



Full wwPDB NMR Structure Validation Report ⓘ

Dec 13, 2023 – 10:13 PM EST

PDB ID : 2JM1
BMRB ID : 15001
Title : Structures and chemical shift assignments for the ADD domain of the ATRX protein
Authors : Yang, J.; Neuhaus, D.
Deposited on : 2006-09-13

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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 : 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) : 2.36

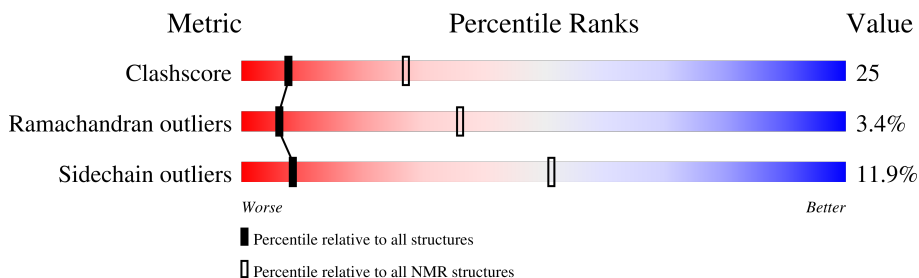
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment was not calculated.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	141	

2 Ensemble composition and analysis i

This entry contains 32 models. Model 3 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:169-A:204, A:218-A:256, A:262-A:288 (102)	0.34	3

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 6 clusters and 3 single-model clusters were found.

Cluster number	Models
1	2, 3, 5, 6, 10, 12, 13, 14, 15, 16, 19, 27, 29, 31
2	7, 11, 17, 18
3	8, 20, 21, 28
4	1, 9, 26
5	22, 23
6	25, 30
Single-model clusters	4; 24; 32

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 2193 atoms, of which 1066 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	141	2190	694	1066	199	213	18	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	156	GLY	-	cloning artifact	UNP P46100
A	157	ALA	-	cloning artifact	UNP P46100
A	158	MET	-	cloning artifact	UNP P46100

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

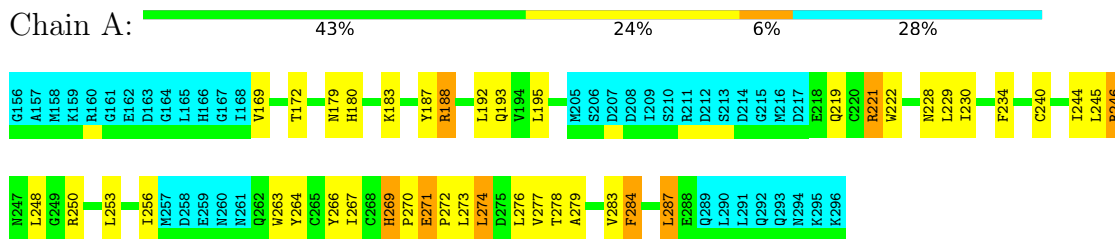
Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	3	3	3

4 Residue-property plots

4.1 Average score per residue in the NMR ensemble

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

- Molecule 1: Transcriptional regulator ATRX

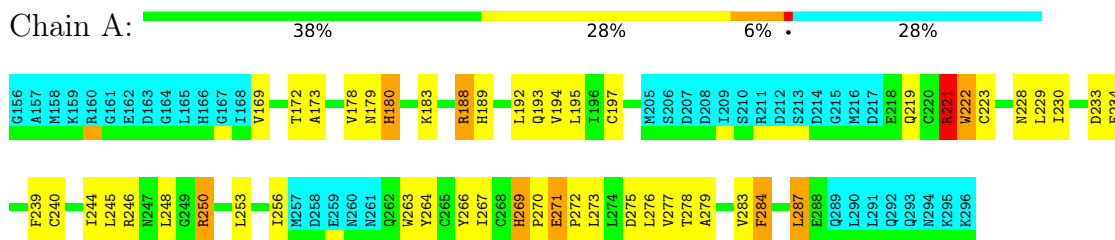


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

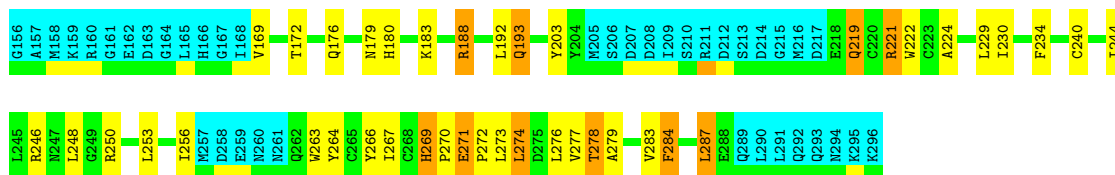
- Molecule 1: Transcriptional regulator ATRX



4.2.2 Score per residue for model 2

- Molecule 1: Transcriptional regulator ATRX





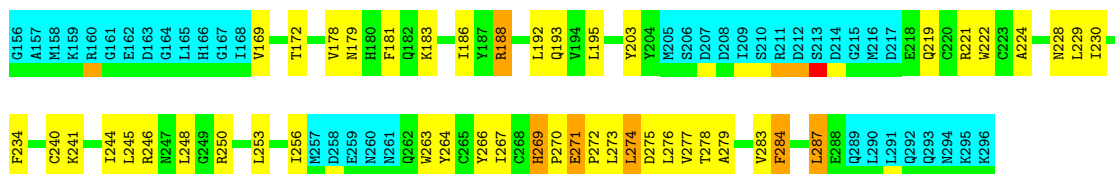
4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Transcriptional regulator ATRX



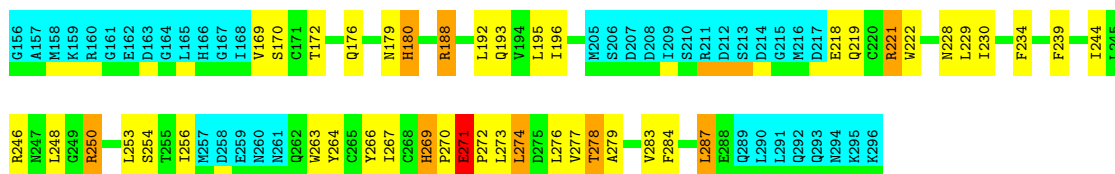
4.2.4 Score per residue for model 4

- Molecule 1: Transcriptional regulator ATRX



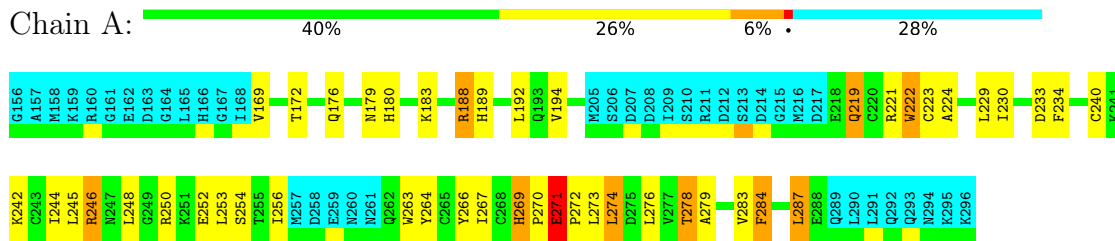
4.2.5 Score per residue for model 5

- Molecule 1: Transcriptional regulator ATRX



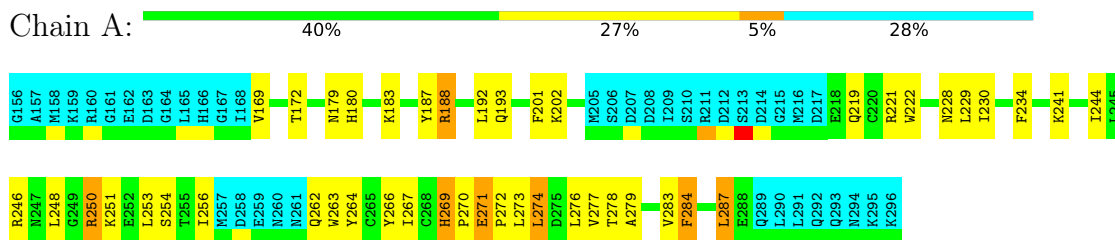
4.2.6 Score per residue for model 6

- Molecule 1: Transcriptional regulator ATRX



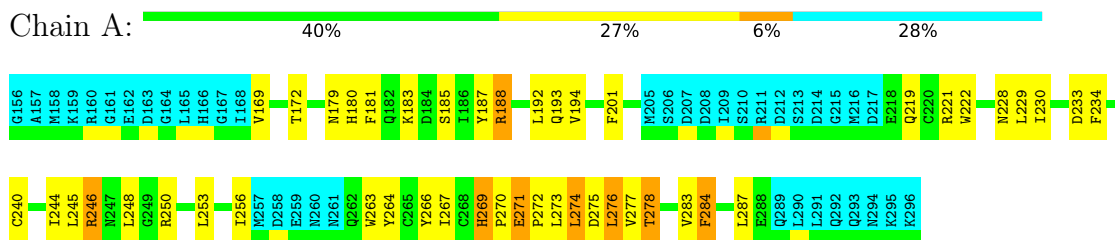
4.2.7 Score per residue for model 7

- Molecule 1: Transcriptional regulator ATRX



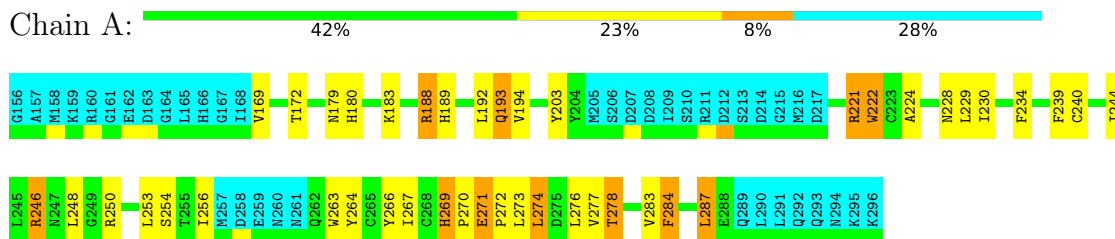
4.2.8 Score per residue for model 8

- Molecule 1: Transcriptional regulator ATRX



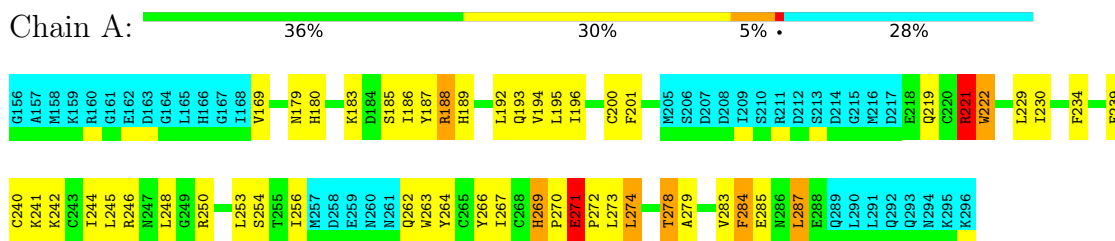
4.2.9 Score per residue for model 9

- Molecule 1: Transcriptional regulator ATRX



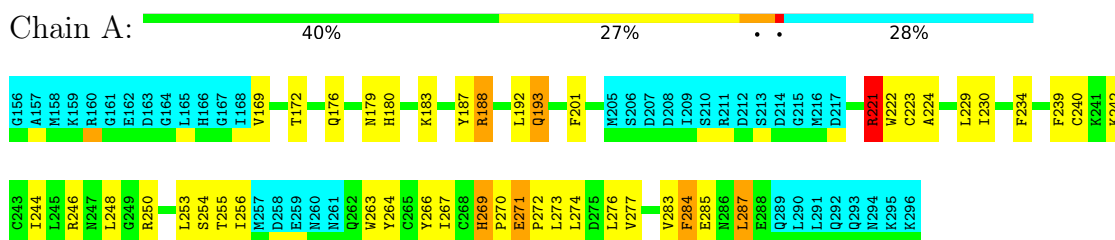
4.2.10 Score per residue for model 10

- Molecule 1: Transcriptional regulator ATRX



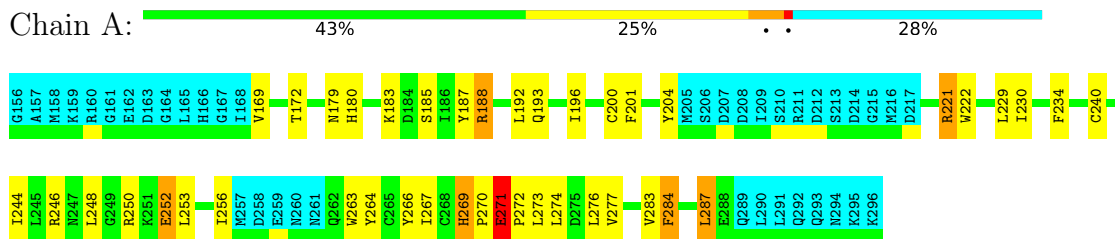
4.2.11 Score per residue for model 11

- Molecule 1: Transcriptional regulator ATRX



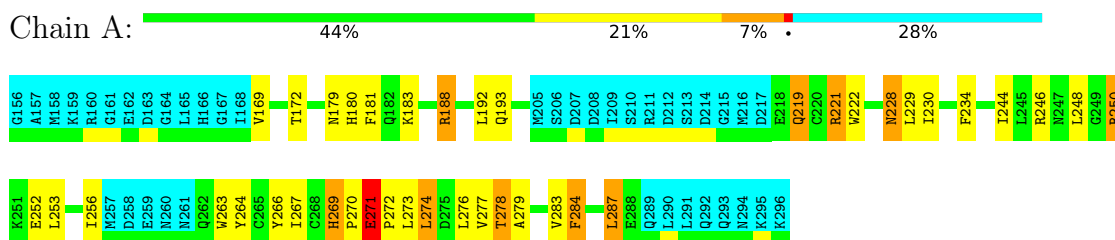
4.2.12 Score per residue for model 12

- Molecule 1: Transcriptional regulator ATRX



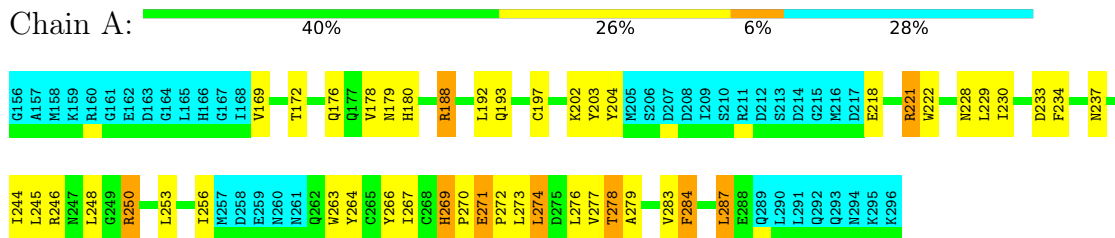
4.2.13 Score per residue for model 13

- Molecule 1: Transcriptional regulator ATRX



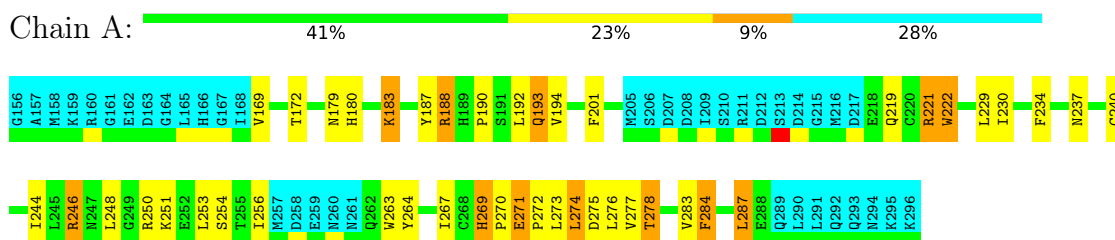
4.2.14 Score per residue for model 14

- Molecule 1: Transcriptional regulator ATRX



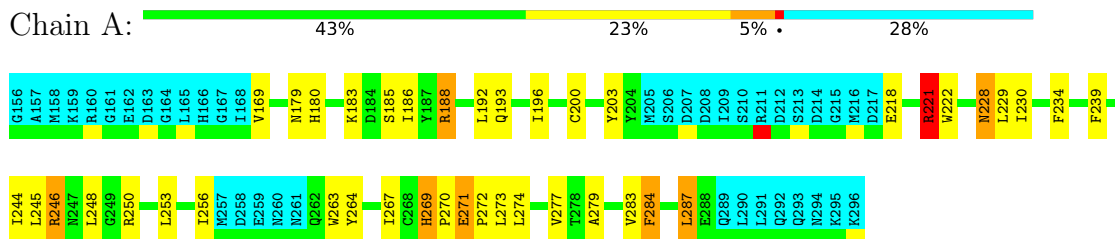
4.2.15 Score per residue for model 15

- Molecule 1: Transcriptional regulator ATRX



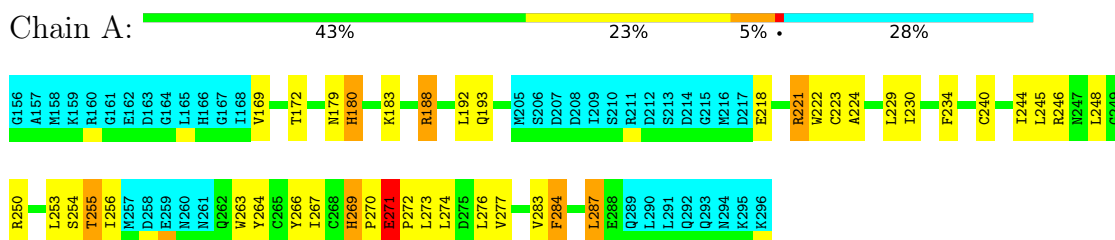
4.2.16 Score per residue for model 16

- Molecule 1: Transcriptional regulator ATRX



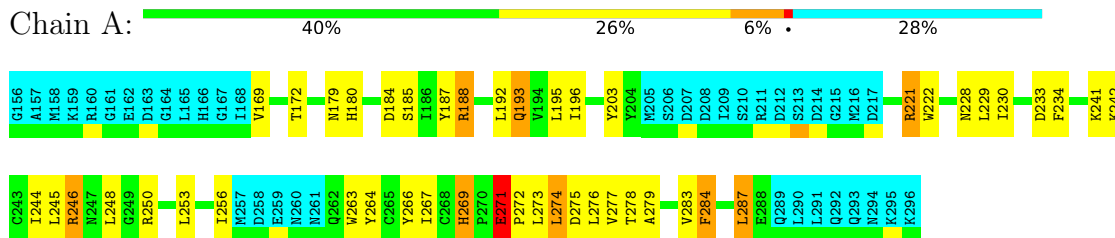
4.2.17 Score per residue for model 17

- Molecule 1: Transcriptional regulator ATRX



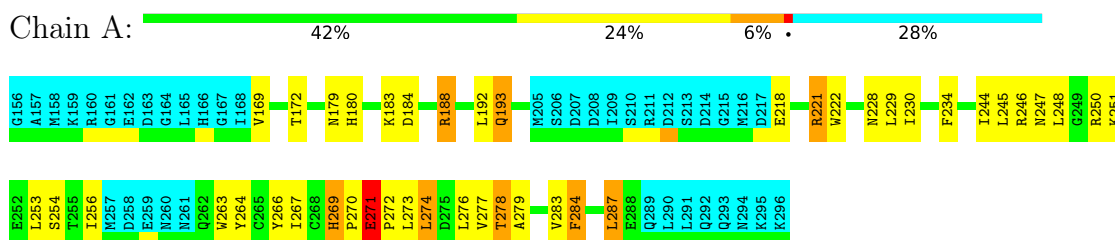
4.2.18 Score per residue for model 18

- Molecule 1: Transcriptional regulator ATRX



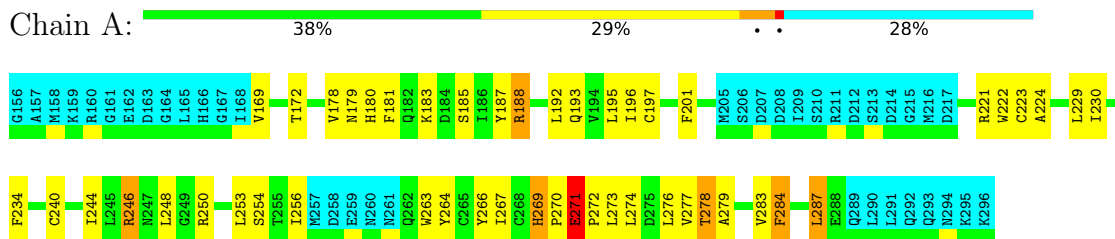
4.2.19 Score per residue for model 19

- Molecule 1: Transcriptional regulator ATRX



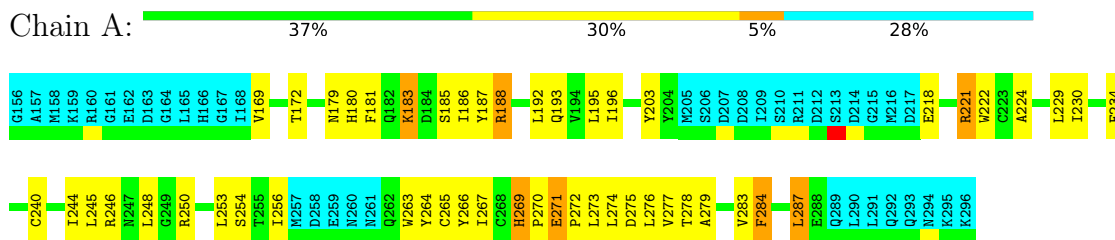
4.2.20 Score per residue for model 20

- Molecule 1: Transcriptional regulator ATRX



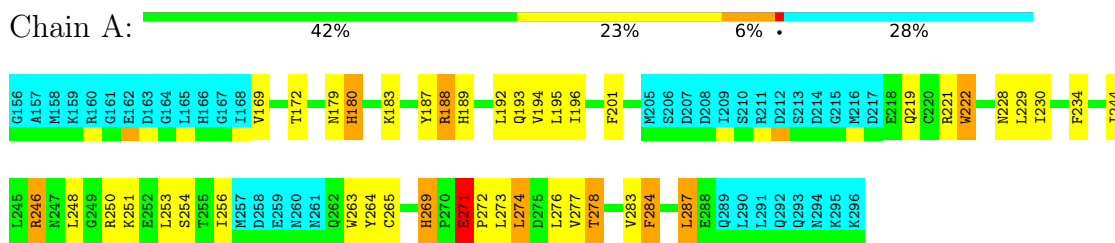
4.2.21 Score per residue for model 21

- Molecule 1: Transcriptional regulator ATRX



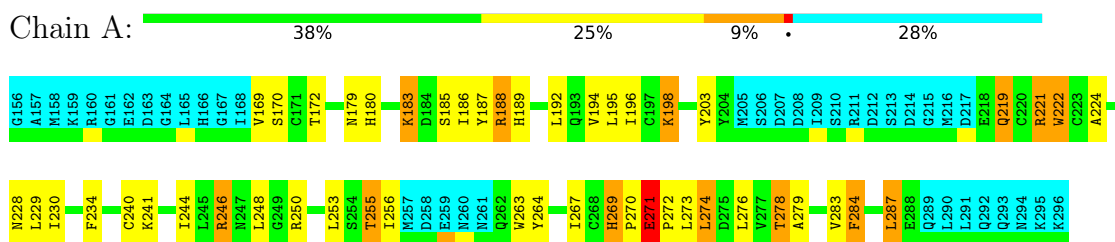
4.2.22 Score per residue for model 22

- Molecule 1: Transcriptional regulator ATRX



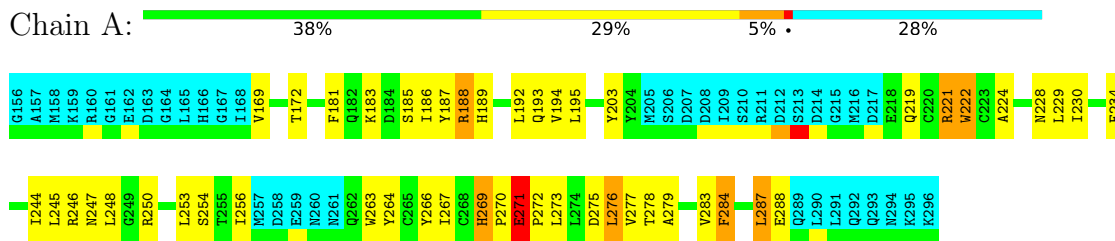
4.2.23 Score per residue for model 23

- Molecule 1: Transcriptional regulator ATRX



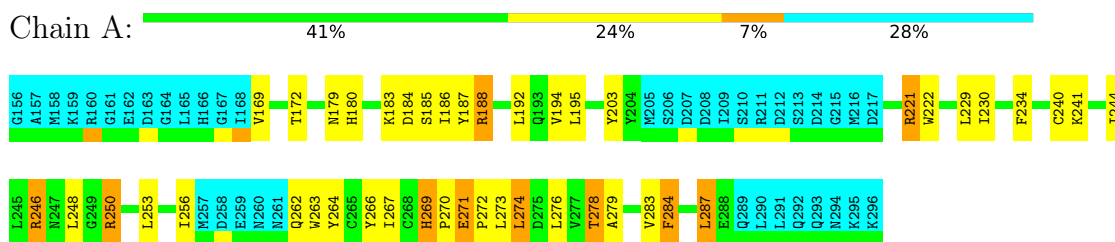
4.2.24 Score per residue for model 24

- Molecule 1: Transcriptional regulator ATRX



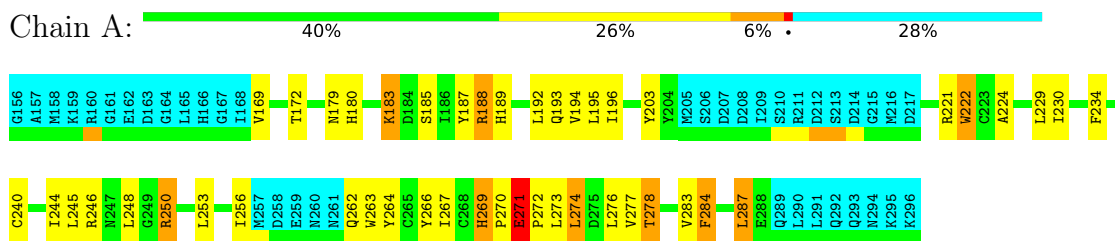
4.2.25 Score per residue for model 25

- Molecule 1: Transcriptional regulator ATRX



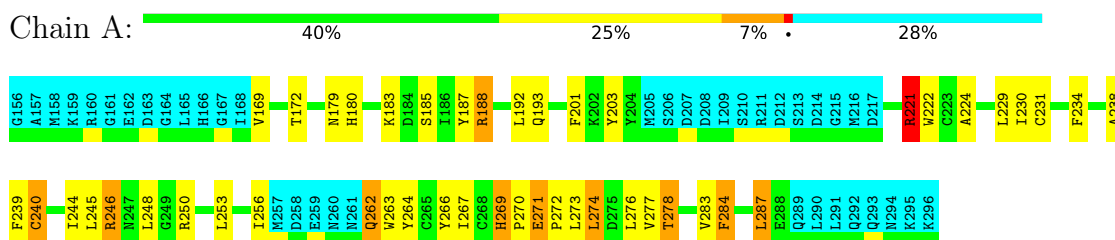
4.2.26 Score per residue for model 26

- Molecule 1: Transcriptional regulator ATRX



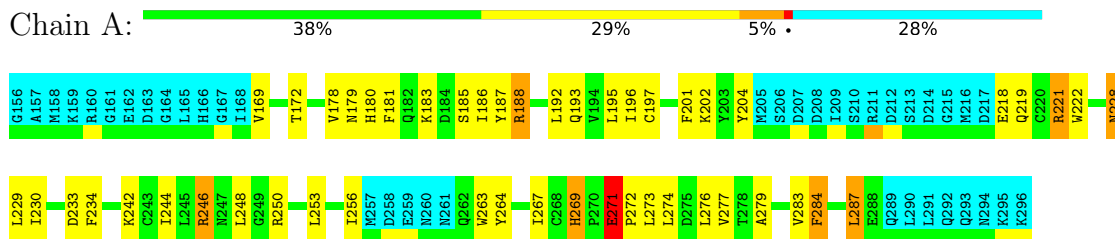
4.2.27 Score per residue for model 27

- Molecule 1: Transcriptional regulator ATRX



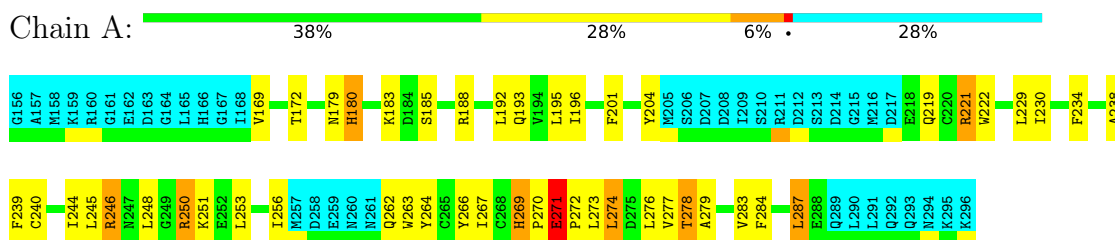
4.2.28 Score per residue for model 28

- Molecule 1: Transcriptional regulator ATRX



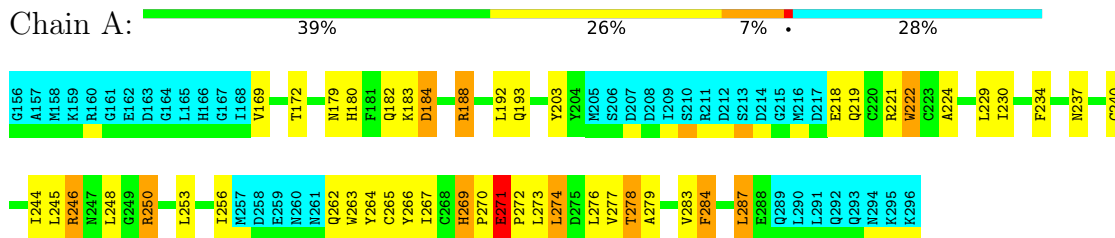
4.2.29 Score per residue for model 29

- Molecule 1: Transcriptional regulator ATRX



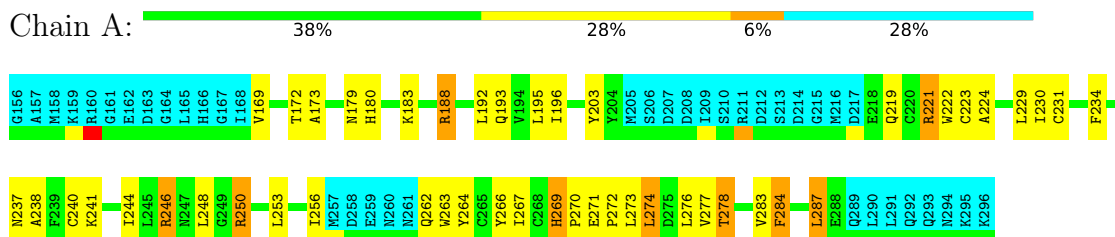
4.2.30 Score per residue for model 30

- Molecule 1: Transcriptional regulator ATRX



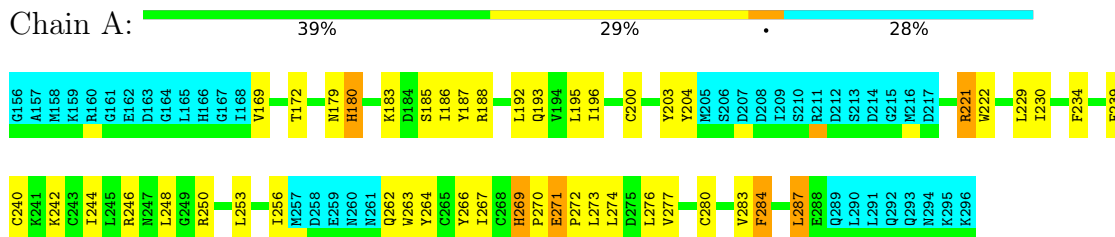
4.2.31 Score per residue for model 31

- Molecule 1: Transcriptional regulator ATRX



4.2.32 Score per residue for model 32

- Molecule 1: Transcriptional regulator ATRX



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 32 were deposited, based on the following criterion: *lowest energy*.

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

Software name	Classification	Version
X-PLOR	structure solution	3.8
X-PLOR	refinement	3.8

No chemical shift data was provided.

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

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

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	Chirality	Planarity
1	A	0.0±0.0	4.0±0.0
All	All	0	128

There are no bond-length outliers.

There are no bond-angle outliers.

There are no chirality outliers.

All unique planar outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	188	ARG	Sidechain	32
1	A	221	ARG	Sidechain	32
1	A	246	ARG	Sidechain	32
1	A	250	ARG	Sidechain	32

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	824	784	784	41±5
All	All	26464	25088	25088	1310

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 25.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:172:THR:OG1	1:A:276:LEU:HD21	0.88	1.68	31	27
1:A:169:VAL:HG23	1:A:283:VAL:HG11	0.86	1.47	26	6
1:A:169:VAL:HG22	1:A:283:VAL:HG13	0.86	1.45	22	24
1:A:195:LEU:HD12	1:A:284:PHE:CD2	0.85	2.06	32	3
1:A:230:ILE:HD11	1:A:253:LEU:CD2	0.82	2.05	26	31
1:A:192:LEU:O	1:A:194:VAL:HG13	0.79	1.78	22	5
1:A:169:VAL:HG23	1:A:283:VAL:CG1	0.78	2.09	25	6
1:A:230:ILE:HD11	1:A:253:LEU:HD21	0.76	1.57	26	31
1:A:193:GLN:O	1:A:277:VAL:HG13	0.75	1.82	1	25
1:A:169:VAL:HG13	1:A:283:VAL:HG11	0.74	1.58	28	16
1:A:244:ILE:CG2	1:A:248:LEU:HD11	0.74	2.13	13	3
1:A:230:ILE:HD12	1:A:244:ILE:CD1	0.71	2.15	18	32
1:A:228:ASN:C	1:A:229:LEU:HD12	0.69	2.08	5	10
1:A:230:ILE:HD11	1:A:253:LEU:CG	0.68	2.19	6	31
1:A:178:VAL:HG21	1:A:186:ILE:HG22	0.67	1.63	4	1
1:A:253:LEU:HA	1:A:256:ILE:HD12	0.67	1.66	23	32
1:A:247:ASN:OD1	1:A:276:LEU:HD13	0.66	1.89	24	1
1:A:256:ILE:HG23	1:A:263:TRP:CD1	0.66	2.26	11	32
1:A:270:PRO:HA	1:A:273:LEU:HD21	0.65	1.67	4	28
1:A:192:LEU:HD13	1:A:222:TRP:CE2	0.65	2.27	22	3
1:A:248:LEU:HD12	1:A:248:LEU:O	0.64	1.92	26	29
1:A:193:GLN:O	1:A:277:VAL:HG22	0.64	1.93	8	20
1:A:192:LEU:HD21	1:A:267:ILE:HD13	0.63	1.71	1	31
1:A:256:ILE:HG23	1:A:263:TRP:CG	0.62	2.30	15	25
1:A:229:LEU:HD23	1:A:240:CYS:HA	0.61	1.71	20	21
1:A:279:ALA:O	1:A:283:VAL:HG23	0.61	1.96	5	21
1:A:187:TYR:O	1:A:195:LEU:HD22	0.61	1.96	10	2
1:A:172:THR:CB	1:A:276:LEU:HD21	0.61	2.25	1	13
1:A:203:TYR:CE2	1:A:224:ALA:HB3	0.61	2.30	4	10
1:A:256:ILE:HG23	1:A:263:TRP:CE2	0.60	2.31	29	13
1:A:245:LEU:HD23	1:A:245:LEU:O	0.60	1.97	30	16
1:A:248:LEU:HD13	1:A:252:GLU:HB3	0.60	1.73	13	2
1:A:192:LEU:O	1:A:194:VAL:HG23	0.59	1.97	25	5
1:A:169:VAL:HG13	1:A:283:VAL:CG1	0.59	2.26	28	12
1:A:230:ILE:HD11	1:A:253:LEU:HG	0.58	1.73	27	31
1:A:192:LEU:HD22	1:A:266:TYR:HB3	0.58	1.74	1	27
1:A:195:LEU:HD23	1:A:196:ILE:N	0.57	2.13	28	9
1:A:253:LEU:HD23	1:A:253:LEU:O	0.57	2.00	31	26
1:A:169:VAL:HG22	1:A:283:VAL:CG1	0.57	2.26	22	2
1:A:194:VAL:HG21	1:A:276:LEU:HD23	0.57	1.77	8	1
1:A:244:ILE:HB	1:A:253:LEU:HD12	0.57	1.76	26	9

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:273:LEU:N	1:A:273:LEU:HD23	0.57	2.15	3	31
1:A:186:ILE:HB	1:A:195:LEU:HD21	0.56	1.77	23	3
1:A:196:ILE:HD12	1:A:200:CYS:HB3	0.56	1.77	10	4
1:A:230:ILE:HD12	1:A:244:ILE:HD12	0.56	1.76	30	12
1:A:230:ILE:HG21	1:A:256:ILE:HG21	0.55	1.77	28	12
1:A:189:HIS:CE1	1:A:192:LEU:HD12	0.55	2.36	22	2
1:A:192:LEU:CD2	1:A:267:ILE:HD13	0.55	2.31	20	31
1:A:287:LEU:HD13	1:A:287:LEU:O	0.55	2.01	25	31
1:A:192:LEU:HD22	1:A:266:TYR:CB	0.55	2.32	1	4
1:A:195:LEU:HD23	1:A:284:PHE:CE2	0.55	2.36	10	1
1:A:194:VAL:HG12	1:A:277:VAL:HG22	0.55	1.79	1	2
1:A:229:LEU:HD23	1:A:240:CYS:CA	0.55	2.31	20	9
1:A:194:VAL:HG11	1:A:273:LEU:HD12	0.54	1.77	26	5
1:A:264:TYR:CD1	1:A:269:HIS:NE2	0.54	2.75	31	30
1:A:195:LEU:HD13	1:A:196:ILE:N	0.54	2.17	26	1
1:A:264:TYR:CD2	1:A:269:HIS:NE2	0.54	2.76	18	2
1:A:194:VAL:HG21	1:A:222:TRP:CZ2	0.54	2.37	1	5
1:A:195:LEU:C	1:A:195:LEU:HD13	0.53	2.23	10	1
1:A:178:VAL:HG22	1:A:197:CYS:HB3	0.53	1.80	20	2
1:A:241:LYS:HG3	1:A:253:LEU:HD13	0.52	1.80	23	1
1:A:244:ILE:HG23	1:A:248:LEU:HD11	0.52	1.82	13	2
1:A:234:PHE:CZ	1:A:264:TYR:CE2	0.52	2.98	13	2
1:A:234:PHE:CE2	1:A:264:TYR:CE2	0.52	2.99	9	28
1:A:256:ILE:HG23	1:A:263:TRP:NE1	0.52	2.20	21	12
1:A:189:HIS:CD2	1:A:222:TRP:CD1	0.51	2.99	3	8
1:A:264:TYR:CD1	1:A:269:HIS:CE1	0.51	2.99	10	30
1:A:275:ASP:HA	1:A:278:THR:OG1	0.51	2.06	1	3
1:A:192:LEU:O	1:A:193:GLN:CB	0.50	2.59	15	1
1:A:234:PHE:CE2	1:A:264:TYR:CE1	0.50	2.99	18	1
1:A:186:ILE:HD12	1:A:195:LEU:HD11	0.50	1.82	4	2
1:A:194:VAL:HG21	1:A:222:TRP:HZ2	0.50	1.67	23	5
1:A:244:ILE:HG22	1:A:248:LEU:HD11	0.50	1.83	28	2
1:A:230:ILE:HD12	1:A:244:ILE:HD11	0.50	1.83	17	7
1:A:229:LEU:HD12	1:A:229:LEU:N	0.50	2.22	24	8
1:A:234:PHE:CZ	1:A:264:TYR:CE1	0.50	3.00	28	1
1:A:169:VAL:HG11	1:A:186:ILE:CG2	0.49	2.38	32	2
1:A:273:LEU:C	1:A:273:LEU:HD12	0.49	2.28	30	1
1:A:195:LEU:HD13	1:A:195:LEU:C	0.49	2.28	26	1
1:A:256:ILE:CG2	1:A:263:TRP:CE2	0.49	2.96	30	6
1:A:264:TYR:CD2	1:A:269:HIS:CE1	0.49	3.00	18	1
1:A:183:LYS:HA	1:A:287:LEU:HD11	0.48	1.83	24	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:195:LEU:C	1:A:195:LEU:HD23	0.48	2.29	32	1
1:A:173:ALA:HB1	1:A:223:CYS:HB3	0.48	1.85	31	2
1:A:192:LEU:CD1	1:A:222:TRP:CE2	0.48	2.97	22	5
1:A:248:LEU:C	1:A:248:LEU:HD12	0.48	2.28	14	3
1:A:245:LEU:HD13	1:A:250:ARG:HB2	0.48	1.86	29	1
1:A:228:ASN:O	1:A:229:LEU:HD12	0.48	2.07	13	2
1:A:192:LEU:CD1	1:A:222:TRP:CD2	0.48	2.97	26	5
1:A:169:VAL:HG11	1:A:186:ILE:HG21	0.47	1.86	16	3
1:A:172:THR:HG21	1:A:276:LEU:HD21	0.47	1.85	24	1
1:A:248:LEU:HD12	1:A:248:LEU:C	0.47	2.30	1	29
1:A:194:VAL:HG12	1:A:277:VAL:CG2	0.47	2.40	1	1
1:A:271:GLU:CB	1:A:272:PRO:HD3	0.47	2.39	22	32
1:A:218:GLU:O	1:A:229:LEU:HD22	0.47	2.10	16	2
1:A:172:THR:HG21	1:A:222:TRP:CZ2	0.47	2.45	1	1
1:A:188:ARG:CG	1:A:284:PHE:CE2	0.47	2.98	25	25
1:A:230:ILE:CD1	1:A:253:LEU:HD21	0.47	2.38	4	2
1:A:183:LYS:HA	1:A:287:LEU:HD21	0.46	1.88	22	23
1:A:187:TYR:CD2	1:A:201:PHE:CG	0.46	3.03	8	5
1:A:192:LEU:HD13	1:A:222:TRP:CD2	0.46	2.46	22	2
1:A:178:VAL:HG13	1:A:197:CYS:HB2	0.46	1.87	28	3
1:A:185:SER:OG	1:A:186:ILE:N	0.46	2.49	28	2
1:A:274:LEU:O	1:A:278:THR:OG1	0.46	2.34	31	22
1:A:247:ASN:ND2	1:A:276:LEU:HD22	0.46	2.26	19	1
1:A:187:TYR:CD1	1:A:201:PHE:CG	0.45	3.04	15	5
1:A:221:ARG:CB	1:A:239:PHE:CZ	0.45	2.99	29	7
1:A:172:THR:OG1	1:A:276:LEU:CD2	0.45	2.64	4	7
1:A:234:PHE:CE2	1:A:264:TYR:CD1	0.45	3.04	18	1
1:A:195:LEU:CD1	1:A:284:PHE:CD2	0.45	3.00	4	2
1:A:270:PRO:HA	1:A:273:LEU:HD11	0.45	1.88	30	1
1:A:187:TYR:CD2	1:A:198:LYS:HA	0.44	2.47	23	1
1:A:230:ILE:HD13	1:A:256:ILE:HG21	0.44	1.88	13	1
1:A:223:CYS:O	1:A:224:ALA:HB3	0.44	2.13	17	4
1:A:178:VAL:HG22	1:A:197:CYS:CB	0.43	2.42	20	1
1:A:222:TRP:CZ3	1:A:266:TYR:CG	0.43	3.06	30	1
1:A:230:ILE:HG22	1:A:263:TRP:CZ3	0.43	2.48	30	1
1:A:230:ILE:HD12	1:A:244:ILE:HD13	0.43	1.87	15	1
1:A:230:ILE:O	1:A:238:ALA:HB1	0.43	2.14	31	3
1:A:275:ASP:OD2	1:A:276:LEU:HD12	0.43	2.14	4	1
1:A:194:VAL:CG1	1:A:273:LEU:HD12	0.43	2.44	26	1
1:A:273:LEU:N	1:A:273:LEU:CD2	0.43	2.82	3	18
1:A:221:ARG:CB	1:A:239:PHE:CE1	0.42	3.03	5	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:185:SER:O	1:A:187:TYR:CD2	0.42	2.72	18	8
1:A:172:THR:CG2	1:A:222:TRP:CE2	0.42	3.02	1	1
1:A:172:THR:HB	1:A:276:LEU:HD21	0.42	1.92	12	1
1:A:181:PHE:O	1:A:181:PHE:CG	0.42	2.71	28	5
1:A:256:ILE:HG23	1:A:263:TRP:CD2	0.42	2.49	31	4
1:A:183:LYS:CA	1:A:287:LEU:HD11	0.42	2.43	24	1
1:A:188:ARG:HG3	1:A:284:PHE:CE2	0.42	2.50	10	28
1:A:195:LEU:HD23	1:A:196:ILE:O	0.42	2.14	23	1
1:A:273:LEU:HD13	1:A:277:VAL:HG23	0.41	1.91	30	1
1:A:269:HIS:NE2	1:A:271:GLU:OE1	0.41	2.53	8	1
1:A:229:LEU:CD2	1:A:240:CYS:CB	0.41	2.99	27	4
1:A:186:ILE:HD11	1:A:287:LEU:HD23	0.41	1.91	25	1
1:A:221:ARG:HB2	1:A:239:PHE:CZ	0.41	2.51	32	4
1:A:230:ILE:CD1	1:A:244:ILE:CD1	0.41	2.98	22	2
1:A:273:LEU:HD23	1:A:273:LEU:H	0.41	1.76	11	8
1:A:275:ASP:O	1:A:278:THR:OG1	0.41	2.38	21	2
1:A:172:THR:HG21	1:A:222:TRP:CE2	0.41	2.50	1	1
1:A:195:LEU:HD22	1:A:283:VAL:HG11	0.41	1.93	4	1
1:A:185:SER:O	1:A:187:TYR:CD1	0.41	2.74	28	2
1:A:194:VAL:HG22	1:A:276:LEU:HB3	0.41	1.93	3	1
1:A:241:LYS:HA	1:A:253:LEU:HD11	0.41	1.92	10	1
1:A:263:TRP:CH2	1:A:265:CYS:CB	0.41	3.04	21	3
1:A:269:HIS:CG	1:A:271:GLU:OE1	0.41	2.74	23	1
1:A:195:LEU:HD23	1:A:284:PHE:CD2	0.41	2.51	26	1
1:A:221:ARG:HB3	1:A:239:PHE:CZ	0.40	2.51	11	1
1:A:269:HIS:CE1	1:A:271:GLU:OE2	0.40	2.74	13	2
1:A:263:TRP:CE2	1:A:264:TYR:O	0.40	2.74	18	2
1:A:195:LEU:HD13	1:A:283:VAL:HB	0.40	1.93	1	2
1:A:248:LEU:HD13	1:A:252:GLU:OE1	0.40	2.16	6	1
1:A:230:ILE:HG21	1:A:256:ILE:CG2	0.40	2.46	28	1
1:A:172:THR:CG2	1:A:222:TRP:NE1	0.40	2.84	1	1
1:A:236:HIS:CD2	1:A:236:HIS:N	0.40	2.90	3	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	102/141 (72%)	83±1 (82±1%)	15±2 (15±2%)	4±1 (3±1%)	6	36
All	All	3264/4512 (72%)	2671 (82%)	481 (15%)	112 (3%)	6	36

All 10 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	179	ASN	31
1	A	271	GLU	31
1	A	180	HIS	30
1	A	228	ASN	8
1	A	262	GLN	6
1	A	184	ASP	2
1	A	181	PHE	1
1	A	190	PRO	1
1	A	193	GLN	1
1	A	218	GLU	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	94/127 (74%)	83±2 (88±2%)	11±2 (12±2%)	8	51
All	All	3008/4064 (74%)	2651 (88%)	357 (12%)	8	51

All 41 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	222	TRP	32
1	A	269	HIS	32
1	A	284	PHE	32
1	A	287	LEU	32
1	A	274	LEU	29
1	A	221	ARG	20
1	A	278	THR	20
1	A	246	ARG	16

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Mol	Chain	Res	Type	Models (Total)
1	A	271	GLU	16
1	A	254	SER	13
1	A	250	ARG	9
1	A	183	LYS	9
1	A	180	HIS	7
1	A	219	GLN	7
1	A	233	ASP	6
1	A	193	GLN	6
1	A	242	LYS	6
1	A	176	GLN	5
1	A	237	ASN	5
1	A	241	LYS	5
1	A	251	LYS	5
1	A	185	SER	5
1	A	204	TYR	5
1	A	262	GLN	4
1	A	218	GLU	4
1	A	202	LYS	3
1	A	275	ASP	3
1	A	184	ASP	3
1	A	170	SER	2
1	A	276	LEU	2
1	A	285	GLU	2
1	A	255	THR	2
1	A	231	CYS	2
1	A	195	LEU	1
1	A	188	ARG	1
1	A	252	GLU	1
1	A	198	LYS	1
1	A	288	GLU	1
1	A	240	CYS	1
1	A	182	GLN	1
1	A	280	CYS	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](#)

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

No chemical shift data were provided