



Full wwPDB NMR Structure Validation Report ⓘ

Mar 27, 2026 – 11:34 AM UTC

PDB ID : 1R36 / pdb_00001r36
BMRB ID : 5991
Title : NMR-based structure of autoinhibited murine Ets-1 deltaN301
Authors : Lee, G.M.; Donaldson, L.W.; Pufall, M.A.; Kang, H.-S.; Pot, I.; Graves, B.J.; McIntosh, L.P.
Deposited on : 2003-09-30

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 : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
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) : 2.49

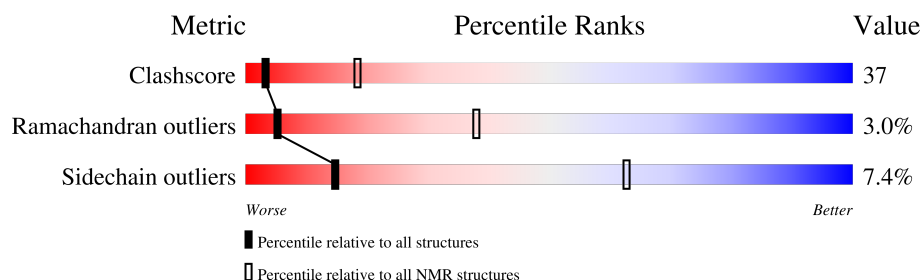
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 93%.

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	229148	14424
Ramachandran outliers	224038	12848
Sidechain outliers	223484	12823

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	140	

2 Ensemble composition and analysis

This entry contains 25 models. Model 11 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:302-A:378, A:384-A:436 (130)	0.33	11

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 4 single-model clusters were found.

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

3 Entry composition

There is only 1 type of molecule in this entry. The entry contains 2291 atoms, of which 1143 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called C-ets-1 protein.

Mol	Chain	Residues	Atoms						Trace
1	A	140	Total	C	H	N	O	S	0
			2291	737	1143	198	210	3	

There is a discrepancy between the modelled and reference sequences:

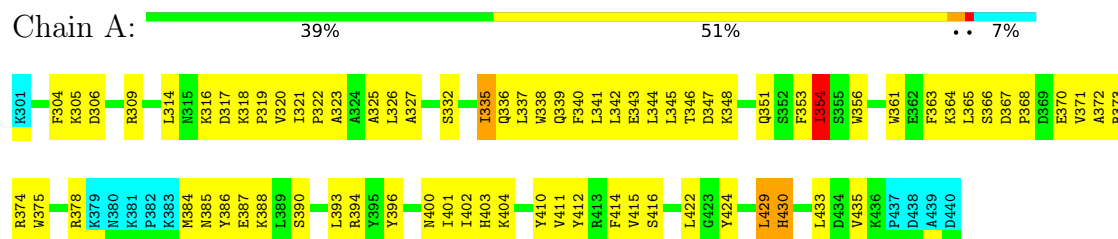
Chain	Residue	Modelled	Actual	Comment	Reference
A	416	SER	CYS	engineered mutation	UNP P27577

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: C-ets-1 protein



4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

4.2.1 Score per residue for model 1

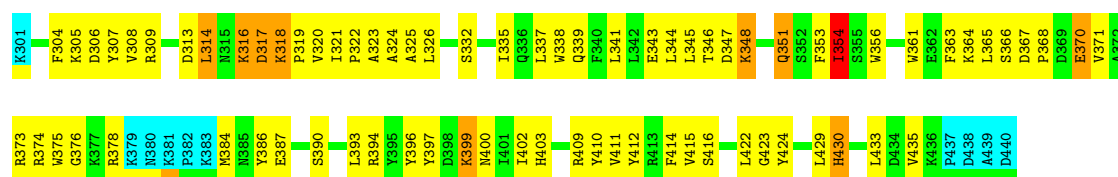
- Molecule 1: C-ets-1 protein



4.2.2 Score per residue for model 2

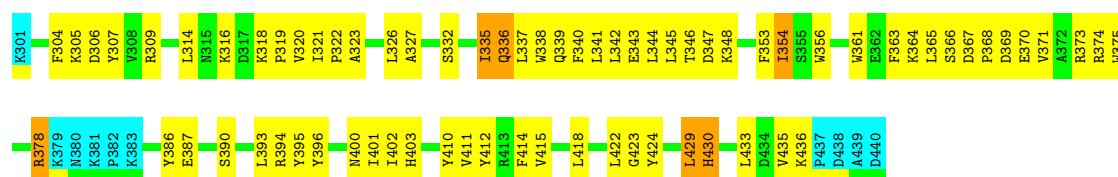
- Molecule 1: C-ets-1 protein





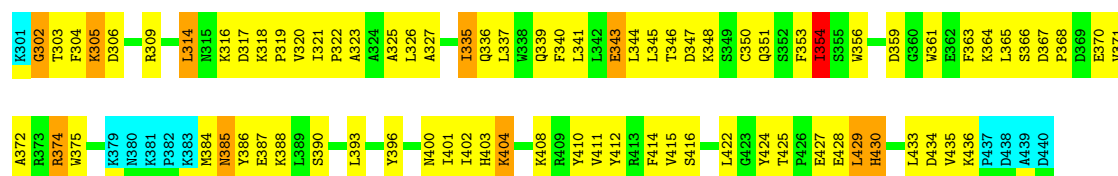
4.2.3 Score per residue for model 3

- Molecule 1: C-ets-1 protein



4.2.4 Score per residue for model 4

- Molecule 1: C-ets-1 protein



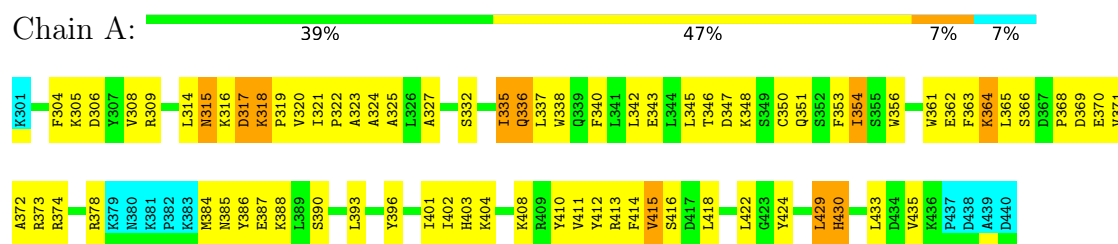
4.2.5 Score per residue for model 5

- Molecule 1: C-ets-1 protein



4.2.6 Score per residue for model 6

- Molecule 1: C-ets-1 protein



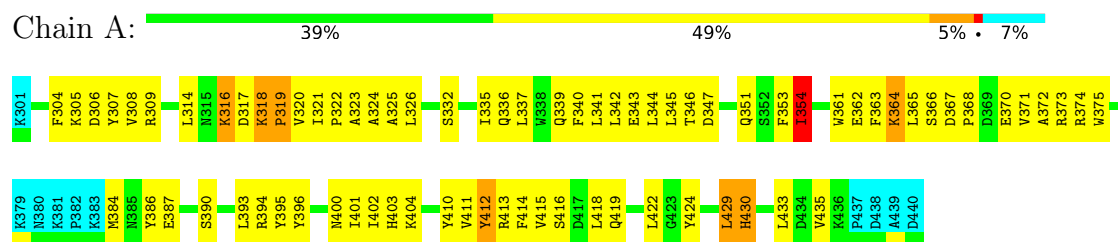
4.2.7 Score per residue for model 7

- Molecule 1: C-ets-1 protein



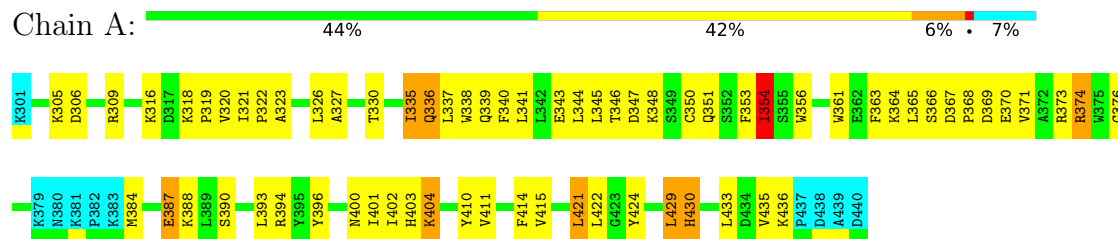
4.2.8 Score per residue for model 8

- Molecule 1: C-ets-1 protein



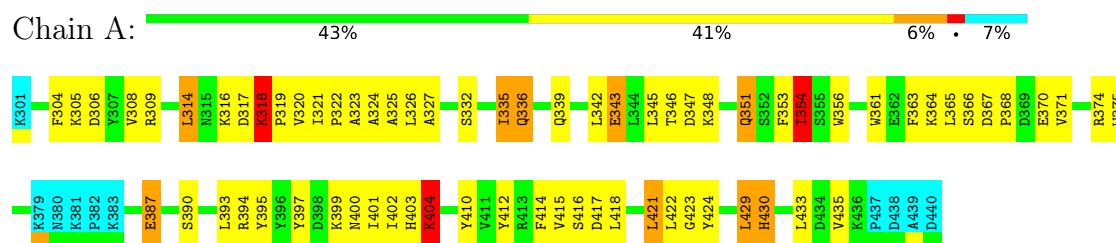
4.2.9 Score per residue for model 9

- Molecule 1: C-ets-1 protein



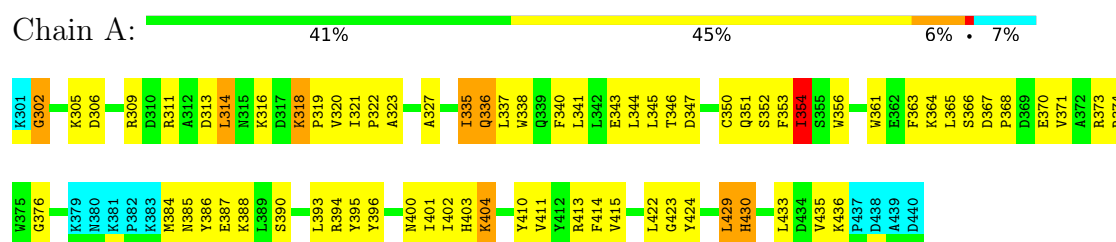
4.2.10 Score per residue for model 10

- Molecule 1: C-ets-1 protein



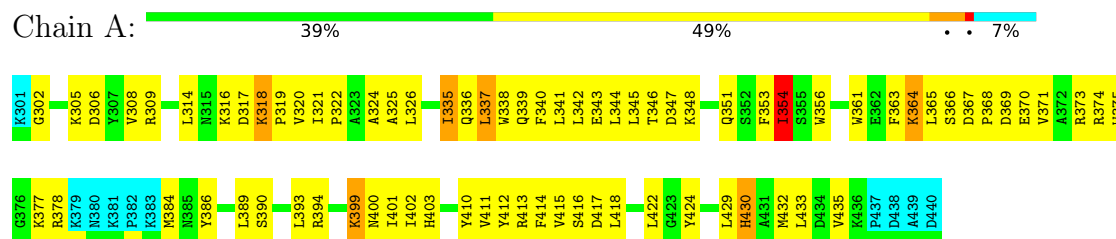
4.2.11 Score per residue for model 11 (medoid)

- Molecule 1: C-ets-1 protein



4.2.12 Score per residue for model 12

- Molecule 1: C-ets-1 protein



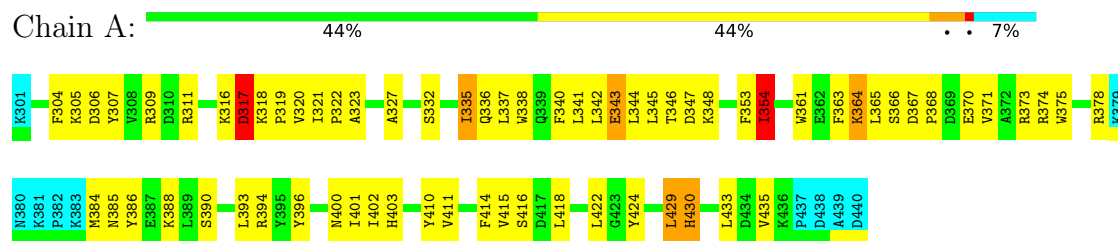
4.2.13 Score per residue for model 13

- Molecule 1: C-ets-1 protein



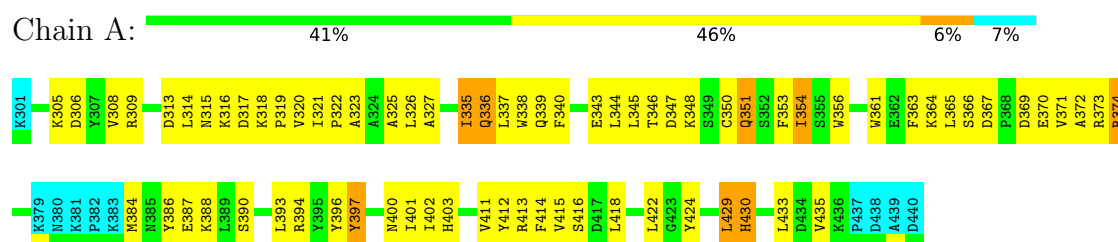
4.2.14 Score per residue for model 14

- Molecule 1: C-ets-1 protein



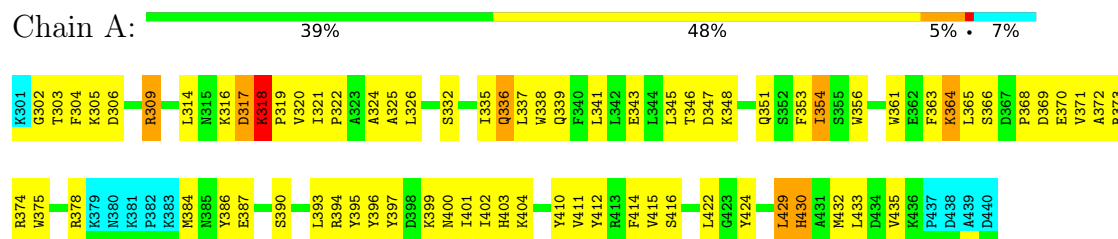
4.2.15 Score per residue for model 15

- Molecule 1: C-ets-1 protein



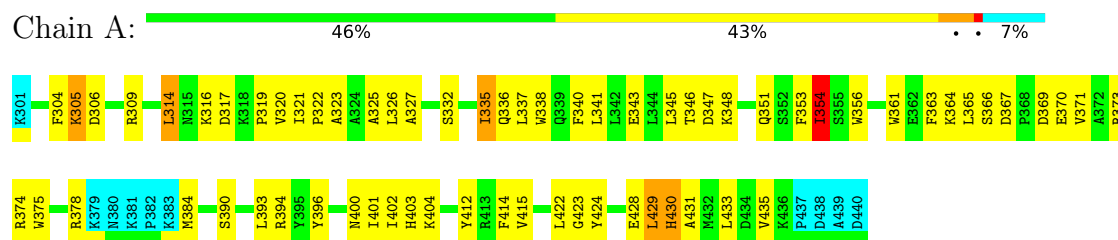
4.2.16 Score per residue for model 16

- Molecule 1: C-ets-1 protein



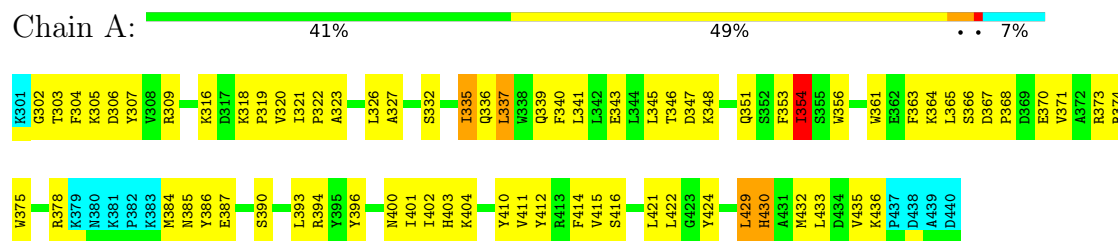
4.2.17 Score per residue for model 17

- Molecule 1: C-ets-1 protein



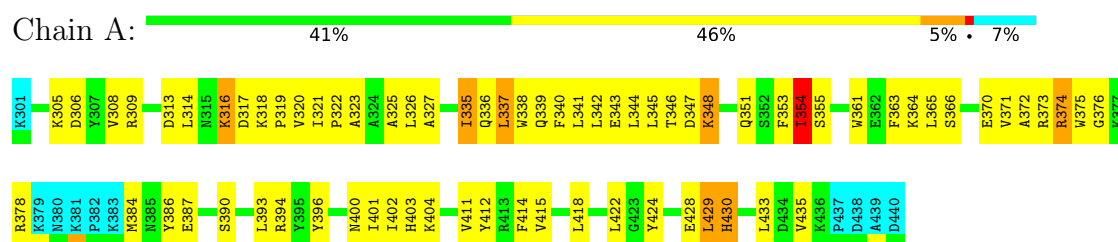
4.2.18 Score per residue for model 18

- Molecule 1: C-ets-1 protein



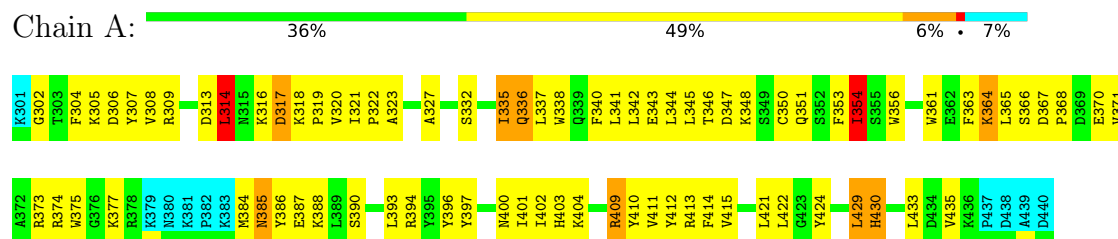
4.2.19 Score per residue for model 19

- Molecule 1: C-ets-1 protein



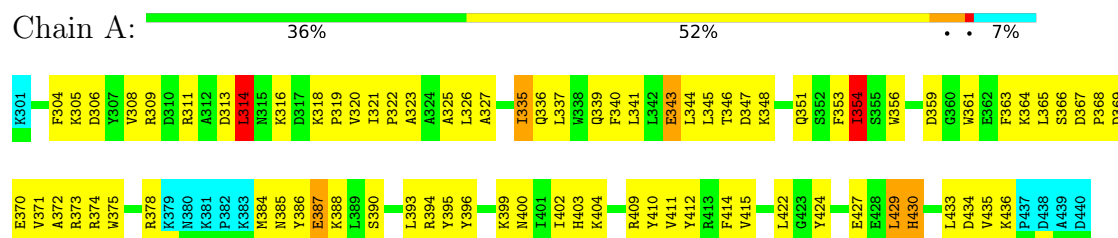
4.2.20 Score per residue for model 20

- Molecule 1: C-ets-1 protein



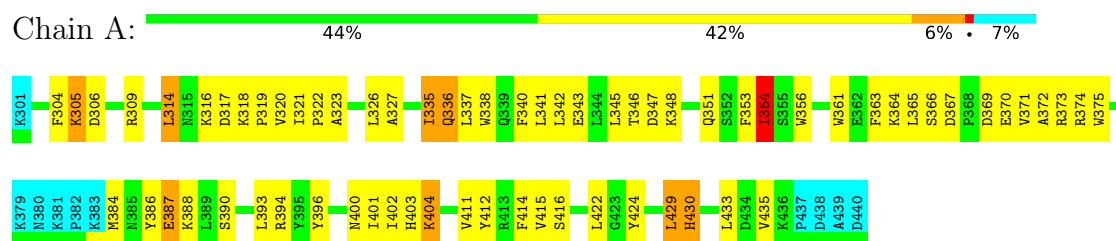
4.2.21 Score per residue for model 21

- Molecule 1: C-ets-1 protein



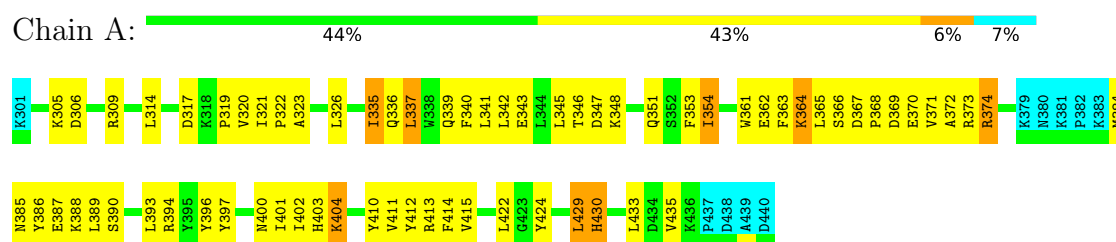
4.2.22 Score per residue for model 22

- Molecule 1: C-ets-1 protein



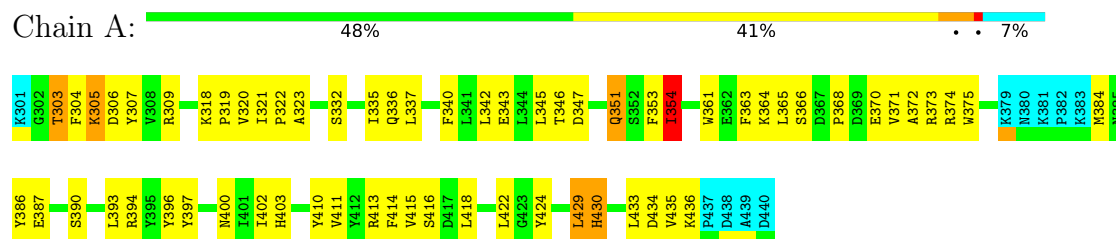
4.2.23 Score per residue for model 23

- Molecule 1: C-ets-1 protein



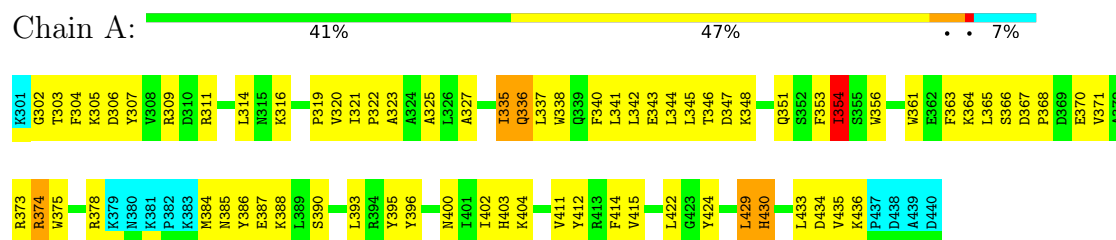
4.2.24 Score per residue for model 24

- Molecule 1: C-ets-1 protein



4.2.25 Score per residue for model 25

- Molecule 1: C-ets-1 protein



5 Refinement protocol and experimental data overview

The models were refined using the following method: *molecular dynamics 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
ARIA	refinement	1.2
CNS	refinement	1.1

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	1838
Number of shifts mapped to atoms	1838
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	93%

6 Model quality

6.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	0.53±0.02	0±0/1097 (0.0± 0.0%)	0.81±0.01	0±0/1484 (0.0± 0.0%)
All	All	0.53	0/27425 (0.0%)	0.81	3/37100 (0.0%)

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	0.0±0.2
All	All	0	1

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	317	ASP	CA-CB-CG	5.15	117.75	112.60	14	1
1	A	318	LYS	CA-C-N	5.03	126.13	119.84	7	1
1	A	318	LYS	C-N-CA	5.03	126.13	119.84	7	1

There are no chirality outliers.

All unique planar outliers are listed below.

Mol	Chain	Res	Type	Group	Models (Total)
1	A	412	TYR	Sidechain	1

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	1068	1056	1054	79±5
All	All	26700	26400	26350	1975

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 37.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:320:VAL:HB	1:A:346:THR:HB	0.99	1.35	2	25
1:A:319:PRO:HG2	1:A:343:GLU:HB2	0.85	1.46	11	7
1:A:319:PRO:HB3	1:A:347:ASP:HB2	0.82	1.51	7	25
1:A:361:TRP:HB3	1:A:414:PHE:HB2	0.82	1.51	16	25
1:A:306:ASP:HA	1:A:309:ARG:HB3	0.81	1.51	7	15
1:A:326:LEU:HG	1:A:339:GLN:HE21	0.80	1.35	2	1
1:A:305:LYS:HA	1:A:424:TYR:CE2	0.79	2.12	17	25
1:A:409:ARG:HA	1:A:409:ARG:HE	0.79	1.37	20	1
1:A:319:PRO:HD2	1:A:322:PRO:HG3	0.78	1.54	15	21
1:A:384:MET:HG3	1:A:388:LYS:HB2	0.77	1.56	7	5
1:A:306:ASP:HA	1:A:309:ARG:HB2	0.76	1.58	15	10
1:A:393:LEU:HD22	1:A:402:ILE:HG21	0.75	1.57	14	25
1:A:319:PRO:HG2	1:A:343:GLU:HA	0.74	1.59	8	4
1:A:390:SER:HA	1:A:393:LEU:HD12	0.74	1.59	7	25
1:A:371:VAL:HA	1:A:374:ARG:HG2	0.74	1.57	5	5
1:A:313:ASP:HA	1:A:317:ASP:CB	0.74	2.13	15	6
1:A:319:PRO:HG2	1:A:343:GLU:HG3	0.73	1.61	17	9
1:A:373:ARG:HA	1:A:384:MET:HB3	0.72	1.59	24	16
1:A:429:LEU:O	1:A:433:LEU:HG	0.71	1.85	3	25
1:A:346:THR:HA	1:A:433:LEU:HD13	0.71	1.62	24	25
1:A:354:ILE:HA	1:A:364:LYS:O	0.70	1.86	6	23
1:A:316:LYS:HB3	1:A:322:PRO:HB3	0.70	1.62	17	7
1:A:365:LEU:HD22	1:A:371:VAL:HG11	0.70	1.64	6	25
1:A:313:ASP:HA	1:A:317:ASP:HB2	0.70	1.62	15	3
1:A:323:ALA:HB2	1:A:340:PHE:HA	0.69	1.62	15	17
1:A:390:SER:O	1:A:394:ARG:HG3	0.69	1.88	5	15
1:A:365:LEU:HB2	1:A:368:PRO:HB3	0.69	1.65	14	6

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:320:VAL:HG12	1:A:321:ILE:HG12	0.68	1.65	9	25
1:A:322:PRO:HA	1:A:343:GLU:HB2	0.68	1.66	4	9
1:A:386:TYR:HE1	1:A:412:TYR:OH	0.68	1.71	8	1
1:A:430:HIS:HB3	1:A:435:VAL:HG21	0.67	1.66	10	25
1:A:323:ALA:CB	1:A:340:PHE:HA	0.67	2.18	17	16
1:A:316:LYS:HB3	1:A:322:PRO:CB	0.67	2.19	22	15
1:A:429:LEU:O	1:A:432:MET:HG2	0.67	1.89	12	1
1:A:316:LYS:HB2	1:A:324:ALA:H	0.67	1.48	1	6
1:A:302:GLY:HA2	1:A:306:ASP:OD2	0.67	1.89	11	3
1:A:309:ARG:HA	1:A:309:ARG:HE	0.67	1.50	16	1
1:A:316:LYS:HB3	1:A:322:PRO:HB2	0.66	1.66	25	8
1:A:323:ALA:N	1:A:343:GLU:HB2	0.66	2.06	17	11
1:A:399:LYS:HB2	1:A:401:ILE:HG13	0.66	1.66	10	3
1:A:316:LYS:O	1:A:322:PRO:HB3	0.66	1.91	2	7
1:A:346:THR:HA	1:A:433:LEU:HD22	0.66	1.68	25	23
1:A:305:LYS:O	1:A:309:ARG:HG2	0.66	1.91	6	6
1:A:337:LEU:HB3	1:A:396:TYR:CE2	0.66	2.26	21	23
1:A:361:TRP:CB	1:A:414:PHE:HB2	0.66	2.20	23	22
1:A:353:PHE:HA	1:A:366:SER:OG	0.65	1.92	2	1
1:A:386:TYR:HE1	1:A:412:TYR:HH	0.65	1.35	8	3
1:A:386:TYR:CE1	1:A:412:TYR:OH	0.65	2.48	8	3
1:A:316:LYS:HG2	1:A:343:GLU:OE1	0.65	1.91	21	11
1:A:374:ARG:HA	1:A:374:ARG:HE	0.65	1.52	19	6
1:A:394:ARG:HA	1:A:397:TYR:HB2	0.64	1.69	15	3
1:A:370:GLU:O	1:A:374:ARG:HG2	0.64	1.93	13	22
1:A:319:PRO:HB2	1:A:346:THR:OG1	0.64	1.92	8	22
1:A:318:LYS:HB3	1:A:319:PRO:HD3	0.64	1.69	14	13
1:A:387:GLU:HA	1:A:390:SER:OG	0.63	1.94	5	18
1:A:323:ALA:H	1:A:343:GLU:HB2	0.63	1.53	17	5
1:A:395:TYR:O	1:A:399:LYS:HG2	0.63	1.93	16	2
1:A:340:PHE:HZ	1:A:374:ARG:HB3	0.62	1.53	7	6
1:A:364:LYS:NZ	1:A:364:LYS:HB3	0.62	2.09	23	6
1:A:367:ASP:HB3	1:A:370:GLU:HG2	0.62	1.69	25	15
1:A:321:ILE:HD11	1:A:424:TYR:CE2	0.62	2.30	17	16
1:A:371:VAL:HA	1:A:374:ARG:CG	0.62	2.24	18	19
1:A:433:LEU:HB2	1:A:435:VAL:HG23	0.62	1.71	11	11
1:A:340:PHE:CZ	1:A:374:ARG:HB3	0.62	2.29	7	8
1:A:348:LYS:HE2	1:A:432:MET:O	0.62	1.95	18	2
1:A:314:LEU:HD23	1:A:325:ALA:HB1	0.62	1.71	1	3
1:A:390:SER:O	1:A:394:ARG:HG2	0.62	1.95	21	6
1:A:335:ILE:HG22	1:A:336:GLN:H	0.61	1.55	25	14

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:401:ILE:HA	1:A:416:SER:HB2	0.61	1.71	15	5
1:A:321:ILE:HD12	1:A:422:LEU:HD22	0.61	1.73	11	23
1:A:368:PRO:HG2	1:A:410:TYR:CG	0.60	2.31	3	12
1:A:403:HIS:CD2	1:A:415:VAL:HG21	0.60	2.31	24	24
1:A:361:TRP:O	1:A:413:ARG:HD3	0.60	1.95	20	3
1:A:308:VAL:HG11	1:A:320:VAL:O	0.60	1.97	19	10
1:A:327:ALA:HB2	1:A:335:ILE:HA	0.59	1.73	19	18
1:A:356:TRP:HB2	1:A:435:VAL:HG11	0.59	1.74	13	15
1:A:319:PRO:CG	1:A:343:GLU:HG3	0.59	2.28	1	13
1:A:351:GLN:NE2	1:A:435:VAL:HA	0.59	2.13	25	15
1:A:322:PRO:HA	1:A:343:GLU:CB	0.58	2.28	9	4
1:A:311:ARG:HB3	1:A:313:ASP:OD1	0.58	1.98	11	2
1:A:371:VAL:O	1:A:374:ARG:HB2	0.58	1.98	8	25
1:A:369:ASP:O	1:A:373:ARG:HG3	0.58	1.99	1	11
1:A:401:ILE:HA	1:A:416:SER:HB3	0.58	1.75	8	1
1:A:336:GLN:HG3	1:A:396:TYR:OH	0.58	1.98	16	5
1:A:326:LEU:HD21	1:A:421:LEU:HD21	0.58	1.75	9	3
1:A:364:LYS:HB2	1:A:411:VAL:HG22	0.58	1.73	23	22
1:A:341:LEU:HD13	1:A:363:PHE:CE2	0.58	2.34	7	9
1:A:314:LEU:H	1:A:317:ASP:HB3	0.57	1.59	13	3
1:A:340:PHE:O	1:A:343:GLU:HG2	0.57	1.99	7	6
1:A:347:ASP:O	1:A:351:GLN:HB3	0.57	1.98	2	12
1:A:378:ARG:HA	1:A:378:ARG:HE	0.57	1.59	18	2
1:A:390:SER:HA	1:A:393:LEU:HB2	0.57	1.76	20	8
1:A:400:ASN:O	1:A:415:VAL:HG23	0.57	2.00	11	6
1:A:323:ALA:HB1	1:A:335:ILE:HG23	0.57	1.76	15	1
1:A:345:LEU:HD21	1:A:363:PHE:HB2	0.57	1.77	6	25
1:A:400:ASN:C	1:A:415:VAL:HG23	0.57	2.24	20	23
1:A:348:LYS:HG2	1:A:433:LEU:HA	0.57	1.75	6	5
1:A:322:PRO:HB2	1:A:325:ALA:CB	0.56	2.29	1	5
1:A:318:LYS:H	1:A:319:PRO:HD3	0.56	1.60	16	12
1:A:319:PRO:HG3	1:A:343:GLU:HG3	0.56	1.77	8	4
1:A:347:ASP:HB3	1:A:350:CYS:HB2	0.56	1.76	9	4
1:A:396:TYR:HB3	1:A:401:ILE:HB	0.56	1.76	7	8
1:A:401:ILE:O	1:A:414:PHE:HA	0.56	1.99	5	14
1:A:306:ASP:HA	1:A:309:ARG:CB	0.55	2.30	7	4
1:A:322:PRO:HB2	1:A:325:ALA:HB2	0.55	1.77	8	6
1:A:393:LEU:CD2	1:A:402:ILE:HG21	0.55	2.31	7	21
1:A:359:ASP:OD1	1:A:427:GLU:HG3	0.55	2.01	4	2
1:A:346:THR:HA	1:A:433:LEU:CD1	0.55	2.30	24	25
1:A:353:PHE:HA	1:A:366:SER:HB3	0.55	1.78	18	17

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:351:GLN:HE22	1:A:435:VAL:HA	0.55	1.62	16	3
1:A:361:TRP:O	1:A:413:ARG:HD2	0.54	2.02	23	2
1:A:327:ALA:CB	1:A:335:ILE:HA	0.54	2.32	19	12
1:A:348:LYS:HG2	1:A:433:LEU:O	0.54	2.02	14	2
1:A:373:ARG:CA	1:A:384:MET:HB3	0.54	2.32	24	9
1:A:394:ARG:HA	1:A:394:ARG:HE	0.54	1.63	8	2
1:A:400:ASN:O	1:A:416:SER:HB2	0.54	2.02	2	4
1:A:394:ARG:HA	1:A:397:TYR:HB3	0.54	1.78	2	3
1:A:341:LEU:HD22	1:A:354:ILE:HD12	0.54	1.80	13	19
1:A:321:ILE:HG21	1:A:342:LEU:HD13	0.54	1.79	25	11
1:A:305:LYS:O	1:A:309:ARG:HB2	0.54	2.03	17	3
1:A:372:ALA:HB1	1:A:384:MET:HG2	0.54	1.79	4	4
1:A:338:TRP:H	1:A:338:TRP:CD1	0.53	2.21	20	11
1:A:323:ALA:HB1	1:A:335:ILE:HG21	0.53	1.79	7	7
1:A:319:PRO:HD2	1:A:322:PRO:CG	0.53	2.31	15	17
1:A:343:GLU:HG3	1:A:344:LEU:N	0.53	2.18	9	6
1:A:348:LYS:HG2	1:A:433:LEU:C	0.53	2.29	14	6
1:A:353:PHE:HA	1:A:366:SER:CB	0.53	2.33	13	4
1:A:322:PRO:HD2	1:A:325:ALA:HB3	0.53	1.81	25	1
1:A:387:GLU:HG3	1:A:388:LYS:N	0.53	2.19	21	3
1:A:313:ASP:HA	1:A:317:ASP:HB3	0.52	1.80	7	1
1:A:368:PRO:HG3	1:A:410:TYR:CG	0.52	2.38	14	4
1:A:409:ARG:HA	1:A:409:ARG:NE	0.52	2.16	20	1
1:A:319:PRO:HD2	1:A:322:PRO:CB	0.52	2.35	25	9
1:A:384:MET:SD	1:A:388:LYS:HB3	0.52	2.44	13	1
1:A:305:LYS:HB2	1:A:422:LEU:O	0.52	2.03	19	16
1:A:395:TYR:O	1:A:399:LYS:HD3	0.52	2.05	21	1
1:A:316:LYS:HG2	1:A:324:ALA:HB3	0.52	1.81	5	1
1:A:368:PRO:HA	1:A:371:VAL:HB	0.52	1.82	3	4
1:A:356:TRP:HD1	1:A:435:VAL:HG21	0.51	1.64	11	9
1:A:318:LYS:H	1:A:319:PRO:CD	0.51	2.18	16	8
1:A:319:PRO:HB3	1:A:347:ASP:CB	0.51	2.33	7	21
1:A:304:PHE:HZ	1:A:325:ALA:HB1	0.51	1.65	2	8
1:A:319:PRO:HG2	1:A:343:GLU:CB	0.51	2.35	7	3
1:A:307:TYR:HA	1:A:311:ARG:NH1	0.51	2.19	14	3
1:A:335:ILE:HG22	1:A:336:GLN:N	0.51	2.19	25	15
1:A:346:THR:HA	1:A:433:LEU:CD2	0.51	2.36	17	16
1:A:374:ARG:O	1:A:378:ARG:HG2	0.51	2.06	17	4
1:A:364:LYS:O	1:A:364:LYS:HD2	0.51	2.06	6	3
1:A:367:ASP:O	1:A:371:VAL:HG23	0.50	2.06	21	9
1:A:356:TRP:CD1	1:A:435:VAL:HG21	0.50	2.41	4	11

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:384:MET:HG3	1:A:388:LYS:CB	0.50	2.36	25	5
1:A:319:PRO:CB	1:A:347:ASP:HB2	0.50	2.32	14	10
1:A:326:LEU:HD23	1:A:339:GLN:HG2	0.50	1.83	3	14
1:A:340:PHE:CE2	1:A:374:ARG:HB3	0.50	2.41	12	6
1:A:340:PHE:CE1	1:A:378:ARG:HG3	0.50	2.41	6	2
1:A:365:LEU:HB3	1:A:371:VAL:HG21	0.50	1.83	10	5
1:A:323:ALA:HB1	1:A:335:ILE:CG2	0.50	2.36	15	6
1:A:367:ASP:HB3	1:A:370:GLU:HB3	0.50	1.84	10	6
1:A:316:LYS:HG2	1:A:323:ALA:HB3	0.50	1.82	8	2
1:A:374:ARG:HA	1:A:374:ARG:NE	0.50	2.21	19	3
1:A:348:LYS:HE3	1:A:434:ASP:HB2	0.50	1.82	21	1
1:A:362:GLU:HB2	1:A:413:ARG:HG3	0.49	1.84	6	2
1:A:344:LEU:O	1:A:351:GLN:HA	0.49	2.07	1	9
1:A:362:GLU:HB2	1:A:413:ARG:CD	0.49	2.36	8	2
1:A:319:PRO:HD2	1:A:322:PRO:HB3	0.49	1.83	25	1
1:A:316:LYS:HG2	1:A:324:ALA:CB	0.49	2.36	5	1
1:A:378:ARG:HA	1:A:378:ARG:NE	0.49	2.22	16	1
1:A:345:LEU:HB3	1:A:356:TRP:NE1	0.49	2.23	7	8
1:A:344:LEU:HD13	1:A:353:PHE:CE2	0.49	2.42	14	3
1:A:324:ALA:HA	1:A:327:ALA:HB3	0.49	1.84	6	2
1:A:353:PHE:HA	1:A:366:SER:HB2	0.49	1.85	1	7
1:A:409:ARG:N	1:A:409:ARG:HD2	0.49	2.22	2	1
1:A:335:ILE:HD12	1:A:378:ARG:HE	0.49	1.67	12	1
1:A:340:PHE:HE2	1:A:374:ARG:HB3	0.49	1.67	12	1
1:A:386:TYR:OH	1:A:404:LYS:HE3	0.49	2.08	25	2
1:A:314:LEU:HD22	1:A:314:LEU:H	0.49	1.68	2	9
1:A:316:LYS:CB	1:A:324:ALA:H	0.48	2.21	8	5
1:A:313:ASP:HA	1:A:317:ASP:CG	0.48	2.33	2	1
1:A:370:GLU:HA	1:A:373:ARG:HD3	0.48	1.84	25	3
1:A:362:GLU:HB2	1:A:413:ARG:HD2	0.48	1.82	8	1
1:A:318:LYS:N	1:A:319:PRO:HD3	0.48	2.22	15	13
1:A:318:LYS:N	1:A:319:PRO:CD	0.48	2.76	3	11
1:A:418:LEU:O	1:A:422:LEU:HB2	0.48	2.08	19	6
1:A:404:LYS:HB2	1:A:404:LYS:NZ	0.48	2.23	11	4
1:A:371:VAL:HA	1:A:374:ARG:HG3	0.48	1.84	2	7
1:A:365:LEU:HD11	1:A:412:TYR:HE2	0.48	1.68	21	17
1:A:402:ILE:HG23	1:A:412:TYR:HB3	0.48	1.85	23	4
1:A:425:THR:OG1	1:A:428:GLU:HB3	0.48	2.09	4	1
1:A:318:LYS:HB3	1:A:319:PRO:CD	0.48	2.37	14	1
1:A:346:THR:CA	1:A:433:LEU:HD22	0.48	2.37	17	15
1:A:387:GLU:HG2	1:A:388:LYS:N	0.48	2.23	9	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:394:ARG:HA	1:A:397:TYR:CB	0.48	2.39	24	2
1:A:375:TRP:CE3	1:A:375:TRP:HA	0.47	2.44	7	5
1:A:335:ILE:HD12	1:A:378:ARG:HB3	0.47	1.85	21	5
1:A:399:LYS:N	1:A:399:LYS:HD2	0.47	2.25	7	1
1:A:323:ALA:HB1	1:A:335:ILE:HD13	0.47	1.85	23	1
1:A:434:ASP:O	1:A:436:LYS:HG3	0.47	2.09	4	4
1:A:385:ASN:ND2	1:A:388:LYS:HG3	0.47	2.25	20	4
1:A:306:ASP:OD1	1:A:309:ARG:HD2	0.47	2.09	18	1
1:A:319:PRO:HB3	1:A:347:ASP:N	0.47	2.24	18	6
1:A:356:TRP:HD1	1:A:435:VAL:CG2	0.47	2.23	4	9
1:A:304:PHE:HA	1:A:307:TYR:HB3	0.46	1.85	3	7
1:A:319:PRO:CD	1:A:322:PRO:HB3	0.46	2.40	25	1
1:A:364:LYS:HD3	1:A:364:LYS:C	0.46	2.35	10	2
1:A:304:PHE:HA	1:A:307:TYR:CB	0.46	2.41	14	4
1:A:385:ASN:OD1	1:A:388:LYS:HE2	0.46	2.11	6	1
1:A:336:GLN:HA	1:A:375:TRP:CH2	0.46	2.45	12	1
1:A:367:ASP:O	1:A:370:GLU:HB3	0.46	2.11	15	1
1:A:348:LYS:HG2	1:A:433:LEU:CA	0.46	2.40	6	2
1:A:399:LYS:HE2	1:A:399:LYS:N	0.46	2.26	2	1
1:A:347:ASP:O	1:A:351:GLN:N	0.46	2.49	17	1
1:A:342:LEU:HD11	1:A:418:LEU:HD13	0.45	1.87	10	5
1:A:321:ILE:HD11	1:A:424:TYR:CD2	0.45	2.46	24	5
1:A:372:ALA:HA	1:A:389:LEU:HD22	0.45	1.88	23	1
1:A:330:THR:HG21	1:A:421:LEU:HD11	0.45	1.88	9	2
1:A:317:ASP:C	1:A:317:ASP:OD1	0.45	2.59	14	1
1:A:316:LYS:C	1:A:322:PRO:HB3	0.45	2.37	2	2
1:A:319:PRO:HB3	1:A:347:ASP:CA	0.45	2.42	6	3
1:A:378:ARG:NE	1:A:378:ARG:HA	0.45	2.27	6	1
1:A:390:SER:HB2	1:A:404:LYS:HD2	0.45	1.88	9	1
1:A:395:TYR:CZ	1:A:399:LYS:HE2	0.45	2.47	16	1
1:A:364:LYS:HE3	1:A:366:SER:HA	0.45	1.89	25	1
1:A:345:LEU:HD21	1:A:363:PHE:CB	0.45	2.42	5	2
1:A:400:ASN:O	1:A:416:SER:HB3	0.45	2.12	22	3
1:A:338:TRP:CD1	1:A:338:TRP:H	0.45	2.30	5	7
1:A:314:LEU:HB2	1:A:325:ALA:CB	0.45	2.42	19	3
1:A:345:LEU:O	1:A:433:LEU:HD13	0.45	2.12	21	2
1:A:309:ARG:NE	1:A:309:ARG:HA	0.45	2.27	10	2
1:A:372:ALA:C	1:A:384:MET:HB3	0.44	2.37	7	2
1:A:408:LYS:HE2	1:A:411:VAL:HG21	0.44	1.88	6	3
1:A:373:ARG:HA	1:A:384:MET:CB	0.44	2.39	2	2
1:A:364:LYS:HB3	1:A:364:LYS:HZ2	0.44	1.72	23	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:353:PHE:O	1:A:365:LEU:HA	0.44	2.13	22	3
1:A:390:SER:HB2	1:A:404:LYS:HD3	0.44	1.89	6	1
1:A:323:ALA:N	1:A:343:GLU:HB3	0.44	2.27	15	3
1:A:397:TYR:HA	1:A:402:ILE:O	0.44	2.12	10	3
1:A:386:TYR:O	1:A:390:SER:N	0.44	2.49	23	20
1:A:318:LYS:HE3	1:A:347:ASP:OD2	0.44	2.12	2	1
1:A:343:GLU:CG	1:A:344:LEU:N	0.44	2.80	13	5
1:A:368:PRO:HG2	1:A:410:TYR:CD1	0.44	2.47	12	2
1:A:305:LYS:HG2	1:A:424:TYR:CD1	0.44	2.48	21	2
1:A:326:LEU:HG	1:A:339:GLN:NE2	0.44	2.17	2	1
1:A:326:LEU:HD22	1:A:422:LEU:HD21	0.44	1.88	8	1
1:A:309:ARG:HA	1:A:309:ARG:CZ	0.44	2.42	10	1
1:A:370:GLU:HG3	1:A:371:VAL:N	0.44	2.28	2	2
1:A:372:ALA:O	1:A:384:MET:HG2	0.43	2.12	8	7
1:A:336:GLN:HE21	1:A:336:GLN:HA	0.43	1.74	13	1
1:A:365:LEU:O	1:A:368:PRO:HD3	0.43	2.12	23	1
1:A:395:TYR:C	1:A:395:TYR:CD1	0.43	2.95	16	1
1:A:320:VAL:CB	1:A:346:THR:HB	0.43	2.29	22	4
1:A:316:LYS:HB2	1:A:324:ALA:N	0.43	2.24	1	1
1:A:351:GLN:OE1	1:A:435:VAL:HA	0.43	2.14	17	3
1:A:344:LEU:HD13	1:A:353:PHE:HE2	0.43	1.73	21	2
1:A:401:ILE:HA	1:A:416:SER:OG	0.43	2.13	10	1
1:A:321:ILE:O	1:A:343:GLU:HA	0.43	2.14	17	1
1:A:344:LEU:CB	1:A:354:ILE:HG21	0.43	2.44	3	2
1:A:305:LYS:HA	1:A:424:TYR:CZ	0.43	2.48	4	1
1:A:342:LEU:HD13	1:A:422:LEU:HD11	0.43	1.90	19	1
1:A:316:LYS:HG3	1:A:323:ALA:HB3	0.43	1.89	1	1
1:A:361:TRP:O	1:A:413:ARG:HG3	0.43	2.13	15	4
1:A:362:GLU:HB2	1:A:413:ARG:NE	0.43	2.29	7	1
1:A:430:HIS:HA	1:A:433:LEU:HD12	0.43	1.90	19	3
1:A:345:LEU:HG	1:A:354:ILE:HG12	0.43	1.91	6	1
1:A:428:GLU:O	1:A:431:ALA:HB3	0.43	2.14	17	1
1:A:366:SER:O	1:A:368:PRO:HD3	0.43	2.14	21	1
1:A:365:LEU:HD13	1:A:371:VAL:HB	0.42	1.89	15	1
1:A:304:PHE:CD2	1:A:326:LEU:HD13	0.42	2.50	22	3
1:A:337:LEU:HD23	1:A:396:TYR:CE2	0.42	2.50	18	1
1:A:395:TYR:CD1	1:A:395:TYR:C	0.42	2.97	8	6
1:A:315:ASN:HB3	1:A:324:ALA:C	0.42	2.40	6	1
1:A:340:PHE:O	1:A:343:GLU:HB3	0.42	2.14	8	1
1:A:315:ASN:HD22	1:A:325:ALA:HA	0.42	1.74	15	1
1:A:343:GLU:HG2	1:A:344:LEU:N	0.42	2.28	21	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:364:LYS:HB3	1:A:364:LYS:HZ3	0.42	1.71	6	1
1:A:371:VAL:CA	1:A:374:ARG:HG2	0.42	2.43	18	1
1:A:318:LYS:HG2	1:A:347:ASP:OD2	0.42	2.14	22	2
1:A:318:LYS:HE3	1:A:350:CYS:SG	0.42	2.54	20	1
1:A:337:LEU:HD11	1:A:389:LEU:HD11	0.42	1.92	12	1
1:A:363:PHE:CE2	1:A:412:TYR:HD2	0.42	2.33	23	1
1:A:341:LEU:HB3	1:A:354:ILE:HD11	0.42	1.92	22	1
1:A:375:TRP:HA	1:A:375:TRP:HE3	0.41	1.75	7	1
1:A:335:ILE:HB	1:A:375:TRP:CZ3	0.41	2.50	19	1
1:A:317:ASP:HA	1:A:322:PRO:CG	0.41	2.45	2	2
1:A:365:LEU:CD1	1:A:412:TYR:HE2	0.41	2.29	10	1
1:A:365:LEU:HD12	1:A:368:PRO:HB3	0.41	1.91	18	1
1:A:356:TRP:HE1	1:A:433:LEU:CD1	0.41	2.28	9	1
1:A:314:LEU:H	1:A:314:LEU:HD22	0.41	1.75	20	1
1:A:308:VAL:HG22	1:A:314:LEU:HD21	0.41	1.91	2	1
1:A:307:TYR:O	1:A:311:ARG:HD2	0.41	2.16	25	1
1:A:374:ARG:O	1:A:378:ARG:HD2	0.41	2.15	3	1
1:A:384:MET:SD	1:A:388:LYS:HE2	0.41	2.56	15	1
1:A:316:LYS:HG3	1:A:343:GLU:OE2	0.41	2.14	8	1
1:A:332:SER:HB2	1:A:336:GLN:HG2	0.41	1.93	7	1
1:A:319:PRO:HG2	1:A:343:GLU:CA	0.41	2.46	2	2
1:A:385:ASN:HD21	1:A:388:LYS:HG3	0.41	1.76	4	1
1:A:370:GLU:HA	1:A:373:ARG:NE	0.41	2.31	14	1
1:A:348:LYS:CG	1:A:433:LEU:HA	0.41	2.46	19	1
1:A:345:LEU:HD13	1:A:356:TRP:CZ2	0.41	2.51	7	1
1:A:364:LYS:HG2	1:A:409:ARG:O	0.41	2.15	21	1
1:A:364:LYS:HD3	1:A:365:LEU:C	0.41	2.41	24	1
1:A:394:ARG:HA	1:A:394:ARG:NE	0.40	2.31	8	1
1:A:424:TYR:CE1	1:A:432:MET:HE1	0.40	2.51	16	1
1:A:348:LYS:N	1:A:348:LYS:HD3	0.40	2.31	2	1
1:A:347:ASP:OD2	1:A:350:CYS:SG	0.40	2.78	4	1
1:A:399:LYS:HE3	1:A:399:LYS:HA	0.40	1.92	12	1
1:A:344:LEU:HB3	1:A:354:ILE:CG2	0.40	2.46	13	1
1:A:305:LYS:HG2	1:A:424:TYR:CG	0.40	2.52	14	1
1:A:320:VAL:O	1:A:322:PRO:HD3	0.40	2.16	22	1
1:A:386:TYR:OH	1:A:404:LYS:HD2	0.40	2.16	4	1
1:A:355:SER:OG	1:A:435:VAL:HG13	0.40	2.17	19	1
1:A:395:TYR:CE1	1:A:396:TYR:CE1	0.40	3.10	16	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	130/140 (93%)	113±2 (87±2%)	13±2 (10±1%)	4±1 (3±1%)	5	38
All	All	3250/3500 (93%)	2837 (87%)	314 (10%)	99 (3%)	5	38

All 13 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	335	ILE	25
1	A	354	ILE	25
1	A	317	ASP	11
1	A	302	GLY	8
1	A	318	LYS	7
1	A	404	LYS	6
1	A	314	LEU	4
1	A	337	LEU	4
1	A	417	ASP	3
1	A	415	VAL	2
1	A	319	PRO	2
1	A	315	ASN	1
1	A	303	THR	1

6.3.2 Protein sidechains

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	112/121 (93%)	104±2 (93±2%)	8±2 (7±2%)	15	63
All	All	2800/3025 (93%)	2592 (93%)	208 (7%)	15	63

All 31 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	430	HIS	25
1	A	429	LEU	23
1	A	354	ILE	18
1	A	336	GLN	16
1	A	332	SER	13
1	A	348	LYS	13
1	A	314	LEU	12
1	A	364	LYS	9
1	A	385	ASN	9
1	A	404	LYS	9
1	A	374	ARG	7
1	A	351	GLN	6
1	A	305	LYS	6
1	A	421	LEU	6
1	A	387	GLU	5
1	A	343	GLU	5
1	A	316	LYS	4
1	A	318	LYS	4
1	A	419	GLN	3
1	A	306	ASP	2
1	A	377	LYS	2
1	A	399	LYS	2
1	A	370	GLU	1
1	A	378	ARG	1
1	A	352	SER	1
1	A	355	SER	1
1	A	317	ASP	1
1	A	397	TYR	1
1	A	309	ARG	1
1	A	428	GLU	1
1	A	409	ARG	1

6.3.3 RNA ⓘ

There are no RNA molecules in this entry.

6.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

There are no ligands in this entry.

6.7 Other polymers [i](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 93% for the well-defined parts and 93% 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

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	1838
Number of shifts mapped to atoms	1838
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	13

7.1.2 Chemical shift referencing

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	140	-0.33 ± 0.09	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	130	0.44 ± 0.12	None needed (< 0.5 ppm)
$^{13}\text{C}'$	127	-0.28 ± 0.10	None needed (< 0.5 ppm)
^{15}N	139	0.68 ± 0.30	Should be applied

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 93%, i.e. 1705 atoms were assigned a chemical shift out of a possible 1837. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	638/650 (98%)	265/265 (100%)	249/260 (96%)	124/125 (99%)
Sidechain	893/992 (90%)	601/641 (94%)	280/306 (92%)	12/45 (27%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	174/195 (89%)	87/93 (94%)	83/94 (88%)	4/8 (50%)
Overall	1705/1837 (93%)	953/999 (95%)	612/660 (93%)	140/178 (79%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 93%, i.e. 1831 atoms were assigned a chemical shift out of a possible 1972. 0 out of 21 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	681/696 (98%)	282/283 (100%)	267/280 (95%)	132/133 (99%)
Sidechain	976/1081 (90%)	656/696 (94%)	307/335 (92%)	13/50 (26%)
Aromatic	174/195 (89%)	87/93 (94%)	83/94 (88%)	4/8 (50%)
Overall	1831/1972 (93%)	1025/1072 (96%)	657/709 (93%)	149/191 (78%)

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	379	LYS	HD3	-0.15	0.54 – 2.65	-8.3
1	A	379	LYS	HD2	0.14	0.58 – 2.64	-7.1
1	A	426	PRO	HG3	-0.09	0.33 – 3.48	-6.3
1	A	339	GLN	CG	26.99	28.36 – 39.21	-6.3
1	A	379	LYS	CD	22.14	23.50 – 34.42	-6.2
1	A	336	GLN	CD	172.17	173.59 – 185.85	-6.2
1	A	351	GLN	CD	172.16	173.59 – 185.85	-6.2
1	A	339	GLN	CD	172.53	173.59 – 185.85	-5.9
1	A	426	PRO	HA	2.64	2.78 – 6.00	-5.4
1	A	345	LEU	HD11	-0.67	-0.61 – 2.12	-5.2
1	A	345	LEU	HD12	-0.67	-0.61 – 2.12	-5.2
1	A	345	LEU	HD13	-0.67	-0.61 – 2.12	-5.2
1	A	379	LYS	HB3	0.45	0.46 – 3.04	-5.0

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:

