



Full wwPDB NMR Structure Validation Report ⓘ

Feb 12, 2017 – 10:23 pm GMT

PDB ID : 2JRI
Title : Solution structure of the Josephin domain of Ataxin-3 in complex with ubiquitin molecule.
Authors : Nicastro, G.; Masino, L.; Esposito, V.; Menon, R.; Pastore, A.
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

<http://wwpdb.org/validation/2016/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:

Cyrange : Kirchner and Güntert (2011)
NmrClust : Kelley et al. (1996)
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : trunk28760
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

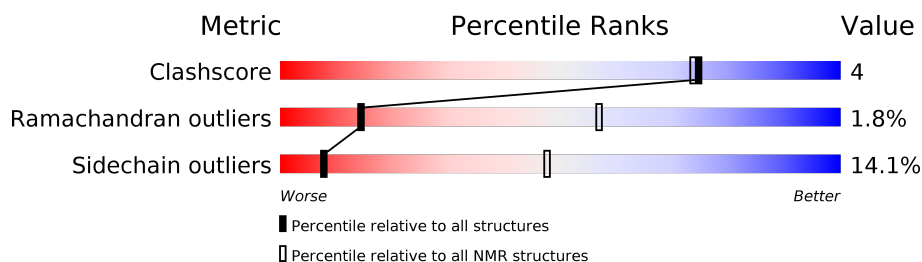
1 Overall quality at a glance

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	125131	11601
Ramachandran outliers	121729	10391
Sidechain outliers	121581	10367

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	182	 64% 21% • 14%
2	B	76	 84% 16%
2	C	76	 87% 13%

2 Ensemble composition and analysis

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
1	A	182	Total	C	H	N	O	S	0
			2915	941	1436	246	283	9	

- Molecule 2 is a protein called UBC protein.

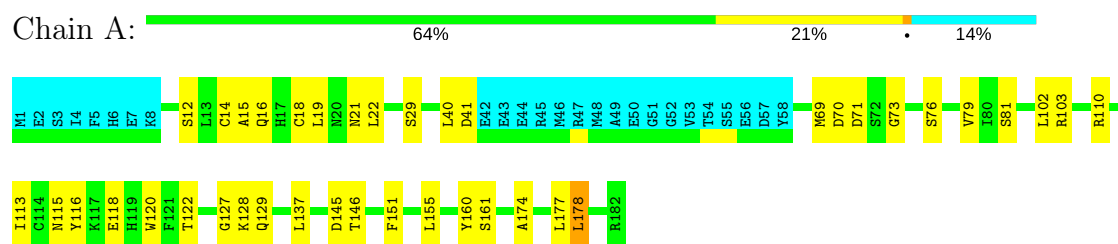
Mol	Chain	Residues	Atoms						Trace
2	B	76	Total	C	H	N	O	S	0
			1230	378	628	105	118	1	
2	C	76	Total	C	H	N	O	S	0
			1232	378	630	105	118	1	

4 Residue-property plots [i](#)

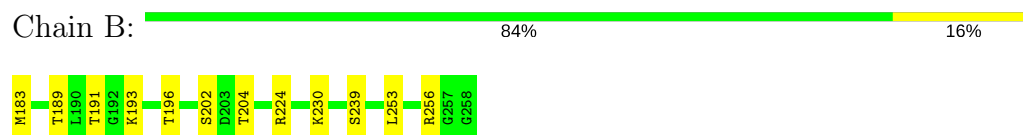
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA and DNA 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.

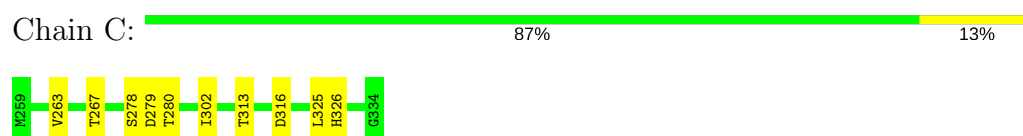
• Molecule 1: Ataxin-3



• Molecule 2: UBC protein



• Molecule 2: UBC protein



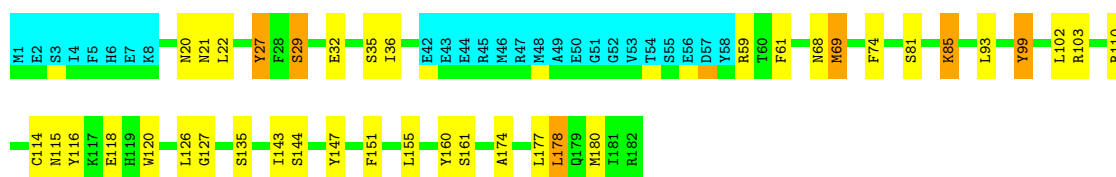
4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

• Molecule 1: Ataxin-3





- Molecule 2: UBC protein

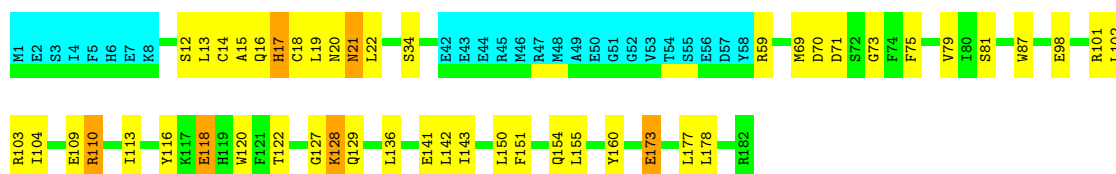


- Molecule 2: UBC protein

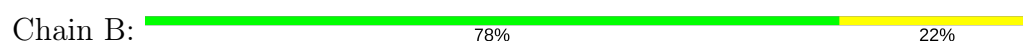


4.2.2 Score per residue for model 2

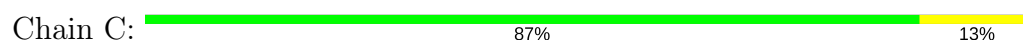
- Molecule 1: Ataxin-3



- Molecule 2: UBC protein

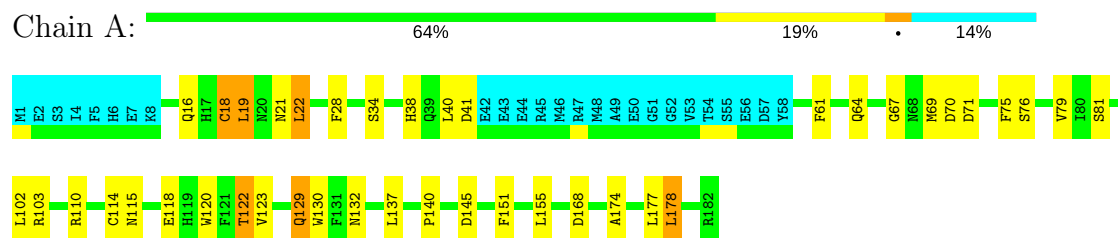


- Molecule 2: UBC protein

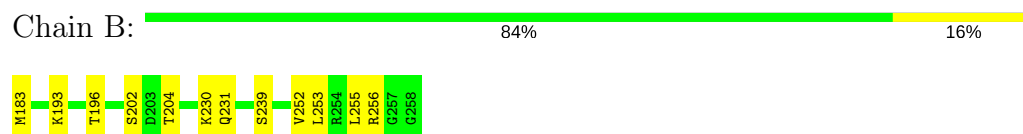


4.2.3 Score per residue for model 3

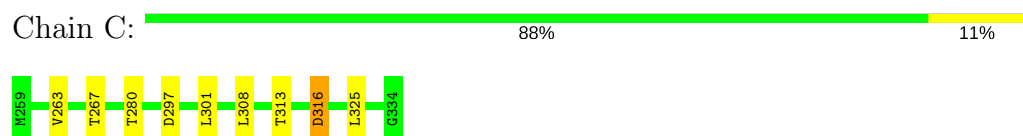
- Molecule 1: Ataxin-3



- Molecule 2: UBC protein

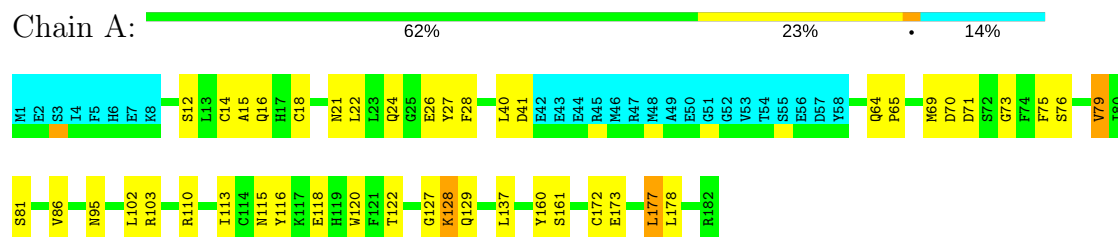


- Molecule 2: UBC protein

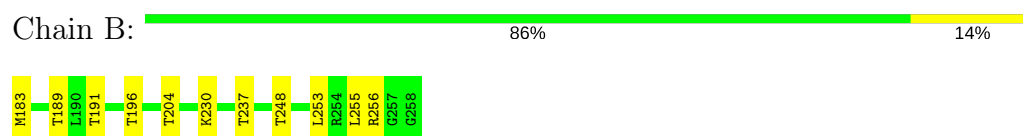


4.2.4 Score per residue for model 4

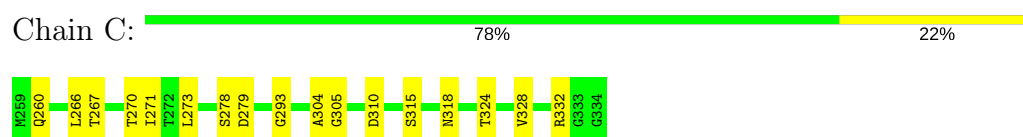
- Molecule 1: Ataxin-3



- Molecule 2: UBC protein

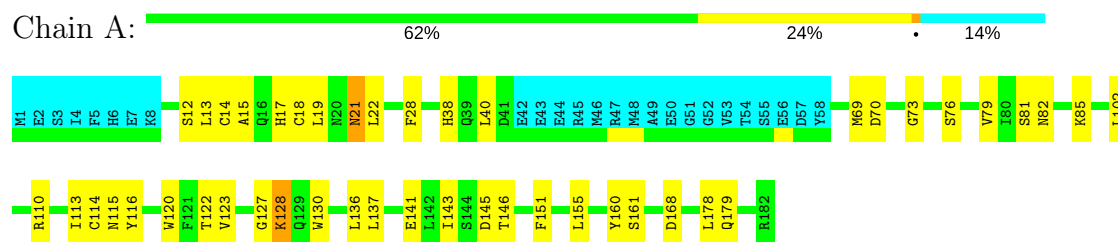


- Molecule 2: UBC protein

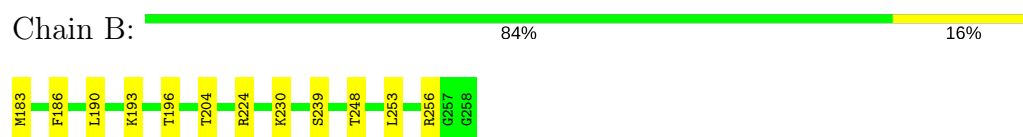


4.2.5 Score per residue for model 5

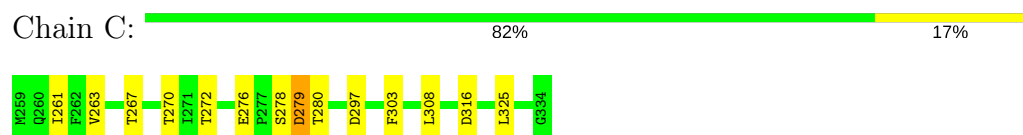
• Molecule 1: Ataxin-3



• Molecule 2: UBC protein

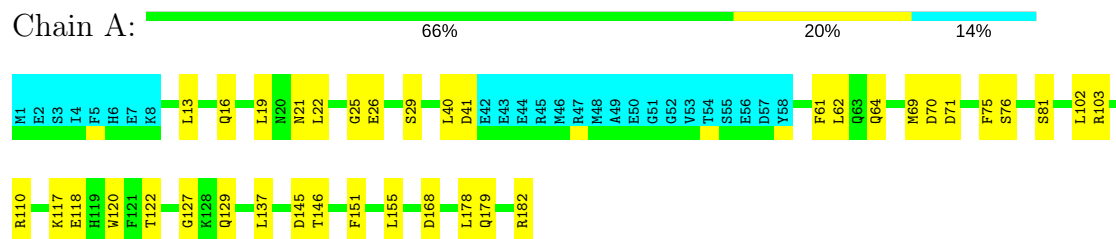


• Molecule 2: UBC protein

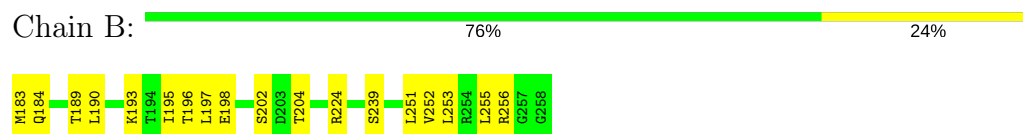


4.2.6 Score per residue for model 6

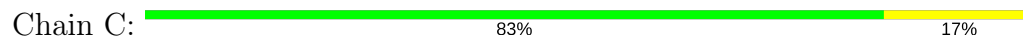
• Molecule 1: Ataxin-3



• Molecule 2: UBC protein



• Molecule 2: UBC protein

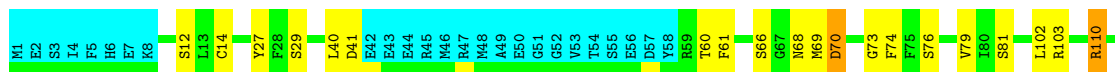




4.2.7 Score per residue for model 7

- Molecule 1: Ataxin-3

Chain A: 63% 22% 14%



- Molecule 2: UBC protein

Chain B: 84% 14% 2%



- Molecule 2: UBC protein

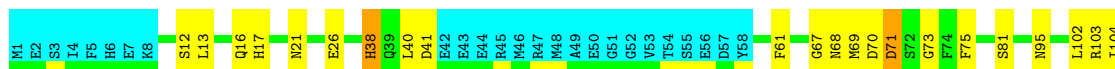
Chain C: 83% 12% 5%



4.2.8 Score per residue for model 8

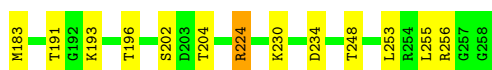
- Molecule 1: Ataxin-3

Chain A: 63% 22% 14%

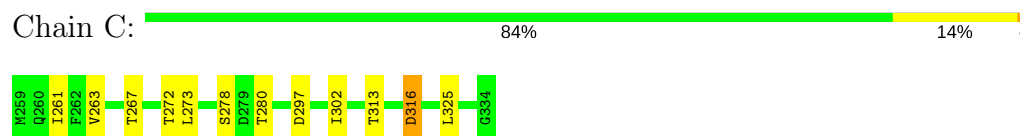


- Molecule 2: UBC protein

Chain B: 83% 16% 1%

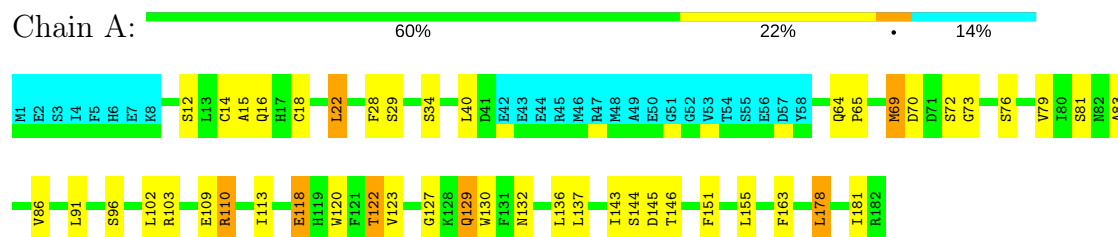


- Molecule 2: UBC protein

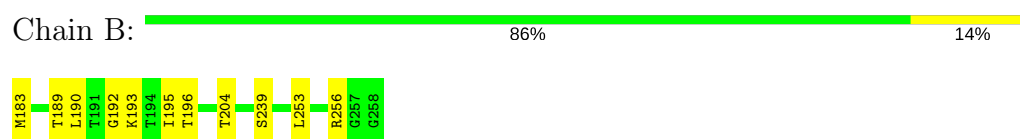


4.2.9 Score per residue for model 9

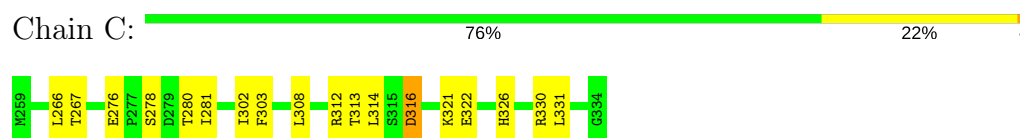
- Molecule 1: Ataxin-3



- Molecule 2: UBC protein

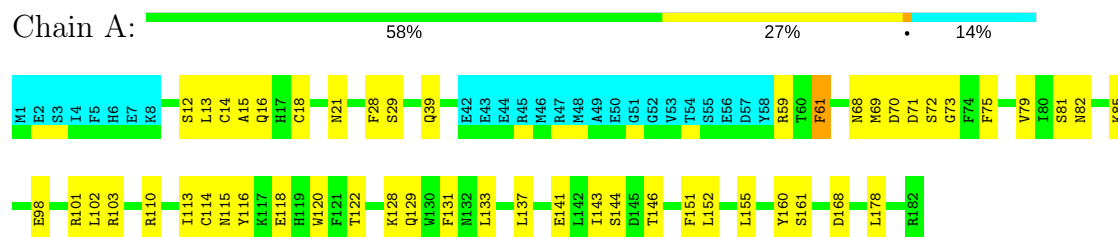


- Molecule 2: UBC protein

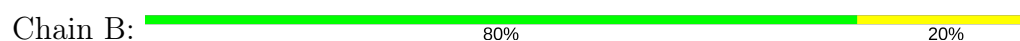


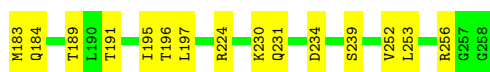
4.2.10 Score per residue for model 10

- Molecule 1: Ataxin-3

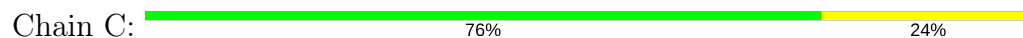


- Molecule 2: UBC protein



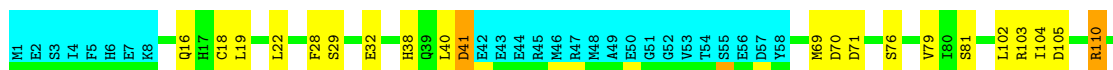


- Molecule 2: UBC protein

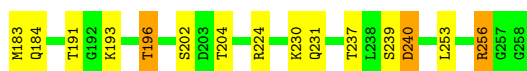


4.2.11 Score per residue for model 11

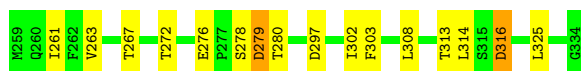
- Molecule 1: Ataxin-3



- Molecule 2: UBC protein

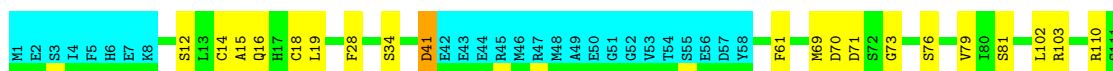


- Molecule 2: UBC protein




4.2.12 Score per residue for model 12

- Molecule 1: Ataxin-3



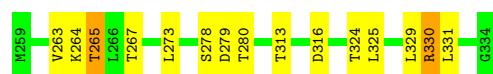
- Molecule 2: UBC protein

Chain B:  82% 18%



- Molecule 2: UBC protein

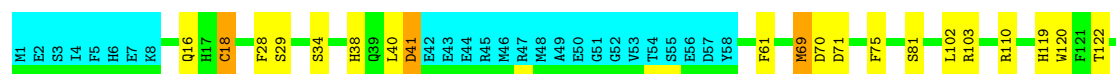
Chain C:  80% 17%




4.2.13 Score per residue for model 13

- Molecule 1: Ataxin-3

Chain A:  69% 14% 14%




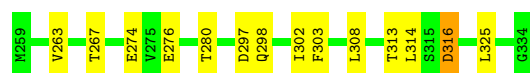
- Molecule 2: UBC protein

Chain B:  79% 21%



- Molecule 2: UBC protein

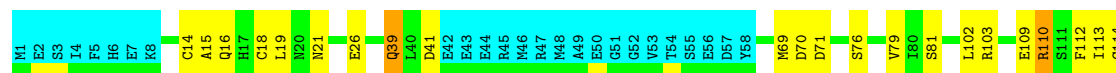
Chain C:  82% 17%



4.2.14 Score per residue for model 14

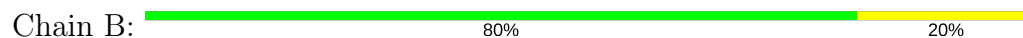
- Molecule 1: Ataxin-3

Chain A:  64% 21% 14%





- Molecule 2: UBC protein

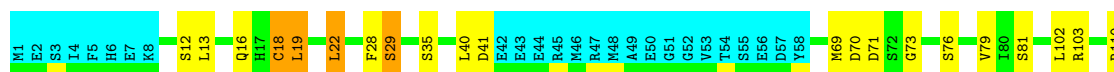


- Molecule 2: UBC protein

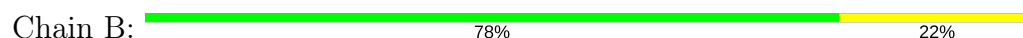


4.2.15 Score per residue for model 15 (medoid)

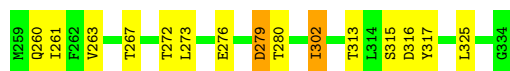
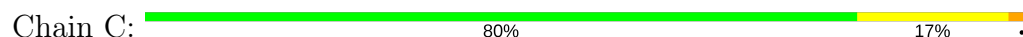
- Molecule 1: Ataxin-3



- Molecule 2: UBC protein



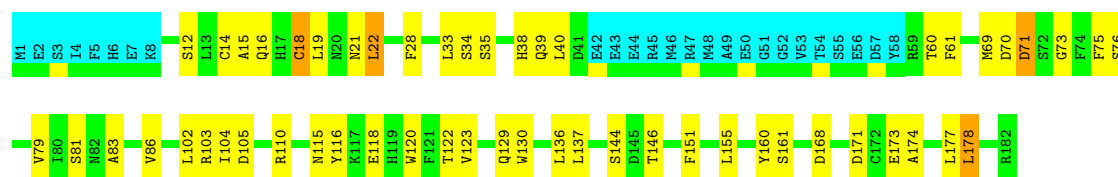
- Molecule 2: UBC protein



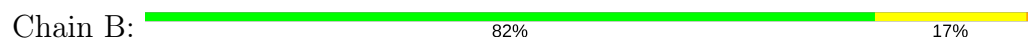
4.2.16 Score per residue for model 16

- Molecule 1: Ataxin-3

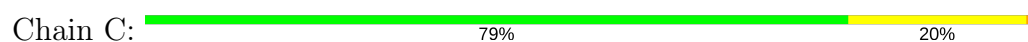




- Molecule 2: UBC protein

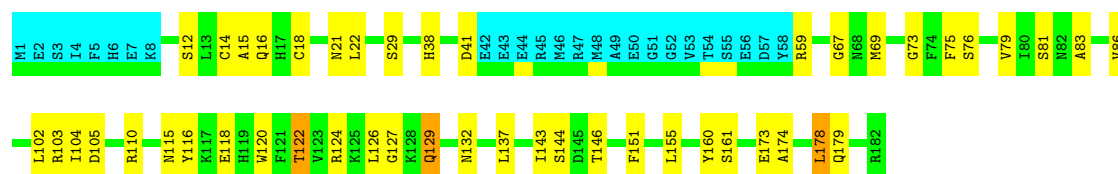


- Molecule 2: UBC protein

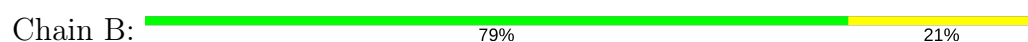


4.2.17 Score per residue for model 17

- Molecule 1: Ataxin-3



- Molecule 2: UBC protein

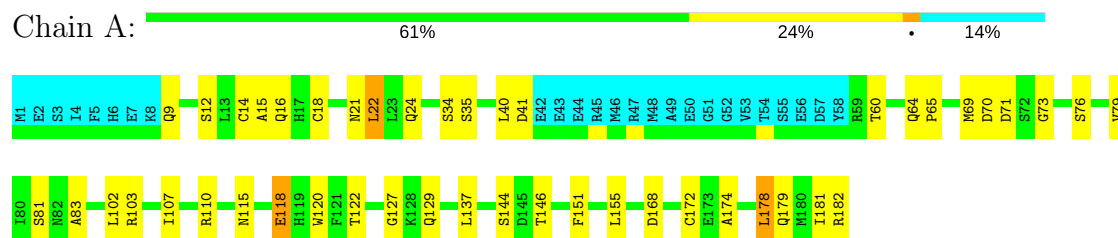


- Molecule 2: UBC protein

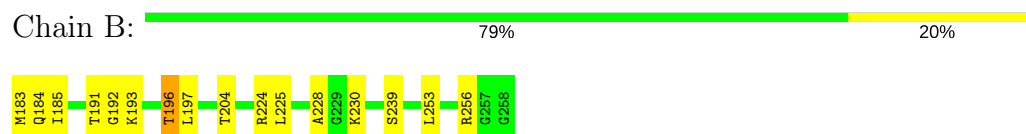


4.2.18 Score per residue for model 18

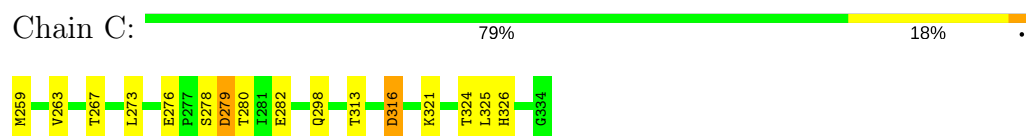
- Molecule 1: Ataxin-3



- Molecule 2: UBC protein

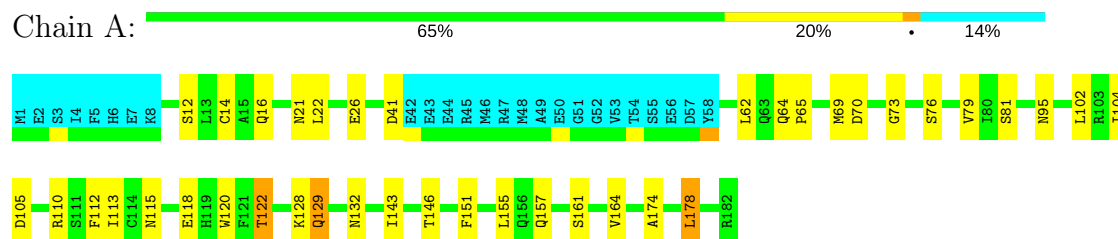


- Molecule 2: UBC protein

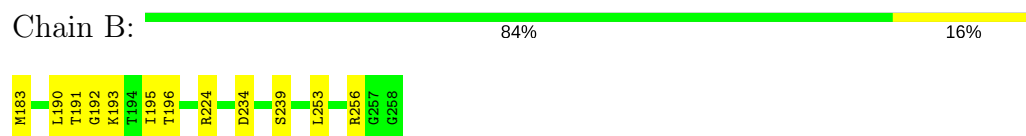


4.2.19 Score per residue for model 19

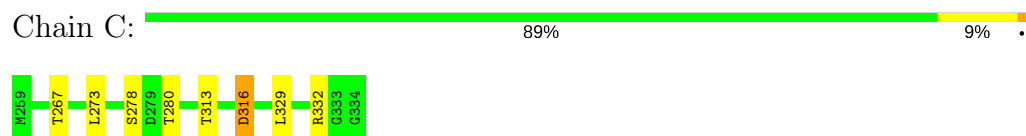
- Molecule 1: Ataxin-3



- Molecule 2: UBC protein

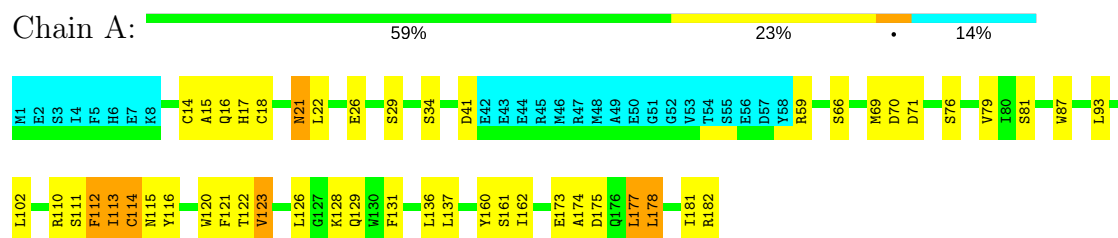


- Molecule 2: UBC protein

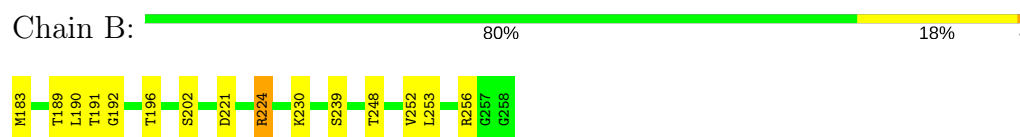


4.2.20 Score per residue for model 20

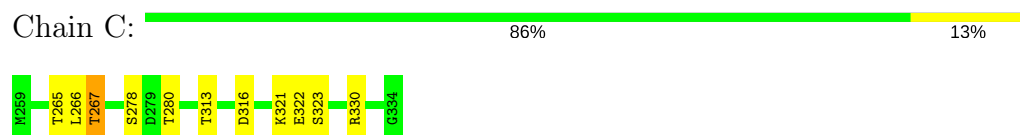
• Molecule 1: Ataxin-3



• Molecule 2: UBC protein



• Molecule 2: UBC protein



5 Refinement protocol and experimental data overview

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. No validations of the models with respect to experimental NMR restraints is performed at this time.

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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 ⓘ

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:303:PHE:HB3	2:C:308:LEU:HD21	0.57	1.75	6	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:C:260:GLN:HA	2:C:273:LEU:O	0.57	1.99	15	2
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
2:C:329:LEU:O	2:C:330:ARG:HD2	0.49	2.07	7	2
1:A:29:SER:HB3	2:C:302:ILE:HG21	0.49	1.83	1	1
2:C:261:ILE:O	2:C:272:THR:HA	0.49	2.07	6	4
1:A:109:GLU:OE1	1:A:110:ARG:HD2	0.49	2.07	2	3
1:A:116:TYR:HB2	1:A:160:TYR:CE1	0.49	2.42	1	1
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:128:LYS:O	1:A:128:LYS:HD2	0.48	2.09	13	1
1:A:91:LEU:HD11	1:A:163:PHE:HB3	0.48	1.86	9	1
1:A:12:SER:HB3	1:A:73:GLY:O	0.47	2.09	5	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:N	1:A:110:ARG:HD2	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
1:A:120:TRP:HB2	2:B:256:ARG:NE	0.46	2.26	19	7
2:B:237:THR:O	2:B:240:ASP:HB2	0.46	2.11	11	2
1:A:150:LEU:O	1:A:154:GLN:HG2	0.45	2.12	8	2
1:A:116:TYR:HB2	1:A:160:TYR:CZ	0.45	2.46	1	1
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:143:ILE:HG23	1:A:147:TYR:CD2	0.45	2.47	14	1
1:A:98:GLU:HA	1:A:101:ARG:CZ	0.45	2.42	2	2
2:C:280:THR:O	2:C:284:VAL:HG23	0.44	2.12	7	1
1:A:126:LEU:HD23	1:A:178:LEU:HG	0.44	1.89	20	1
2:C:264:LYS:HB2	2:C:326:HIS:CD2	0.44	2.47	16	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:104:ILE:HG22	1:A:105:ASP:N	0.43	2.27	17	5
1:A:32:GLU:O	1:A:36:ILE:HG12	0.43	2.13	1	1
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:129:GLN:HG3	1:A:143:ILE:O	0.43	2.13	19	4
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:38:HIS:O	1:A:41:ASP:HB3	0.43	2.13	13	2
1:A:113:ILE:HA	1:A:121:PHE:O	0.43	2.14	7	1
2:C:264:LYS:HA	2:C:269:LYS:O	0.43	2.13	2	2
1:A:112:PHE:CB	1:A:164:VAL:HA	0.43	2.43	12	2
2:B:186:PHE:O	2:B:248:THR:HA	0.43	2.14	5	1
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:110:ARG:HD3	1:A:165:VAL:O	0.43	2.14	7	2
1:A:68:ASN:HA	2:C:332:ARG:CD	0.43	2.44	7	1
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:128:LYS:HD2	1:A:128:LYS:O	0.42	2.15	12	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
2:B:189:THR:HG22	2:B:251:LEU:HD23	0.41	1.90	6	2
1:A:24:GLN:HB3	1:A:172:CYS:SG	0.41	2.55	4	1
1:A:114:CYS:HA	1:A:161:SER:O	0.41	2.16	7	2
1:A:68:ASN:HA	2:C:332:ARG:HD2	0.41	1.92	7	1
2:B:208:VAL:O	2:B:212:ILE:HG13	0.41	2.15	2	2
1:A:39:GLN:HG3	2:C:266:LEU:O	0.41	2.16	14	1
2:C:266:LEU:HD11	2:C:328:VAL:HG13	0.41	1.91	4	1
1:A:68:ASN:O	1:A:69:MET:HB3	0.41	2.15	1	1
2:C:317:TYR:O	2:C:319:ILE:HG13	0.41	2.16	14	1
1:A:93:LEU:O	1:A:99:TYR:HB3	0.41	2.16	1	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 ⓘ

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	156/182 (86%)	131±4 (84±2%)	21±4 (14±2%)	4±2 (3±1%)	10	45
2	B	74/76 (97%)	68±2 (92±2%)	5±2 (7±2%)	0±0 (1±1%)	33	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	74/76 (97%)	67±3 (91±5%)	6±3 (8±4%)	1±1 (1±2%)	23	70
All	All	6080/6680 (91%)	5324 (88%)	649 (11%)	107 (2%)	14	57

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	118	GLU	2
1	A	127	GLY	2
1	A	123	VAL	2
1	A	112	PHE	2
2	C	267	THR	2
2	C	293	GLY	2
2	C	319	ILE	2
2	C	261	ILE	2
1	A	17	HIS	1
1	A	104	ILE	1
2	C	271	ILE	1
1	A	113	ILE	1
2	C	266	LEU	1
1	A	145	ASP	1
2	C	323	SER	1
2	C	333	GLY	1
2	C	318	ASN	1
2	C	305	GLY	1
2	C	316	ASP	1
1	A	27	TYR	1
1	A	174	ALA	1
1	A	175	ASP	1
1	A	142	LEU	1
2	B	191	THR	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	142/164 (87%)	122±2 (86±2%)	20±2 (14±2%)	7	47
2	B	68/68 (100%)	57±2 (84±3%)	11±2 (16±3%)	6	44
2	C	68/68 (100%)	60±3 (88±4%)	8±3 (12±4%)	10	52
All	All	5560/6000 (93%)	4776 (86%)	784 (14%)	8	47

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

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Mol	Chain	Res	Type	Models (Total)
1	A	40	LEU	12
1	A	145	ASP	11
2	B	230	LYS	11
2	C	297	ASP	10
1	A	29	SER	10
2	B	195	ILE	10
2	B	189	THR	10
2	C	316	ASP	10
2	B	252	VAL	10
2	C	326	HIS	9
2	B	231	GLN	8
2	C	279	ASP	8
1	A	19	LEU	8
2	C	273	LEU	8
1	A	182	ARG	8
2	C	302	ILE	8
1	A	113	ILE	8
1	A	144	SER	8
1	A	28	PHE	8
1	A	61	PHE	7
1	A	168	ASP	7
1	A	34	SER	6
1	A	26	GLU	6
1	A	13	LEU	6
2	C	324	THR	6
2	C	313	THR	5
2	C	315	SER	5
1	A	59	ARG	5
2	B	248	THR	5
2	C	330	ARG	5
1	A	18	CYS	5
1	A	115	ASN	5
2	B	234	ASP	5
2	C	332	ARG	4
2	C	331	LEU	4
2	C	265	THR	4
1	A	128	LYS	4
2	C	270	THR	3
2	B	237	THR	3
2	C	310	ASP	3
1	A	114	CYS	3
1	A	95	ASN	3

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Mol	Chain	Res	Type	Models (Total)
1	A	118	GLU	3
2	C	272	THR	3
1	A	38	HIS	3
1	A	39	GLN	3
1	A	126	LEU	3
1	A	177	LEU	3
2	C	298	GLN	2
2	C	274	GLU	2
1	A	119	HIS	2
1	A	72	SER	2
2	C	329	LEU	2
1	A	20	ASN	2
1	A	27	TYR	2
2	B	221	ASP	2
1	A	87	TRP	2
2	C	318	ASN	2
1	A	35	SER	2
1	A	173	GLU	2
1	A	171	ASP	2
1	A	157	GLN	1
1	A	161	SER	1
2	C	328	VAL	1
1	A	99	TYR	1
2	C	289	GLN	1
1	A	96	SER	1
1	A	64	GLN	1
1	A	60	THR	1
2	C	262	PHE	1
1	A	75	PHE	1
2	C	323	SER	1
2	C	301	LEU	1
2	C	271	ILE	1
1	A	68	ASN	1
1	A	33	LEU	1
2	C	314	LEU	1
1	A	9	GLN	1
2	B	200	GLU	1
2	C	325	LEU	1
2	C	306	LYS	1
2	B	225	LEU	1
1	A	85	LYS	1
1	A	107	ILE	1

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Mol	Chain	Res	Type	Models (Total)
1	A	135	SER	1
2	C	282	GLU	1
2	B	240	ASP	1
1	A	152	LEU	1
2	C	317	TYR	1
2	C	266	LEU	1
1	A	117	LYS	1
2	B	256	ARG	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 carbohydrates 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