER:HA	0.48	2.08	19	3
1:A:173:GLU:CG	1:A:232:ILE:HB	0.48	2.38	17	1
1:A:156:LEU:HD21	1:A:216:GLU:CG	0.48	2.39	1	3
1:A:175:GLN:O	1:A:175:GLN:HG3	0.47	2.09	3	1
1:A:187:ARG:HA	1:A:187:ARG:NE	0.47	2.24	3	1
1:A:174:GLY:O	1:A:230:PHE:HD1	0.46	1.94	6	4
1:A:173:GLU:O	1:A:197:LYS:HG3	0.46	2.11	12	2
1:A:187:ARG:C	1:A:187:ARG:HD3	0.46	2.31	14	1
1:A:154:ARG:HD3	1:A:216:GLU:OE2	0.46	2.11	1	1
1:A:228:ILE:HA	1:A:237:GLU:O	0.46	2.10	15	5
1:A:175:GLN:HG2	1:A:197:LYS:HG2	0.46	1.86	1	1
1:A:155:ALA:HB1	1:A:158:ARG:HG3	0.45	1.88	12	2
1:A:161:PRO:HB2	1:A:230:PHE:CZ	0.45	2.46	13	3
1:A:197:LYS:CB	1:A:198:PRO:CD	0.45	2.94	1	2
1:A:160:GLN:HA	1:A:238:ILE:HD11	0.45	1.89	2	3
1:A:173:GLU:HB3	1:A:232:ILE:N	0.45	2.26	13	1
1:A:194:LEU:HD22	1:A:194:LEU:N	0.45	2.26	17	1
1:A:172:ILE:HG22	1:A:173:GLU:N	0.45	2.26	2	3
1:A:219:LYS:HE3	1:A:219:LYS:HA	0.45	1.87	18	1
1:A:165:ALA:O	1:A:168:GLN:HG3	0.44	2.12	3	1
1:A:160:GLN:OE1	1:A:238:ILE:HD12	0.44	2.13	6	1
1:A:166:ARG:O	1:A:170:LEU:HD13	0.44	2.13	8	1
1:A:179:LYS:HE2	1:A:223:GLY:CA	0.44	2.43	3	1
1:A:171:ARG:HD2	1:A:232:ILE:HD11	0.44	1.89	10	1
1:A:232:ILE:O	1:A:232:ILE:HD13	0.44	2.12	9	1
1:A:179:LYS:CE	1:A:223:GLY:HA2	0.44	2.43	3	1
1:A:206:VAL:HG12	1:A:210:MET:SD	0.43	2.52	16	3
1:A:177:LYS:NZ	1:A:177:LYS:HB2	0.43	2.28	20	1
1:A:165:ALA:HA	1:A:168:GLN:CG	0.43	2.42	16	1
1:A:176:VAL:HG21	1:A:206:VAL:HG21	0.43	1.90	17	1
1:A:156:LEU:HD22	1:A:156:LEU:N	0.43	2.28	16	3
1:A:197:LYS:HE3	1:A:201:MET:HB2	0.43	1.89	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:227:ASN:HB3	1:A:239:GLN:HE21	0.43	1.73	8	1
1:A:176:VAL:CG2	1:A:228:ILE:HB	0.43	2.43	10	1
1:A:164:PRO:HB2	1:A:166:ARG:HG2	0.42	1.89	15	1
1:A:166:ARG:HD2	1:A:201:MET:SD	0.42	2.54	1	1
1:A:181:ASP:OD2	1:A:190:ASN:HB2	0.42	2.14	6	1
1:A:197:LYS:CE	1:A:201:MET:HB2	0.42	2.45	20	1
1:A:161:PRO:HB3	1:A:205:GLU:O	0.42	2.15	2	1
1:A:174:GLY:HA3	1:A:202:PHE:CE2	0.42	2.50	13	1
1:A:183:THR:CB	1:A:184:PRO:CD	0.41	2.96	1	1
1:A:173:GLU:O	1:A:197:LYS:HD3	0.41	2.14	3	1
1:A:176:VAL:HG12	1:A:196:ALA:CB	0.41	2.45	10	3
1:A:165:ALA:O	1:A:168:GLN:HG2	0.41	2.15	11	1
1:A:228:ILE:HG12	1:A:238:ILE:HG12	0.41	1.92	11	1
1:A:231:LYS:HB2	1:A:235:THR:OG1	0.41	2.16	10	1
1:A:187:ARG:NE	1:A:187:ARG:HA	0.41	2.30	15	1
1:A:184:PRO:O	1:A:218:GLY:N	0.41	2.53	15	1
1:A:229:LEU:HD22	1:A:229:LEU:N	0.41	2.31	3	1
1:A:231:LYS:HE2	1:A:231:LYS:HA	0.41	1.92	4	1
1:A:198:PRO:HB2	1:A:201:MET:HB3	0.41	1.92	16	1
1:A:165:ALA:HA	1:A:168:GLN:OE1	0.40	2.15	6	1
1:A:216:GLU:HA	1:A:217:PRO:HD3	0.40	1.78	12	1
1:A:156:LEU:HD12	1:A:156:LEU:N	0.40	2.30	18	1
1:A:163:TYR:CD1	1:A:230:PHE:HB3	0.40	2.52	3	1
1:A:161:PRO:HB2	1:A:230:PHE:HZ	0.40	1.77	13	1
1:A:160:GLN:NE2	1:A:237:GLU:HA	0.40	2.32	2	1

6.3 Torsion angles (i)

6.3.1 Protein backbone (i)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	85/144 (59%)	80±1 (94±1%)	4±1 (5±1%)	1±1 (1±1%)	21	69
All	All	1700/2880 (59%)	1605 (94%)	79 (5%)	16 (1%)	21	69

All 3 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	198	PRO	11
1	A	199	ALA	3
1	A	197	LYS	2

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	73/123 (59%)	69±2 (95±2%)	4±2 (5±2%)	26 75
All	All	1460/2460 (59%)	1383 (95%)	77 (5%)	26 75

All 26 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	227	ASN	12
1	A	205	GLU	10
1	A	160	GLN	8
1	A	214	ARG	6
1	A	173	GLU	5
1	A	156	LEU	3
1	A	197	LYS	3
1	A	168	GLN	3
1	A	203	GLU	3
1	A	194	LEU	2
1	A	187	ARG	2
1	A	181	ASP	2
1	A	226	VAL	2
1	A	171	ARG	2
1	A	233	ASN	2
1	A	154	ARG	2
1	A	200	ASN	1
1	A	238	ILE	1
1	A	175	GLN	1
1	A	232	ILE	1
1	A	182	VAL	1
1	A	179	LYS	1
1	A	158	ARG	1

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Mol	Chain	Res	Type	Models (Total)
1	A	185	ASP	1
1	A	208	ASN	1
1	A	219	LYS	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 (i)

No chemical shift data were provided