Full wwPDB NMR Structure Validation Report (i)

Mar 3, 2022 – 09:36 AM EST

PDB ID	:	2JRI
Title	:	Solution structure of the Josephin domain of Ataxin-3 in complex with ubiquitin molecule.
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Deposited on	:	2007-06-27

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:

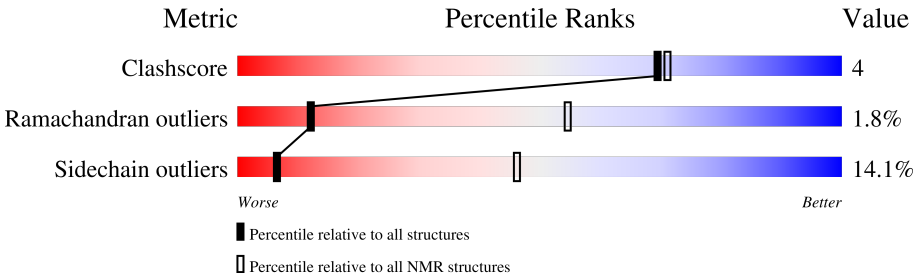
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.27
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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	182	65% 21% • 14%
2	B	76	84% 16%
2	C	76	88% 12%

2 Ensemble composition and analysis (i)

This entry contains 20 models. Model 15 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:9-A:41, A:59-A:182, B:183-B:258, C:259-C:334 (309)	0.50	15

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 1 single-model cluster was found.

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

3 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5377 atoms, of which 2694 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Ataxin-3.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	182	2915	941	1436	246	283	9	0

- Molecule 2 is a protein called UBC protein.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
2	B	76	1230	378	628	105	118	1	0
2	C	76	1232	378	630	105	118	1	0

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: Ataxin-3

Chain A: 65% 21% • 14%

M1 E2 S3 I4 F5 H6 E7 K8 S12 L13 C14 A15 Q16 H17 C18 L19 N20 N21 L22 S29 L40 D41 E42 E43 E44 R45 M46 R47 M48 A49 E50 G51 G52 V53 T54 S55 E56 D57 Y58 M69 D70 D71 S72 G73 S76 V79 I80 S81 L102 R103 R110

N115 Y116 K117 E118 H119 W120 F121 T122 G127 K128 Q129 L137 D145 T146 F151 L155 Y160 S161 A174 L177 L178 R182

• Molecule 2: UBC protein

Chain B: 84% 16%

M183 T189 L190 T191 G192 K193 T196 S202 D203 T204 R224 K230 S239 L253 R256 G257 G258

• Molecule 2: UBC protein

Chain C: 88% 12%

M259 V263 T267 S278 D279 T280 I302 T313 D316 L325 G334

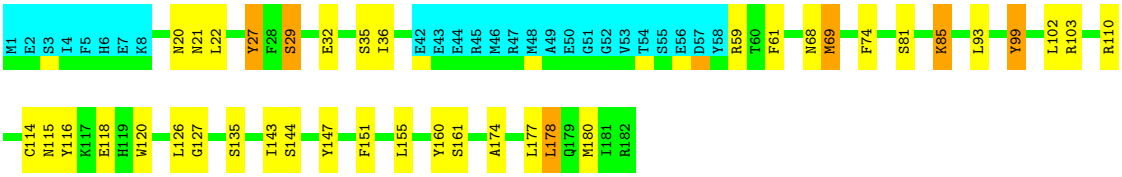
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Ataxin-3

Chain A: 65% 18% • 14%



• Molecule 2: UBC protein

Chain B:

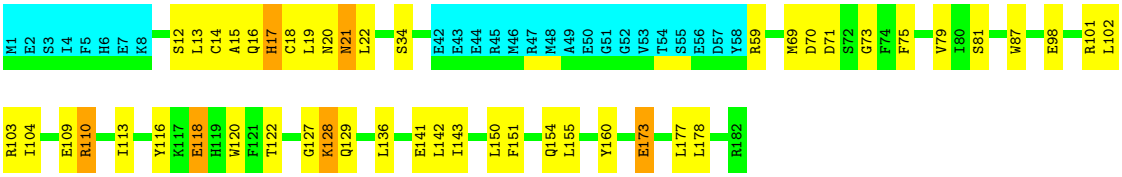
• Molecule 2: UBC protein

Chain C:

4.2.2 Score per residue for model 2

• Molecule 1: Ataxin-3

Chain A:



• Molecule 2: UBC protein

Chain B:

• Molecule 2: UBC protein

Chain C:

4.2.3 Score per residue for model 3

• Molecule 1: Ataxin-3

Chain A: 64% 19% • 14%

M1 E2 S3 I4 F5 H6 E7 K8 Q16 H17 C18 L19 N20 N21 L22 F28 S34 H38 Q39 L40 D41 E42 E43 E44 R45 M46 R47 M48 A49 E50 G51 G52 V53 T54 S55 E56 D57 Y58 F61 Q64 G67 M68 M69 D70 D71 F75 S76 V79 I80 S81

L102 R103 R110 C114 N115 E118 H119 W120 F121 T122 V123 Q129 W130 F131 N132 L137 P140 D145 F151 L155 D168 A174 L177 L178 R182

• Molecule 2: UBC protein

Chain B: 84% 16%

M183 K193 T196 S202 D203 T204 K230 Q231 S239 V252 L253 R254 L255 R256 G257 G258

• Molecule 2: UBC protein

Chain C: 88% 11% •

M259 V263 T267 T280 D297 L301 L308 T313 D316 L325 G334

4.2.4 Score per residue for model 4

• Molecule 1: Ataxin-3

Chain A: 62% 23% • 14%

M1 E2 S3 I4 F5 H6 E7 K8 S12 L13 C14 A15 Q16 H17 C18 N21 L22 L23 Q24 G25 E26 Y27 F28 L40 D41 E42 E43 E44 R45 M46 R47 M48 A49 E50 G51 G52 V53 T54 S55 E56 D57 Y58 Q64 P65 M69 D70 D71 S72 G73 F74 F75 S76 V79 I80

S81 V86 N95 L102 R103 R110 I113 C114 N115 Y116 K117 E118 H119 W120 F121 T122 G127 K128 Q129 L137 Y160 S161 C172 E173 L177 L178 R182

• Molecule 2: UBC protein

Chain B: 86% 14%

M183 T189 L190 T191 T196 T204 K230 T237 T248 L253 R254 L255 R256 G257 G258

• Molecule 2: UBC protein

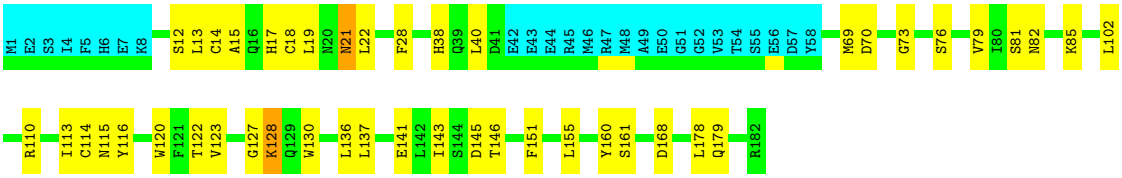
Chain C: 78% 22%

M259 Q260 L266 T267 T270 I271 T272 L273 S278 D279 G293 A304 G305 D310 S315 N318 T324 V328 R332 G333 G334

4.2.5 Score per residue for model 5

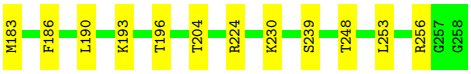
- Molecule 1: Ataxin-3

Chain A: 62% 24% • 14%



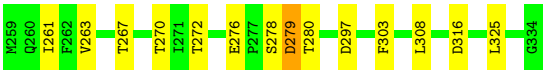
- Molecule 2: UBC protein

Chain B: 84% 16%



- Molecule 2: UBC protein

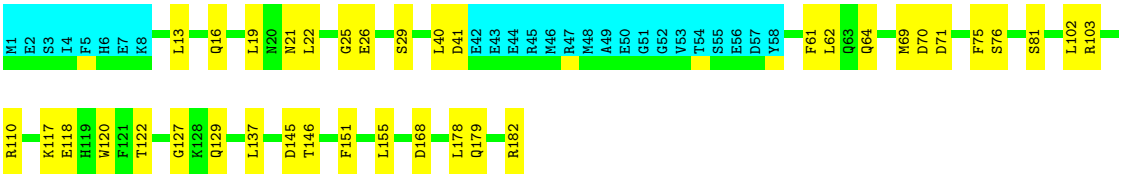
Chain C: 82% 17% •



4.2.6 Score per residue for model 6

- Molecule 1: Ataxin-3

Chain A: 66% 20% 14%

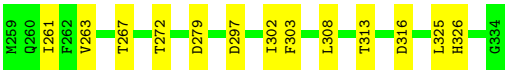


- Molecule 2: UBC protein

Chain B: 76% 24%

- Molecule 2: UBC protein

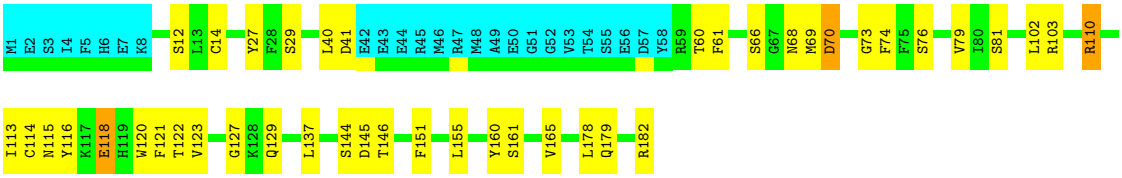
Chain C: 83% 17%



4.2.7 Score per residue for model 7

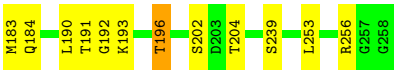
- Molecule 1: Ataxin-3

Chain A:



- Molecule 2: UBC protein

Chain B:



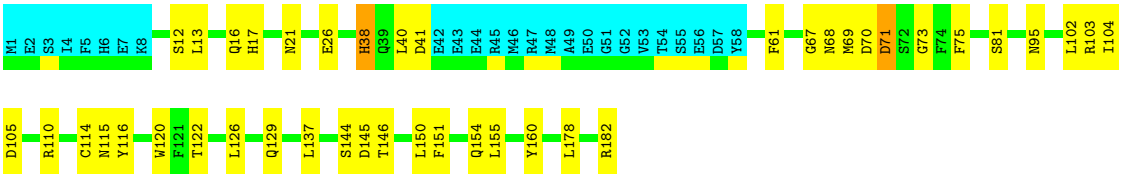
- Molecule 2: UBC protein

Chain C:

4.2.8 Score per residue for model 8

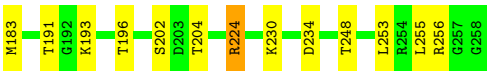
- Molecule 1: Ataxin-3

Chain A:



- Molecule 2: UBC protein

Chain B:



- Molecule 2: UBC protein

Chain C: 84% 14% •

M259 Q260 I261 F262 V263 T267 T272 L273 S278 D279 T280 D297 I302 T313 D316 L325 G334

4.2.9 Score per residue for model 9

- Molecule 1: Ataxin-3

Chain A: 60% 22% • 14%

M1 E2 S3 I4 F5 H6 E7 K8 S12 L13 C14 A15 Q16 H17 C18 L22 F28 S29 S34 L40 D41 E42 E43 E44 R45 M46 R47 M48 A49 E50 G51 G52 V53 T54 S55 E56 D57 Y58 Q64 P65 M69 D70 D71 S72 G73 S76 V79 I80 S81 N82 A83

V86 L91 S96 L102 R103 E109 R110 I113 E118 H119 W120 F121 T122 V123 G127 K128 Q129 W130 F131 N132 L136 L137 I143 S144 D145 T146 F151 L155 F163 L178 I181 R182

- Molecule 2: UBC protein

Chain B: 86% 14%

M183 T189 L190 T191 G192 K193 T194 I195 T196 T204 S239 L253 R256 G257 G258

- Molecule 2: UBC protein

Chain C: 76% 22% •

M259 L266 T267 E276 P277 S278 D279 T280 I281 I302 F303 L308 R312 T313 L314 S315 D316 K321 E322 H326 R330 L331 G334

4.2.10 Score per residue for model 10

- Molecule 1: Ataxin-3

Chain A: 58% 27% • 14%

M1 E2 S3 I4 F5 H6 E7 K8 S12 L13 C14 A15 Q16 H17 C18 N21 F28 S29 Q39 E42 E43 E44 R45 M46 R47 M48 A49 E50 G51 G52 V53 T54 S55 E56 D57 Y58 R59 T60 F61 N68 M69 D70 D71 S72 G73 F74 F75 V79 I80 S81 N82 K85

E98 R101 L102 R103 R110 I113 C114 N115 Y116 K117 E118 H119 W120 F121 T122 K128 Q129 W130 F131 N132 L133 L137 E141 L142 I143 S144 D145 T146 F151 L152 L155 Y160 S161 D168 L178 R182

- Molecule 2: UBC protein

Chain B: 80% 20%

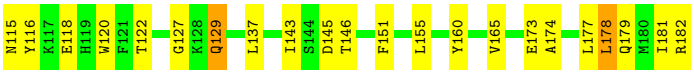
• Molecule 2: UBC protein

Chain C:

4.2.11 Score per residue for model 11

• Molecule 1: Ataxin-3

Chain A:

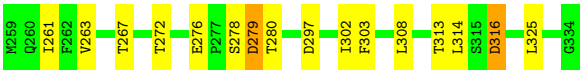


• Molecule 2: UBC protein

Chain B:

• Molecule 2: UBC protein

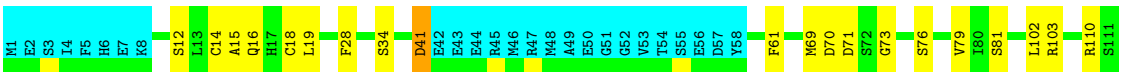
Chain C:



4.2.12 Score per residue for model 12

• Molecule 1: Ataxin-3

Chain A:



• Molecule 2: UBC protein

Chain B: 82% 18%

M183 L190 T191 G192 K193 T194 I195 T196 E200 P201 S202 D203 T204 K230 Q231 V252 L253 R256 G257 G258

• Molecule 2: UBC protein

Chain C: 80% 17% •

M259 V263 K264 T265 L266 T267 L273 S278 D279 T280 T313 D316 T324 L325 L329 R330 L331 G334

4.2.13 Score per residue for model 13

• Molecule 1: Ataxin-3

Chain A: 69% 14% • 14%

M1 E2 S3 I4 F5 H6 E7 K8 Q16 H17 C18 F28 S29 S34 H38 Q39 L40 D41 E42 E43 E44 R45 M46 R47 M48 A49 E50 G51 G52 V53 T54 S55 E56 D57 Y58 F61 M69 D70 D71 F75 S81 L102 R103 R110 H119 W120 F121 T122

G127 K128 Q129 L137 D145 F151 L155 A174 L178 Q179 M180 I181 R182

• Molecule 2: UBC protein

Chain B: 79% 21%

M183 T189 G192 K193 T194 I195 T196 S202 D203 T204 R224 Q231 T237 L238 S239 T248 L253 R254 L255 R256 G257 G258

• Molecule 2: UBC protein

Chain C: 82% 17% •

M259 V263 T267 E274 V275 E276 T280 D297 Q298 I302 F303 L308 T313 L314 S315 D316 L325 G334

4.2.14 Score per residue for model 14

• Molecule 1: Ataxin-3

Chain A: 64% 21% • 14%

M1 E2 S3 I4 F5 H6 E7 K8 C14 A15 Q16 H17 C18 L19 N20 N21 E26 Q39 L40 D41 E42 E43 E44 R45 M46 R47 M48 A49 E50 G51 G52 V53 T54 S55 E56 D57 Y58 M69 D70 D71 S76 V79 I80 S81 L102 R103 E109 R110 S111 F112 I113 C114

• Molecule 2: UBC protein

Chain B: 80% 20%

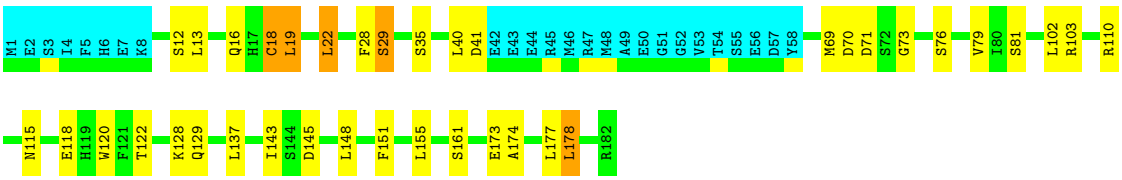
• Molecule 2: UBC protein

Chain C: 78% 20% •

4.2.15 Score per residue for model 15 (medoid)

• Molecule 1: Ataxin-3

Chain A: 65% 18% • 14%

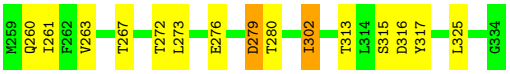


• Molecule 2: UBC protein

Chain B: 78% 22%

• Molecule 2: UBC protein

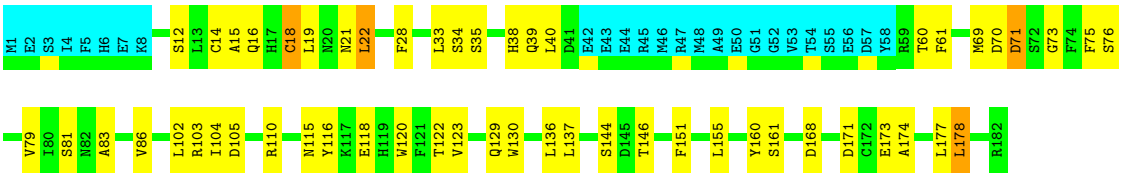
Chain C: 80% 17% •



4.2.16 Score per residue for model 16

• Molecule 1: Ataxin-3

Chain A: 57% 27% • 14%

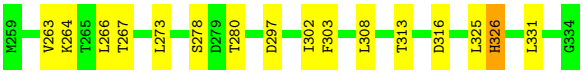


- Molecule 2: UBC protein

Chain B:

- Molecule 2: UBC protein

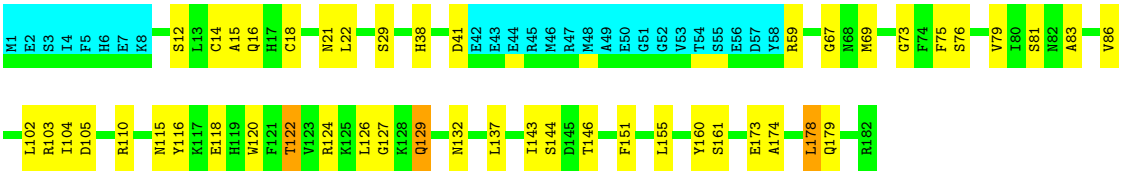
Chain C:



4.2.17 Score per residue for model 17

- Molecule 1: Ataxin-3

Chain A:

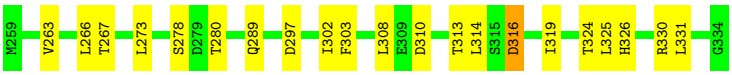


- Molecule 2: UBC protein

Chain B:

- Molecule 2: UBC protein

Chain C:



4.2.18 Score per residue for model 18

- Molecule 1: Ataxin-3

Chain A: 61% 24% • 14%

M1 E2 S3 I4 F5 H6 E7 K8 Q9 S12 L13 C14 A15 Q16 H17 C18 N21 L22 I23 Q24 S34 S35 L40 D41 E42 E43 E44 R45 M46 R47 M48 A49 E50 G51 G52 V53 T54 S55 E56 D57 Y58 R59 T60 Q64 P65 M69 D70 D71 S72 G73 S76 V79

I80 S81 N82 A83 L102 R103 I107 R110 N115 E118 H119 W120 F121 T122 G127 K128 Q129 L137 S144 D145 T146 F151 L155 D168 C172 E173 A174 L178 Q179 M180 I181 R182

• Molecule 2: UBC protein

Chain B: 79% 20% •

M183 Q184 I185 T191 G192 K193 T196 L197 T204 R224 L225 A228 G229 K230 S239 L253 R256 G257 G258

• Molecule 2: UBC protein

Chain C: 79% 18% •

M259 V263 T267 L273 E276 P277 S278 D279 T280 I281 E282 Q298 T313 D316 K321 T324 L325 H326 G334

4.2.19 Score per residue for model 19

• Molecule 1: Ataxin-3

Chain A: 65% 20% • 14%

M1 E2 S3 I4 F5 H6 E7 K8 S12 L13 C14 A15 Q16 N21 L22 E26 D41 E42 E43 E44 R45 M46 R47 M48 A49 E50 G51 G52 V53 T54 S55 E56 D57 Y58 L62 Q63 Q64 P65 M69 D70 G73 S76 V79 I80 S81 N95 L102 R103 I104

D105 R110 S111 F112 I113 C114 N115 E118 H119 W120 F121 T122 K128 Q129 N132 I143 T146 F151 L155 Q156 Q157 S161 V164 A174 L178 H182

• Molecule 2: UBC protein

Chain B: 84% 16%

M183 L190 T191 G192 K193 T194 I195 T196 R224 D234 S239 L253 R256 G257 G258

• Molecule 2: UBC protein

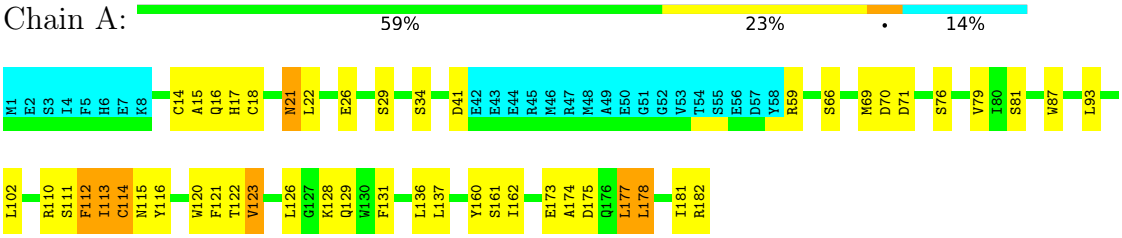
Chain C: 89% 9% •

M259 T267 L273 S278 D279 T280 T313 D316 L329 R332 G333 G334

4.2.20 Score per residue for model 20

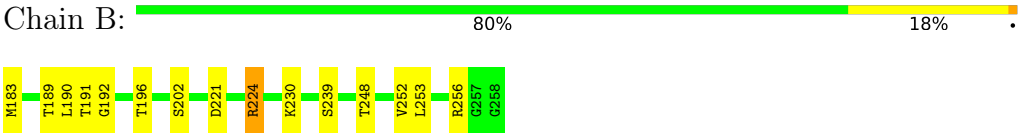
- Molecule 1: Ataxin-3

Chain A:



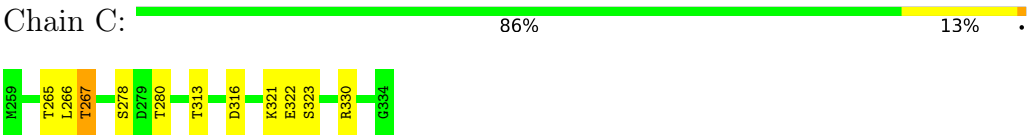
- Molecule 2: UBC protein

Chain B:



- Molecule 2: UBC protein

Chain C:



5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *torsion angle dynamics*.

Of the 100 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
ARIA	structure solution	2.1
HADDOCK	structure solution	2.0
HADDOCK	refinement	2.0

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	1273	1248	1245	14±3
2	B	602	628	626	4±1
2	C	602	630	626	4±2
All	All	49540	50120	49940	364

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 4.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:263:VAL:HA	2:C:325:LEU:O	0.67	1.90	13	11
1:A:19:LEU:HD21	1:A:83:ALA:HB1	0.65	1.69	16	1
1:A:120:TRP:CD1	2:B:256:ARG:HB3	0.64	2.28	9	19
1:A:27:TYR:HA	2:C:304:ALA:O	0.60	1.96	4	1
1:A:76:SER:HA	2:B:190:LEU:HD13	0.60	1.71	14	6
1:A:99:TYR:O	1:A:102:LEU:HG	0.59	1.98	1	1
1:A:126:LEU:HD22	1:A:131:PHE:CD1	0.58	2.33	20	1
1:A:151:PHE:O	1:A:155:LEU:HG	0.58	1.98	6	18
1:A:74:PHE:CE1	2:B:256:ARG:HB2	0.57	2.34	1	1
1:A:15:ALA:HA	1:A:18:CYS:SG	0.57	2.40	10	11
1:A:19:LEU:HD21	1:A:28:PHE:HB3	0.57	1.77	3	2
2:C:260:GLN:HA	2:C:273:LEU:O	0.57	1.99	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:303:PHE:HB3	2:C:308:LEU:HD21	0.57	1.75	6	7
2:C:301:LEU:HB3	2:C:308:LEU:HD12	0.57	1.74	3	1
1:A:174:ALA:O	1:A:178:LEU:HB2	0.55	2.01	11	10
1:A:120:TRP:CD1	2:B:256:ARG:HG3	0.55	2.36	1	1
1:A:118:GLU:O	2:B:256:ARG:HA	0.54	2.02	2	15
1:A:75:PHE:O	2:B:255:LEU:HB2	0.54	2.02	6	8
1:A:122:THR:O	1:A:132:ASN:HA	0.53	2.04	9	5
2:C:314:LEU:O	2:C:319:ILE:HB	0.52	2.04	17	1
2:C:313:THR:O	2:C:316:ASP:HB2	0.52	2.05	9	11
2:C:276:GLU:O	2:C:279:ASP:HB2	0.52	2.05	18	6
1:A:178:LEU:HD13	1:A:181:ILE:HB	0.52	1.81	18	4
1:A:116:TYR:HB2	1:A:160:TYR:CE2	0.52	2.40	5	11
1:A:173:GLU:O	1:A:177:LEU:HG	0.52	2.05	15	7
1:A:71:ASP:OD2	2:B:224:ARG:HD3	0.52	2.04	16	1
1:A:111:SER:O	1:A:112:PHE:HB3	0.51	2.05	20	1
1:A:38:HIS:HA	1:A:67:GLY:O	0.50	2.05	8	3
2:C:263:VAL:O	2:C:270:THR:HA	0.50	2.07	14	2
1:A:29:SER:HB3	2:C:302:ILE:HG21	0.49	1.83	1	1
2:C:329:LEU:O	2:C:330:ARG:HD2	0.49	2.07	7	2
1:A:116:TYR:HB2	1:A:160:TYR:CE1	0.49	2.42	1	1
1:A:109:GLU:OE1	1:A:110:ARG:HD2	0.49	2.07	2	3
2:C:261:ILE:O	2:C:272:THR:HA	0.49	2.07	6	4
1:A:104:ILE:HG22	1:A:105:ASP:H	0.49	1.66	17	2
1:A:115:ASN:ND2	1:A:161:SER:HB2	0.49	2.22	15	9
1:A:86:VAL:HG12	2:C:266:LEU:O	0.49	2.07	17	4
1:A:127:GLY:HA2	1:A:179:GLN:NE2	0.48	2.23	14	8
1:A:114:CYS:SG	1:A:155:LEU:HD13	0.48	2.48	3	3
1:A:70:ASP:OD2	1:A:74:PHE:HB2	0.48	2.09	7	1
1:A:61:PHE:O	1:A:64:GLN:HB2	0.48	2.08	6	1
1:A:141:GLU:O	1:A:143:ILE:HG13	0.48	2.09	2	3
1:A:115:ASN:HB3	1:A:120:TRP:CD2	0.48	2.44	8	1
1:A:91:LEU:HD11	1:A:163:PHE:HB3	0.48	1.86	9	1
1:A:128:LYS:HD2	1:A:128:LYS:O	0.48	2.09	13	2
1:A:12:SER:HB3	1:A:73:GLY:O	0.47	2.09	4	13
1:A:35:SER:OG	2:C:328:VAL:HG13	0.47	2.09	1	1
1:A:81:SER:O	1:A:85:LYS:HB2	0.47	2.09	1	1
2:C:276:GLU:O	2:C:314:LEU:HD12	0.47	2.10	9	3
1:A:35:SER:HA	2:C:331:LEU:HD11	0.47	1.86	16	1
1:A:143:ILE:HG21	1:A:148:LEU:HD13	0.47	1.87	15	1
1:A:76:SER:O	1:A:79:VAL:HG22	0.47	2.10	7	14
1:A:18:CYS:SG	2:B:256:ARG:HD2	0.47	2.50	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:321:LYS:O	2:C:322:GLU:HB2	0.46	2.11	20	3
1:A:127:GLY:O	1:A:128:LYS:HB2	0.46	2.10	2	2
1:A:64:GLN:OE1	1:A:65:PRO:HD2	0.46	2.09	19	4
1:A:110:ARG:HD2	1:A:110:ARG:N	0.46	2.25	11	1
1:A:79:VAL:O	1:A:83:ALA:HB2	0.46	2.10	18	4
1:A:178:LEU:HD22	1:A:181:ILE:HG13	0.46	1.88	9	1
2:B:237:THR:O	2:B:240:ASP:HB2	0.46	2.11	11	2
1:A:120:TRP:HB2	2:B:256:ARG:NE	0.46	2.26	19	7
1:A:116:TYR:HB2	1:A:160:TYR:CZ	0.45	2.46	1	1
1:A:150:LEU:O	1:A:154:GLN:HG2	0.45	2.12	8	2
1:A:71:ASP:OD1	2:B:224:ARG:HD3	0.45	2.11	20	1
1:A:38:HIS:CE1	1:A:68:ASN:HA	0.45	2.46	8	1
1:A:177:LEU:O	1:A:180:MET:HG2	0.45	2.12	1	1
2:B:184:GLN:OE1	2:B:196:THR:HB	0.45	2.11	7	2
1:A:18:CYS:O	1:A:22:LEU:HB2	0.45	2.12	18	5
1:A:22:LEU:O	1:A:124:ARG:HD3	0.45	2.12	17	1
1:A:98:GLU:HA	1:A:101:ARG:CZ	0.45	2.42	2	2
1:A:143:ILE:HG23	1:A:147:TYR:CD2	0.45	2.47	14	1
2:C:280:THR:O	2:C:284:VAL:HG23	0.44	2.12	7	1
2:C:264:LYS:HB2	2:C:326:HIS:CD2	0.44	2.47	16	1
1:A:126:LEU:HD23	1:A:178:LEU:HG	0.44	1.89	20	1
1:A:131:PHE:O	1:A:133:LEU:HG	0.44	2.12	10	1
2:B:184:GLN:HA	2:B:197:LEU:O	0.44	2.13	15	4
1:A:143:ILE:HG23	1:A:147:TYR:HD2	0.44	1.72	1	1
1:A:32:GLU:OE2	2:C:302:ILE:HG21	0.44	2.12	11	1
1:A:32:GLU:O	1:A:36:ILE:HG12	0.43	2.13	1	1
1:A:104:ILE:HG22	1:A:105:ASP:N	0.43	2.27	17	5
2:C:259:MET:SD	2:C:321:LYS:HA	0.43	2.53	18	1
1:A:71:ASP:OD1	2:B:224:ARG:HD2	0.43	2.13	8	1
1:A:34:SER:HB3	1:A:69:MET:SD	0.43	2.52	9	2
1:A:17:HIS:O	1:A:21:ASN:HB2	0.43	2.13	8	4
1:A:82:ASN:OD1	1:A:85:LYS:HE2	0.43	2.13	10	2
1:A:129:GLN:HG3	1:A:143:ILE:O	0.43	2.13	19	4
1:A:38:HIS:O	1:A:41:ASP:HB3	0.43	2.13	13	2
2:C:264:LYS:HA	2:C:269:LYS:O	0.43	2.13	2	2
1:A:113:ILE:HA	1:A:121:PHE:O	0.43	2.14	7	1
2:B:186:PHE:O	2:B:248:THR:HA	0.43	2.14	5	1
1:A:112:PHE:CB	1:A:164:VAL:HA	0.43	2.43	12	2
1:A:102:LEU:HD12	1:A:103:ARG:N	0.43	2.29	1	1
1:A:123:VAL:HG12	1:A:130:TRP:HE3	0.43	1.74	9	3
1:A:112:PHE:CZ	1:A:123:VAL:HB	0.43	2.49	20	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:123:VAL:HG12	1:A:130:TRP:HB3	0.43	1.91	5	1
1:A:24:GLN:O	1:A:172:CYS:HB3	0.43	2.14	18	1
2:B:185:ILE:O	2:B:196:THR:HA	0.43	2.13	18	1
1:A:68:ASN:HA	2:C:332:ARG:CD	0.43	2.44	7	1
1:A:110:ARG:HD3	1:A:165:VAL:O	0.43	2.14	7	2
1:A:129:GLN:HA	1:A:129:GLN:NE2	0.42	2.30	3	1
1:A:60:THR:HG23	2:B:228:ALA:HB2	0.42	1.91	18	1
1:A:29:SER:OG	2:C:302:ILE:HG12	0.42	2.15	15	1
1:A:112:PHE:CE1	1:A:123:VAL:HB	0.42	2.49	20	1
1:A:24:GLN:HB3	1:A:172:CYS:SG	0.41	2.55	4	1
2:B:189:THR:HG22	2:B:251:LEU:HD23	0.41	1.90	6	2
1:A:114:CYS:HA	1:A:161:SER:O	0.41	2.16	7	2
2:B:208:VAL:O	2:B:212:ILE:HG13	0.41	2.15	2	2
1:A:68:ASN:HA	2:C:332:ARG:HD2	0.41	1.92	7	1
2:C:266:LEU:HD11	2:C:328:VAL:HG13	0.41	1.91	4	1
1:A:39:GLN:HG3	2:C:266:LEU:O	0.41	2.16	14	1
1:A:68:ASN:O	1:A:69:MET:HB3	0.41	2.15	1	1
1:A:93:LEU:O	1:A:99:TYR:HB3	0.41	2.16	1	1
2:C:317:TYR:O	2:C:319:ILE:HG13	0.41	2.16	14	1
1:A:93:LEU:HD12	1:A:162:ILE:O	0.41	2.16	20	1
2:B:184:GLN:NE2	2:B:198:GLU:HB2	0.41	2.30	6	1
2:C:281:ILE:HG12	2:C:312:ARG:O	0.40	2.16	9	1
1:A:131:PHE:HA	1:A:141:GLU:O	0.40	2.16	14	1
1:A:66:SER:OG	2:B:190:LEU:HD21	0.40	2.16	7	2
2:C:264:LYS:O	2:C:265:THR:HG23	0.40	2.16	12	1
1:A:114:CYS:SG	1:A:121:PHE:HB2	0.40	2.56	20	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	156/182 (86%)	131±4 (84±2%)	21±4 (14±2%)	4±2 (3±1%)	8	43
2	B	74/76 (97%)	68±2 (92±2%)	5±2 (7±2%)	0±0 (1±1%)	29	74
2	C	74/76 (97%)	67±3 (91±5%)	6±3 (8±4%)	1±1 (1±2%)	20	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	6080/6680 (91%)	5324 (88%)	649 (11%)	107 (2%)	12 54

All 31 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	69	MET	20
1	A	70	ASP	18
1	A	71	ASP	13
2	B	192	GLY	8
1	A	128	LYS	7
1	A	136	LEU	6
1	A	79	VAL	3
1	A	127	GLY	2
2	C	261	ILE	2
2	C	319	ILE	2
2	C	293	GLY	2
1	A	123	VAL	2
1	A	118	GLU	2
1	A	112	PHE	2
2	C	267	THR	2
1	A	27	TYR	1
2	B	191	THR	1
1	A	17	HIS	1
1	A	104	ILE	1
1	A	142	LEU	1
2	C	271	ILE	1
2	C	305	GLY	1
2	C	318	ASN	1
2	C	316	ASP	1
2	C	333	GLY	1
1	A	145	ASP	1
2	C	323	SER	1
1	A	113	ILE	1
1	A	174	ALA	1
1	A	175	ASP	1
2	C	266	LEU	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	142/164 (87%)	122±2 (86±2%)	20±2 (14±2%)	6 46
2	B	68/68 (100%)	57±2 (84±3%)	11±2 (16±3%)	5 43
2	C	68/68 (100%)	60±3 (88±4%)	8±3 (12±4%)	8 50
All	All	5560/6000 (93%)	4776 (86%)	784 (14%)	6 46

All 118 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	110	ARG	20
1	A	178	LEU	20
2	B	183	MET	20
2	B	253	LEU	20
2	C	267	THR	20
1	A	81	SER	19
1	A	102	LEU	19
1	A	122	THR	19
2	B	196	THR	19
2	C	280	THR	18
1	A	129	GLN	18
1	A	16	GLN	17
1	A	137	LEU	17
2	B	204	THR	16
1	A	103	ARG	16
2	B	193	LYS	15
2	B	239	SER	15
2	B	191	THR	14
1	A	41	ASP	14
1	A	21	ASN	13
1	A	22	LEU	13
2	B	224	ARG	13
2	C	278	SER	13
1	A	14	CYS	13
2	B	202	SER	12
1	A	40	LEU	12
1	A	146	THR	12
1	A	145	ASP	11
2	B	230	LYS	11
1	A	29	SER	10

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Mol	Chain	Res	Type	Models (Total)
2	B	189	THR	10
2	B	195	ILE	10
2	B	252	VAL	10
2	C	297	ASP	10
2	C	316	ASP	10
2	C	326	HIS	9
1	A	144	SER	8
1	A	19	LEU	8
1	A	113	ILE	8
2	B	231	GLN	8
2	C	302	ILE	8
1	A	28	PHE	8
2	C	279	ASP	8
1	A	182	ARG	8
2	C	273	LEU	8
1	A	61	PHE	7
1	A	168	ASP	7
2	C	324	THR	6
1	A	13	LEU	6
1	A	34	SER	6
1	A	26	GLU	6
1	A	59	ARG	5
1	A	115	ASN	5
2	B	248	THR	5
2	C	313	THR	5
2	C	315	SER	5
1	A	18	CYS	5
2	C	330	ARG	5
2	B	234	ASP	5
2	C	332	ARG	4
1	A	128	LYS	4
2	C	265	THR	4
2	C	331	LEU	4
1	A	114	CYS	3
1	A	118	GLU	3
1	A	126	LEU	3
2	C	270	THR	3
2	C	272	THR	3
1	A	177	LEU	3
1	A	95	ASN	3
2	B	237	THR	3
2	C	310	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	A	38	HIS	3
1	A	39	GLN	3
1	A	20	ASN	2
1	A	27	TYR	2
2	B	221	ASP	2
2	C	318	ASN	2
2	C	329	LEU	2
1	A	87	TRP	2
1	A	173	GLU	2
1	A	72	SER	2
1	A	119	HIS	2
1	A	171	ASP	2
2	C	274	GLU	2
2	C	298	GLN	2
1	A	35	SER	2
1	A	85	LYS	1
1	A	99	TYR	1
1	A	135	SER	1
1	A	161	SER	1
2	C	262	PHE	1
2	C	325	LEU	1
2	C	306	LYS	1
2	C	314	LEU	1
1	A	64	GLN	1
1	A	117	LYS	1
1	A	96	SER	1
1	A	68	ASN	1
1	A	75	PHE	1
1	A	152	LEU	1
2	C	266	LEU	1
2	C	271	ILE	1
2	C	301	LEU	1
2	B	240	ASP	1
2	B	256	ARG	1
2	B	200	GLU	1
2	C	328	VAL	1
2	C	317	TYR	1
1	A	33	LEU	1
1	A	60	THR	1
2	C	289	GLN	1
1	A	9	GLN	1
1	A	107	ILE	1

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Mol	Chain	Res	Type	Models (Total)
2	B	225	LEU	1
2	C	282	GLU	1
1	A	157	GLN	1
2	C	323	SER	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