Full wwPDB NMR Structure Validation Report (i)

Jun 16, 2024 – 08:18 AM EDT

PDB ID	:	2LBM
Title	:	Solution structure of the ADD domain of ATRX complexed with histone tail H3 1-15 K9me3
Authors	:	Eustermann, S.; Yang, J.; Neuhaus, D.
Deposited on	:	2011-04-08

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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

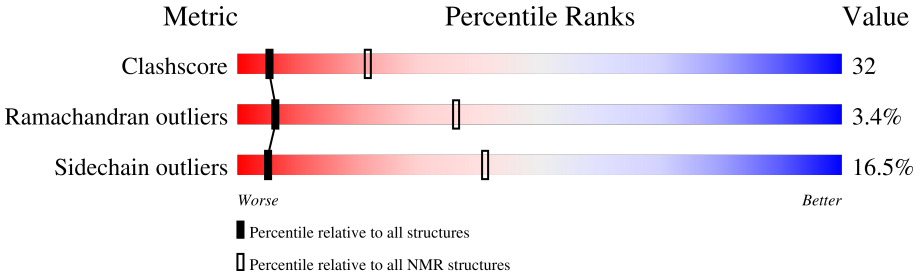
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
wwPDB-ShiftChecker	:	v1.2
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 is 77%.

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	142	37% 28% 5% • 30%
2	C	15	13% 13% 73%

2 Ensemble composition and analysis (i)

This entry contains 25 models. Model 4 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:170-A:178, A:185-A:208, A:218-A:284, C:3-C:6 (104)	0.29	4

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 5 clusters and 2 single-model clusters were found.

Cluster number	Models
1	2, 4, 9, 11, 14, 15, 16, 17, 19
2	5, 7, 12, 13, 18, 20, 22, 25
3	1, 8
4	6, 10
5	21, 23
Single-model clusters	3; 24

3 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 2440 atoms, of which 1197 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Transcriptional regulator ATRX.

Mol	Chain	Residues	Atoms						Trace
			Total	C	H	N	O	S	
1	A	142	2197	696	1069	200	214	18	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	GLY	-	EXPRESSION TAG	UNP P46100
A	156	ALA	-	EXPRESSION TAG	UNP P46100
A	157	MET	-	EXPRESSION TAG	UNP P46100
A	158	ALA	-	EXPRESSION TAG	UNP P46100
A	159	ASP	-	EXPRESSION TAG	UNP P46100
A	?	-	GLU	DELETION	UNP P46100

- Molecule 2 is a protein called histone tail H3 K9me3.

Mol	Chain	Residues	Atoms					Trace
			Total	C	H	N	O	
2	C	15	240	66	128	25	21	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	
			Total	Zn
3	A	3	3	3

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: Transcriptional regulator ATRX

Chain A: 37% 28% 5% • 30%

G155 A156 M157 A158 D159 K160 R161 G162 D163 G164 L165 H166 G167 I168 V169 S170 C171 T172 Q177 V178 N179 H180 F181 Q182 K183 D184 S185 I186 Y187 R188 H189 P190 S191 L192 Q193 V194 L195 I196 C200 F201 Y204 I209 S210 R211 D212 S213 D214 G215 M216 D217 E218 Q219 W222 C223 A224

N228 L229 I230 D233 F234 F239 C240 K241 K242 C243 I244 L245 R246 N247 L248 L253 I256 W263 Y264 C265 Y266 I267 C268 H269 P270 E271 P272 L273 L274 D275 L276 V277 V283 F284 E285 N286 L287 E288 Q289 L290 L291 Q292 Q293 N294 K295 K296

• Molecule 2: histone tail H3 K9me3

Chain C: 13% 13% 73%

A1 R2 T3 K4 A7 R8 K9 S10 T11 G12 G13 K14 A15

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: Transcriptional regulator ATRX

Chain A: 39% 27% • • 30%

G155 A156 M157 A158 D159 K160 R161 G162 D163 G164 L165 H166 G167 I168 V169 S170 C171 T172 Q177 V178 N179 H180 F181 Q182 K183 D184 S185 I186 H189 P190 S191 L192 Q193 V194 C200 F201 Y204 I209 S210 R211 D212 S213 D214 G215 M216 D217 E218 Q219 W222 C223 A224 N228 L229

I230 D233 F234 F239 C240 K241 K242 C243 I244 L245 R246 N247 L248 L253 I256 N260 W263 Y264 C265 Y266 I267 C268 H269 P270 E271 P272 L273 L274 D275 L276 A279 V283 F284 E285 N286 L287 E288 Q289 L290 L291 Q292 Q293 N294 K295 K296

• Molecule 2: histone tail H3 K9me3

Chain C: 13% 13% 73%

A1 R2 T3 K4 A7 R8 K9 S10 T11 G12 G13 K14 A15

4.2.2 Score per residue for model 2

- Molecule 1: Transcriptional regulator ATRX

Chain A: 37% 28% 5% • 30%

G155 A156 M157 A158 D159 K160 R161 G162 D163 G164 L165 H166 G167 I168 V169 T172 Q177 V178 N179 H180 F181 Q182 K183 D184 S185 I186 Y187 R188 H189 P190 S191 L192 Q193 V194 L195 I196 C200 F201 Y204 I209 S210 R211 D212 S213 D214 G215 M216 D217 E218 Q219 W222 E225

N228 L229 I230 D233 F234 F239 C240 K241 K242 C243 I244 L245 L248 L253 I256 E259 W263 Y264 C265 Y266 I267 C268 H269 P270 E271 P272 L273 L276 V277 V283 F284 E285 N286 L287 E288 Q289 L290 L291 Q292 Q293 N294 K295 K296

- Molecule 2: histone tail H3 K9me3

Chain C: 7% 20% 73%

A1 R2 T3 K4 Q5 T6 A7 R8 K9 S10 T11 G12 G13 K14 A15

4.2.3 Score per residue for model 3

- Molecule 1: Transcriptional regulator ATRX

Chain A: 32% 33% • • 30%

G155 A156 M157 A158 D159 K160 R161 G162 D163 G164 L165 H166 G167 I168 V169 S170 C171 T172 A173 Q177 V178 N179 H180 F181 Q182 K183 D184 S185 I186 Y187 R188 H189 P190 S191 L192 Q193 V194 L195 C200 F201 Y204 I209 S210 R211 D212 S213 D214 G215 M216 D217 E218 Q219 C220 R221 W222 C223

A224 N228 L229 I230 D233 F234 F239 C240 K241 K242 C243 I244 L245 R246 N247 L248 K251 E252 L253 I256 M257 W263 Y264 C265 Y266 I267 C268 H269 P270 E271 P272 L273 L274 D275 L276 V277 T278 V283 F284 E285 N286 L287 E288 Q289 L290 L291 Q292 Q293 N294 K295 K296

- Molecule 2: histone tail H3 K9me3

Chain C: 13% 13% 73%

A1 R2 T3 T6 A7 R8 K9 S10 T11 G12 G13 K14 A15

4.2.4 Score per residue for model 4 (medoid)

- Molecule 1: Transcriptional regulator ATRX

Chain A: 37% 27% 6% • 30%

G155 A156 M157 A158 D159 K160 R161 G162 D163 G164 L165 H166 G167 I168 V169 T172 A173 Q177 V178 N179 H180 F181 Q182 K183 D184 S185 I186 Y187 R188 H189 P190 S191 L192 Q193 V194 L195 I196 C200 F201 Y204 D207 D208 I209 S210 R211 D212 S213 D214 G215 M216 D217 E218 Q219 C220 R221

W222 C223 A224 L229 I230 D233 F234 C235 H236 W237 A238 F239 C240 K241 K242 C243 I244 L245 R246 N247 L248 I256 W263 Y264 C265 Y266 I267 C268 H269 P270 E271 P272 L273 L276 V277 V283 F284 E285 N286 L287 E288 Q289 L290 L291 Q292 Q293 N294 K295 K296

• Molecule 2: histone tail H3 K9me3

Chain C: 13% 13% 73%

A1 R2 T3 T6 A7 R8 K9 S10 T11 G12 G13 K14 A15

4.2.5 Score per residue for model 5

• Molecule 1: Transcriptional regulator ATRX

Chain A: 37% 28% 5% • 30%

G155 A156 M157 A158 D159 K160 R161 G162 D163 G164 L165 H166 G167 I168 V169 T172 V178 N179 H180 F181 Q182 K183 D184 S185 I186 Y187 R188 H189 P190 S191 L192 Q193 V194 L195 I196 C197 K198 F201 I209 S210 R211 D212 S213 D214 G215 M216 D217 E218 Q219 C220 R221 W222 C223 A224 N228

L229 I230 D233 F234 N237 A238 F239 C240 K241 K242 C243 I244 L245 R246 N247 L248 G249 R250 L253 I256 W263 Y264 C265 Y266 I267 C268 H269 P270 E271 P272 L273 L274 D275 L276 V277 T278 V283 F284 E285 N286 L287 E288 Q289 L290 L291 Q292 Q293 N294 K295 K296

• Molecule 2: histone tail H3 K9me3

Chain C: 13% 13% 73%

A1 R2 T3 K4 A7 R8 K9 S10 T11 G12 G13 K14 A15

4.2.6 Score per residue for model 6

• Molecule 1: Transcriptional regulator ATRX

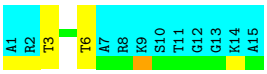
Chain A: 39% 25% 6% • 30%

G155 A156 M157 A158 D159 K160 R161 G162 D163 G164 L165 H166 G167 I168 V169 S170 C171 T172 Q177 V178 N179 H180 F181 Q182 K183 D184 S185 I186 Y187 R188 H189 P190 S191 L192 Q193 V194 C200 F201 Y204 D207 D208 I209 S210 R211 D212 S213 D214 G215 M216 D217 E218 Q219 W222 C223 A224

N228 L229 I230 D233 F234 A238 F239 C240 K241 K242 C243 I244 N247 L248 K251 E252 L253 I256 W263 Y264 C265 Y266 I267 C268 H269 P270 E271 P272 L273 L274 D275 L276 V283 F284 E285 N286 L287 E288 Q289 L290 L291 Q292 Q293 N294 K295 K296

• Molecule 2: histone tail H3 K9me3

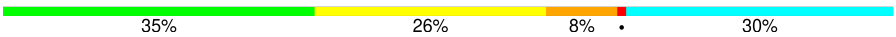
Chain C: 13% 13% 73%

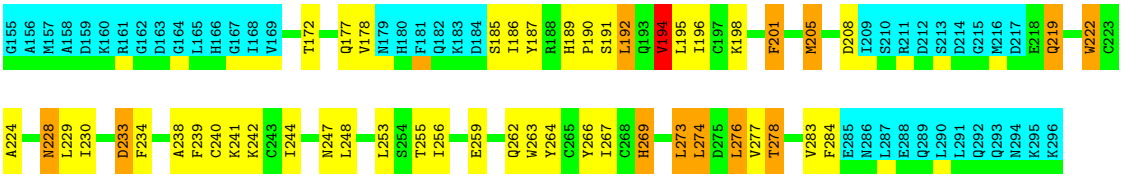


4.2.7 Score per residue for model 7

- Molecule 1: Transcriptional regulator ATRX

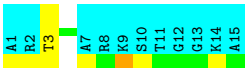
Chain A:





- Molecule 2: histone tail H3 K9me3

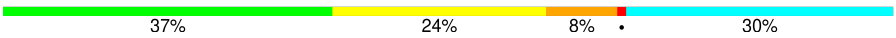
Chain C:

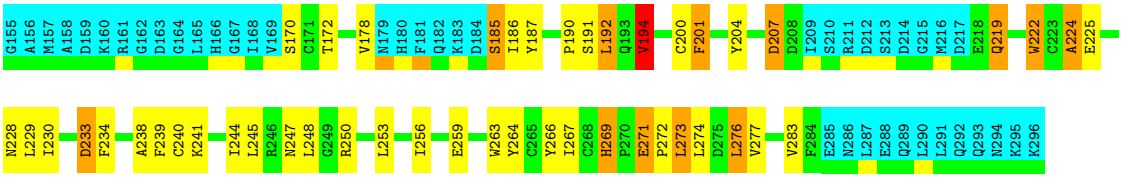


4.2.8 Score per residue for model 8

- Molecule 1: Transcriptional regulator ATRX

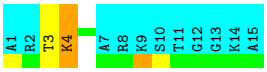
Chain A:





- Molecule 2: histone tail H3 K9me3

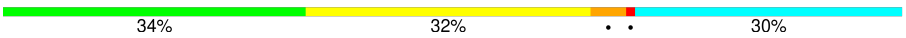
Chain C:

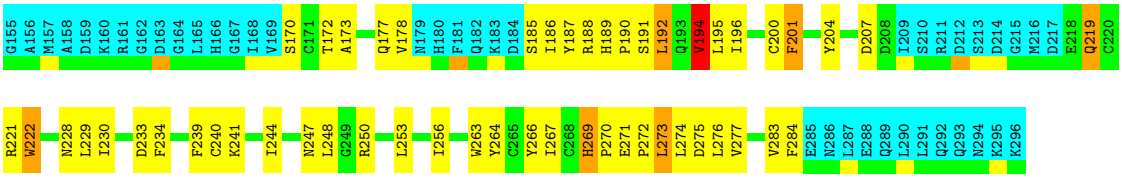


4.2.9 Score per residue for model 9

- Molecule 1: Transcriptional regulator ATRX

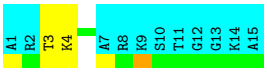
Chain A:





- Molecule 2: histone tail H3 K9me3

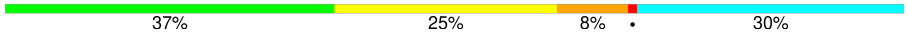
Chain C:

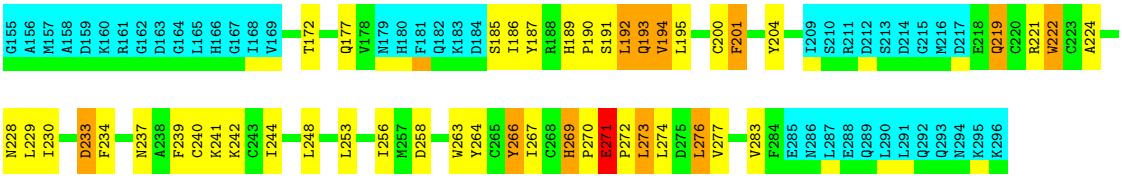


4.2.10 Score per residue for model 10

- Molecule 1: Transcriptional regulator ATRX

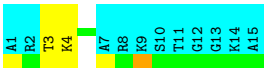
Chain A:





- Molecule 2: histone tail H3 K9me3

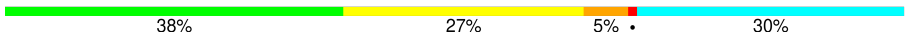
Chain C:

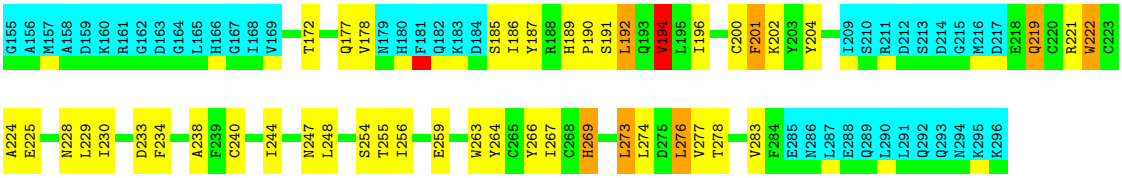


4.2.11 Score per residue for model 11

- Molecule 1: Transcriptional regulator ATRX

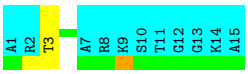
Chain A:





- Molecule 2: histone tail H3 K9me3

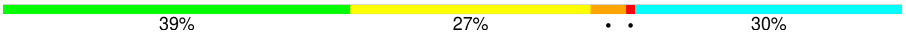
Chain C:



4.2.12 Score per residue for model 12

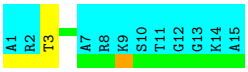
- Molecule 1: Transcriptional regulator ATRX

Chain A:



- Molecule 2: histone tail H3 K9me3

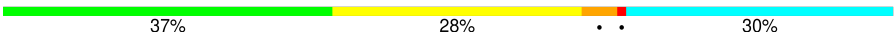
Chain C:

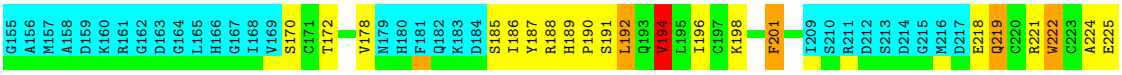


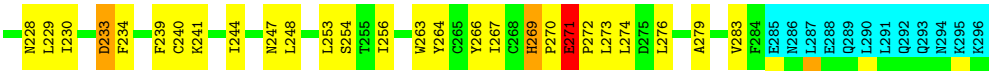
4.2.13 Score per residue for model 13

- Molecule 1: Transcriptional regulator ATRX

Chain A:

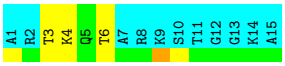






- Molecule 2: histone tail H3 K9me3

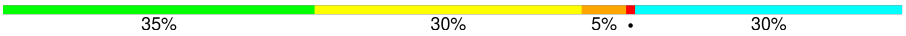
Chain C:

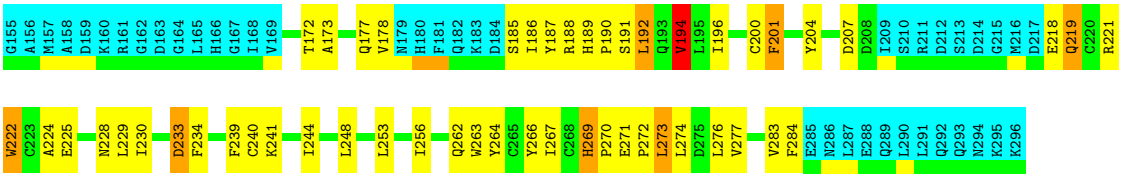


4.2.14 Score per residue for model 14

- Molecule 1: Transcriptional regulator ATRX

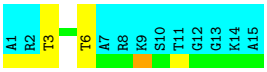
Chain A:





• Molecule 2: histone tail H3 K9me3

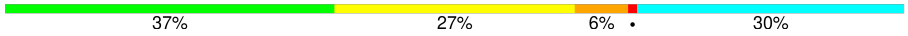
Chain C:

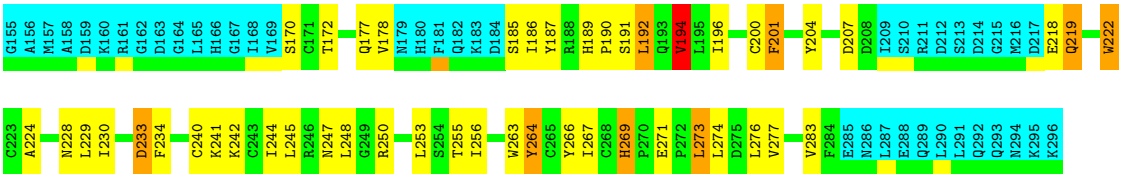


4.2.15 Score per residue for model 15

• Molecule 1: Transcriptional regulator ATRX

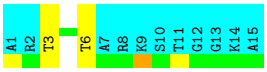
Chain A:





• Molecule 2: histone tail H3 K9me3

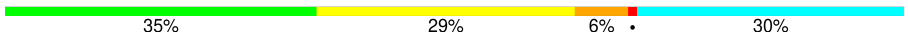
Chain C:

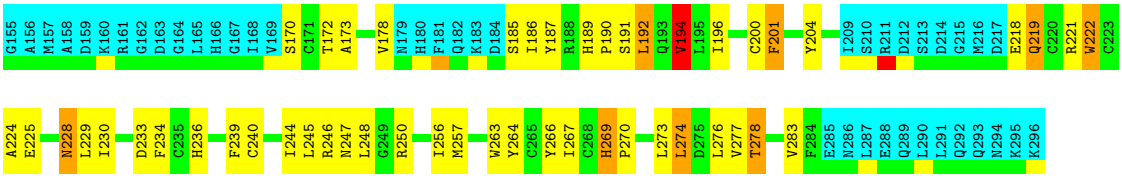


4.2.16 Score per residue for model 16

• Molecule 1: Transcriptional regulator ATRX

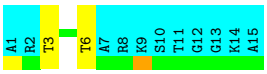
Chain A:





• Molecule 2: histone tail H3 K9me3

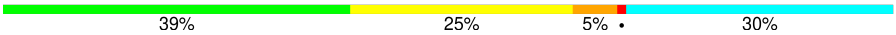
Chain C:



4.2.17 Score per residue for model 17

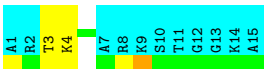
• Molecule 1: Transcriptional regulator ATRX

Chain A:



• Molecule 2: histone tail H3 K9me3

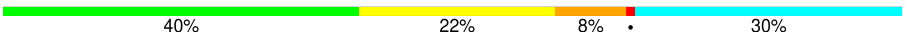
Chain C:

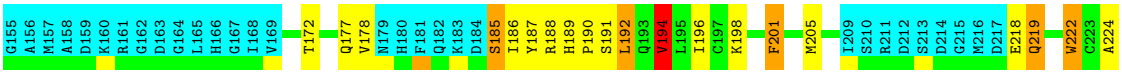


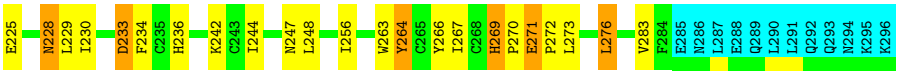
4.2.18 Score per residue for model 18

• Molecule 1: Transcriptional regulator ATRX

Chain A:

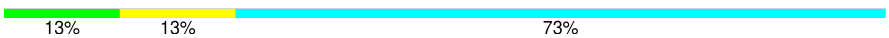


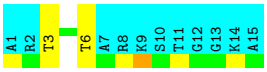




• Molecule 2: histone tail H3 K9me3

Chain C:

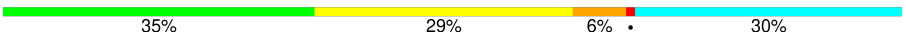


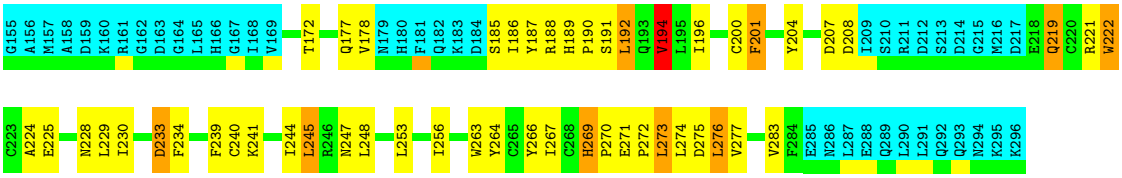


4.2.19 Score per residue for model 19

• Molecule 1: Transcriptional regulator ATRX

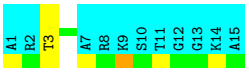
Chain A:





- Molecule 2: histone tail H3 K9me3

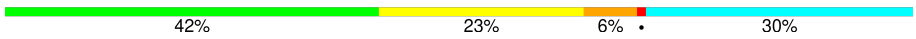
Chain C:

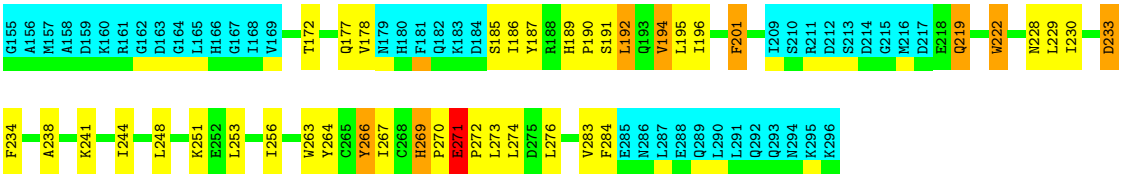


4.2.20 Score per residue for model 20

- Molecule 1: Transcriptional regulator ATRX

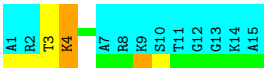
Chain A:





- Molecule 2: histone tail H3 K9me3

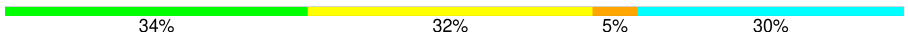
Chain C:

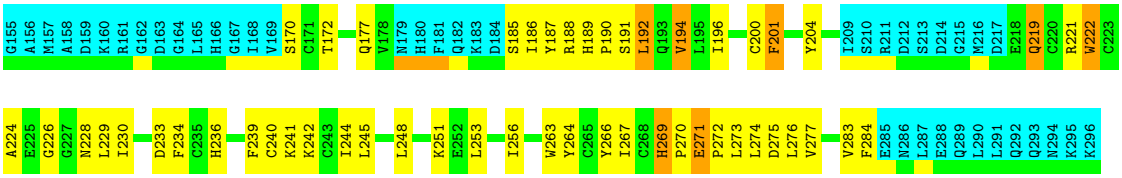


4.2.21 Score per residue for model 21

- Molecule 1: Transcriptional regulator ATRX

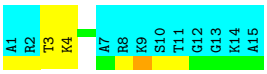
Chain A:





- Molecule 2: histone tail H3 K9me3

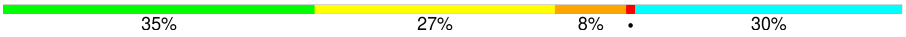
Chain C:

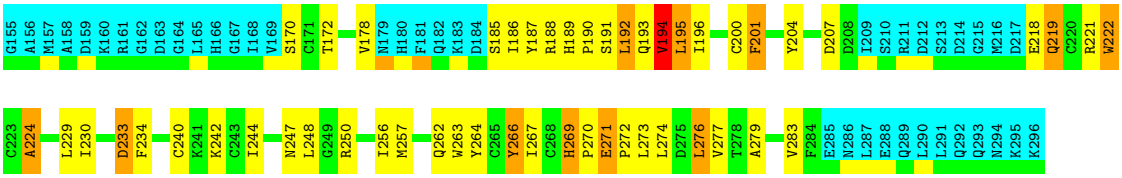


4.2.22 Score per residue for model 22

- Molecule 1: Transcriptional regulator ATRX

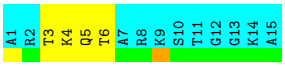
Chain A:





- Molecule 2: histone tail H3 K9me3

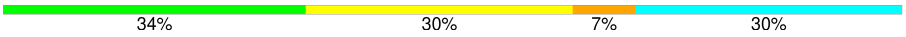
Chain C:

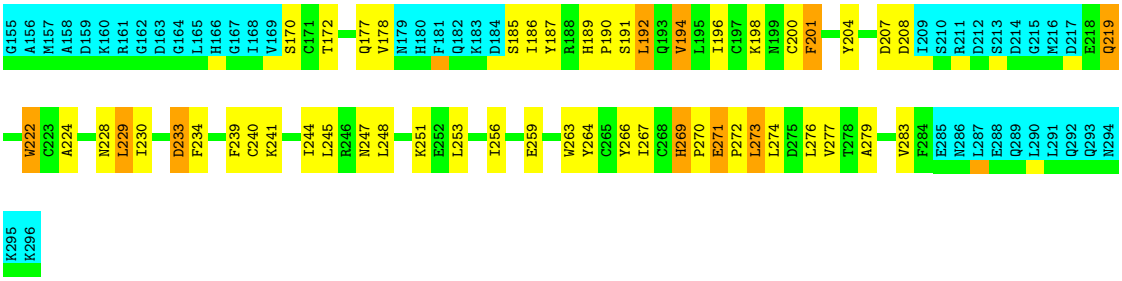


4.2.23 Score per residue for model 23

- Molecule 1: Transcriptional regulator ATRX

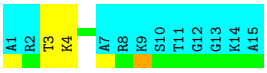
Chain A:





- Molecule 2: histone tail H3 K9me3

Chain C:



4.2.24 Score per residue for model 24

- Molecule 1: Transcriptional regulator ATRX

Chain A: 38% 25% 6% • 30%

G155 A156 M157 A158 D159 K160 R161 G162 D163 G164 L165 H166 G167 I168 V169 T172 Q177 V178 N179 H180 F181 Q182 K183 D184 S185 I186 Y187 R188 H189 P190 S191 L192 Q193 V194 L195 I196 C197 K198 F201 I209 S210 R211 D212 S213 D214 G215 M216 D217 E218 Q219 W222 C223 A224 M228

L229 I230 D233 F234 F239 C240 K241 I244 L245 R246 N247 L248 K251 I256 M257 D258 E259 W263 Y264 C265 Y266 I267 C268 H269 P270 E271 P272 L273 L274 D275 L276 V283 F284 E285 N286 L287 E288 Q289 L290 L291 Q292 Q293 N294 K295 K296

• Molecule 2: histone tail H3 K9me3

Chain C: 7% 20% 73%

A1 R2 T3 K4 Q5 T6 A7 R8 K9 S10 T11 G12 G13 K14 A15

4.2.25 Score per residue for model 25

• Molecule 1: Transcriptional regulator ATRX

Chain A: 37% 28% 5% • 30%

G155 A156 M157 A158 D159 K160 R161 G162 D163 G164 L165 H166 G167 I168 V169 S170 C171 T172 Q177 V178 N179 H180 F181 Q182 K183 D184 S185 I186 Y187 R188 H189 P190 S191 L192 Q193 V194 L195 I196 C197 K198 F201 D207 D208 I209 S210 R211 D212 S213 D214 G215 M216 D217 E218 Q219 W222 C223

A224 E225 N228 L229 I230 D233 F234 F239 C240 K241 K242 C243 I244 L245 L248 L253 S254 T255 I256 Q262 W263 Y264 C265 Y266 I267 C268 H269 P270 E271 P272 L273 L274 D275 L276 V277 T278 V283 F284 E285 N286 L287 E288 Q289 L290 L291 Q292 Q293 N294 K295 K296

• Molecule 2: histone tail H3 K9me3

Chain C: 20% 7% 73%

A1 R2 T3 A7 R8 K9 S10 T11 G12 G13 K14 A15

5 Refinement protocol and experimental data overview (i)

The models were refined using the following method: *simulated annealing*.

Of the 50 calculated structures, 25 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
xplor-nih	structure solution	2.19
xplor-nih	refinement	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	1
Total number of shifts	1483
Number of shifts mapped to atoms	1483
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	77%

6 Model quality (i)

6.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, M3L

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	799	752	752	52±4
2	C	32	35	35	2±1
All	All	20850	19675	19675	1289

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 32.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:194:VAL:HG21	1:A:276:LEU:HD23	0.92	1.41	11	15
1:A:172:THR:OG1	1:A:276:LEU:HD21	0.87	1.69	10	22
1:A:189:HIS:CD2	1:A:196:ILE:HD13	0.85	2.07	16	20
1:A:248:LEU:HD22	1:A:256:ILE:HD11	0.83	1.50	10	2
1:A:266:TYR:O	1:A:267:ILE:HD13	0.81	1.75	8	25
1:A:256:ILE:HG23	1:A:263:TRP:CD1	0.78	2.13	11	25
1:A:218:GLU:HG2	2:C:6:THR:HG21	0.73	1.60	14	5
1:A:248:LEU:HD23	1:A:256:ILE:HD11	0.73	1.58	11	22
1:A:192:LEU:HD22	1:A:267:ILE:CD1	0.73	2.14	3	25
1:A:248:LEU:CD2	1:A:256:ILE:HD11	0.72	2.15	11	14
1:A:256:ILE:HG23	1:A:263:TRP:CG	0.72	2.20	11	25

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:247:ASN:OD1	1:A:276:LEU:HD12	0.72	1.85	7	5
1:A:229:LEU:HD23	1:A:240:CYS:CA	0.71	2.15	8	20
1:A:178:VAL:HG21	1:A:186:ILE:HG22	0.71	1.61	11	7
1:A:178:VAL:HG11	1:A:185:SER:O	0.68	1.89	17	18
1:A:194:VAL:CG2	1:A:276:LEU:HD22	0.68	2.18	7	2
1:A:178:VAL:HG21	1:A:186:ILE:CG2	0.67	2.18	11	3
1:A:264:TYR:CD2	1:A:269:HIS:NE2	0.67	2.63	24	1
1:A:218:GLU:CG	2:C:6:THR:HG21	0.67	2.19	22	9
1:A:240:CYS:O	1:A:244:ILE:HD12	0.67	1.90	24	17
1:A:228:ASN:C	1:A:229:LEU:HD12	0.67	2.10	24	5
1:A:230:ILE:HG13	1:A:244:ILE:HD13	0.66	1.67	14	14
1:A:244:ILE:HD13	1:A:266:TYR:OH	0.66	1.90	18	8
1:A:194:VAL:HG22	1:A:276:LEU:HD22	0.65	1.67	7	1
1:A:270:PRO:HA	1:A:273:LEU:HD21	0.65	1.69	10	18
1:A:218:GLU:HG3	2:C:6:THR:HG21	0.64	1.69	2	3
1:A:229:LEU:HB3	1:A:238:ALA:HB1	0.63	1.71	7	6
1:A:241:LYS:HG3	1:A:253:LEU:HD11	0.62	1.71	13	13
1:A:239:PHE:HB3	1:A:244:ILE:HD11	0.62	1.71	4	17
1:A:247:ASN:OD1	1:A:276:LEU:HD13	0.62	1.94	19	9
1:A:192:LEU:HD12	1:A:222:TRP:CE2	0.61	2.31	13	25
1:A:230:ILE:HG12	2:C:3:THR:HG22	0.61	1.73	1	25
1:A:229:LEU:HD23	1:A:240:CYS:HA	0.61	1.71	15	20
1:A:194:VAL:HG11	1:A:222:TRP:CZ2	0.60	2.31	3	25
1:A:266:TYR:C	1:A:267:ILE:HD13	0.59	2.18	10	25
1:A:172:THR:OG1	1:A:276:LEU:HD11	0.59	1.96	7	4
1:A:241:LYS:HG2	1:A:253:LEU:HD11	0.59	1.75	21	2
1:A:194:VAL:CG2	1:A:276:LEU:HD23	0.58	2.23	11	2
1:A:192:LEU:N	1:A:192:LEU:HD23	0.57	2.13	10	21
1:A:187:TYR:CE1	1:A:196:ILE:HD11	0.57	2.35	12	14
1:A:264:TYR:CG	1:A:269:HIS:NE2	0.57	2.73	23	24
1:A:247:ASN:OD1	1:A:276:LEU:HD22	0.56	2.00	18	2
1:A:218:GLU:HB3	2:C:6:THR:HG21	0.56	1.76	18	1
1:A:187:TYR:CE1	1:A:201:PHE:CD1	0.56	2.93	22	14
1:A:187:TYR:CE2	1:A:201:PHE:CD1	0.56	2.94	19	6
1:A:238:ALA:HB2	2:C:4:LYS:NZ	0.56	2.15	8	1
1:A:191:SER:C	1:A:192:LEU:HD23	0.55	2.21	23	25
1:A:187:TYR:CE2	1:A:196:ILE:HD11	0.55	2.37	24	6
1:A:279:ALA:O	1:A:283:VAL:HG23	0.55	2.01	23	4
1:A:173:ALA:HB2	1:A:222:TRP:CD1	0.55	2.37	16	5
1:A:273:LEU:HD12	1:A:277:VAL:HG23	0.55	1.76	3	16
1:A:245:LEU:HD23	1:A:245:LEU:O	0.55	2.02	24	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:185:SER:O	1:A:186:ILE:HG23	0.54	2.02	25	20
1:A:234:PHE:CD2	1:A:264:TYR:CE1	0.54	2.96	7	25
1:A:248:LEU:HD11	1:A:266:TYR:HE1	0.54	1.62	10	1
1:A:248:LEU:HD12	1:A:248:LEU:N	0.54	2.18	16	24
1:A:172:THR:CB	1:A:276:LEU:HD21	0.54	2.32	1	6
1:A:192:LEU:HD23	1:A:192:LEU:N	0.54	2.17	25	4
1:A:248:LEU:HD11	1:A:266:TYR:CE1	0.54	2.38	10	1
1:A:234:PHE:CE2	1:A:264:TYR:CE2	0.53	2.97	7	24
1:A:229:LEU:HD12	1:A:229:LEU:N	0.53	2.19	7	5
1:A:192:LEU:HD22	1:A:267:ILE:HD11	0.53	1.81	20	25
1:A:241:LYS:HE3	1:A:245:LEU:HD12	0.53	1.79	19	1
1:A:195:LEU:HD22	1:A:283:VAL:HG21	0.52	1.82	20	5
1:A:273:LEU:HD12	1:A:273:LEU:O	0.52	2.04	21	10
1:A:186:ILE:HD12	1:A:284:PHE:CE1	0.51	2.39	14	3
1:A:192:LEU:CD1	1:A:222:TRP:CD2	0.51	2.94	21	25
1:A:270:PRO:CA	1:A:273:LEU:HD21	0.51	2.36	18	5
1:A:241:LYS:CG	1:A:253:LEU:HD11	0.50	2.37	19	5
1:A:193:GLN:O	1:A:277:VAL:HG22	0.50	2.06	10	2
1:A:230:ILE:HD11	1:A:253:LEU:HG	0.50	1.84	8	4
1:A:229:LEU:CB	1:A:238:ALA:HB1	0.50	2.37	12	2
1:A:234:PHE:CE2	1:A:264:TYR:CZ	0.49	3.00	22	24
1:A:178:VAL:HG11	1:A:186:ILE:HG23	0.49	1.82	22	7
1:A:172:THR:HB	1:A:276:LEU:HD21	0.49	1.83	12	2
1:A:192:LEU:HD12	1:A:222:TRP:CD2	0.48	2.42	6	24
1:A:229:LEU:HD23	1:A:240:CYS:CB	0.48	2.37	17	3
1:A:266:TYR:HD1	1:A:273:LEU:HD22	0.48	1.69	1	7
1:A:248:LEU:CD1	1:A:266:TYR:OH	0.48	2.62	11	15
1:A:187:TYR:CZ	1:A:201:PHE:CD1	0.48	3.02	7	15
1:A:239:PHE:CB	1:A:244:ILE:HD11	0.48	2.38	1	5
1:A:222:TRP:CZ2	1:A:276:LEU:HD23	0.48	2.43	18	3
1:A:187:TYR:CE1	1:A:201:PHE:CE1	0.47	3.03	7	14
1:A:241:LYS:CE	1:A:245:LEU:HD12	0.47	2.39	19	1
1:A:187:TYR:HE1	1:A:196:ILE:HD11	0.47	1.66	17	14
1:A:244:ILE:CD1	1:A:266:TYR:OH	0.47	2.62	6	8
1:A:187:TYR:CD2	1:A:201:PHE:CD2	0.47	3.03	3	4
1:A:263:TRP:CD2	1:A:264:TYR:O	0.46	2.68	19	15
1:A:172:THR:OG1	1:A:276:LEU:CD2	0.46	2.64	14	1
1:A:187:TYR:HE2	1:A:196:ILE:HD11	0.46	1.67	24	5
1:A:248:LEU:HD13	1:A:266:TYR:OH	0.46	2.11	17	9
1:A:187:TYR:CE1	1:A:196:ILE:CD1	0.46	2.99	7	14
1:A:170:SER:OG	1:A:177:GLN:N	0.45	2.49	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:187:TYR:CE2	1:A:196:ILE:CD1	0.45	3.00	14	6
1:A:234:PHE:CE2	1:A:264:TYR:CE1	0.45	3.04	24	1
1:A:236:HIS:CD2	1:A:236:HIS:N	0.45	2.85	4	1
1:A:234:PHE:CD2	1:A:264:TYR:CZ	0.44	3.05	7	20
1:A:178:VAL:CG1	1:A:185:SER:OG	0.44	2.65	7	1
1:A:269:HIS:CD2	1:A:269:HIS:O	0.44	2.70	9	25
1:A:187:TYR:OH	1:A:201:PHE:CD1	0.44	2.71	7	5
1:A:204:TYR:OH	1:A:222:TRP:O	0.44	2.35	19	1
1:A:172:THR:HG21	1:A:222:TRP:CZ2	0.44	2.48	3	1
1:A:201:PHE:CD2	1:A:205:MET:CE	0.44	3.00	7	1
1:A:264:TYR:CB	1:A:269:HIS:HE2	0.44	2.25	10	12
1:A:192:LEU:CD2	1:A:267:ILE:CD1	0.44	2.95	20	15
1:A:264:TYR:CD1	1:A:269:HIS:NE2	0.44	2.86	6	6
1:A:271:GLU:CB	1:A:272:PRO:HD3	0.44	2.43	23	20
1:A:248:LEU:HD22	1:A:256:ILE:CD1	0.44	2.34	10	1
1:A:192:LEU:N	1:A:192:LEU:CD2	0.44	2.80	19	17
1:A:229:LEU:N	1:A:229:LEU:CD1	0.43	2.81	7	3
1:A:194:VAL:HG11	1:A:222:TRP:HZ2	0.43	1.72	16	6
1:A:195:LEU:HD12	1:A:284:PHE:CE2	0.43	2.49	9	6
1:A:173:ALA:HB1	1:A:223:CYS:HB3	0.43	1.89	3	1
1:A:273:LEU:O	1:A:273:LEU:HD12	0.43	2.13	6	1
1:A:195:LEU:CD1	1:A:284:PHE:CE2	0.43	3.01	2	1
1:A:273:LEU:CD1	1:A:277:VAL:HG23	0.43	2.44	15	2
1:A:230:ILE:HG22	1:A:263:TRP:CZ3	0.42	2.49	5	1
1:A:248:LEU:N	1:A:248:LEU:CD1	0.42	2.82	16	14
1:A:189:HIS:HB3	1:A:194:VAL:HG12	0.42	1.90	10	2
1:A:244:ILE:HG23	1:A:248:LEU:HD22	0.42	1.91	5	2
1:A:233:ASP:O	1:A:234:PHE:CG	0.42	2.72	24	1
1:A:274:LEU:O	1:A:278:THR:OG1	0.42	2.38	7	3
1:A:178:VAL:HG12	1:A:185:SER:OG	0.42	2.14	16	1
1:A:233:ASP:O	1:A:234:PHE:CD1	0.42	2.73	19	24
1:A:200:CYS:O	1:A:204:TYR:CD2	0.42	2.73	10	16
1:A:263:TRP:CE2	1:A:264:TYR:O	0.41	2.73	10	12
1:A:269:HIS:CD2	1:A:269:HIS:N	0.41	2.88	15	6
1:A:266:TYR:HB3	1:A:273:LEU:HD22	0.41	1.92	19	2
1:A:219:GLN:C	1:A:229:LEU:HD21	0.41	2.36	20	1
1:A:189:HIS:CB	1:A:194:VAL:HG12	0.41	2.44	3	3
1:A:229:LEU:O	2:C:4:LYS:N	0.41	2.53	21	2
1:A:253:LEU:HA	1:A:256:ILE:HD12	0.41	1.93	25	1
1:A:170:SER:OG	1:A:177:GLN:CA	0.41	2.68	6	1
1:A:185:SER:O	1:A:185:SER:OG	0.41	2.38	6	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:187:TYR:CE2	1:A:201:PHE:CE1	0.41	3.09	19	2
1:A:248:LEU:CD1	1:A:248:LEU:N	0.41	2.84	15	2
1:A:247:ASN:CG	1:A:276:LEU:HD12	0.40	2.37	7	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	100/142 (70%)	76±2 (76±2%)	21±2 (21±2%)	4±1 (4±1%)	6 34
2	C	4/15 (27%)	3±1 (81±15%)	1±1 (19±15%)	0±0 (0±0%)	100 100
All	All	2600/3925 (66%)	1979 (76%)	532 (20%)	89 (3%)	6 36

All 8 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	190	PRO	25
1	A	194	VAL	24
1	A	228	ASN	20
1	A	271	GLU	12
1	A	264	TYR	4
1	A	224	ALA	2
1	A	262	GLN	1
1	A	226	GLY	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	92/127 (72%)	77±2 (83±2%)	15±2 (17±2%)	5 41
2	C	4/9 (44%)	3±1 (87±14%)	1±1 (13±14%)	7 48
All	All	2400/3400 (71%)	2003 (83%)	397 (17%)	5 41

All 47 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	192	LEU	25
1	A	201	PHE	25
1	A	269	HIS	25
1	A	222	TRP	24
1	A	219	GLN	23
1	A	274	LEU	22
1	A	194	VAL	21
1	A	233	ASP	17
1	A	242	LYS	15
1	A	170	SER	14
1	A	271	GLU	12
1	A	221	ARG	12
1	A	273	LEU	12
1	A	225	GLU	11
2	C	4	LYS	10
1	A	188	ARG	10
1	A	177	GLN	9
1	A	198	LYS	9
1	A	207	ASP	7
1	A	250	ARG	7
1	A	276	LEU	7
1	A	259	GLU	6
1	A	251	LYS	6
1	A	278	THR	6
1	A	185	SER	5
1	A	246	ARG	5
1	A	245	LEU	5
1	A	257	MET	5
1	A	255	THR	4
1	A	275	ASP	4
1	A	266	TYR	4
1	A	218	GLU	3
2	C	5	GLN	3
1	A	208	ASP	3

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Mol	Chain	Res	Type	Models (Total)
1	A	262	GLN	3
1	A	254	SER	3
1	A	237	ASN	2
1	A	205	MET	2
1	A	258	ASP	2
1	A	236	HIS	2
1	A	260	ASN	1
1	A	193	GLN	1
1	A	202	LYS	1
1	A	228	ASN	1
1	A	195	LEU	1
1	A	229	LEU	1
1	A	241	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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	M3L	C	9	2	10,11,12	0.59±0.01	0±0 (0±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of angles that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Bond angles		
					Counts	RMSZ	#Z>2
2	M3L	C	9	2	9,14,16	0.85±0.02	1±0 (11±0%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	M3L	C	9	2	-	0±0,9,10,12	-

There are no bond-length outliers.

All unique angle outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})	Models	
								Worst	Total
2	C	9	M3L	CD-CE-NZ	2.22	107.84	115.97	23	25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6.5 Carbohydrates (i)

There are no monosaccharides in this entry.

6.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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)

The completeness of assignment taking into account all chemical shift lists is 77% for the well-defined parts and 71% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chem_shift_list_1*

7.1.1 Bookkeeping (i)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	1483
Number of shifts mapped to atoms	1483
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	3

7.1.2 Chemical shift referencing (i)

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction ± precision, *ppm*	Suggested action
$^{13}C_{\alpha}$	136	-0.56 ± 0.14	Should be checked
$^{13}C_{\beta}$	117	0.24 ± 0.20	None needed (< 0.5 ppm)
$^{13}C'$	0	—	None (insufficient data)
^{15}N	133	-0.22 ± 0.35	None needed (< 0.5 ppm)

7.1.3 Completeness of resonance assignments (i)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 77%, i.e. 1073 atoms were assigned a chemical shift out of a possible 1392. 0 out of 13 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	401/518 (77%)	207/209 (99%)	98/208 (47%)	96/101 (95%)
Sidechain	556/744 (75%)	404/481 (84%)	142/232 (61%)	10/31 (32%)

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	Total	^{1}H	^{13}C	^{15}N
Aromatic	116/130 (89%)	58/64 (91%)	56/61 (92%)	2/5 (40%)
Overall	1073/1392 (77%)	669/754 (89%)	296/501 (59%)	108/137 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 71%, i.e. 1476 atoms were assigned a chemical shift out of a possible 2071. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^{1}H	^{13}C	^{15}N
Backbone	564/785 (72%)	295/320 (92%)	136/312 (44%)	133/153 (87%)
Sidechain	778/1132 (69%)	573/727 (79%)	192/350 (55%)	13/55 (24%)
Aromatic	134/154 (87%)	67/77 (87%)	65/70 (93%)	2/7 (29%)
Overall	1476/2071 (71%)	935/1124 (83%)	393/732 (54%)	148/215 (69%)

7.1.4 Statistically unusual chemical shifts (i)

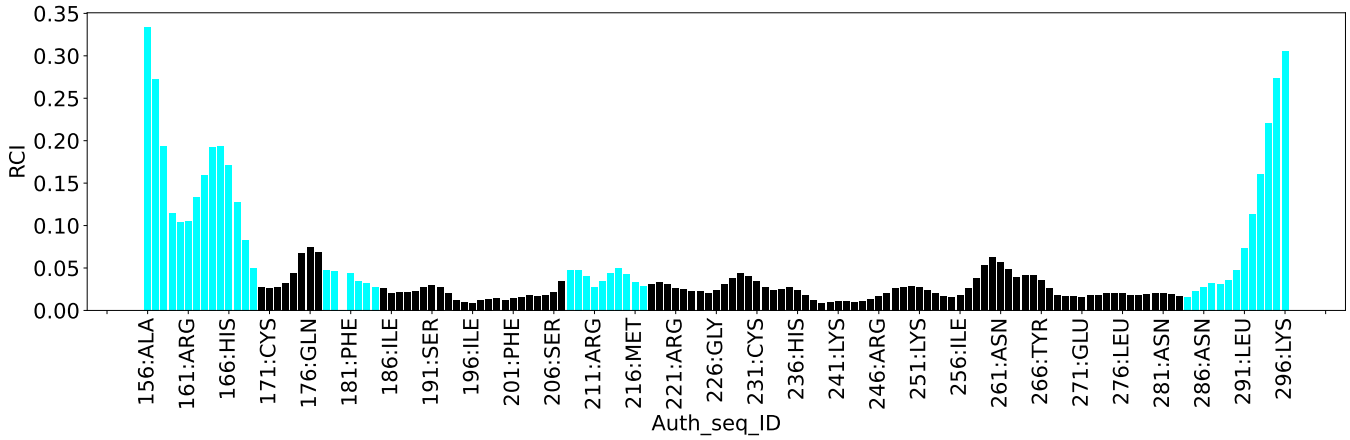
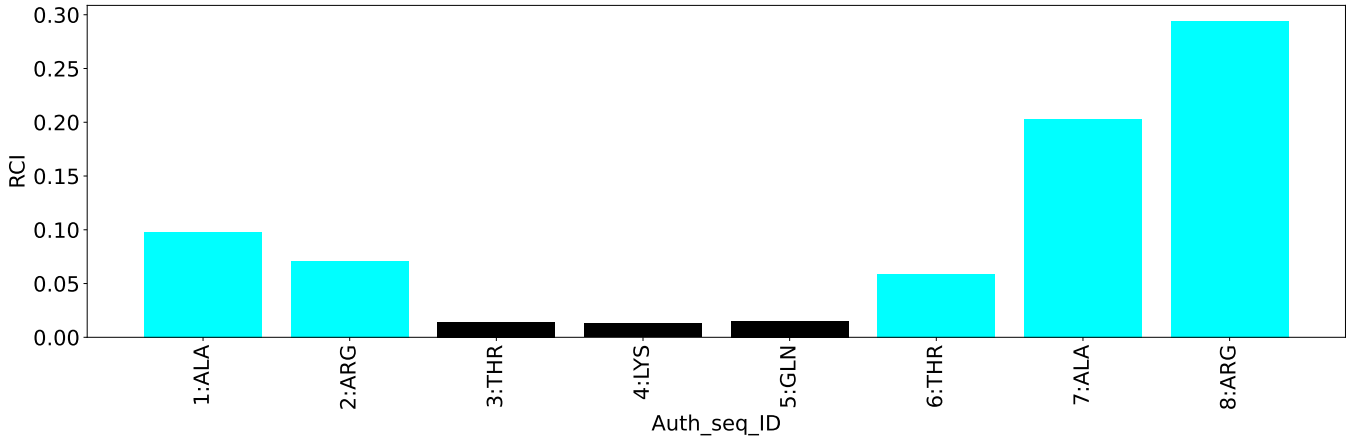
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

List Id	Chain	Res	Type	Atom	Shift, *ppm*	Expected range, *ppm*	Z-score
1	A	192	LEU	HD11	-0.63	-0.61 – 2.12	-5.1
1	A	192	LEU	HD12	-0.63	-0.61 – 2.12	-5.1
1	A	192	LEU	HD13	-0.63	-0.61 – 2.12	-5.1

7.1.5 Random Coil Index (RCI) plots (i)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.If well-defined core and ill-defined regions are not identified then it is shown as gray bars.

Random coil index (RCI) for chain A:



Random coil index (RCI) for chain C: