



Full wwPDB NMR Structure Validation Report ⓘ

Mar 5, 2026 – 10:02 AM UTC

PDB ID : 8BA1 / pdb_00008ba1
BMRB ID : 51624
Title : CTD12-CTD12 heterodimer from CPSF73 and CPSF100
Authors : Thore, S.; Mackereth, C.
Deposited on : 2022-10-10

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

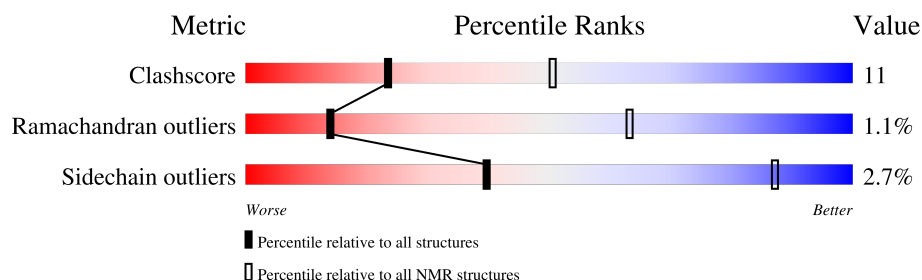
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

The overall completeness of chemical shifts assignment is 45%.

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	119	
2	B	116	

2 Ensemble composition and analysis

This entry contains 20 models. Model 3 is the overall representative, medoid model (most similar to other models). The authors have identified model 1 as representative, based on the following criterion: *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:455-A:566, B:530-B:620, B:624-B:639 (219)	0.96	3

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 2 clusters. No single-model clusters were found.

Cluster number	Models
1	1, 2, 3, 4, 5, 6, 7, 8, 9, 11, 12, 13, 14, 16, 19, 20
2	10, 15, 17, 18

3 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3664 atoms, of which 1824 are hydrogens and 0 are deuteriums.

- Molecule 1 is a protein called Cleavage and polyadenylation specificity factor subunit 3.

Mol	Chain	Residues	Atoms						Trace
1	A	119	Total	C	H	N	O	S	0
			1895	603	947	150	190	5	

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	449	GLY	-	expression tag	UNP Q8SUE4
A	450	HIS	-	expression tag	UNP Q8SUE4
A	451	MET	-	expression tag	UNP Q8SUE4

- Molecule 2 is a protein called Cleavage and polyadenylation specificity factor subunit 2.

Mol	Chain	Residues	Atoms						Trace
2	B	116	Total	C	H	N	O	S	0
			1769	548	877	161	173	10	

There is a discrepancy between the modelled and reference sequences:

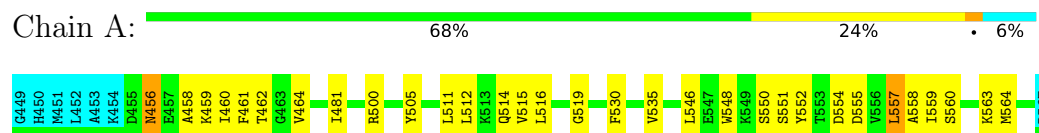
Chain	Residue	Modelled	Actual	Comment	Reference
B	524	MET	-	initiating methionine	UNP M1JIZ1

4 Residue-property plots

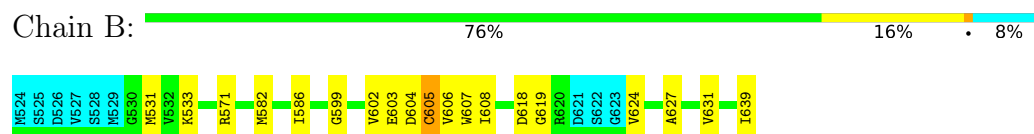
4.1 Average score per residue in the NMR ensemble

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: Cleavage and polyadenylation specificity factor subunit 3



- Molecule 2: Cleavage and polyadenylation specificity factor subunit 2

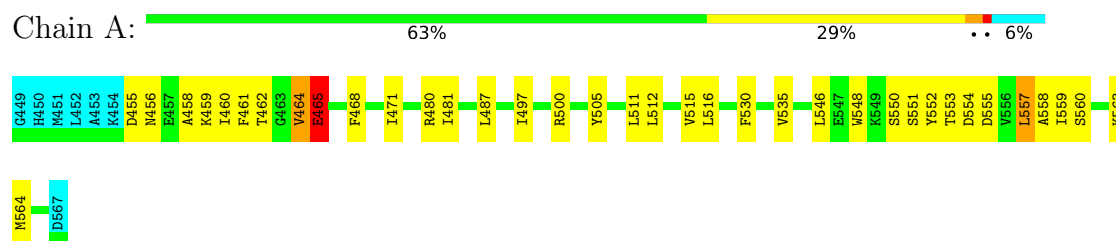


4.2 Scores per residue for each member of the ensemble

Colouring as in section 4.1 above.

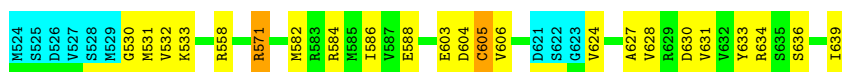
4.2.1 Score per residue for model 1

- Molecule 1: Cleavage and polyadenylation specificity factor subunit 3



- Molecule 2: Cleavage and polyadenylation specificity factor subunit 2





4.2.2 Score per residue for model 2

- Molecule 1: Cleavage and polyadenylation specificity factor subunit 3

Chain A: 70% 23% 6%



- Molecule 2: Cleavage and polyadenylation specificity factor subunit 2

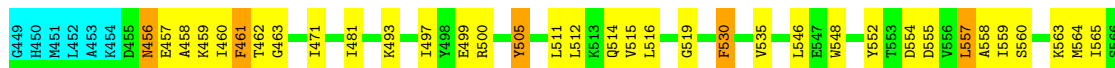
Chain B: 76% 16% 8%



4.2.3 Score per residue for model 3 (medoid)

- Molecule 1: Cleavage and polyadenylation specificity factor subunit 3

Chain A: 65% 25% 6%



- Molecule 2: Cleavage and polyadenylation specificity factor subunit 2

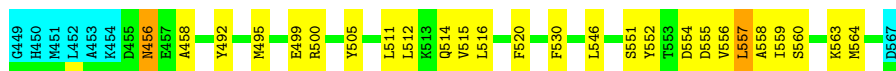
Chain B: 75% 16% 8%



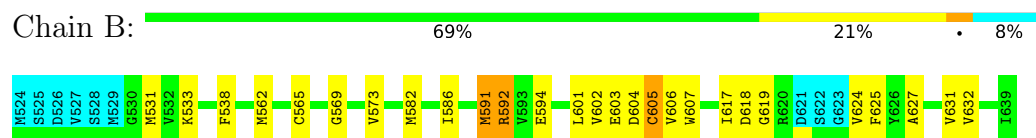
4.2.4 Score per residue for model 4

- Molecule 1: Cleavage and polyadenylation specificity factor subunit 3

Chain A: 72% 20% 6%

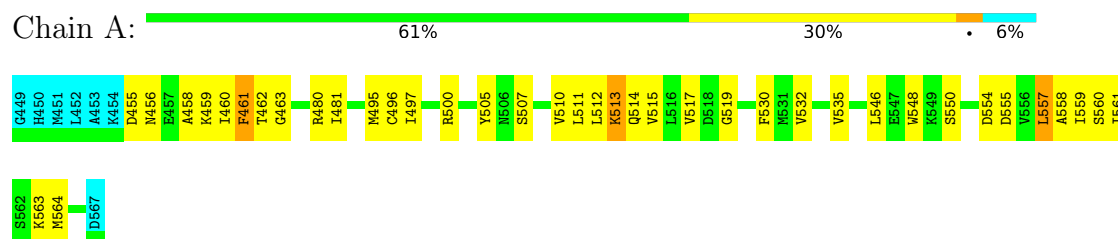


- Molecule 2: Cleavage and polyadenylation specificity factor subunit 2

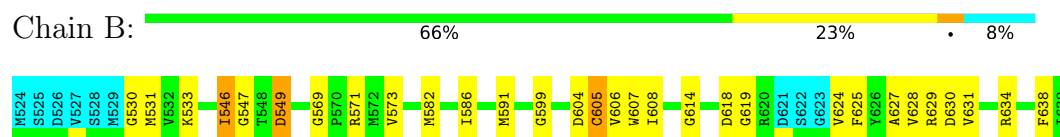


4.2.5 Score per residue for model 5

- Molecule 1: Cleavage and polyadenylation specificity factor subunit 3

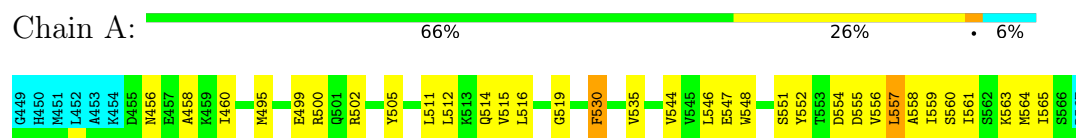


- Molecule 2: Cleavage and polyadenylation specificity factor subunit 2

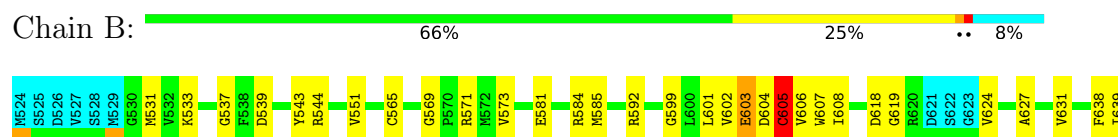


4.2.6 Score per residue for model 6

- Molecule 1: Cleavage and polyadenylation specificity factor subunit 3



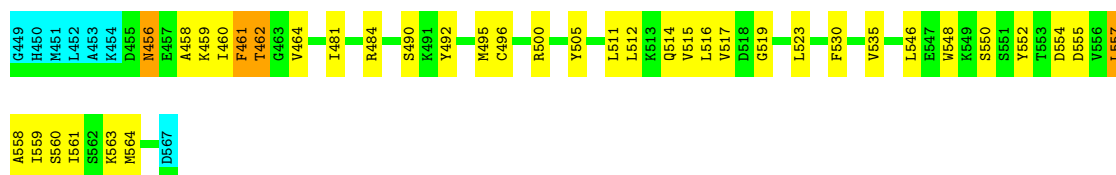
- Molecule 2: Cleavage and polyadenylation specificity factor subunit 2



4.2.7 Score per residue for model 7

- Molecule 1: Cleavage and polyadenylation specificity factor subunit 3





- Molecule 2: Cleavage and polyadenylation specificity factor subunit 2

Chain B: 70% 22% 8%



4.2.8 Score per residue for model 8

- Molecule 1: Cleavage and polyadenylation specificity factor subunit 3

Chain A: 62% 27% 5% 6%



- Molecule 2: Cleavage and polyadenylation specificity factor subunit 2

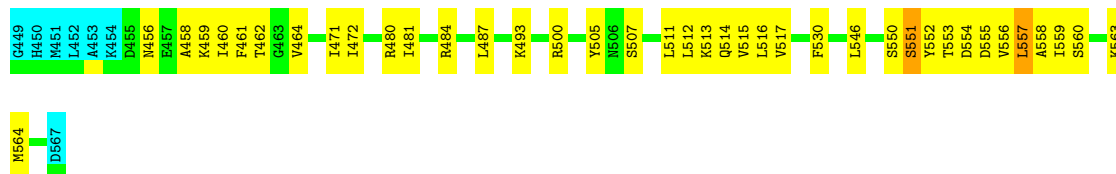
Chain B: 72% 17% 8%



4.2.9 Score per residue for model 9

- Molecule 1: Cleavage and polyadenylation specificity factor subunit 3

Chain A: 61% 31% 6%



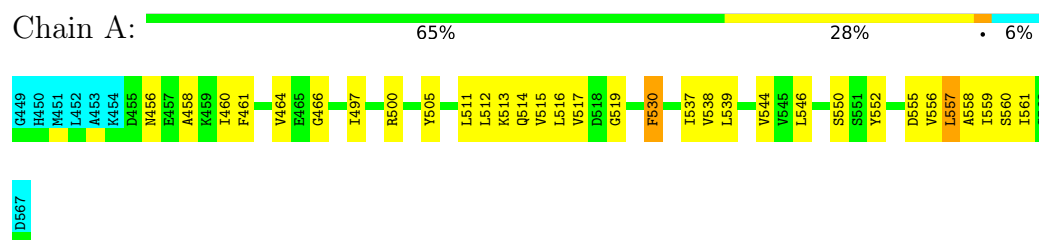
- Molecule 2: Cleavage and polyadenylation specificity factor subunit 2

Chain B: 63% 28% 8%

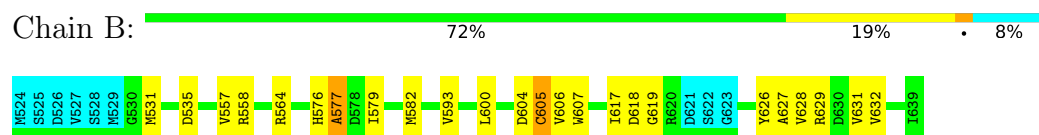


4.2.10 Score per residue for model 10

- Molecule 1: Cleavage and polyadenylation specificity factor subunit 3

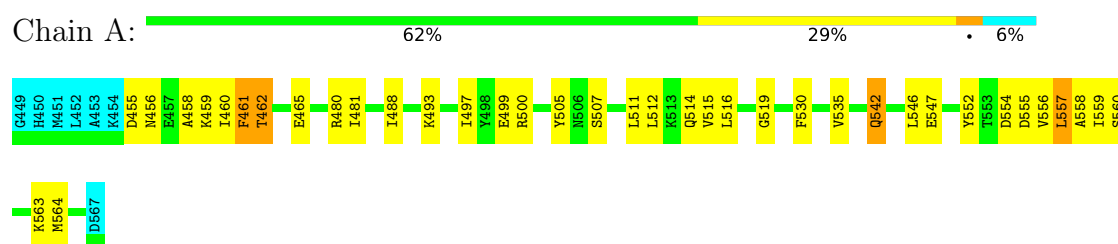


- Molecule 2: Cleavage and polyadenylation specificity factor subunit 2

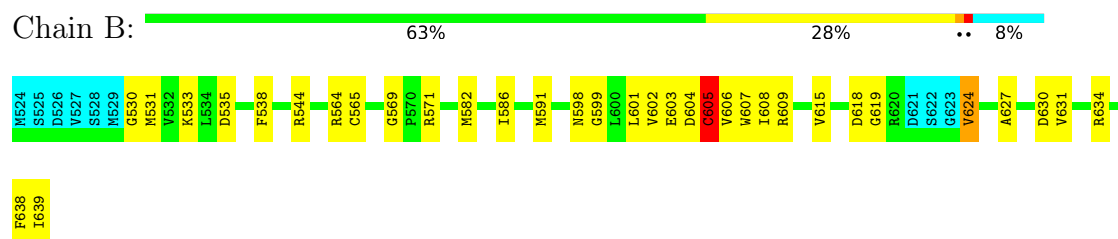


4.2.11 Score per residue for model 11

- Molecule 1: Cleavage and polyadenylation specificity factor subunit 3

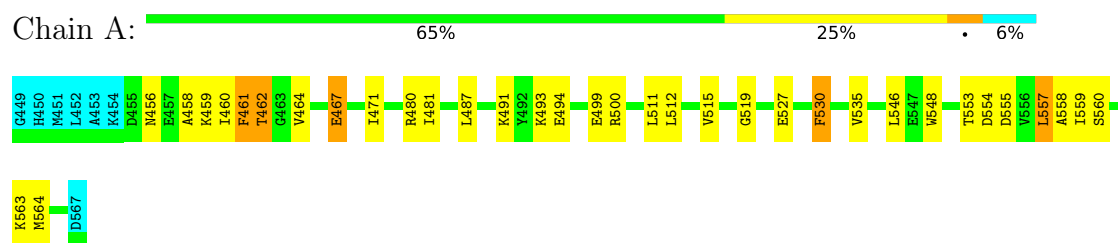


- Molecule 2: Cleavage and polyadenylation specificity factor subunit 2

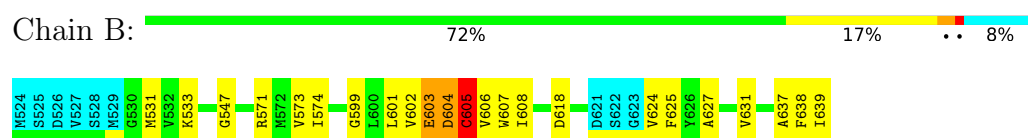


4.2.12 Score per residue for model 12

- Molecule 1: Cleavage and polyadenylation specificity factor subunit 3

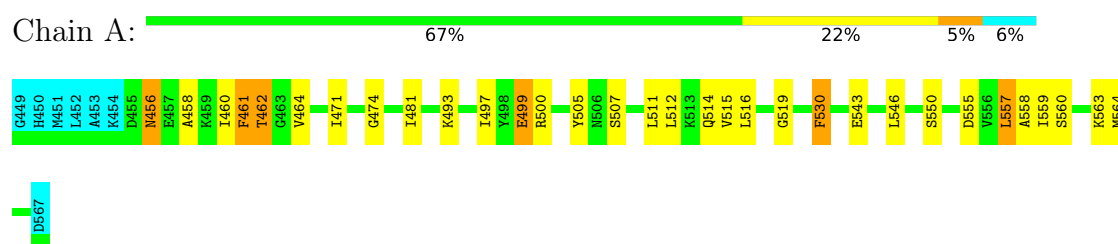


- Molecule 2: Cleavage and polyadenylation specificity factor subunit 2

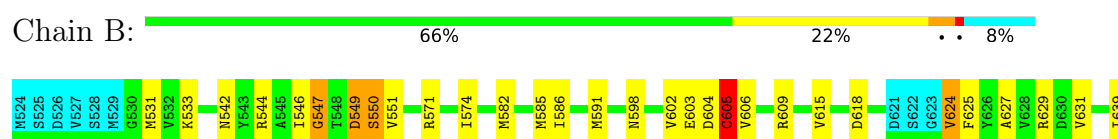


4.2.13 Score per residue for model 13

- Molecule 1: Cleavage and polyadenylation specificity factor subunit 3

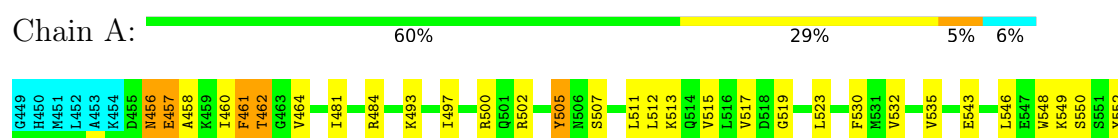


- Molecule 2: Cleavage and polyadenylation specificity factor subunit 2



4.2.14 Score per residue for model 14

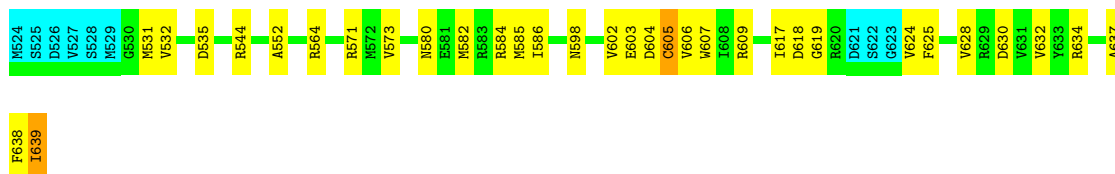
- Molecule 1: Cleavage and polyadenylation specificity factor subunit 3





- Molecule 2: Cleavage and polyadenylation specificity factor subunit 2

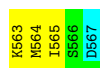
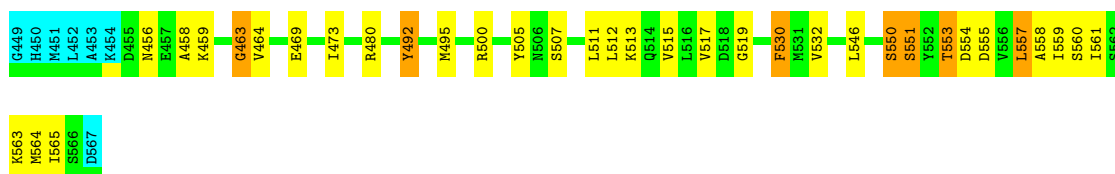
Chain B: 64% 27% 8%



4.2.15 Score per residue for model 15

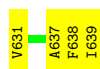
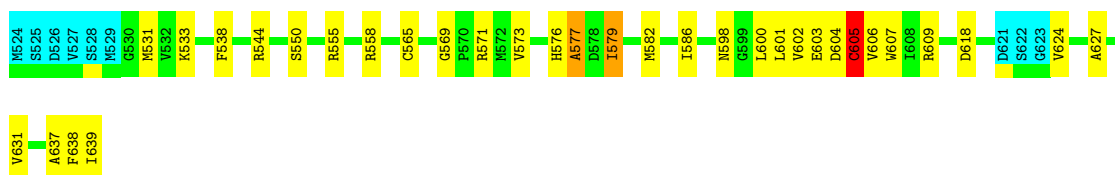
- Molecule 1: Cleavage and polyadenylation specificity factor subunit 3

Chain A: 65% 24% 6% 6%



- Molecule 2: Cleavage and polyadenylation specificity factor subunit 2

Chain B: 64% 26% 8%



4.2.16 Score per residue for model 16

- Molecule 1: Cleavage and polyadenylation specificity factor subunit 3

Chain A: 66% 24% 6%



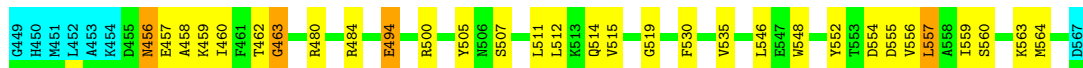
- Molecule 2: Cleavage and polyadenylation specificity factor subunit 2

Chain B: 74% 16% 8%

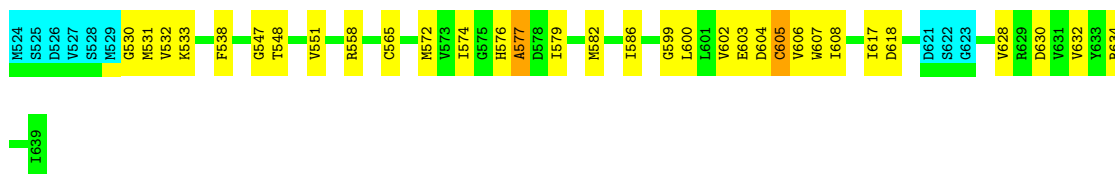


4.2.17 Score per residue for model 17

- Molecule 1: Cleavage and polyadenylation specificity factor subunit 3

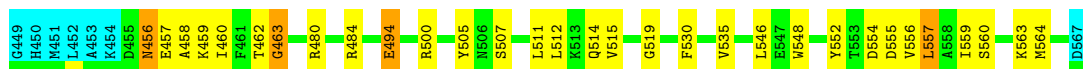


- Molecule 2: Cleavage and polyadenylation specificity factor subunit 2

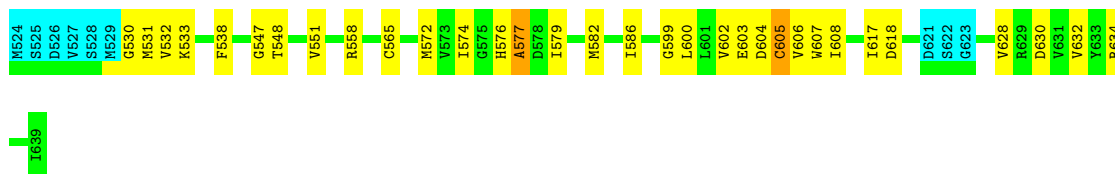


4.2.18 Score per residue for model 18

- Molecule 1: Cleavage and polyadenylation specificity factor subunit 3



- Molecule 2: Cleavage and polyadenylation specificity factor subunit 2



4.2.19 Score per residue for model 19

- Molecule 1: Cleavage and polyadenylation specificity factor subunit 3





- Molecule 2: Cleavage and polyadenylation specificity factor subunit 2

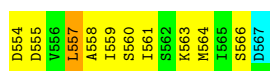
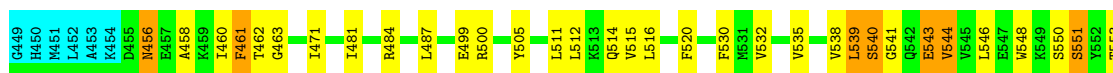
Chain B: 66% 23% 8%



4.2.20 Score per residue for model 20

- Molecule 1: Cleavage and polyadenylation specificity factor subunit 3

Chain A: 58% 29% 7% 6%



- Molecule 2: Cleavage and polyadenylation specificity factor subunit 2

Chain B: 69% 22% 8%



5 Refinement protocol and experimental data overview

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

Of the 250 calculated structures, 20 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
CNS	refinement	1.2
ARIA	structure calculation	2.3

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	1407
Number of shifts mapped to atoms	1407
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	45%

6 Model quality (i)

6.1 Standard geometry (i)

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	0.49±0.02	0±0/908 (0.0± 0.0%)	0.82±0.06	1±3/1225 (0.1± 0.2%)
2	B	0.46±0.04	0±0/841 (0.0± 0.0%)	0.81±0.05	2±2/1127 (0.1± 0.2%)
All	All	0.48	1/34980 (0.0%)	0.81	52/47040 (0.1%)

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	1.6±1.1
2	B	0.0±0.0	1.2±0.4
All	All	0	56

All unique bond outliers are listed below.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	B	603	GLU	N-CA	5.14	1.52	1.46	12	1

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
2	B	605	CYS	N-CA-C	-7.65	98.32	108.34	19	9
2	B	620	ARG	N-CA-C	-6.34	107.39	114.62	19	1
1	A	539	LEU	N-CA-C	6.27	120.10	110.20	20	1
1	A	464	VAL	N-CA-C	6.25	117.41	107.98	19	1
1	A	543	GLU	CA-C-N	-6.21	114.96	122.90	20	1
1	A	543	GLU	C-N-CA	-6.21	114.96	122.90	20	1
2	B	604	ASP	CA-C-N	5.71	131.75	122.39	19	8
2	B	604	ASP	C-N-CA	5.71	131.75	122.39	19	8

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	463	GLY	CA-C-N	-5.56	115.42	122.43	20	3
1	A	463	GLY	C-N-CA	-5.56	115.42	122.43	20	3
1	A	463	GLY	N-CA-C	-5.56	106.86	114.64	17	3
1	A	541	GLY	N-CA-C	-5.39	100.41	113.18	20	1
2	B	605	CYS	CA-C-N	5.39	131.67	121.97	12	1
2	B	605	CYS	C-N-CA	5.39	131.67	121.97	12	1
1	A	539	LEU	CA-C-N	5.35	130.62	122.65	20	1
1	A	539	LEU	C-N-CA	5.35	130.62	122.65	20	1
1	A	541	GLY	CA-C-N	-5.33	113.05	122.26	20	1
1	A	541	GLY	C-N-CA	-5.33	113.05	122.26	20	1
1	A	544	VAL	N-CA-CB	5.24	117.34	111.21	20	1
1	A	543	GLU	O-C-N	-5.13	115.77	122.59	20	1
2	B	549	ASP	CA-C-N	-5.02	113.77	121.40	13	1
2	B	549	ASP	C-N-CA	-5.02	113.77	121.40	13	1
2	B	550	SER	CA-C-N	-5.01	115.17	122.58	13	1
2	B	550	SER	C-N-CA	-5.01	115.17	122.58	13	1

There are no chirality outliers.

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

Mol	Chain	Res	Type	Group	Models (Total)
2	B	605	CYS	Peptide	20
1	A	461	PHE	Peptide	10
1	A	462	THR	Peptide	9
1	A	463	GLY	Peptide	3
1	A	464	VAL	Peptide	2
1	A	465	GLU	Peptide	2
1	A	547	GLU	Peptide	2
1	A	550	SER	Peptide	2
2	B	591	MET	Peptide	1
2	B	546	ILE	Peptide	1
2	B	604	ASP	Peptide	1
1	A	457	GLU	Peptide	1
2	B	619	GLY	Peptide	1
1	A	540	SER	Peptide	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	895	892	891	25±4
2	B	831	822	821	18±3
All	All	34520	34280	34240	758

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 11.

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

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:540:SER:HB2	1:A:544:VAL:N	0.86	1.85	20	1
1:A:505:TYR:CE2	1:A:544:VAL:HB	0.81	2.09	10	1
1:A:535:VAL:HG21	1:A:558:ALA:HB2	0.76	1.57	6	4
1:A:499:GLU:O	1:A:548:TRP:HB2	0.76	1.79	2	1
2:B:606:VAL:HG21	2:B:625:PHE:HA	0.74	1.59	12	1
1:A:500:ARG:HA	1:A:546:LEU:O	0.73	1.84	16	20
2:B:586:ILE:O	2:B:591:MET:HB2	0.72	1.85	4	1
1:A:462:THR:O	1:A:464:VAL:HG23	0.71	1.85	13	5
1:A:461:PHE:O	1:A:462:THR:HG23	0.70	1.87	3	12
1:A:557:LEU:HD22	1:A:558:ALA:N	0.69	2.03	11	12
2:B:535:ASP:OD2	2:B:564:ARG:HA	0.69	1.87	9	5
1:A:460:ILE:O	2:B:530:GLY:HA2	0.69	1.88	17	2
2:B:546:ILE:HB	2:B:549:ASP:CB	0.68	2.18	13	1
2:B:576:HIS:CG	2:B:577:ALA:H	0.67	2.07	15	4
1:A:538:VAL:O	1:A:544:VAL:HA	0.67	1.90	20	1
1:A:460:ILE:HG12	1:A:461:PHE:N	0.67	2.05	9	1
1:A:458:ALA:O	2:B:531:MET:HA	0.66	1.90	17	20
1:A:519:GLY:HA3	1:A:564:MET:HE2	0.66	1.66	11	6
1:A:557:LEU:HD12	1:A:558:ALA:N	0.66	2.04	16	1
1:A:516:LEU:HD23	1:A:564:MET:SD	0.65	2.32	2	11
1:A:560:SER:O	1:A:563:LYS:HG2	0.65	1.91	20	20
1:A:516:LEU:HA	1:A:564:MET:SD	0.65	2.32	11	5
1:A:512:LEU:HD23	1:A:530:PHE:CE2	0.64	2.27	20	20
1:A:460:ILE:HG13	1:A:481:ILE:O	0.63	1.93	9	1
2:B:591:MET:SD	2:B:624:VAL:HG23	0.63	2.34	16	2
1:A:505:TYR:OH	1:A:565:ILE:HD13	0.63	1.93	10	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:456:ASN:O	2:B:533:LYS:HA	0.63	1.94	2	18
1:A:465:GLU:CG	2:B:558:ARG:HG3	0.62	2.24	1	1
1:A:505:TYR:CZ	1:A:565:ILE:HD13	0.62	2.29	10	1
2:B:585:MET:SD	2:B:634:ARG:HD2	0.62	2.34	7	3
2:B:605:CYS:O	2:B:606:VAL:HG23	0.62	1.94	12	1
1:A:464:VAL:HG12	1:A:465:GLU:H	0.62	1.55	1	1
1:A:560:SER:O	1:A:564:MET:HG2	0.62	1.94	15	9
2:B:606:VAL:HG13	2:B:618:ASP:O	0.62	1.93	8	7
2:B:571:ARG:HA	2:B:639:ILE:O	0.62	1.95	8	9
1:A:457:GLU:HA	2:B:532:VAL:O	0.61	1.95	19	3
1:A:473:ILE:HA	2:B:550:SER:O	0.61	1.96	15	1
2:B:606:VAL:HA	2:B:618:ASP:O	0.61	1.96	12	1
1:A:519:GLY:HA3	1:A:564:MET:HE1	0.60	1.73	19	9
1:A:548:TRP:CE3	1:A:558:ALA:HB1	0.60	2.32	1	5
2:B:546:ILE:HB	2:B:549:ASP:HB2	0.60	1.72	13	2
2:B:601:LEU:HD13	2:B:607:TRP:CE2	0.60	2.31	20	7
2:B:592:ARG:HD3	2:B:602:VAL:HG13	0.59	1.73	4	1
1:A:505:TYR:CE1	1:A:544:VAL:HG21	0.59	2.32	10	1
2:B:619:GLY:HA2	2:B:625:PHE:CD1	0.58	2.33	5	5
2:B:602:VAL:HB	2:B:606:VAL:HB	0.58	1.75	4	1
1:A:540:SER:CB	1:A:544:VAL:HG23	0.57	2.28	20	1
1:A:457:GLU:HB2	2:B:532:VAL:O	0.57	1.99	14	1
1:A:495:MET:O	2:B:573:VAL:HB	0.57	1.99	16	7
1:A:497:ILE:HA	2:B:615:VAL:O	0.57	2.00	11	6
2:B:592:ARG:H	2:B:592:ARG:CD	0.57	2.13	4	1
2:B:585:MET:HB3	2:B:631:VAL:HG13	0.57	1.77	13	1
1:A:505:TYR:CZ	1:A:544:VAL:HB	0.56	2.35	10	1
2:B:584:ARG:O	2:B:588:GLU:HG2	0.56	2.01	20	2
2:B:592:ARG:H	2:B:592:ARG:HD2	0.56	1.59	4	1
2:B:599:GLY:HA3	2:B:608:ILE:O	0.56	1.99	5	11
1:A:535:VAL:HG13	1:A:548:TRP:HB3	0.56	1.78	7	8
1:A:511:LEU:O	1:A:514:GLN:HG3	0.56	2.01	2	1
2:B:579:ILE:HA	2:B:582:MET:SD	0.56	2.40	2	1
1:A:540:SER:HB3	1:A:544:VAL:HG23	0.56	1.78	20	1
2:B:533:LYS:HD3	2:B:562:MET:SD	0.55	2.42	4	1
1:A:552:TYR:O	1:A:556:VAL:HG23	0.55	2.01	11	7
2:B:617:ILE:HD11	2:B:632:VAL:HG21	0.55	1.79	10	6
1:A:456:ASN:HD22	1:A:456:ASN:N	0.55	2.00	16	5
1:A:505:TYR:CE2	1:A:565:ILE:HG21	0.55	2.36	10	1
1:A:505:TYR:CZ	1:A:507:SER:HB2	0.55	2.37	13	9
1:A:474:GLY:H	2:B:550:SER:HB2	0.55	1.62	13	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:466:GLY:O	2:B:557:VAL:HA	0.54	2.02	8	3
2:B:607:TRP:HB2	2:B:618:ASP:O	0.54	2.01	19	1
1:A:459:LYS:O	1:A:480:ARG:HA	0.54	2.02	15	10
1:A:555:ASP:O	1:A:559:ILE:HG13	0.54	2.02	10	20
2:B:572:MET:O	2:B:639:ILE:HG13	0.54	2.01	8	1
1:A:460:ILE:HB	1:A:481:ILE:HB	0.53	1.80	5	12
1:A:474:GLY:N	2:B:550:SER:HB2	0.53	2.18	13	1
2:B:594:GLU:HB2	2:B:601:LEU:O	0.53	2.03	4	1
1:A:494:GLU:HG2	2:B:572:MET:SD	0.53	2.43	17	2
1:A:460:ILE:HA	1:A:481:ILE:O	0.53	2.03	19	2
2:B:571:ARG:HA	2:B:639:ILE:OXT	0.53	2.03	11	1
1:A:459:LYS:HA	2:B:530:GLY:O	0.53	2.03	1	6
1:A:497:ILE:H	1:A:550:SER:HB3	0.53	1.64	14	6
2:B:630:ASP:O	2:B:634:ARG:HG3	0.53	2.04	3	7
1:A:511:LEU:O	1:A:515:VAL:HG23	0.53	2.03	2	20
2:B:627:ALA:O	2:B:631:VAL:HG23	0.53	2.04	9	13
1:A:557:LEU:C	1:A:557:LEU:HD22	0.53	2.28	1	7
2:B:539:ASP:HA	2:B:543:TYR:OH	0.53	2.04	6	1
2:B:573:VAL:HG22	2:B:638:PHE:CD1	0.53	2.39	6	8
1:A:466:GLY:HA2	2:B:558:ARG:O	0.53	2.03	16	2
2:B:538:PHE:O	2:B:541:LEU:HG	0.53	2.03	9	1
2:B:582:MET:O	2:B:586:ILE:HG13	0.53	2.04	2	12
1:A:554:ASP:HA	1:A:557:LEU:CD1	0.53	2.34	11	14
2:B:602:VAL:C	2:B:605:CYS:HB2	0.53	2.29	6	8
2:B:601:LEU:HD13	2:B:607:TRP:NE1	0.52	2.19	19	1
1:A:519:GLY:HA3	1:A:564:MET:CE	0.52	2.34	10	6
2:B:585:MET:SD	2:B:631:VAL:HA	0.52	2.45	19	2
2:B:546:ILE:CB	2:B:549:ASP:HB2	0.52	2.34	13	1
2:B:546:ILE:HB	2:B:549:ASP:OD2	0.52	2.05	19	1
2:B:606:VAL:HG11	2:B:628:VAL:HG21	0.52	1.81	2	7
1:A:505:TYR:CE1	1:A:544:VAL:CG2	0.51	2.93	10	1
2:B:573:VAL:HA	2:B:637:ALA:O	0.51	2.06	15	5
1:A:535:VAL:HG11	1:A:561:ILE:HD12	0.51	1.82	7	2
1:A:465:GLU:HG2	2:B:558:ARG:HG3	0.51	1.82	1	1
1:A:539:LEU:HD13	1:A:544:VAL:HG23	0.51	1.82	10	1
2:B:602:VAL:O	2:B:604:ASP:N	0.51	2.38	12	1
2:B:571:ARG:HG3	2:B:639:ILE:OXT	0.51	2.06	15	1
1:A:540:SER:HA	1:A:543:GLU:N	0.51	2.21	20	1
2:B:602:VAL:HB	2:B:624:VAL:N	0.51	2.20	12	1
2:B:604:ASP:O	2:B:605:CYS:SG	0.50	2.69	10	11
1:A:500:ARG:O	2:B:619:GLY:HA3	0.50	2.06	4	5

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:552:TYR:HA	1:A:555:ASP:OD2	0.50	2.07	4	1
2:B:538:PHE:CE2	2:B:565:CYS:HB2	0.50	2.41	17	7
1:A:501:GLN:HA	2:B:619:GLY:HA2	0.50	1.84	16	1
1:A:540:SER:HB2	1:A:543:GLU:C	0.50	2.32	20	1
2:B:607:TRP:HB2	2:B:618:ASP:HB2	0.49	1.84	17	4
2:B:592:ARG:CG	2:B:602:VAL:HG13	0.49	2.38	4	1
2:B:544:ARG:NH1	2:B:639:ILE:HG23	0.49	2.22	8	1
1:A:499:GLU:HG2	2:B:629:ARG:CZ	0.49	2.38	13	2
2:B:558:ARG:C	2:B:558:ARG:HD2	0.49	2.33	9	1
2:B:547:GLY:C	2:B:549:ASP:H	0.49	2.16	13	1
1:A:460:ILE:CG1	1:A:461:PHE:N	0.49	2.76	9	1
1:A:461:PHE:CE2	2:B:530:GLY:HA2	0.49	2.43	8	1
1:A:505:TYR:CB	1:A:540:SER:HB3	0.48	2.38	20	1
1:A:468:PHE:CE1	2:B:558:ARG:HB2	0.48	2.43	1	1
1:A:532:VAL:HB	1:A:561:ILE:HD11	0.48	1.84	5	5
2:B:598:ASN:O	2:B:609:ARG:HA	0.48	2.07	13	6
2:B:592:ARG:CD	2:B:602:VAL:HG13	0.48	2.39	4	1
2:B:624:VAL:HB	2:B:627:ALA:HB3	0.48	1.86	6	1
1:A:493:LYS:HG2	1:A:494:GLU:N	0.48	2.24	12	1
2:B:607:TRP:HB2	2:B:618:ASP:HB3	0.48	1.85	16	5
1:A:552:TYR:O	1:A:555:ASP:HB2	0.48	2.09	6	5
2:B:592:ARG:HB3	2:B:603:GLU:HG2	0.48	1.86	4	1
2:B:591:MET:SD	2:B:624:VAL:HG13	0.48	2.48	13	4
1:A:505:TYR:CE2	1:A:507:SER:HB2	0.48	2.43	8	1
1:A:471:ILE:HG12	1:A:487:LEU:HD22	0.48	1.84	12	5
2:B:579:ILE:O	2:B:600:LEU:HD11	0.48	2.07	15	1
1:A:505:TYR:HB3	1:A:540:SER:HB3	0.48	1.85	20	1
1:A:505:TYR:CZ	1:A:565:ILE:HG21	0.47	2.43	10	1
1:A:465:GLU:OE1	1:A:483:LYS:HE3	0.47	2.08	16	1
2:B:607:TRP:HB2	2:B:618:ASP:CB	0.47	2.39	16	5
2:B:544:ARG:HB2	2:B:551:VAL:HG23	0.47	1.84	6	1
1:A:469:GLU:OE1	1:A:484:ARG:HD3	0.47	2.08	8	1
2:B:542:ASN:HB2	2:B:544:ARG:NH1	0.47	2.24	13	1
1:A:496:CYS:O	2:B:614:GLY:HA3	0.47	2.10	5	1
2:B:576:HIS:CG	2:B:577:ALA:N	0.47	2.79	17	4
1:A:548:TRP:HE1	1:A:555:ASP:CG	0.47	2.18	6	1
2:B:579:ILE:HG12	2:B:600:LEU:CD1	0.47	2.39	10	4
2:B:582:MET:SD	2:B:632:VAL:HG22	0.47	2.49	10	3
1:A:488:ILE:O	1:A:493:LYS:HE2	0.47	2.10	11	1
1:A:474:GLY:CA	2:B:550:SER:HB2	0.47	2.39	13	1
2:B:580:ASN:O	2:B:584:ARG:HG3	0.47	2.09	14	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:505:TYR:CG	1:A:565:ILE:HG23	0.47	2.45	15	2
2:B:581:GLU:OE2	2:B:584:ARG:HD3	0.47	2.09	6	1
1:A:499:GLU:OE2	2:B:617:ILE:HB	0.46	2.10	3	1
2:B:546:ILE:CG2	2:B:549:ASP:HB2	0.46	2.40	13	1
1:A:462:THR:O	1:A:464:VAL:N	0.46	2.48	19	1
1:A:499:GLU:HB2	1:A:548:TRP:NE1	0.46	2.25	20	1
2:B:625:PHE:O	2:B:629:ARG:HG3	0.46	2.09	5	2
1:A:465:GLU:O	2:B:558:ARG:HB3	0.46	2.09	8	2
1:A:460:ILE:HG22	2:B:530:GLY:O	0.46	2.10	2	1
2:B:546:ILE:HG22	2:B:547:GLY:H	0.46	1.70	5	1
1:A:469:GLU:HG3	2:B:555:ARG:HE	0.46	1.71	15	1
1:A:553:THR:O	1:A:557:LEU:HD13	0.46	2.11	15	4
1:A:467:GLU:H	1:A:467:GLU:CD	0.46	2.19	12	1
2:B:571:ARG:HG2	2:B:639:ILE:OXT	0.46	2.10	12	1
1:A:554:ASP:O	1:A:557:LEU:HD13	0.46	2.11	17	2
2:B:576:HIS:CD2	2:B:577:ALA:H	0.46	2.28	17	4
1:A:557:LEU:HD13	1:A:558:ALA:N	0.46	2.26	14	1
1:A:496:CYS:HA	1:A:550:SER:HB3	0.46	1.87	7	1
1:A:557:LEU:HD13	1:A:558:ALA:H	0.46	1.71	14	1
2:B:625:PHE:CE2	2:B:629:ARG:HD2	0.45	2.46	9	2
1:A:459:LYS:O	1:A:480:ARG:HG3	0.45	2.11	12	1
2:B:592:ARG:HB2	2:B:603:GLU:CD	0.45	2.36	6	1
1:A:500:ARG:HD2	2:B:618:ASP:OD1	0.45	2.12	16	2
1:A:557:LEU:H	1:A:557:LEU:HD13	0.45	1.72	4	4
1:A:484:ARG:NH1	2:B:570:PRO:HG3	0.45	2.27	20	2
1:A:464:VAL:O	2:B:558:ARG:HD3	0.45	2.10	10	1
1:A:502:ARG:HD3	1:A:543:GLU:OE2	0.45	2.11	14	1
1:A:468:PHE:CD1	2:B:558:ARG:HB2	0.45	2.46	1	1
1:A:539:LEU:HA	1:A:544:VAL:HG22	0.45	1.87	10	1
2:B:633:TYR:HA	2:B:636:SER:OG	0.45	2.12	1	1
2:B:592:ARG:CB	2:B:603:GLU:HG2	0.45	2.41	4	1
1:A:510:VAL:O	1:A:513:LYS:HG3	0.44	2.11	5	1
2:B:538:PHE:CE2	2:B:565:CYS:HB3	0.44	2.48	7	1
2:B:538:PHE:CZ	2:B:554:PHE:CD1	0.44	3.06	9	1
2:B:546:ILE:O	2:B:547:GLY:C	0.44	2.60	19	1
2:B:537:GLY:HA3	2:B:565:CYS:SG	0.44	2.52	7	2
2:B:602:VAL:O	2:B:605:CYS:HB2	0.44	2.13	16	2
2:B:606:VAL:HG21	2:B:625:PHE:CA	0.44	2.39	12	1
1:A:484:ARG:HD3	1:A:484:ARG:C	0.44	2.38	14	3
2:B:552:ALA:HA	2:B:639:ILE:HG21	0.44	1.89	14	1
1:A:558:ALA:O	1:A:561:ILE:HB	0.43	2.13	10	2

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:540:SER:HB2	1:A:544:VAL:H	0.43	1.70	20	1
2:B:602:VAL:HG12	2:B:603:GLU:HG2	0.43	1.89	17	3
1:A:505:TYR:CZ	1:A:544:VAL:CB	0.43	3.01	10	1
2:B:544:ARG:HD2	2:B:638:PHE:O	0.43	2.12	15	3
1:A:557:LEU:HD12	1:A:557:LEU:C	0.43	2.39	16	1
1:A:513:LYS:O	1:A:517:VAL:HG23	0.43	2.14	15	6
2:B:533:LYS:HB2	2:B:533:LYS:NZ	0.43	2.29	3	1
1:A:505:TYR:OH	1:A:565:ILE:CD1	0.43	2.66	10	1
1:A:550:SER:O	1:A:551:SER:C	0.43	2.61	20	5
1:A:464:VAL:HG12	1:A:465:GLU:N	0.42	2.25	1	1
1:A:551:SER:HB3	1:A:554:ASP:OD1	0.42	2.13	1	1
1:A:554:ASP:HA	1:A:557:LEU:HD11	0.42	1.90	3	5
2:B:618:ASP:OD2	2:B:620:ARG:HG2	0.42	2.14	3	1
2:B:607:TRP:O	2:B:617:ILE:HA	0.42	2.14	7	1
1:A:542:GLN:HE21	1:A:542:GLN:HA	0.42	1.74	11	1
1:A:549:LYS:HB2	1:A:554:ASP:OD2	0.42	2.14	14	1
1:A:553:THR:O	1:A:557:LEU:HD12	0.42	2.15	14	2
2:B:629:ARG:HB3	2:B:633:TYR:CE2	0.42	2.49	19	1
2:B:628:VAL:O	2:B:632:VAL:HG23	0.42	2.14	20	1
2:B:551:VAL:CG1	2:B:574:ILE:HD11	0.42	2.45	13	1
1:A:520:PHE:CE1	1:A:564:MET:HE1	0.42	2.50	4	3
1:A:512:LEU:O	1:A:516:LEU:HG	0.42	2.15	10	1
1:A:513:LYS:HB3	1:A:530:PHE:CD1	0.42	2.50	10	1
1:A:539:LEU:C	1:A:543:GLU:O	0.42	2.63	20	1
1:A:494:GLU:HA	2:B:574:ILE:HA	0.42	1.92	12	1
2:B:532:VAL:HG11	2:B:558:ARG:NH1	0.42	2.29	1	1
2:B:603:GLU:C	2:B:605:CYS:H	0.42	2.23	7	2
1:A:512:LEU:HD21	1:A:537:ILE:CG2	0.42	2.45	10	1
1:A:455:ASP:C	1:A:456:ASN:HD22	0.41	2.22	1	3
1:A:538:VAL:O	1:A:544:VAL:HG13	0.41	2.14	10	1
2:B:538:PHE:CE1	2:B:565:CYS:HB2	0.41	2.50	11	1
2:B:558:ARG:HD3	2:B:558:ARG:C	0.41	2.40	8	1
1:A:513:LYS:HG3	1:A:523:LEU:HD21	0.41	1.91	14	1
1:A:505:TYR:HB3	1:A:540:SER:C	0.41	2.40	20	1
2:B:586:ILE:CG2	2:B:592:ARG:HD2	0.41	2.44	4	1
1:A:499:GLU:O	1:A:548:TRP:HB3	0.41	2.16	6	1
1:A:544:VAL:HG21	1:A:565:ILE:HD13	0.41	1.93	6	1
2:B:583:ARG:HD2	2:B:595:GLN:HG3	0.41	1.92	9	1
1:A:505:TYR:CE1	1:A:512:LEU:HD13	0.41	2.51	10	1
2:B:571:ARG:N	2:B:571:ARG:HD2	0.41	2.31	7	1
1:A:555:ASP:CG	2:B:629:ARG:HH22	0.41	2.23	3	1

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Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
1:A:461:PHE:O	1:A:462:THR:CG2	0.41	2.69	11	2
1:A:475:THR:HG22	2:B:549:ASP:OD2	0.41	2.16	2	1
1:A:490:SER:C	1:A:492:TYR:N	0.41	2.79	7	1
2:B:551:VAL:HB	2:B:574:ILE:HD11	0.41	1.93	17	2
2:B:606:VAL:HA	2:B:619:GLY:HA3	0.41	1.92	19	1
1:A:472:ILE:HG13	1:A:481:ILE:HG12	0.41	1.93	9	1
1:A:557:LEU:HD22	1:A:557:LEU:C	0.41	2.41	11	1
1:A:460:ILE:HG12	1:A:461:PHE:O	0.40	2.16	10	1
1:A:505:TYR:CZ	1:A:544:VAL:CG2	0.40	3.04	10	1
2:B:626:TYR:O	2:B:629:ARG:HG2	0.40	2.16	10	1
1:A:548:TRP:CZ3	1:A:558:ALA:HB1	0.40	2.51	1	1
2:B:547:GLY:C	2:B:549:ASP:N	0.40	2.79	13	1
1:A:464:VAL:O	2:B:558:ARG:HD2	0.40	2.16	15	1
2:B:573:VAL:CG1	2:B:636:SER:HB2	0.40	2.46	20	1
1:A:499:GLU:O	1:A:548:TRP:CB	0.40	2.69	12	1
1:A:492:TYR:N	1:A:492:TYR:CD2	0.40	2.88	15	1
1:A:517:VAL:HG23	1:A:523:LEU:HD23	0.40	1.93	7	1
2:B:544:ARG:NH2	2:B:639:ILE:HG12	0.40	2.32	8	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	112/119 (94%)	109±1 (98±1%)	2±1 (2±1%)	1±1 (0±1%)	26	74
2	B	106/116 (91%)	100±2 (95±2%)	4±1 (4±1%)	2±1 (2±1%)	9	52
All	All	4360/4700 (93%)	4191 (96%)	120 (3%)	49 (1%)	14	63

All 12 unique Ramachandran outliers are listed below. They are sorted by the frequency of occurrence in the ensemble.

Mol	Chain	Res	Type	Models (Total)
2	B	603	GLU	10
1	A	551	SER	7
2	B	624	VAL	7

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Mol	Chain	Res	Type	Models (Total)
2	B	547	GLY	7
2	B	569	GLY	6
2	B	577	ALA	4
2	B	548	THR	3
1	A	465	GLU	1
1	A	466	GLY	1
2	B	619	GLY	1
1	A	463	GLY	1
1	A	566	SER	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	101/106 (95%)	96±2 (96±2%)	4±2 (4±2%)	26	77
2	B	88/96 (92%)	87±1 (99±1%)	1±1 (1±1%)	73	96
All	All	3780/4040 (94%)	3678 (97%)	102 (3%)	40	87

All 33 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	557	LEU	19
1	A	514	GLN	15
1	A	456	ASN	11
1	A	505	TYR	7
1	A	530	PHE	6
1	A	552	TYR	5
1	A	493	LYS	4
1	A	553	THR	3
1	A	499	GLU	3
2	B	571	ARG	2
1	A	471	ILE	2
1	A	492	TYR	2
2	B	639	ILE	2
1	A	494	GLU	2
1	A	459	LYS	1

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Mol	Chain	Res	Type	Models (Total)
1	A	457	GLU	1
2	B	533	LYS	1
2	B	558	ARG	1
2	B	592	ARG	1
1	A	513	LYS	1
2	B	549	ASP	1
1	A	502	ARG	1
1	A	484	ARG	1
2	B	544	ARG	1
2	B	564	ARG	1
2	B	593	VAL	1
1	A	542	GLN	1
1	A	467	GLU	1
1	A	491	LYS	1
1	A	527	GLU	1
1	A	543	GLU	1
2	B	579	ILE	1
1	A	500	ARG	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 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 ⓘ

There are no chain breaks in this entry.

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 45% for the well-defined parts and 44% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_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	1407
Number of shifts mapped to atoms	1407
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

The following table shows the suggested chemical shift referencing corrections.

Nucleus	# values	Correction $\pm$ precision, ppm	Suggested action
$^{13}\text{C}_\alpha$	116	-0.09 ± 0.06	None needed (< 0.5 ppm)
$^{13}\text{C}_\beta$	105	0.07 ± 0.14	None needed (< 0.5 ppm)
$^{13}\text{C}'$	113	0.20 ± 0.12	None needed (< 0.5 ppm)
^{15}N	111	-0.41 ± 0.36	None needed (< 0.5 ppm)

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 45%, i.e. 1364 atoms were assigned a chemical shift out of a possible 3006. 0 out of 39 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	^1H	^{13}C	^{15}N
Backbone	558/1112 (50%)	229/457 (50%)	221/438 (50%)	108/217 (50%)
Sidechain	746/1702 (44%)	524/1106 (47%)	216/529 (41%)	6/67 (9%)

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	Total	¹ H	¹³ C	¹⁵ N
Aromatic	60/192 (31%)	46/92 (50%)	13/94 (14%)	1/6 (17%)
Overall	1364/3006 (45%)	799/1655 (48%)	450/1061 (42%)	115/290 (40%)

The following table shows the completeness of the chemical shift assignments for the full structure. The overall completeness is 44%, i.e. 1407 atoms were assigned a chemical shift out of a possible 3190. 0 out of 41 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	576/1194 (48%)	236/491 (48%)	229/470 (49%)	111/233 (48%)
Sidechain	771/1796 (43%)	539/1168 (46%)	226/560 (40%)	6/68 (9%)
Aromatic	60/200 (30%)	46/96 (48%)	13/96 (14%)	1/8 (12%)
Overall	1407/3190 (44%)	821/1755 (47%)	468/1126 (42%)	118/309 (38%)

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	499	GLU	HB2	-0.10	1.00 – 3.05	-10.4
1	A	499	GLU	HB3	0.84	0.95 – 3.05	-5.5

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:

