



Full wwPDB NMR Structure Validation Report ⓘ

May 28, 2020 – 11:08 pm BST

PDB ID : 2LD1
Title : Structures and chemical shift assignments for the ADD domain of the ATRX protein
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Deposited on : 2011-05-13

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 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)
RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
ShiftChecker : 2.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

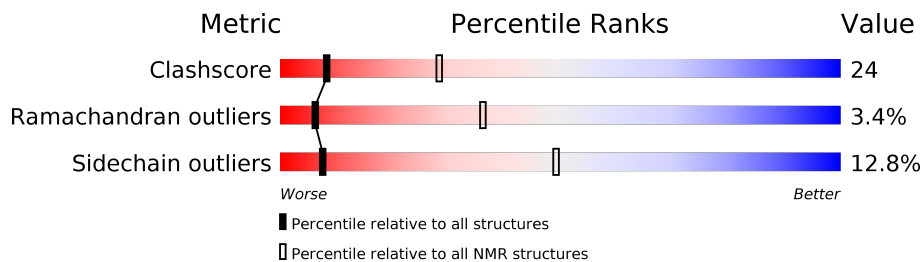
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 74%.

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	142	

2 Ensemble composition and analysis

This entry contains 34 models. Model 2 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:257, A:262-A:288 (103)	0.18	2

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 4 clusters and 12 single-model clusters were found.

Cluster number	Models
1	2, 4, 5, 6, 10, 12, 16, 24, 31
2	9, 13, 14, 17, 22, 23
3	1, 8, 11, 21, 29
4	3, 7
Single-model clusters	15; 18; 19; 20; 25; 26; 27; 28; 30; 32; 33; 34

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2200 atoms, of which 1069 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 ZINC ION (three-letter code: ZN) (formula: Zn).

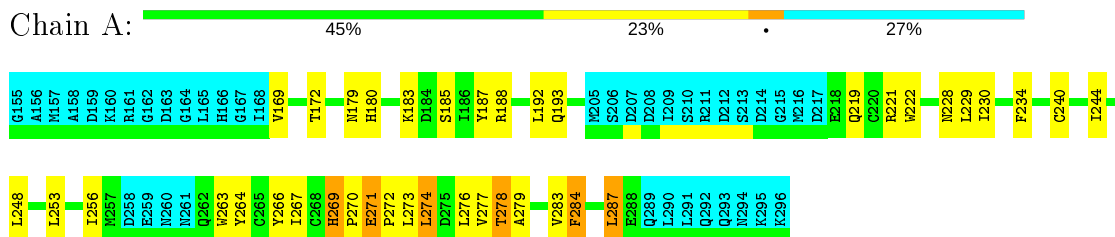
Mol	Chain	Residues	Atoms	
			Total	Zn
2	A	3	3	3

4 Residue-property plots [i](#)

4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA 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: Transcriptional regulator ATRX

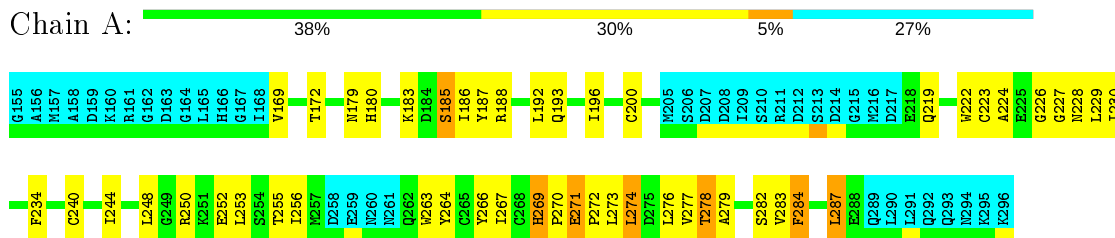


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

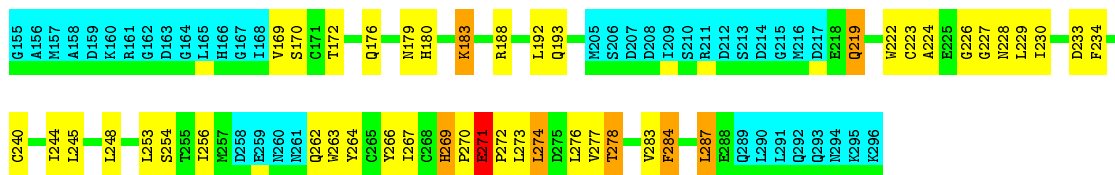
- Molecule 1: Transcriptional regulator ATRX



4.2.2 Score per residue for model 2 (medoid)

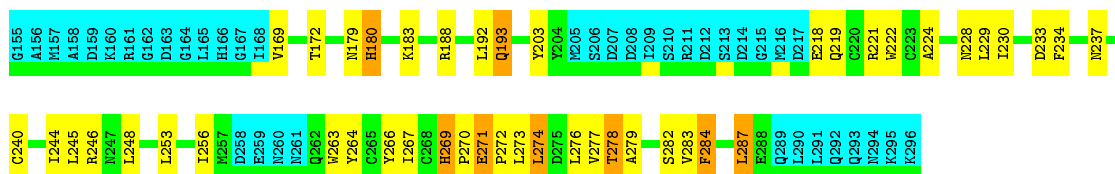
- Molecule 1: Transcriptional regulator ATRX





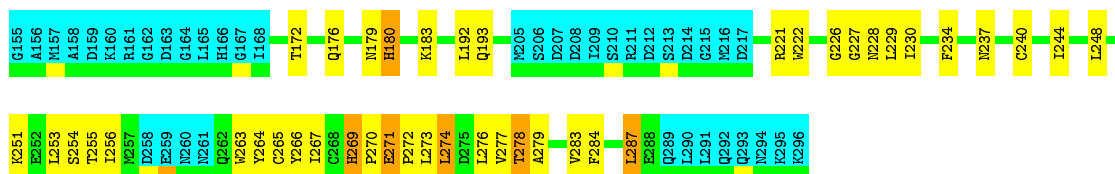
4.2.3 Score per residue for model 3

- Molecule 1: Transcriptional regulator ATRX



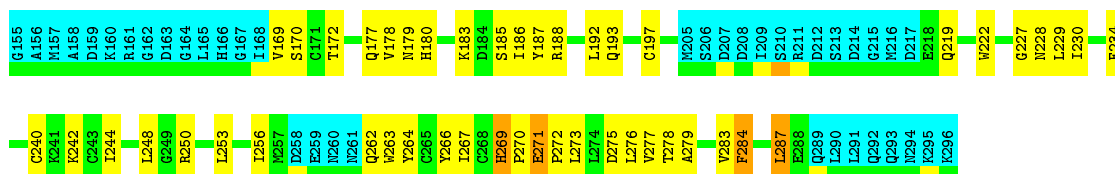
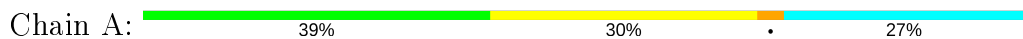
4.2.4 Score per residue for model 4

- Molecule 1: Transcriptional regulator ATRX



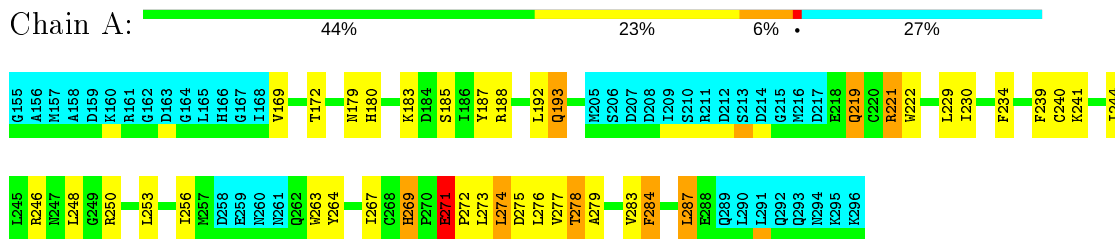
4.2.5 Score per residue for model 5

- Molecule 1: Transcriptional regulator ATRX



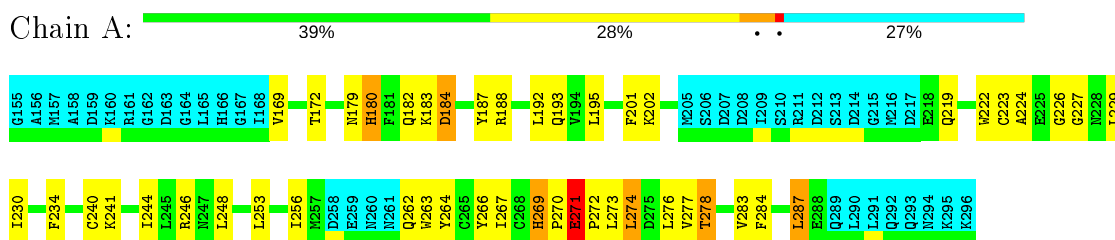
4.2.6 Score per residue for model 6

- Molecule 1: Transcriptional regulator ATRX



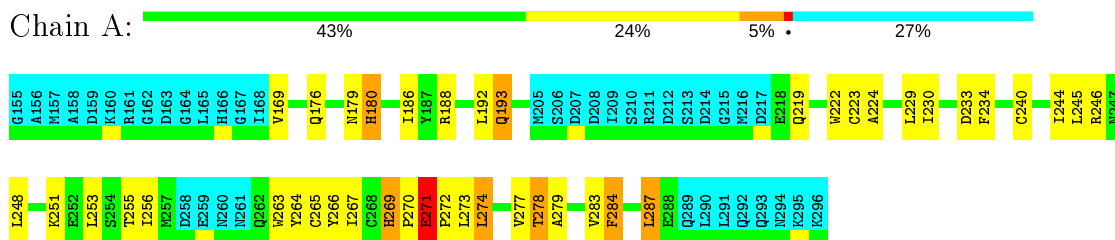
4.2.7 Score per residue for model 7

- Molecule 1: Transcriptional regulator ATRX



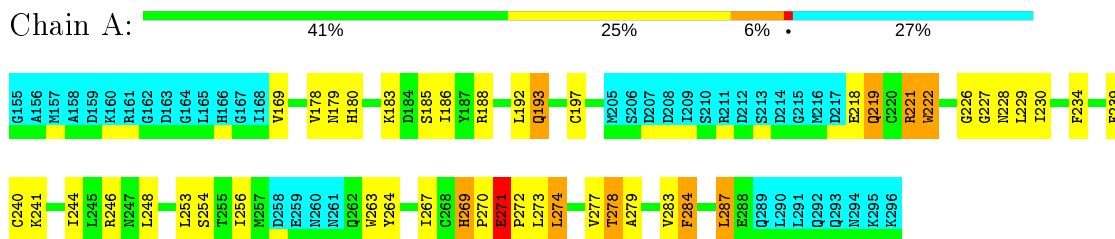
4.2.8 Score per residue for model 8

- Molecule 1: Transcriptional regulator ATRX



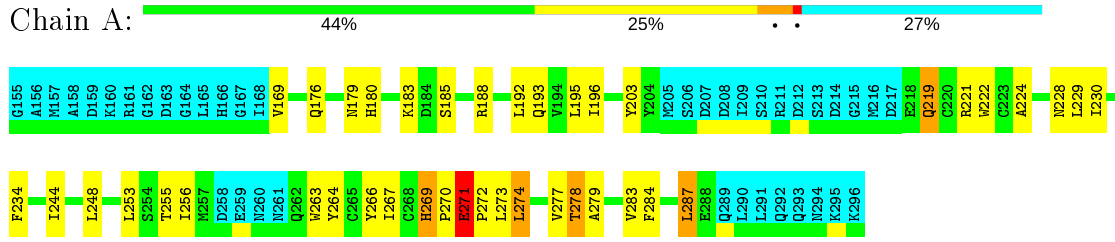
4.2.9 Score per residue for model 9

- Molecule 1: Transcriptional regulator ATRX



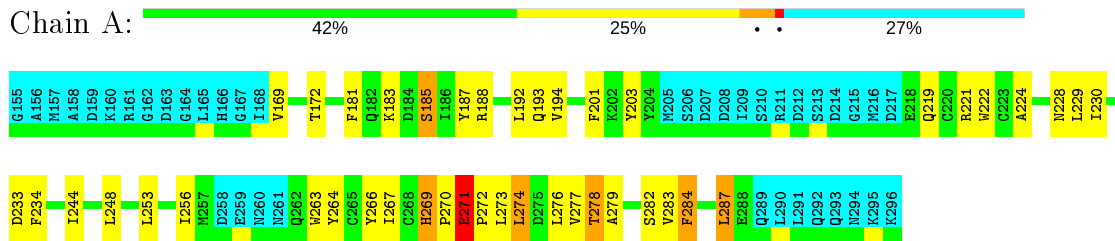
4.2.10 Score per residue for model 10

- Molecule 1: Transcriptional regulator ATRX



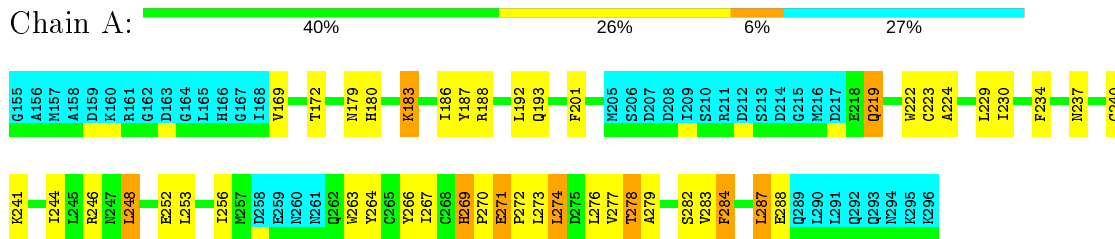
4.2.11 Score per residue for model 11

- Molecule 1: Transcriptional regulator ATRX



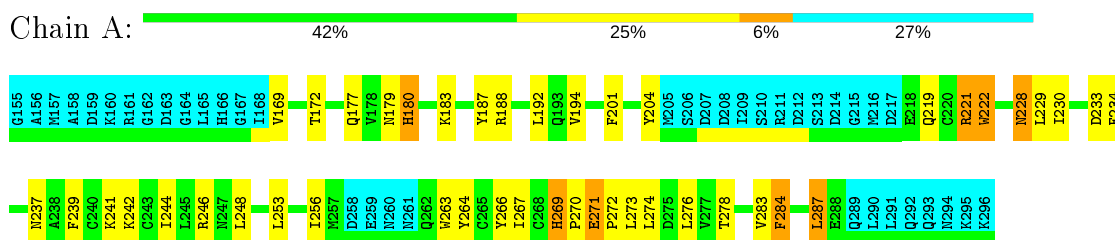
4.2.12 Score per residue for model 12

- Molecule 1: Transcriptional regulator ATRX



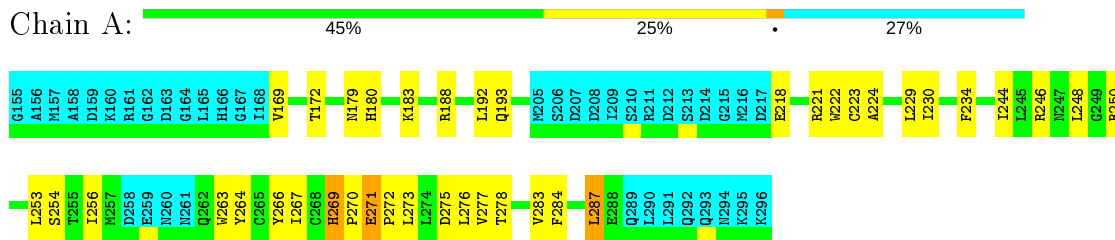
4.2.13 Score per residue for model 13

- Molecule 1: Transcriptional regulator ATRX



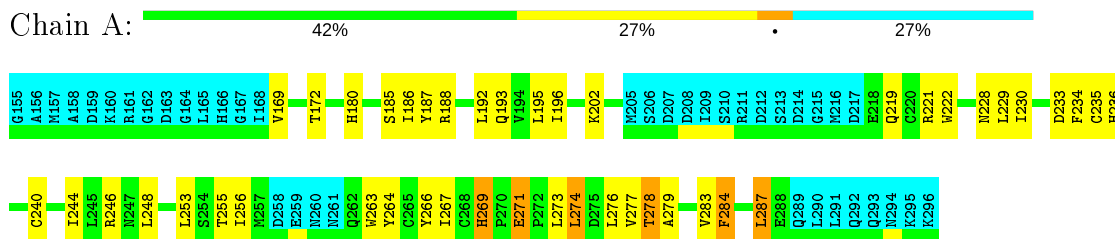
4.2.14 Score per residue for model 14

- Molecule 1: Transcriptional regulator ATRX



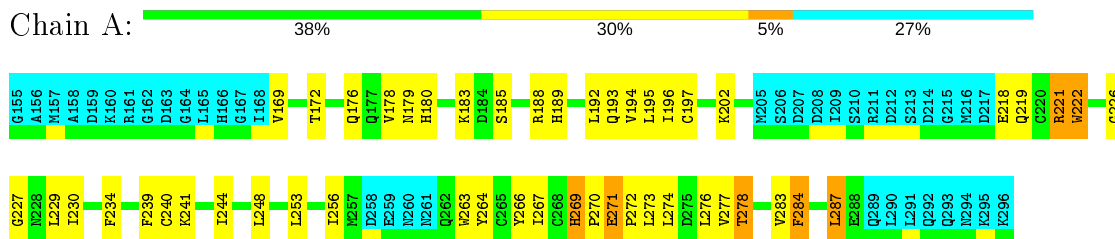
4.2.15 Score per residue for model 15

- Molecule 1: Transcriptional regulator ATRX



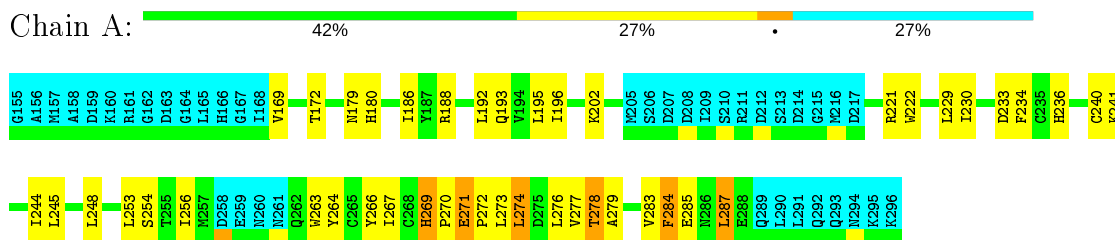
4.2.16 Score per residue for model 16

- Molecule 1: Transcriptional regulator ATRX



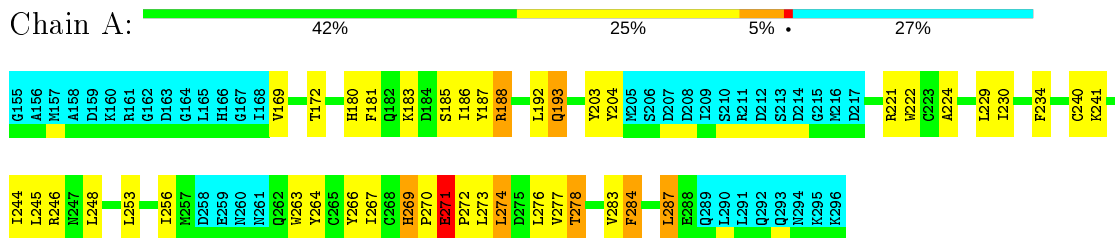
4.2.17 Score per residue for model 17

- Molecule 1: Transcriptional regulator ATRX



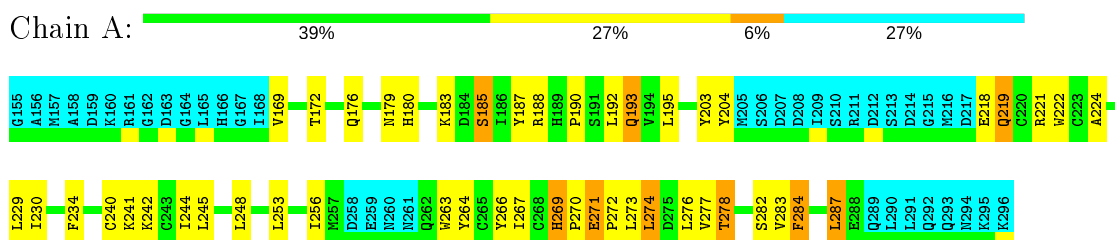
4.2.18 Score per residue for model 18

- Molecule 1: Transcriptional regulator ATRX



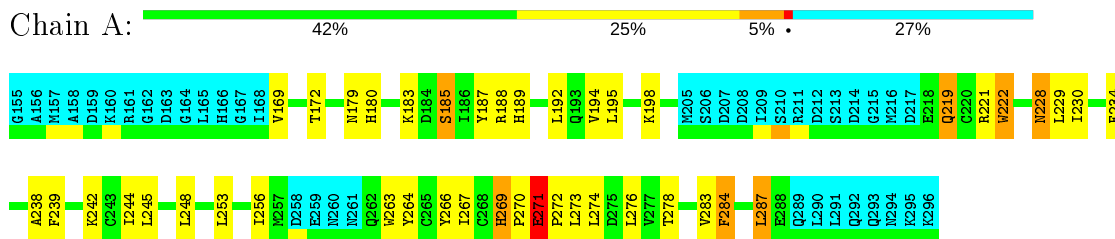
4.2.19 Score per residue for model 19

- Molecule 1: Transcriptional regulator ATRX



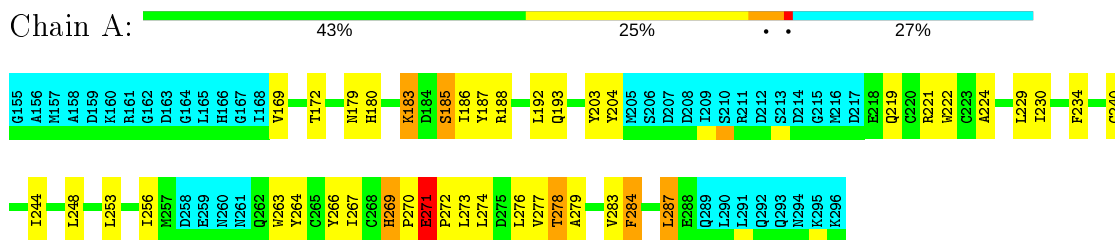
4.2.20 Score per residue for model 20

- Molecule 1: Transcriptional regulator ATRX



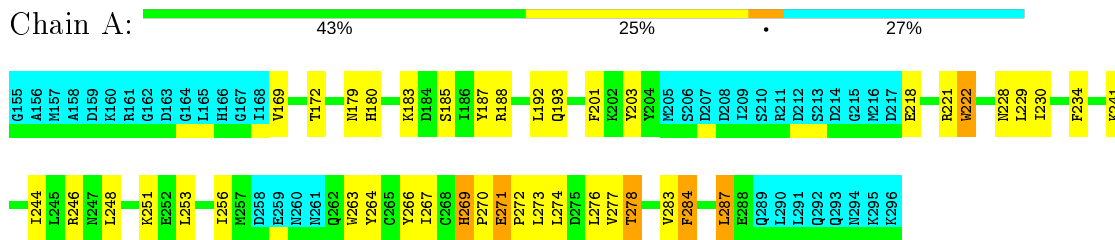
4.2.21 Score per residue for model 21

- Molecule 1: Transcriptional regulator ATRX



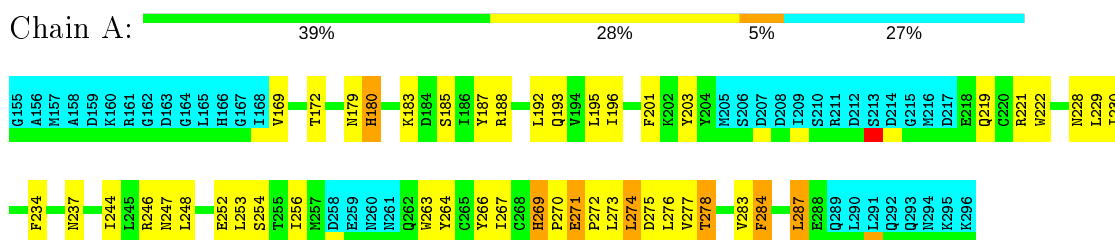
4.2.22 Score per residue for model 22

- Molecule 1: Transcriptional regulator ATRX



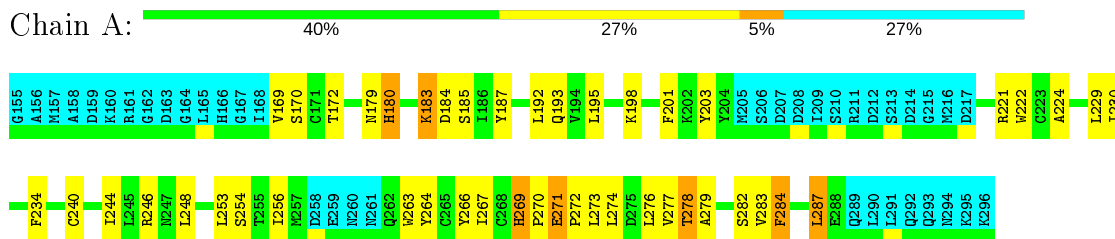
4.2.23 Score per residue for model 23

- Molecule 1: Transcriptional regulator ATRX



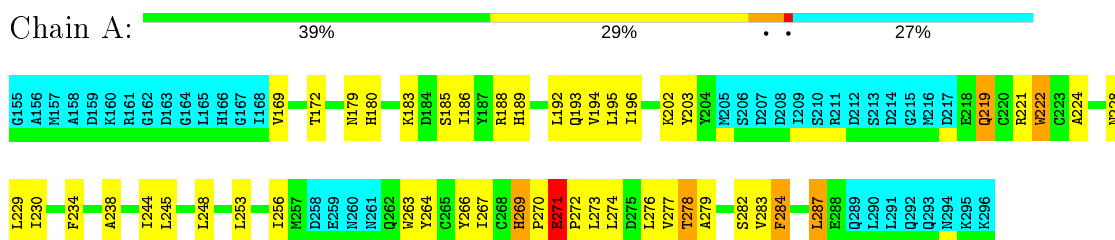
4.2.24 Score per residue for model 24

- Molecule 1: Transcriptional regulator ATRX



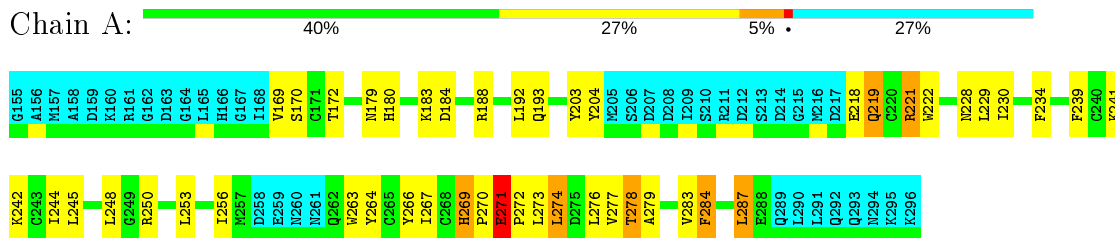
4.2.25 Score per residue for model 25

- Molecule 1: Transcriptional regulator ATRX



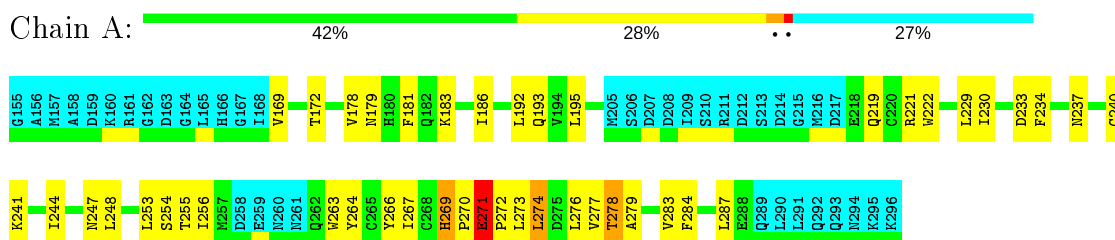
4.2.26 Score per residue for model 26

- Molecule 1: Transcriptional regulator ATRX



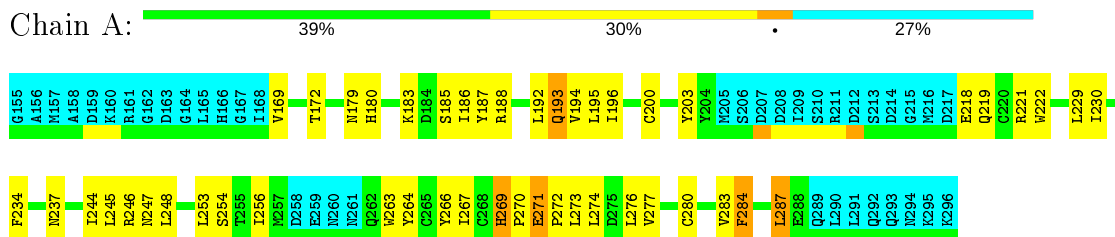
4.2.27 Score per residue for model 27

- Molecule 1: Transcriptional regulator ATRX



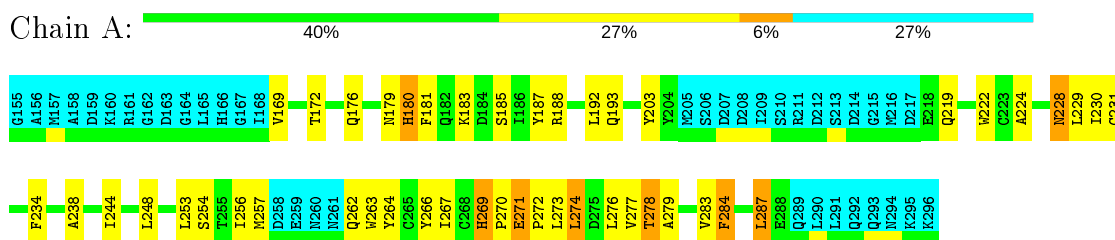
4.2.28 Score per residue for model 28

- Molecule 1: Transcriptional regulator ATRX



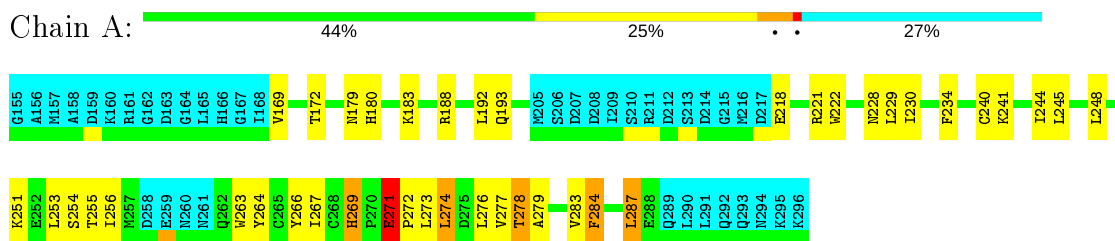
4.2.29 Score per residue for model 29

- Molecule 1: Transcriptional regulator ATRX



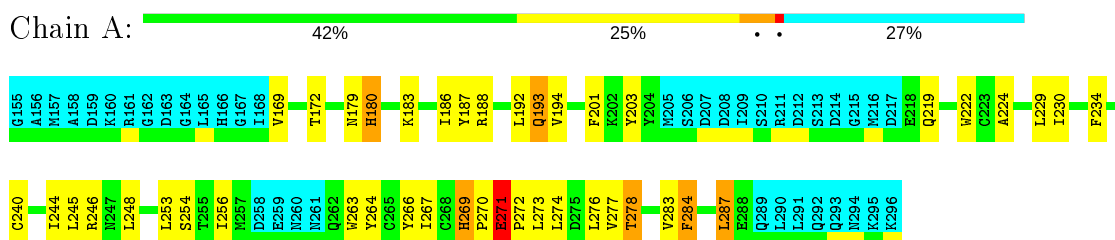
4.2.30 Score per residue for model 30

- Molecule 1: Transcriptional regulator ATRX



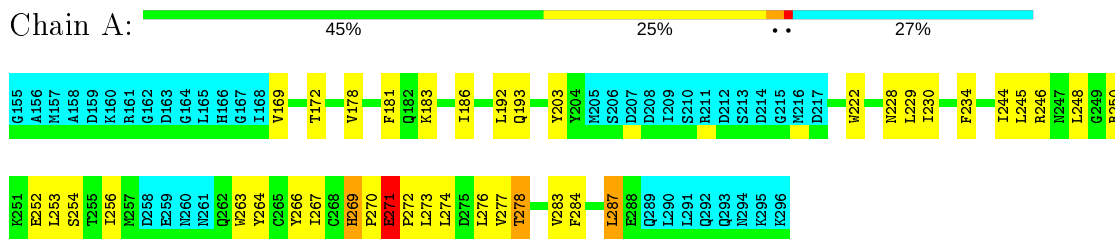
4.2.31 Score per residue for model 31

- Molecule 1: Transcriptional regulator ATRX



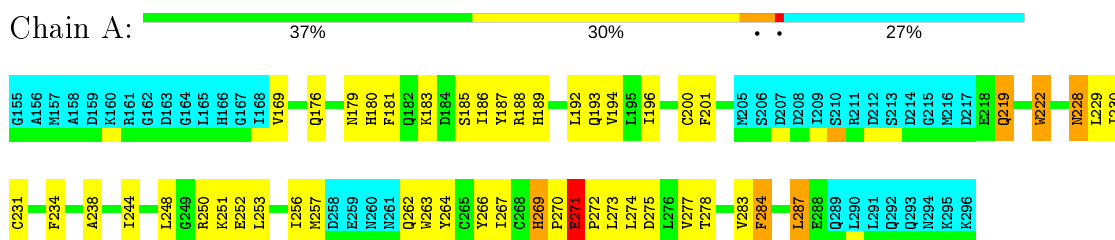
4.2.32 Score per residue for model 32

- Molecule 1: Transcriptional regulator ATRX



4.2.33 Score per residue for model 33

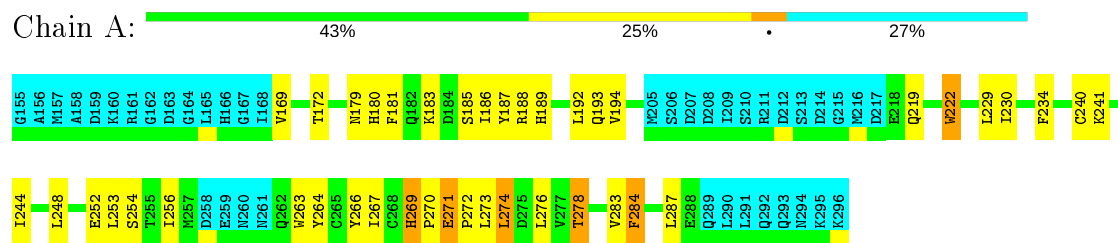
- Molecule 1: Transcriptional regulator ATRX



4.2.34 Score per residue for model 34

- Molecule 1: Transcriptional regulator ATRX

Chain A:



5 Refinement protocol and experimental data overview

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

Of the 100 calculated structures, 34 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
X-PLOR	structure solution	3.8
X-PLOR	refinement	3.8

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)	input_cs.cif
Number of chemical shift lists	1
Total number of shifts	1390
Number of shifts mapped to atoms	1390
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	74%

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

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.

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	832	793	793	40±4
All	All	28390	26962	26962	1350

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 24.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:244:ILE:HG23	1:A:248:LEU:HD21	1.04	1.28	12	1
1:A:195:LEU:HD12	1:A:284:PHE:CD2	0.89	2.03	28	3
1:A:172:THR:OG1	1:A:276:LEU:HD21	0.88	1.68	23	25
1:A:169:VAL:HG22	1:A:283:VAL:HG13	0.81	1.48	13	29
1:A:192:LEU:O	1:A:194:VAL:HG13	0.79	1.78	25	4
1:A:169:VAL:HG13	1:A:283:VAL:HG11	0.78	1.56	14	19
1:A:230:ILE:HD11	1:A:253:LEU:CD2	0.78	2.09	25	34
1:A:193:GLN:O	1:A:277:VAL:HG13	0.75	1.82	6	29
1:A:230:ILE:HD11	1:A:253:LEU:HD21	0.74	1.57	8	33
1:A:169:VAL:HG13	1:A:283:VAL:CG1	0.73	2.14	27	10
1:A:244:ILE:CG2	1:A:248:LEU:HD11	0.73	2.14	9	2
1:A:230:ILE:HD12	1:A:244:ILE:CD1	0.71	2.15	9	34

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:230:ILE:HD11	1:A:253:LEU:CG	0.70	2.17	19	34
1:A:228:ASN:C	1:A:229:LEU:HD12	0.69	2.08	25	11
1:A:229:LEU:HD23	1:A:240:CYS:HA	0.69	1.63	19	20
1:A:248:LEU:HD12	1:A:252:GLU:HB2	0.68	1.66	12	1
1:A:193:GLN:O	1:A:277:VAL:HG22	0.67	1.88	10	20
1:A:256:ILE:HG23	1:A:263:TRP:CD1	0.67	2.25	15	34
1:A:203:TYR:CE2	1:A:224:ALA:HB3	0.66	2.25	21	10
1:A:253:LEU:HA	1:A:256:ILE:HD12	0.66	1.68	32	34
1:A:256:ILE:HG23	1:A:263:TRP:CE2	0.65	2.25	26	9
1:A:248:LEU:HD13	1:A:252:GLU:HB3	0.65	1.68	23	3
1:A:192:LEU:HD13	1:A:222:TRP:CE2	0.65	2.27	25	1
1:A:248:LEU:O	1:A:248:LEU:HD12	0.65	1.92	28	13
1:A:270:PRO:HA	1:A:273:LEU:HD21	0.65	1.70	33	31
1:A:218:GLU:O	1:A:229:LEU:HD22	0.64	1.92	28	4
1:A:226:GLY:HA2	1:A:229:LEU:HD11	0.64	1.68	16	6
1:A:248:LEU:HD12	1:A:248:LEU:O	0.64	1.93	1	18
1:A:192:LEU:O	1:A:194:VAL:HG23	0.63	1.93	33	2
1:A:253:LEU:HD23	1:A:253:LEU:O	0.63	1.92	12	13
1:A:194:VAL:HG11	1:A:273:LEU:HD12	0.63	1.71	13	3
1:A:229:LEU:HD23	1:A:240:CYS:CA	0.63	2.24	19	8
1:A:256:ILE:HG23	1:A:263:TRP:CG	0.62	2.30	24	30
1:A:172:THR:OG1	1:A:276:LEU:HD11	0.61	1.95	11	3
1:A:244:ILE:CG2	1:A:248:LEU:HD21	0.61	2.19	12	1
1:A:169:VAL:HG11	1:A:186:ILE:HG21	0.61	1.73	5	9
1:A:196:ILE:HD12	1:A:200:CYS:HB3	0.60	1.74	28	3
1:A:248:LEU:HD12	1:A:252:GLU:CB	0.60	2.25	12	1
1:A:279:ALA:O	1:A:283:VAL:HG23	0.60	1.97	1	19
1:A:245:LEU:HD23	1:A:245:LEU:O	0.59	1.98	19	8
1:A:192:LEU:HD22	1:A:266:TYR:HB3	0.59	1.74	19	32
1:A:192:LEU:HD21	1:A:267:ILE:HD13	0.59	1.74	9	34
1:A:192:LEU:HD22	1:A:266:TYR:CB	0.59	2.28	19	11
1:A:256:ILE:HG23	1:A:263:TRP:NE1	0.59	2.13	26	8
1:A:230:ILE:HD11	1:A:253:LEU:HG	0.59	1.75	33	33
1:A:172:THR:CB	1:A:276:LEU:HD21	0.58	2.29	30	16
1:A:169:VAL:HG11	1:A:186:ILE:CG2	0.58	2.28	5	6
1:A:244:ILE:HG23	1:A:248:LEU:CD2	0.57	2.18	12	1
1:A:245:LEU:O	1:A:245:LEU:HD23	0.57	2.00	26	5
1:A:273:LEU:N	1:A:273:LEU:HD23	0.56	2.16	29	17
1:A:194:VAL:HG21	1:A:222:TRP:CZ2	0.56	2.35	34	3
1:A:273:LEU:HD23	1:A:273:LEU:N	0.56	2.15	33	17
1:A:287:LEU:O	1:A:287:LEU:HD13	0.55	2.01	18	16

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:195:LEU:HD23	1:A:196:ILE:N	0.55	2.17	15	4
1:A:264:TYR:CD2	1:A:269:HIS:NE2	0.55	2.75	15	5
1:A:192:LEU:CD2	1:A:267:ILE:HD13	0.54	2.31	24	33
1:A:228:ASN:O	1:A:229:LEU:HD12	0.54	2.02	33	4
1:A:169:VAL:HG23	1:A:283:VAL:HG11	0.54	1.77	28	1
1:A:264:TYR:CD1	1:A:269:HIS:NE2	0.54	2.76	30	29
1:A:186:ILE:HD12	1:A:195:LEU:HD11	0.54	1.78	27	3
1:A:287:LEU:HD13	1:A:287:LEU:O	0.53	2.03	15	15
1:A:189:HIS:CE1	1:A:192:LEU:HD12	0.53	2.38	25	1
1:A:169:VAL:HG22	1:A:283:VAL:CG1	0.52	2.28	13	2
1:A:195:LEU:HD13	1:A:196:ILE:N	0.52	2.18	16	1
1:A:244:ILE:HB	1:A:253:LEU:HD12	0.52	1.82	29	3
1:A:253:LEU:O	1:A:253:LEU:HD23	0.52	2.05	30	11
1:A:234:PHE:CE2	1:A:264:TYR:CE2	0.52	2.98	10	26
1:A:172:THR:HB	1:A:276:LEU:HD21	0.52	1.82	11	2
1:A:234:PHE:CE2	1:A:264:TYR:CE1	0.51	2.99	22	4
1:A:230:ILE:HD12	1:A:244:ILE:HD11	0.51	1.81	24	14
1:A:234:PHE:CZ	1:A:264:TYR:CE2	0.51	2.99	27	3
1:A:275:ASP:HA	1:A:278:THR:OG1	0.51	2.06	14	2
1:A:247:ASN:OD1	1:A:276:LEU:HD13	0.51	2.04	28	1
1:A:264:TYR:CD1	1:A:269:HIS:CE1	0.51	2.99	34	29
1:A:234:PHE:CZ	1:A:264:TYR:CE1	0.51	2.99	17	1
1:A:189:HIS:CD2	1:A:222:TRP:CD1	0.50	2.99	20	5
1:A:187:TYR:CD2	1:A:201:PHE:CG	0.50	3.00	7	1
1:A:264:TYR:CD2	1:A:269:HIS:CE1	0.50	2.99	15	5
1:A:195:LEU:C	1:A:195:LEU:HD13	0.50	2.27	16	1
1:A:230:ILE:HD12	1:A:244:ILE:HD12	0.50	1.83	28	10
1:A:221:ARG:HB3	1:A:267:ILE:HD11	0.49	1.84	28	1
1:A:178:VAL:HG21	1:A:186:ILE:HG22	0.49	1.83	27	2
1:A:169:VAL:HG11	1:A:181:PHE:CD1	0.49	2.42	27	1
1:A:244:ILE:HG22	1:A:248:LEU:HD11	0.49	1.83	9	2
1:A:194:VAL:HG21	1:A:222:TRP:HZ2	0.49	1.67	34	5
1:A:194:VAL:CG2	1:A:276:LEU:HD22	0.49	2.38	31	2
1:A:248:LEU:HD12	1:A:248:LEU:C	0.49	2.28	27	17
1:A:229:LEU:N	1:A:229:LEU:HD12	0.48	2.23	22	3
1:A:230:ILE:HG21	1:A:256:ILE:HG21	0.48	1.85	27	18
1:A:256:ILE:CG2	1:A:263:TRP:CE2	0.48	2.97	29	3
1:A:192:LEU:CD1	1:A:222:TRP:CD2	0.47	2.97	20	2
1:A:229:LEU:HD12	1:A:229:LEU:N	0.47	2.24	10	4
1:A:271:GLU:CB	1:A:272:PRO:HD3	0.47	2.39	33	33
1:A:195:LEU:C	1:A:195:LEU:HD23	0.47	2.30	28	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:248:LEU:C	1:A:248:LEU:HD12	0.47	2.30	23	16
1:A:241:LYS:HG3	1:A:253:LEU:HD13	0.47	1.86	7	2
1:A:188:ARG:CG	1:A:284:PHE:CE2	0.46	2.98	7	23
1:A:247:ASN:ND2	1:A:276:LEU:HD22	0.46	2.25	27	1
1:A:172:THR:HG21	1:A:222:TRP:CZ2	0.46	2.45	34	1
1:A:230:ILE:CD1	1:A:253:LEU:HD21	0.46	2.37	19	1
1:A:192:LEU:CD1	1:A:222:TRP:CE2	0.46	2.99	25	3
1:A:248:LEU:HD13	1:A:252:GLU:CB	0.46	2.40	34	2
1:A:230:ILE:HD12	1:A:244:ILE:HD13	0.46	1.87	17	6
1:A:172:THR:OG1	1:A:276:LEU:CD1	0.46	2.64	20	1
1:A:172:THR:HG1	1:A:276:LEU:HD21	0.46	1.68	12	2
1:A:204:TYR:OH	1:A:221:ARG:CD	0.46	2.64	19	1
1:A:195:LEU:HD23	1:A:284:PHE:CD2	0.45	2.46	16	1
1:A:221:ARG:CB	1:A:239:PHE:CZ	0.45	2.99	9	5
1:A:244:ILE:HG23	1:A:248:LEU:HD11	0.45	1.87	9	2
1:A:195:LEU:HD12	1:A:284:PHE:CE2	0.45	2.46	24	2
1:A:194:VAL:HG21	1:A:276:LEU:HD23	0.45	1.87	28	1
1:A:274:LEU:O	1:A:278:THR:OG1	0.45	2.34	24	28
1:A:183:LYS:CA	1:A:287:LEU:HD11	0.45	2.42	32	1
1:A:183:LYS:HA	1:A:287:LEU:HD21	0.45	1.88	20	27
1:A:182:GLN:O	1:A:287:LEU:HD21	0.45	2.12	7	1
1:A:195:LEU:CD1	1:A:284:PHE:CD2	0.44	3.00	24	4
1:A:221:ARG:CB	1:A:239:PHE:CE1	0.44	3.01	26	3
1:A:186:ILE:HB	1:A:195:LEU:HD21	0.44	1.88	15	1
1:A:219:GLN:C	1:A:229:LEU:HD21	0.44	2.32	28	1
1:A:223:CYS:O	1:A:224:ALA:HB3	0.44	2.13	12	6
1:A:194:VAL:CG1	1:A:273:LEU:HD12	0.44	2.39	13	1
1:A:187:TYR:CD1	1:A:201:PHE:CG	0.44	3.05	12	8
1:A:230:ILE:O	1:A:238:ALA:HB1	0.44	2.13	33	4
1:A:204:TYR:OH	1:A:221:ARG:NH2	0.44	2.50	21	1
1:A:235:CYS:O	1:A:236:HIS:CG	0.43	2.71	15	1
1:A:172:THR:OG1	1:A:276:LEU:CD2	0.43	2.62	15	2
1:A:203:TYR:CE2	1:A:224:ALA:CB	0.43	3.01	21	1
1:A:234:PHE:CE2	1:A:264:TYR:CD1	0.43	3.07	22	2
1:A:273:LEU:N	1:A:273:LEU:CD2	0.43	2.82	33	8
1:A:229:LEU:CD2	1:A:240:CYS:CB	0.43	2.97	9	7
1:A:195:LEU:CD2	1:A:284:PHE:CE2	0.43	3.02	16	1
1:A:194:VAL:HG11	1:A:276:LEU:HD23	0.43	1.90	25	1
1:A:266:TYR:CD1	1:A:273:LEU:HD13	0.42	2.48	25	1
1:A:189:HIS:HD2	1:A:196:ILE:HG21	0.42	1.74	25	1
1:A:273:LEU:CD2	1:A:273:LEU:N	0.42	2.82	29	7

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:183:LYS:HA	1:A:287:LEU:HD11	0.42	1.90	32	2
1:A:204:TYR:OH	1:A:221:ARG:HD3	0.42	2.14	19	1
1:A:181:PHE:CG	1:A:181:PHE:O	0.42	2.71	32	1
1:A:253:LEU:HD23	1:A:253:LEU:C	0.42	2.35	12	2
1:A:172:THR:HG21	1:A:276:LEU:HD21	0.42	1.91	28	1
1:A:269:HIS:NE2	1:A:271:GLU:OE1	0.42	2.53	2	3
1:A:181:PHE:O	1:A:181:PHE:CG	0.42	2.73	34	1
1:A:172:THR:HB	1:A:276:LEU:HD22	0.41	1.92	20	1
1:A:256:ILE:HG23	1:A:263:TRP:CD2	0.41	2.50	26	1
1:A:188:ARG:HG3	1:A:284:PHE:CE2	0.41	2.51	20	22
1:A:178:VAL:HG13	1:A:197:CYS:HB2	0.41	1.91	5	3
1:A:263:TRP:CE2	1:A:264:TYR:O	0.41	2.73	21	5
1:A:221:ARG:HB3	1:A:239:PHE:CZ	0.41	2.50	9	3
1:A:222:TRP:CZ3	1:A:266:TYR:CG	0.41	3.08	33	2
1:A:221:ARG:HB2	1:A:239:PHE:CZ	0.41	2.50	20	1
1:A:185:SER:O	1:A:187:TYR:CD2	0.41	2.74	28	12
1:A:248:LEU:CD1	1:A:252:GLU:CB	0.41	2.99	12	1
1:A:230:ILE:CD1	1:A:244:ILE:CD1	0.41	2.99	19	3
1:A:269:HIS:CG	1:A:271:GLU:OE1	0.41	2.74	20	1
1:A:263:TRP:CH2	1:A:265:CYS:CB	0.41	3.04	8	2
1:A:203:TYR:CD2	1:A:224:ALA:HB3	0.41	2.50	21	1
1:A:234:PHE:CE2	1:A:264:TYR:CD2	0.40	3.10	24	2
1:A:269:HIS:N	1:A:269:HIS:CD2	0.40	2.89	27	1
1:A:273:LEU:HD23	1:A:273:LEU:H	0.40	1.77	17	1
1:A:241:LYS:CG	1:A:253:LEU:HD13	0.40	2.46	7	1
1:A:185:SER:OG	1:A:186:ILE:N	0.40	2.54	18	1
1:A:195:LEU:HD13	1:A:283:VAL:HB	0.40	1.91	20	1
1:A:273:LEU:H	1:A:273:LEU:HD23	0.40	1.76	34	1
1:A:204:TYR:CE1	1:A:221:ARG:O	0.40	2.75	19	1
1:A:230:ILE:HG21	1:A:256:ILE:CG2	0.40	2.46	26	1
1:A:269:HIS:CE1	1:A:271:GLU:OE1	0.40	2.75	31	1
1:A:229:LEU:HD23	1:A:240:CYS:CB	0.40	2.47	34	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	103/142 (73%)	85±2 (82±2%)	15±2 (14±2%)	3±1 (3±1%)	6	36
All	All	3502/4828 (73%)	2883 (82%)	501 (14%)	118 (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	271	GLU	34
1	A	179	ASN	30
1	A	180	HIS	30
1	A	228	ASN	11
1	A	227	GLY	7
1	A	262	GLN	2
1	A	184	ASP	1
1	A	190	PRO	1
1	A	186	ILE	1
1	A	222	TRP	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	95/127 (75%)	83±2 (87±2%)	12±2 (13±2%)	7	49
All	All	3230/4318 (75%)	2816 (87%)	414 (13%)	7	49

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	269	HIS	34
1	A	222	TRP	34
1	A	287	LEU	34
1	A	284	PHE	33
1	A	278	THR	31
1	A	274	LEU	25
1	A	221	ARG	19
1	A	271	GLU	18

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Mol	Chain	Res	Type	Models (Total)
1	A	246	ARG	16
1	A	254	SER	14
1	A	185	SER	13
1	A	219	GLN	13
1	A	241	LYS	12
1	A	180	HIS	10
1	A	193	GLN	9
1	A	176	GLN	8
1	A	233	ASP	8
1	A	183	LYS	8
1	A	250	ARG	7
1	A	282	SER	7
1	A	237	ASN	7
1	A	218	GLU	5
1	A	202	LYS	5
1	A	251	LYS	5
1	A	242	LYS	5
1	A	170	SER	4
1	A	188	ARG	4
1	A	204	TYR	3
1	A	262	GLN	3
1	A	275	ASP	3
1	A	184	ASP	3
1	A	252	GLU	2
1	A	231	CYS	2
1	A	198	LYS	2
1	A	257	MET	2
1	A	280	CYS	1
1	A	247	ASN	1
1	A	248	LEU	1
1	A	285	GLU	1
1	A	288	GLU	1
1	A	228	ASN	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](#)

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 74% for the well-defined parts and 72% for the entire structure.

7.1 Chemical shift list 1

File name: input_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	1390
Number of shifts mapped to atoms	1390
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 \pm precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	140	-0.45 ± 0.18	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	130	0.35 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	0	—	None (insufficient data)
^{15}N	134	-0.47 ± 0.24	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 74%, i.e. 955 atoms were assigned a chemical shift out of a possible 1293. 0 out of 15 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	397/509 (78%)	198/203 (98%)	102/206 (50%)	97/100 (97%)
Sidechain	447/647 (69%)	285/384 (74%)	159/232 (69%)	3/31 (10%)

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	Total	¹H	¹³C	¹⁵N
Aromatic	111/137 (81%)	65/73 (89%)	44/58 (76%)	2/6 (33%)
Overall	955/1293 (74%)	548/660 (83%)	305/496 (61%)	102/137 (74%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 72%, i.e. 1250 atoms were assigned a chemical shift out of a possible 1745. 0 out of 18 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹H	¹³C	¹⁵N
Backbone	547/704 (78%)	273/281 (97%)	140/284 (49%)	134/139 (96%)
Sidechain	588/897 (66%)	378/530 (71%)	207/321 (64%)	3/46 (7%)
Aromatic	115/144 (80%)	67/77 (87%)	46/60 (77%)	2/7 (29%)
Overall	1250/1745 (72%)	718/888 (81%)	393/665 (59%)	139/192 (72%)

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.

Mol	Chain	Res	Type	Atom	Shift, ppm	Expected range, ppm	Z-score
1	A	192	LEU	HD12	-0.65	2.16 – -0.64	-5.0
1	A	192	LEU	HD13	-0.65	2.16 – -0.64	-5.0
1	A	192	LEU	HD11	-0.65	2.16 – -0.64	-5.0

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.

Random coil index (RCI) for chain A:

