



Full wwPDB NMR Structure Validation Report ⓘ

Jun 17, 2024 – 10:54 PM EDT

PDB ID : 5YZ9
BMRB ID : 36143
Title : zinc finger domain of METTL3-METTL14 N6-methyladenosine methyltransferase
Authors : Dong, X.; Tang, C.; Gong, Z.; Yin, P.; Huang, J.B.
Deposited on : 2017-12-13

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:

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) : 2.37.1

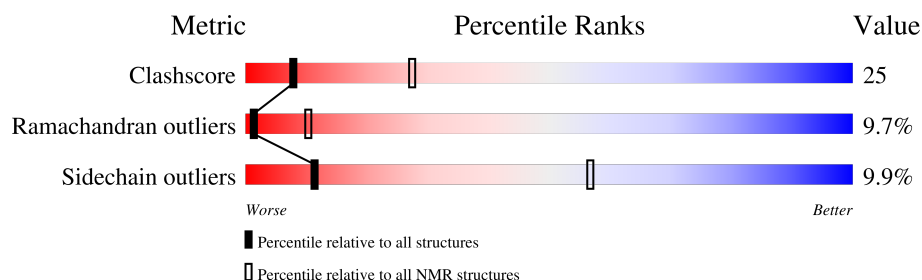
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR, SOLUTION SCATTERING

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	102	

2 Ensemble composition and analysis

This entry contains 25 models. Model 18 is the overall representative, medoid model (most similar to other models). The authors have identified model 15 as representative, based on the following criterion: *closest to the average*.

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:259-A:335 (77)	0.65	18

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 1 single-model cluster was found.

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

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1543 atoms, of which 747 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called N6-adenosine-methyltransferase catalytic subunit.

Mol	Chain	Residues	Atoms						Trace
1	A	99	Total	C	H	N	O	S	0
			1541	484	747	143	158	9	

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	256	ALA	-	expression tag	UNP Q86U44
A	257	HIS	-	expression tag	UNP Q86U44
A	258	MET	-	expression tag	UNP Q86U44
A	336	SER	CYS	engineered mutation	UNP Q86U44

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

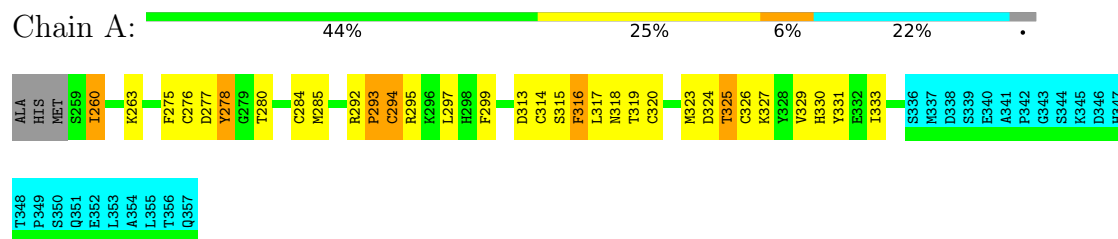
Mol	Chain	Residues	Atoms	
2	A	2	Total	Zn
			2	2

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: N6-adenosine-methyltransferase catalytic subunit

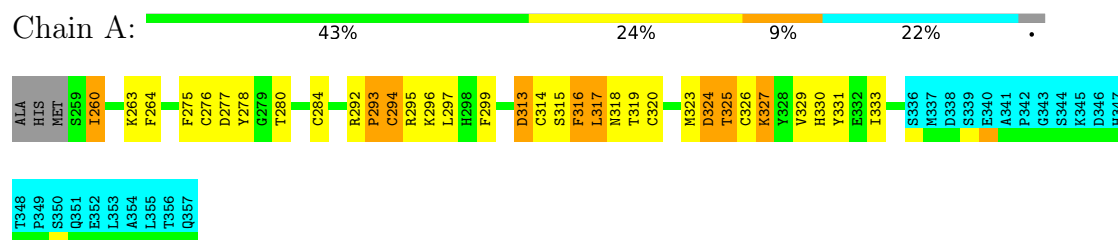


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

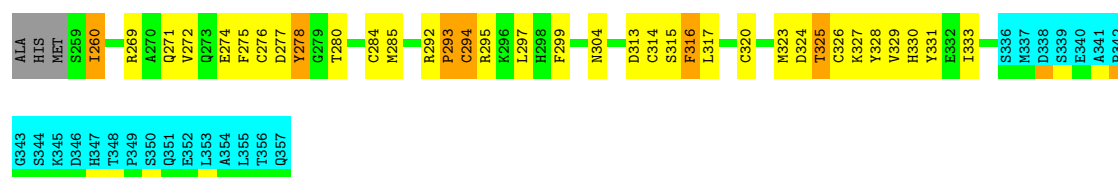
- Molecule 1: N6-adenosine-methyltransferase catalytic subunit



4.2.2 Score per residue for model 2

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit

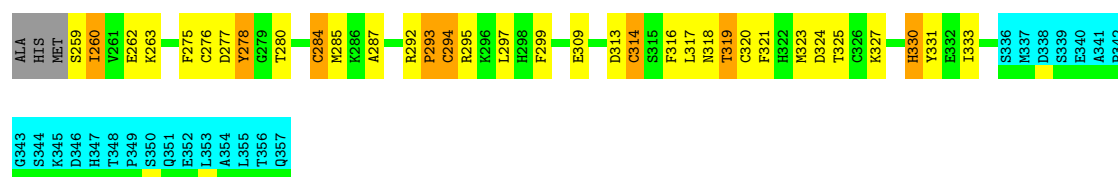




4.2.3 Score per residue for model 3

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit

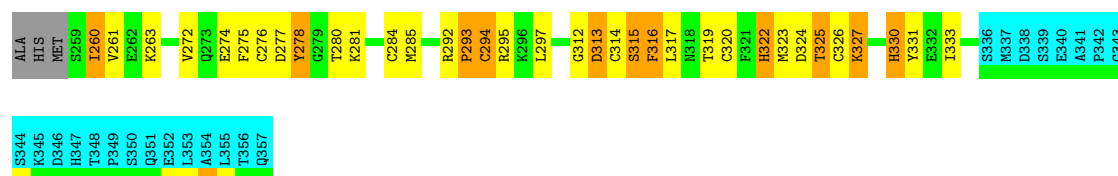
Chain A: 42% 25% 8% 22%



4.2.4 Score per residue for model 4

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit

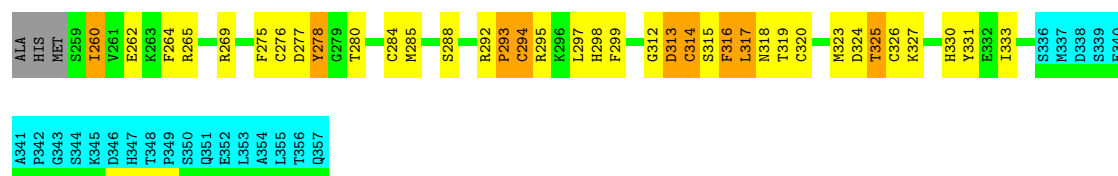
Chain A: 41% 24% 11% 22%



4.2.5 Score per residue for model 5

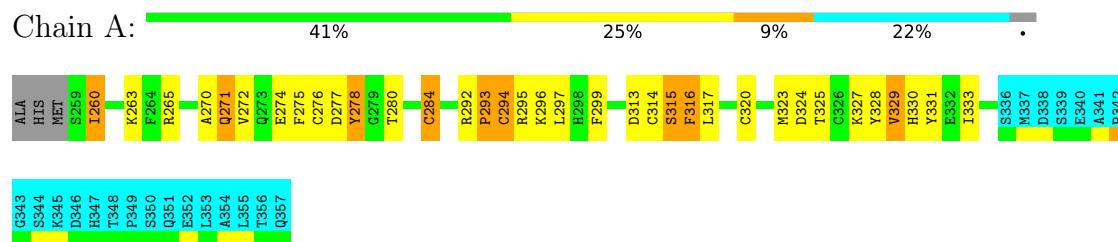
- Molecule 1: N6-adenosine-methyltransferase catalytic subunit

Chain A: 39% 27% 9% 22%



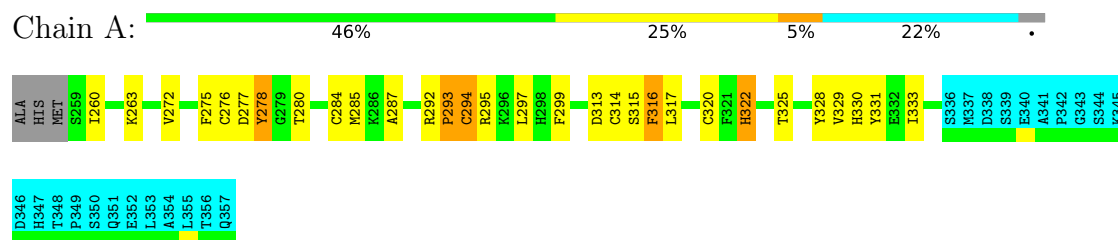
4.2.6 Score per residue for model 6

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit



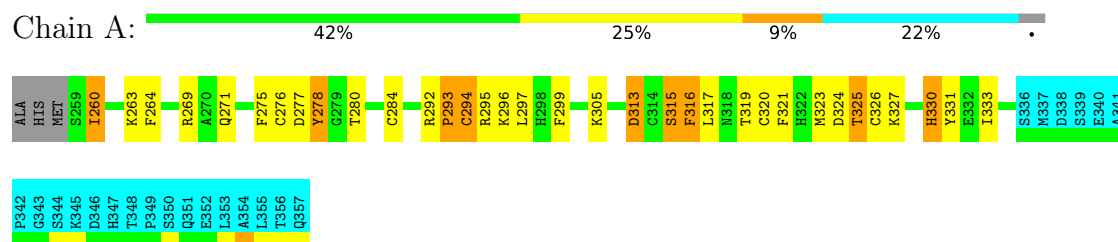
4.2.7 Score per residue for model 7

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit



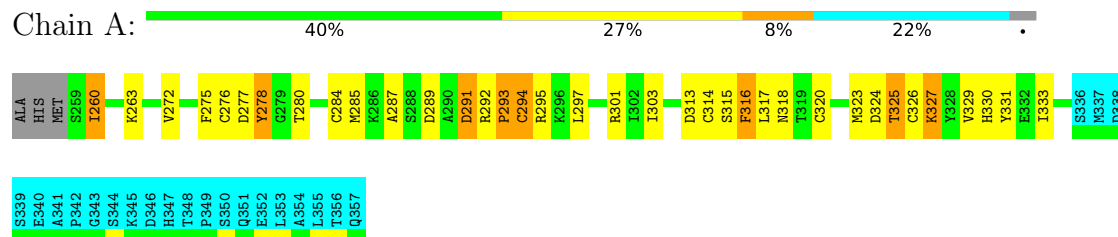
4.2.8 Score per residue for model 8

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit



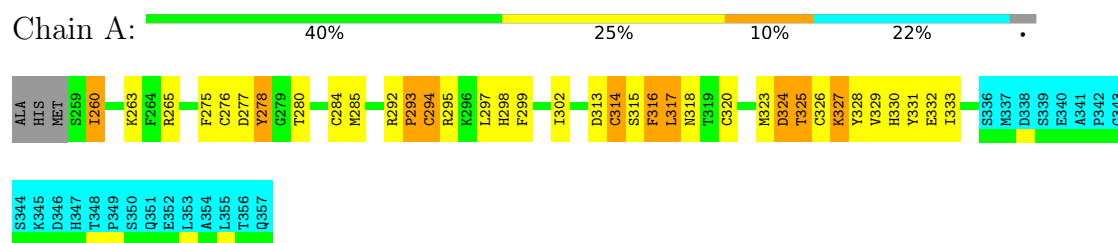
4.2.9 Score per residue for model 9

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit



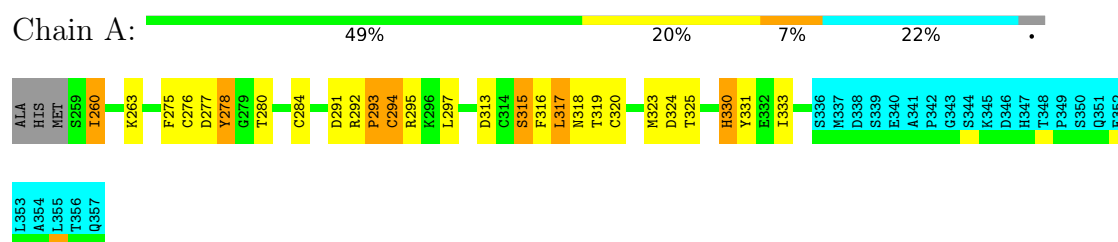
4.2.10 Score per residue for model 10

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit



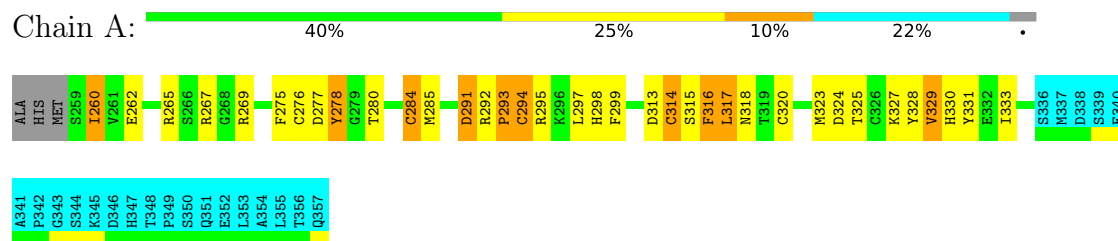
4.2.11 Score per residue for model 11

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit



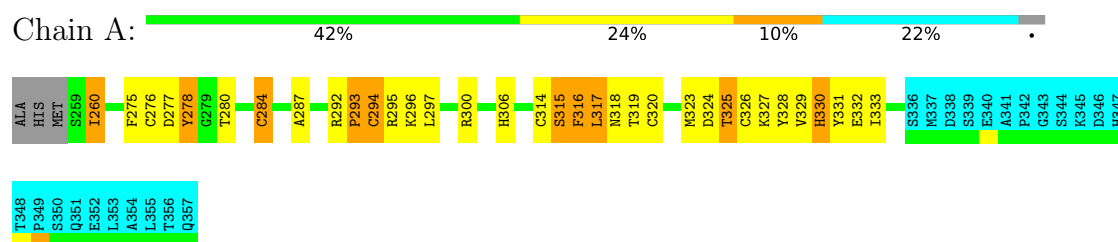
4.2.12 Score per residue for model 12

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit



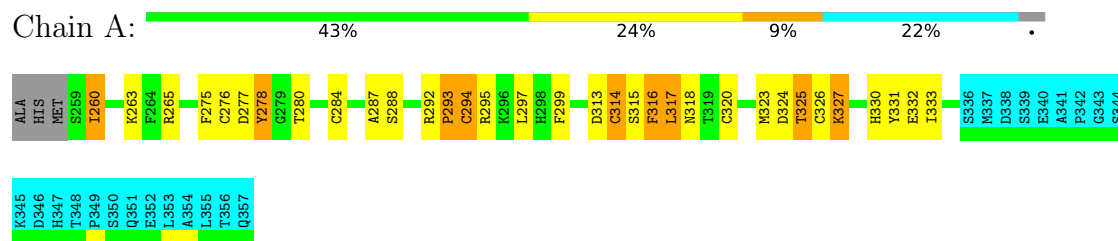
4.2.13 Score per residue for model 13

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit



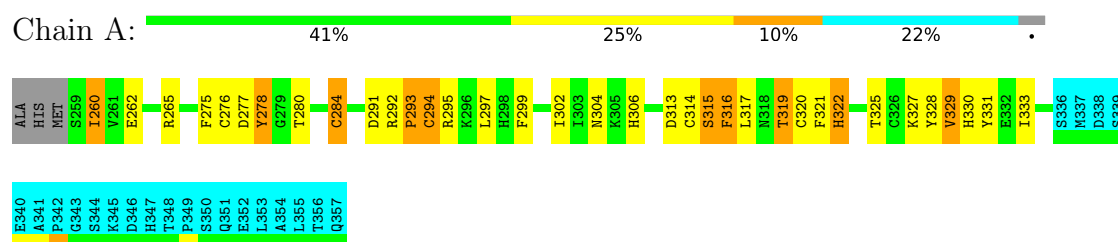
4.2.14 Score per residue for model 14

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit



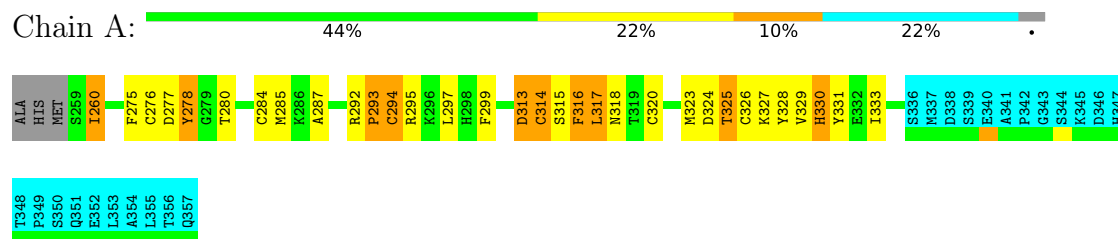
4.2.15 Score per residue for model 15

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit



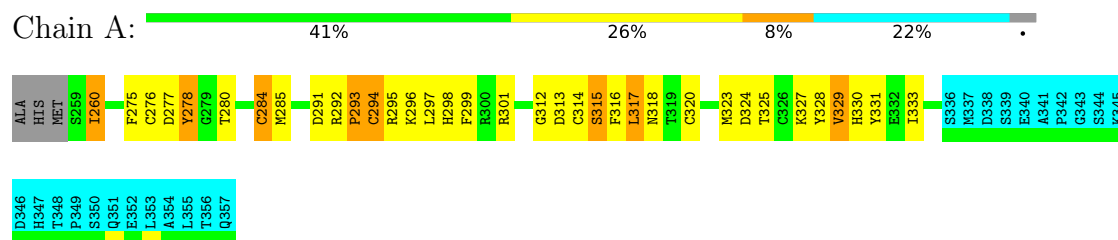
4.2.16 Score per residue for model 16

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit



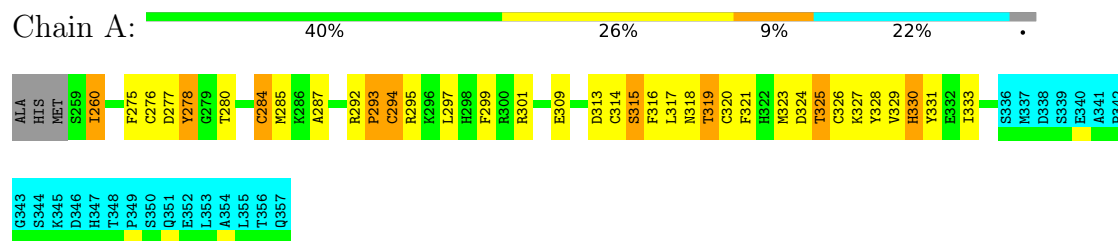
4.2.17 Score per residue for model 17

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit



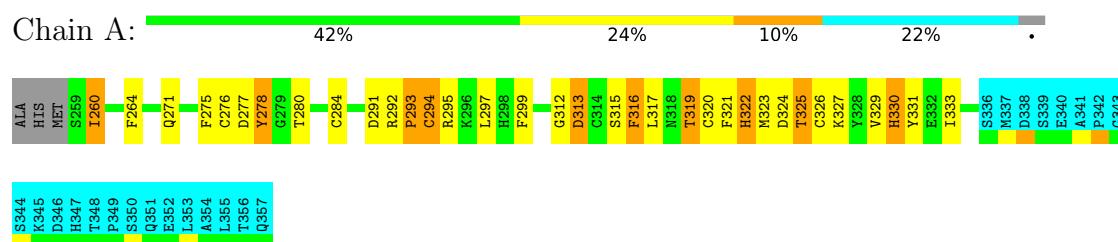
4.2.18 Score per residue for model 18 (medoid)

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit



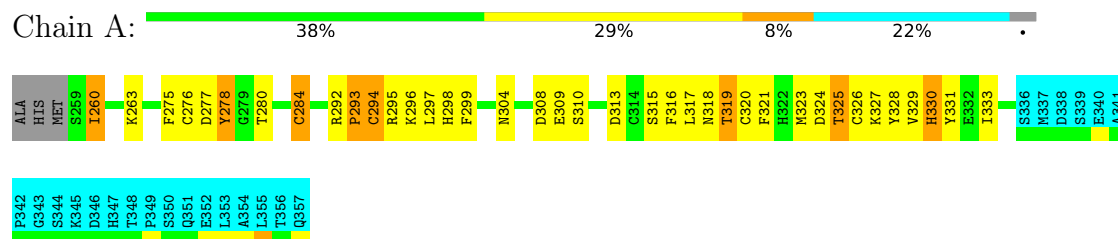
4.2.19 Score per residue for model 19

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit



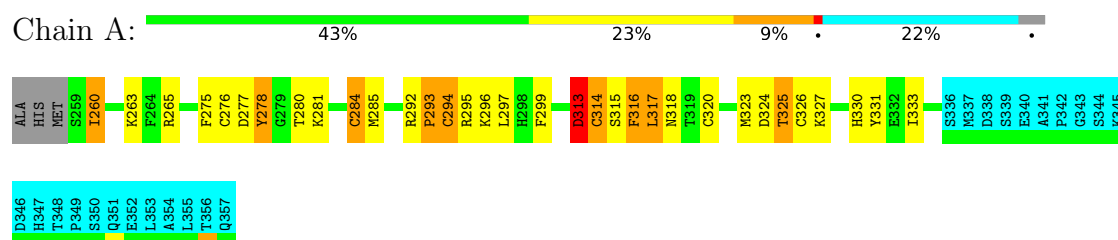
4.2.20 Score per residue for model 20

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit



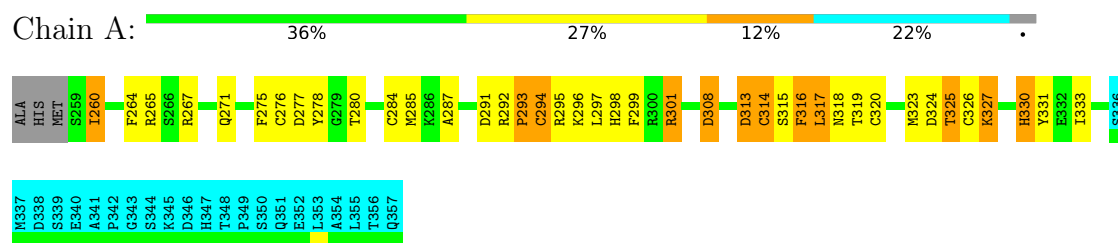
4.2.21 Score per residue for model 21

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit



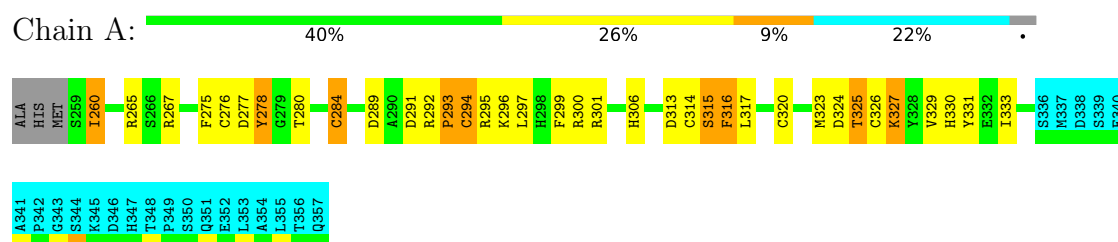
4.2.22 Score per residue for model 22

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit



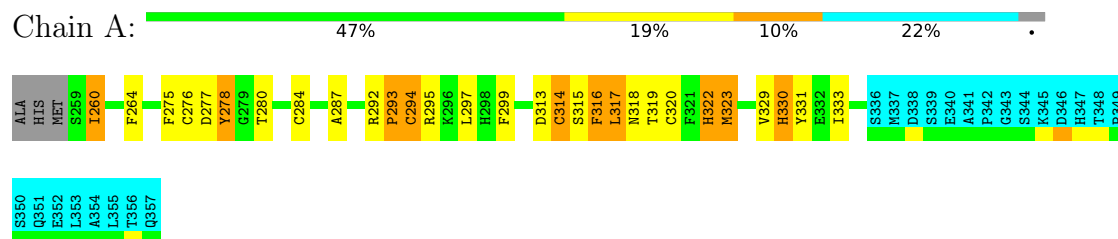
4.2.23 Score per residue for model 23

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit



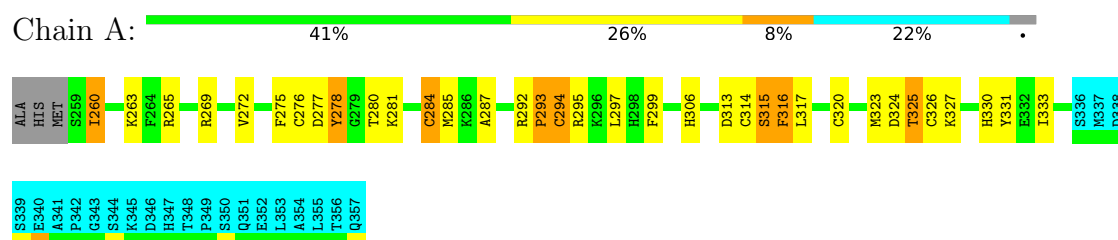
4.2.24 Score per residue for model 24

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit



4.2.25 Score per residue for model 25

- Molecule 1: N6-adenosine-methyltransferase catalytic subunit



5 Refinement protocol and experimental data overview

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

Of the 960 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
X-PLOR NIH	refinement	
X-PLOR NIH	structure calculation	

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	961
Number of shifts mapped to atoms	961
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%

6 Model quality ⓘ

6.1 Standard geometry ⓘ

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 ⓘ

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	632	598	595	31±3
All	All	15850	14950	14875	774

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:265:ARG:HH12	1:A:295:ARG:NH2	1.09	1.44	21	1
1:A:265:ARG:NH1	1:A:295:ARG:NH2	0.93	2.15	21	1
1:A:272:VAL:HG22	1:A:295:ARG:NH2	0.76	1.96	25	1
1:A:301:ARG:HE	1:A:301:ARG:H	0.70	1.28	22	1
1:A:322:HIS:H	1:A:322:HIS:CD2	0.67	2.05	19	3
1:A:272:VAL:CG2	1:A:295:ARG:NH2	0.67	2.58	25	1
1:A:301:ARG:H	1:A:301:ARG:NE	0.65	1.89	22	1
1:A:292:ARG:O	1:A:293:PRO:O	0.64	2.15	5	25
1:A:322:HIS:CD2	1:A:322:HIS:N	0.61	2.69	24	3
1:A:294:CYS:SG	1:A:295:ARG:N	0.60	2.74	17	24
1:A:265:ARG:NH1	1:A:295:ARG:HH21	0.60	1.92	21	1
1:A:278:TYR:OH	1:A:294:CYS:N	0.59	2.36	23	23

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:276:CYS:SG	1:A:277:ASP:N	0.59	2.76	1	25
1:A:272:VAL:HG22	1:A:295:ARG:HH22	0.58	1.58	25	1
1:A:331:TYR:CD1	1:A:331:TYR:N	0.58	2.71	15	24
1:A:315:SER:O	1:A:317:LEU:N	0.58	2.37	16	20
1:A:280:THR:OG1	1:A:284:CYS:N	0.57	2.37	17	25
1:A:323:MET:O	1:A:325:THR:N	0.57	2.38	25	22
1:A:329:VAL:O	1:A:330:HIS:CD2	0.57	2.57	1	8
1:A:299:PHE:CE1	1:A:301:ARG:CZ	0.56	2.88	17	1
1:A:261:VAL:HG12	1:A:295:ARG:HE	0.56	1.59	4	1
1:A:264:PHE:CD1	1:A:269:ARG:NH2	0.56	2.74	5	1
1:A:265:ARG:NH1	1:A:297:LEU:CD1	0.56	2.69	10	3
1:A:304:ASN:ND2	1:A:328:TYR:O	0.55	2.39	15	3
1:A:276:CYS:HA	1:A:295:ARG:CZ	0.55	2.32	25	2
1:A:301:ARG:NE	1:A:301:ARG:O	0.55	2.39	22	1
1:A:260:ILE:CD1	1:A:264:PHE:CE1	0.55	2.90	8	4
1:A:328:TYR:O	1:A:330:HIS:N	0.55	2.39	16	10
1:A:313:ASP:O	1:A:314:CYS:SG	0.55	2.65	12	11
1:A:295:ARG:O	1:A:297:LEU:N	0.54	2.40	21	25
1:A:274:GLU:CD	1:A:274:GLU:N	0.54	2.61	6	1
1:A:275:PHE:CD1	1:A:276:CYS:O	0.54	2.60	11	25
1:A:313:ASP:O	1:A:315:SER:N	0.54	2.41	1	5
1:A:316:PHE:O	1:A:318:ASN:N	0.54	2.41	12	15
1:A:323:MET:N	1:A:323:MET:SD	0.54	2.81	8	4
1:A:260:ILE:HD12	1:A:260:ILE:C	0.54	2.23	2	24
1:A:274:GLU:N	1:A:274:GLU:OE1	0.53	2.40	6	1
1:A:269:ARG:HH21	1:A:271:GLN:NE2	0.53	2.02	8	1
1:A:262:GLU:OE1	1:A:265:ARG:NH1	0.53	2.42	5	1
1:A:293:PRO:O	1:A:296:LYS:NZ	0.53	2.41	22	4
1:A:262:GLU:OE1	1:A:265:ARG:NH2	0.53	2.42	12	2
1:A:262:GLU:OE2	1:A:265:ARG:NH2	0.53	2.42	12	1
1:A:295:ARG:C	1:A:297:LEU:H	0.53	2.05	21	23
1:A:299:PHE:CD1	1:A:299:PHE:O	0.53	2.62	21	21
1:A:289:ASP:OD2	1:A:301:ARG:NH2	0.53	2.42	9	1
1:A:281:LYS:N	1:A:281:LYS:CD	0.53	2.72	4	3
1:A:325:THR:O	1:A:325:THR:HG23	0.53	2.03	12	2
1:A:325:THR:OG1	1:A:326:CYS:N	0.52	2.42	19	11
1:A:316:PHE:CD2	1:A:316:PHE:O	0.52	2.62	21	11
1:A:316:PHE:CE1	1:A:332:GLU:OE2	0.52	2.62	13	2
1:A:316:PHE:O	1:A:316:PHE:CD2	0.52	2.63	12	5
1:A:330:HIS:C	1:A:331:TYR:CD1	0.52	2.84	2	25
1:A:261:VAL:HG12	1:A:295:ARG:NE	0.52	2.19	4	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:265:ARG:NE	1:A:297:LEU:CD1	0.52	2.72	6	1
1:A:304:ASN:ND2	1:A:330:HIS:H	0.52	2.02	15	1
1:A:302:ILE:HD11	1:A:332:GLU:OE1	0.52	2.04	10	1
1:A:317:LEU:N	1:A:317:LEU:CD2	0.51	2.72	16	1
1:A:308:ASP:O	1:A:310:SER:N	0.51	2.42	20	1
1:A:291:ASP:OD1	1:A:291:ASP:N	0.51	2.43	12	2
1:A:329:VAL:O	1:A:329:VAL:HG23	0.51	2.04	23	4
1:A:277:ASP:OD1	1:A:295:ARG:N	0.51	2.44	23	1
1:A:330:HIS:C	1:A:331:TYR:CG	0.51	2.84	5	18
1:A:271:GLN:NE2	1:A:274:GLU:OE2	0.51	2.44	2	1
1:A:267:ARG:NH2	1:A:269:ARG:CZ	0.51	2.73	12	1
1:A:260:ILE:O	1:A:263:LYS:N	0.50	2.45	9	13
1:A:314:CYS:SG	1:A:325:THR:O	0.50	2.70	6	5
1:A:329:VAL:O	1:A:330:HIS:CG	0.50	2.65	9	4
1:A:299:PHE:CE1	1:A:301:ARG:NE	0.50	2.80	17	3
1:A:271:GLN:H	1:A:271:GLN:CD	0.50	2.10	6	2
1:A:313:ASP:OD1	1:A:314:CYS:N	0.50	2.44	12	2
1:A:325:THR:HG23	1:A:326:CYS:H	0.49	1.68	10	5
1:A:295:ARG:HG3	1:A:297:LEU:HB2	0.49	1.82	1	1
1:A:259:SER:O	1:A:262:GLU:CG	0.49	2.61	3	1
1:A:317:LEU:N	1:A:317:LEU:HD12	0.49	2.23	5	3
1:A:317:LEU:HD12	1:A:317:LEU:N	0.49	2.23	11	2
1:A:314:CYS:SG	1:A:325:THR:HG23	0.48	2.48	21	3
1:A:319:THR:CG2	1:A:321:PHE:CZ	0.48	2.97	8	1
1:A:269:ARG:HH21	1:A:271:GLN:HE22	0.48	1.51	8	1
1:A:317:LEU:N	1:A:317:LEU:HD22	0.48	2.22	16	1
1:A:284:CYS:O	1:A:287:ALA:N	0.47	2.47	9	10
1:A:285:MET:O	1:A:288:SER:N	0.47	2.47	5	1
1:A:301:ARG:O	1:A:301:ARG:CZ	0.47	2.61	22	1
1:A:275:PHE:CE1	1:A:276:CYS:O	0.47	2.67	25	15
1:A:314:CYS:SG	1:A:326:CYS:N	0.47	2.88	4	6
1:A:316:PHE:CD1	1:A:332:GLU:OE2	0.47	2.68	13	1
1:A:313:ASP:OD1	1:A:313:ASP:N	0.47	2.47	14	1
1:A:317:LEU:CD2	1:A:317:LEU:H	0.46	2.23	16	1
1:A:326:CYS:O	1:A:327:LYS:O	0.46	2.33	9	7
1:A:319:THR:HG23	1:A:321:PHE:CE1	0.46	2.46	20	5
1:A:271:GLN:CD	1:A:271:GLN:N	0.46	2.69	6	2
1:A:315:SER:O	1:A:315:SER:OG	0.46	2.33	10	5
1:A:318:ASN:N	1:A:318:ASN:OD1	0.46	2.48	1	1
1:A:313:ASP:O	1:A:325:THR:OG1	0.46	2.34	19	5
1:A:322:HIS:CD2	1:A:322:HIS:H	0.46	2.26	15	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:318:ASN:CG	1:A:319:THR:H	0.46	2.14	1	1
1:A:261:VAL:CG1	1:A:295:ARG:HE	0.45	2.25	4	1
1:A:265:ARG:HE	1:A:297:LEU:CD1	0.45	2.24	6	1
1:A:293:PRO:O	1:A:294:CYS:O	0.45	2.34	1	20
1:A:316:PHE:CD2	1:A:316:PHE:C	0.45	2.90	11	7
1:A:269:ARG:NH2	1:A:271:GLN:NE2	0.45	2.63	8	1
1:A:278:TYR:CD2	1:A:278:TYR:N	0.45	2.84	20	1
1:A:295:ARG:C	1:A:297:LEU:N	0.45	2.70	23	7
1:A:271:GLN:N	1:A:271:GLN:CD	0.45	2.70	22	1
1:A:315:SER:O	1:A:316:PHE:C	0.45	2.56	7	14
1:A:323:MET:C	1:A:325:THR:N	0.45	2.70	17	22
1:A:313:ASP:O	1:A:325:THR:O	0.45	2.35	6	1
1:A:285:MET:C	1:A:285:MET:SD	0.45	2.96	5	1
1:A:284:CYS:O	1:A:285:MET:C	0.44	2.55	7	13
1:A:330:HIS:O	1:A:331:TYR:CG	0.44	2.69	5	1
1:A:264:PHE:N	1:A:264:PHE:CD2	0.44	2.86	19	1
1:A:308:ASP:OD1	1:A:308:ASP:N	0.44	2.51	22	1
1:A:270:ALA:O	1:A:274:GLU:OE1	0.44	2.35	6	1
1:A:272:VAL:O	1:A:275:PHE:O	0.44	2.36	7	2
1:A:319:THR:HG23	1:A:319:THR:O	0.44	2.13	11	1
1:A:314:CYS:SG	1:A:329:VAL:HG23	0.44	2.52	24	1
1:A:315:SER:C	1:A:317:LEU:N	0.44	2.72	14	14
1:A:301:ARG:NH1	1:A:303:ILE:HG21	0.44	2.28	9	1
1:A:302:ILE:HD12	1:A:302:ILE:O	0.43	2.13	15	1
1:A:323:MET:C	1:A:325:THR:H	0.43	2.17	17	4
1:A:305:LYS:CD	1:A:305:LYS:N	0.43	2.81	8	1
1:A:269:ARG:O	1:A:272:VAL:HG12	0.43	2.14	2	2
1:A:260:ILE:CD1	1:A:264:PHE:CZ	0.43	3.02	19	2
1:A:312:GLY:O	1:A:313:ASP:OD1	0.43	2.35	19	1
1:A:319:THR:HG23	1:A:321:PHE:CZ	0.42	2.49	19	1
1:A:325:THR:O	1:A:326:CYS:C	0.42	2.56	25	13
1:A:312:GLY:O	1:A:313:ASP:CG	0.42	2.57	4	3
1:A:264:PHE:CE1	1:A:269:ARG:NH2	0.42	2.87	5	1
1:A:332:GLU:N	1:A:332:GLU:CD	0.42	2.73	10	1
1:A:313:ASP:O	1:A:314:CYS:CB	0.42	2.67	3	1
1:A:295:ARG:O	1:A:296:LYS:CB	0.42	2.66	17	1
1:A:315:SER:OG	1:A:319:THR:O	0.42	2.36	8	2
1:A:289:ASP:N	1:A:289:ASP:OD1	0.41	2.52	23	1
1:A:316:PHE:CD1	1:A:316:PHE:C	0.41	2.94	6	1
1:A:316:PHE:O	1:A:317:LEU:C	0.41	2.59	10	2
1:A:262:GLU:CD	1:A:265:ARG:NH2	0.41	2.73	12	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:265:ARG:CZ	1:A:297:LEU:CD1	0.41	2.98	23	2
1:A:280:THR:OG1	1:A:284:CYS:CB	0.41	2.68	20	1
1:A:272:VAL:C	1:A:274:GLU:H	0.41	2.18	4	1
1:A:297:LEU:O	1:A:298:HIS:C	0.41	2.59	22	3
1:A:291:ASP:O	1:A:291:ASP:OD1	0.41	2.38	11	1
1:A:262:GLU:OE2	1:A:265:ARG:CZ	0.41	2.69	12	1
1:A:316:PHE:C	1:A:318:ASN:N	0.41	2.74	18	1
1:A:316:PHE:O	1:A:316:PHE:CG	0.41	2.73	21	2
1:A:317:LEU:N	1:A:317:LEU:CD1	0.40	2.85	11	2
1:A:262:GLU:OE2	1:A:265:ARG:NE	0.40	2.54	15	1
1:A:299:PHE:CD1	1:A:301:ARG:NE	0.40	2.90	17	1
1:A:314:CYS:O	1:A:315:SER:OG	0.40	2.36	7	1
1:A:272:VAL:O	1:A:272:VAL:CG1	0.40	2.69	9	1

6.3 Torsion angles

6.3.1 Protein backbone

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	76/102 (75%)	52±2 (69±2%)	16±2 (22±2%)	7±1 (10±2%)	1	10
All	All	1900/2550 (75%)	1305 (69%)	410 (22%)	185 (10%)	1	10

All 15 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	293	PRO	25
1	A	294	CYS	25
1	A	324	ASP	22
1	A	327	LYS	22
1	A	316	PHE	20
1	A	317	LEU	15
1	A	329	VAL	11
1	A	313	ASP	10
1	A	314	CYS	10

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Mol	Chain	Res	Type	Models (Total)
1	A	315	SER	10
1	A	296	LYS	4
1	A	306	HIS	4
1	A	309	GLU	3
1	A	298	HIS	3
1	A	271	GLN	1

6.3.2 Protein sidechains ⓘ

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	70/91 (77%)	63±2 (90±2%)	7±2 (10±2%)	11	57
All	All	1750/2275 (77%)	1577 (90%)	173 (10%)	11	57

All 19 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	278	TYR	25
1	A	320	CYS	25
1	A	333	ILE	25
1	A	260	ILE	24
1	A	325	THR	17
1	A	284	CYS	11
1	A	330	HIS	11
1	A	319	THR	9
1	A	291	ASP	7
1	A	322	HIS	5
1	A	313	ASP	3
1	A	324	ASP	2
1	A	300	ARG	2
1	A	267	ARG	2
1	A	318	ASN	1
1	A	288	SER	1
1	A	301	ARG	1
1	A	308	ASP	1
1	A	323	MET	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 2 ligands modelled in this entry, 2 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 73% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *zfd_ass.tab*

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	961
Number of shifts mapped to atoms	961
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	2

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
$^{13}\text{C}_\alpha$	99	-0.35 ± 0.22	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	94	0.13 ± 0.17	None needed (< 0.5 ppm)
$^{13}\text{C}'$	94	-0.11 ± 0.18	None needed (< 0.5 ppm)
^{15}N	95	-0.54 ± 0.31	None needed (imprecise)

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. 788 atoms were assigned a chemical shift out of a possible 1060. 0 out of 6 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	380/386 (98%)	153/156 (98%)	152/154 (99%)	75/76 (99%)
Sidechain	382/567 (67%)	250/361 (69%)	132/175 (75%)	0/31 (0%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	26/107 (24%)	20/53 (38%)	6/48 (12%)	0/6 (0%)
Overall	788/1060 (74%)	423/570 (74%)	290/377 (77%)	75/113 (66%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 73%, i.e. 961 atoms were assigned a chemical shift out of a possible 1319. 0 out of 8 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	484/493 (98%)	196/199 (98%)	193/198 (97%)	95/96 (99%)
Sidechain	451/711 (63%)	285/454 (63%)	166/223 (74%)	0/34 (0%)
Aromatic	26/115 (23%)	20/57 (35%)	6/50 (12%)	0/8 (0%)
Overall	961/1319 (73%)	501/710 (71%)	365/471 (77%)	95/138 (69%)

7.1.4 Statistically unusual chemical shifts ⓘ

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	336	SER	CB	27.86	56.28 – 71.32	-23.9
1	A	312	GLY	N	130.54	91.59 – 127.52	5.8

7.1.5 Random Coil Index (RCI) plots ⓘ

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:

