



Full wwPDB EM Validation Report ⓘ

Jul 15, 2025 – 10:07 PM JST

PDB ID : 8HMY / pdb_00008hmy
EMDB ID : EMD-34904
Title : Cryo-EM structure of the human pre-catalytic TSEN/pre-tRNA complex
Authors : Zhang, X.; Yang, F.; Zhan, X.; Shi, Y.
Deposited on : 2022-12-06
Resolution : 2.94 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

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:

EMDB validation analysis : **FAILED**
MolProbity : 4-5-2 with Phenix2.0rc1
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

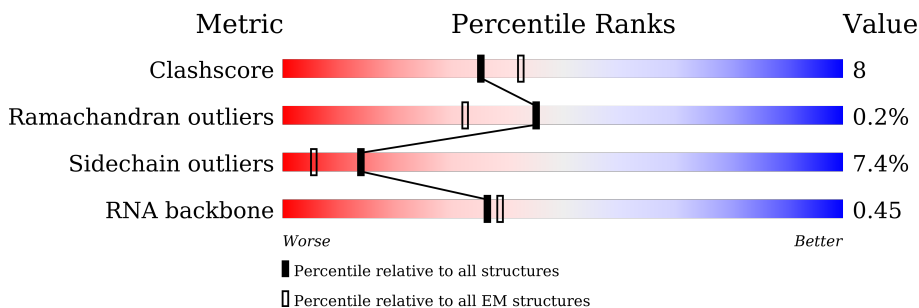
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.94 Å.

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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	485	<div> <div>43%</div> <div>20%</div> <div>.</div> <div>35%</div> </div>
2	B	330	<div> <div>62%</div> <div>17%</div> <div>.</div> <div>20%</div> </div>
3	T	114	<div> <div>45%</div> <div>28%</div> <div>6%</div> <div>21%</div> </div>
4	C	546	<div> <div>38%</div> <div>13%</div> <div>.</div> <div>48%</div> </div>
5	D	213	<div> <div>39%</div> <div>18%</div> <div>.</div> <div>41%</div> </div>
6	E	445	<div> <div>85%</div> <div>15%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11675 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called tRNA-splicing endonuclease subunit Sen2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	314	Total	C	N	O	S	0	0
			2608	1683	445	467	13		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q8NCE0
A	-18	ALA	-	expression tag	UNP Q8NCE0
A	-17	SER	-	expression tag	UNP Q8NCE0
A	-16	ASP	-	expression tag	UNP Q8NCE0
A	-15	TYR	-	expression tag	UNP Q8NCE0
A	-14	LYS	-	expression tag	UNP Q8NCE0
A	-13	ASP	-	expression tag	UNP Q8NCE0
A	-12	ASP	-	expression tag	UNP Q8NCE0
A	-11	ASP	-	expression tag	UNP Q8NCE0
A	-10	ASP	-	expression tag	UNP Q8NCE0
A	-9	LYS	-	expression tag	UNP Q8NCE0
A	-8	ALA	-	expression tag	UNP Q8NCE0
A	-7	SER	-	expression tag	UNP Q8NCE0
A	-6	ASP	-	expression tag	UNP Q8NCE0
A	-5	GLU	-	expression tag	UNP Q8NCE0
A	-4	VAL	-	expression tag	UNP Q8NCE0
A	-3	ASP	-	expression tag	UNP Q8NCE0
A	-2	ALA	-	expression tag	UNP Q8NCE0
A	-1	GLY	-	expression tag	UNP Q8NCE0
A	0	THR	-	expression tag	UNP Q8NCE0
A	377	ALA	HIS	engineered mutation	UNP Q8NCE0

- Molecule 2 is a protein called tRNA-splicing endonuclease subunit Sen34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	264	Total	C	N	O	S	0	0
			2057	1298	386	369	4		

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	MET	-	initiating methionine	UNP Q9BSV6
B	-18	ALA	-	expression tag	UNP Q9BSV6
B	-17	SER	-	expression tag	UNP Q9BSV6
B	-16	ASP	-	expression tag	UNP Q9BSV6
B	-15	TYR	-	expression tag	UNP Q9BSV6
B	-14	LYS	-	expression tag	UNP Q9BSV6
B	-13	ASP	-	expression tag	UNP Q9BSV6
B	-12	ASP	-	expression tag	UNP Q9BSV6
B	-11	ASP	-	expression tag	UNP Q9BSV6
B	-10	ASP	-	expression tag	UNP Q9BSV6
B	-9	LYS	-	expression tag	UNP Q9BSV6
B	-8	ALA	-	expression tag	UNP Q9BSV6
B	-7	SER	-	expression tag	UNP Q9BSV6
B	-6	ASP	-	expression tag	UNP Q9BSV6
B	-5	GLU	-	expression tag	UNP Q9BSV6
B	-4	VAL	-	expression tag	UNP Q9BSV6
B	-3	ASP	-	expression tag	UNP Q9BSV6
B	-2	ALA	-	expression tag	UNP Q9BSV6
B	-1	GLY	-	expression tag	UNP Q9BSV6
B	0	THR	-	expression tag	UNP Q9BSV6
B	255	ALA	HIS	engineered mutation	UNP Q9BSV6

- Molecule 3 is a RNA chain called Pre-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	90	Total	C	N	O	P	0	0
			1888	838	336	624	90		

- Molecule 4 is a protein called tRNA-splicing endonuclease subunit Sen54.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	285	Total	C	N	O	S	0	0
			2263	1440	405	412	6		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	MET	-	initiating methionine	UNP Q7Z6J9
C	-18	ALA	-	expression tag	UNP Q7Z6J9
C	-17	SER	-	expression tag	UNP Q7Z6J9
C	-16	ASP	-	expression tag	UNP Q7Z6J9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-15	TYR	-	expression tag	UNP Q7Z6J9
C	-14	LYS	-	expression tag	UNP Q7Z6J9
C	-13	ASP	-	expression tag	UNP Q7Z6J9
C	-12	ASP	-	expression tag	UNP Q7Z6J9
C	-11	ASP	-	expression tag	UNP Q7Z6J9
C	-10	ASP	-	expression tag	UNP Q7Z6J9
C	-9	LYS	-	expression tag	UNP Q7Z6J9
C	-8	ALA	-	expression tag	UNP Q7Z6J9
C	-7	SER	-	expression tag	UNP Q7Z6J9
C	-6	ASP	-	expression tag	UNP Q7Z6J9
C	-5	GLU	-	expression tag	UNP Q7Z6J9
C	-4	VAL	-	expression tag	UNP Q7Z6J9
C	-3	ASP	-	expression tag	UNP Q7Z6J9
C	-2	ALA	-	expression tag	UNP Q7Z6J9
C	-1	GLY	-	expression tag	UNP Q7Z6J9
C	0	THR	-	expression tag	UNP Q7Z6J9

- Molecule 5 is a protein called Chromosome 1 open reading frame 19, isoform CRA_a.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	D	126	Total	C	N	O	S	
			984	631	154	191	8	
							0	0

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-37	MET	-	initiating methionine	UNP A0A2U3TZM3
D	-36	ALA	-	expression tag	UNP A0A2U3TZM3
D	-35	SER	-	expression tag	UNP A0A2U3TZM3
D	-34	SER	-	expression tag	UNP A0A2U3TZM3
D	-33	ALA	-	expression tag	UNP A0A2U3TZM3
D	-32	TRP	-	expression tag	UNP A0A2U3TZM3
D	-31	SER	-	expression tag	UNP A0A2U3TZM3
D	-30	HIS	-	expression tag	UNP A0A2U3TZM3
D	-29	PRO	-	expression tag	UNP A0A2U3TZM3
D	-28	GLN	-	expression tag	UNP A0A2U3TZM3
D	-27	PHE	-	expression tag	UNP A0A2U3TZM3
D	-26	GLU	-	expression tag	UNP A0A2U3TZM3
D	-25	LYS	-	expression tag	UNP A0A2U3TZM3
D	-24	GLY	-	expression tag	UNP A0A2U3TZM3
D	-23	GLY	-	expression tag	UNP A0A2U3TZM3
D	-22	GLY	-	expression tag	UNP A0A2U3TZM3

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-21	SER	-	expression tag	UNP A0A2U3TZM3
D	-20	GLY	-	expression tag	UNP A0A2U3TZM3
D	-19	GLY	-	expression tag	UNP A0A2U3TZM3
D	-18	GLY	-	expression tag	UNP A0A2U3TZM3
D	-17	SER	-	expression tag	UNP A0A2U3TZM3
D	-16	GLY	-	expression tag	UNP A0A2U3TZM3
D	-15	GLY	-	expression tag	UNP A0A2U3TZM3
D	-14	SER	-	expression tag	UNP A0A2U3TZM3
D	-13	ALA	-	expression tag	UNP A0A2U3TZM3
D	-12	TRP	-	expression tag	UNP A0A2U3TZM3
D	-11	SER	-	expression tag	UNP A0A2U3TZM3
D	-10	HIS	-	expression tag	UNP A0A2U3TZM3
D	-9	PRO	-	expression tag	UNP A0A2U3TZM3
D	-8	GLN	-	expression tag	UNP A0A2U3TZM3
D	-7	PHE	-	expression tag	UNP A0A2U3TZM3
D	-6	GLU	-	expression tag	UNP A0A2U3TZM3
D	-5	LYS	-	expression tag	UNP A0A2U3TZM3
D	-4	GLY	-	expression tag	UNP A0A2U3TZM3
D	-3	SER	-	expression tag	UNP A0A2U3TZM3
D	-2	ALA	-	expression tag	UNP A0A2U3TZM3
D	-1	ALA	-	expression tag	UNP A0A2U3TZM3
D	0	ALA	-	expression tag	UNP A0A2U3TZM3

- Molecule 6 is a protein called Polyribonucleotide 5'-hydroxyl-kinase Clp1.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	379	Total	C	N	O	0	0
			1869	1111	379	379		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	MET	-	initiating methionine	UNP Q92989
E	-18	ALA	-	expression tag	UNP Q92989
E	-17	SER	-	expression tag	UNP Q92989
E	-16	ASP	-	expression tag	UNP Q92989
E	-15	TYR	-	expression tag	UNP Q92989
E	-14	LYS	-	expression tag	UNP Q92989
E	-13	ASP	-	expression tag	UNP Q92989
E	-12	ASP	-	expression tag	UNP Q92989
E	-11	ASP	-	expression tag	UNP Q92989
E	-10	ASP	-	expression tag	UNP Q92989

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-9	LYS	-	expression tag	UNP Q92989
E	-8	ALA	-	expression tag	UNP Q92989
E	-7	SER	-	expression tag	UNP Q92989
E	-6	ASP	-	expression tag	UNP Q92989
E	-5	GLU	-	expression tag	UNP Q92989
E	-4	VAL	-	expression tag	UNP Q92989
E	-3	ASP	-	expression tag	UNP Q92989
E	-2	ALA	-	expression tag	UNP Q92989
E	-1	GLY	-	expression tag	UNP Q92989
E	0	THR	-	expression tag	UNP Q92989

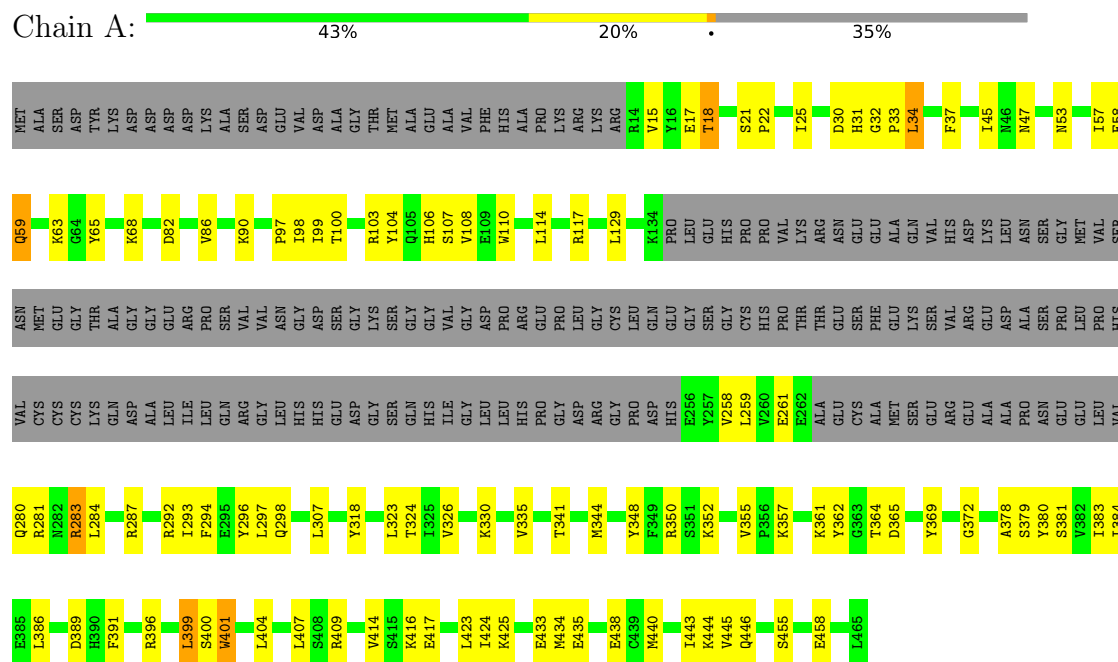
- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
7	T	6	Total Mg 6 6	0

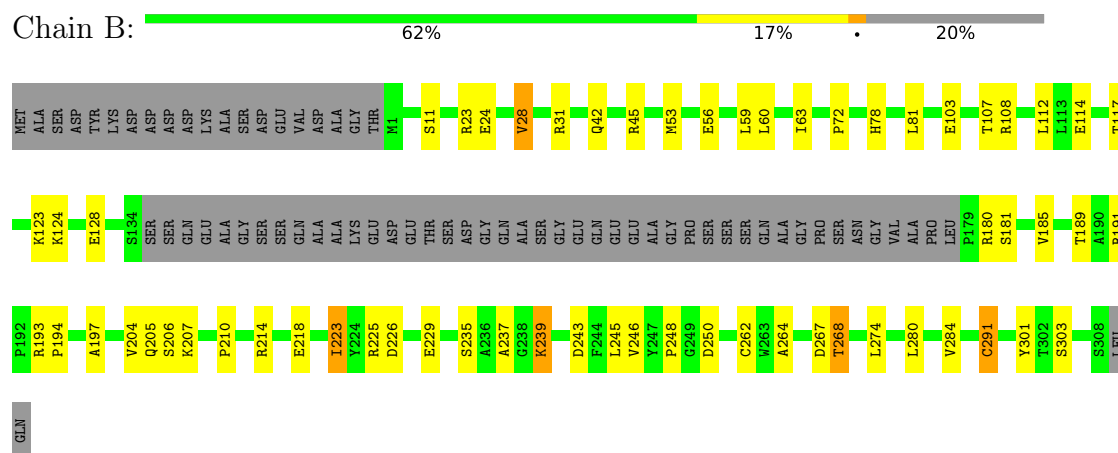
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-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 outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

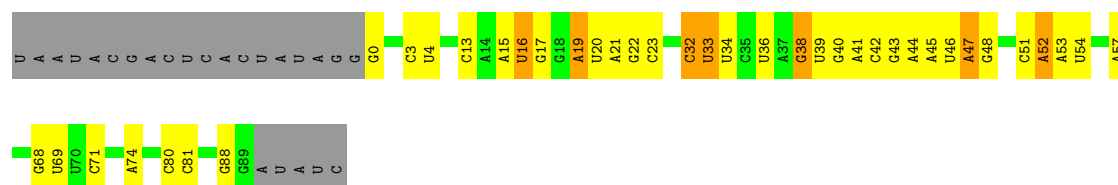
- Molecule 1: tRNA-splicing endonuclease subunit Sen2



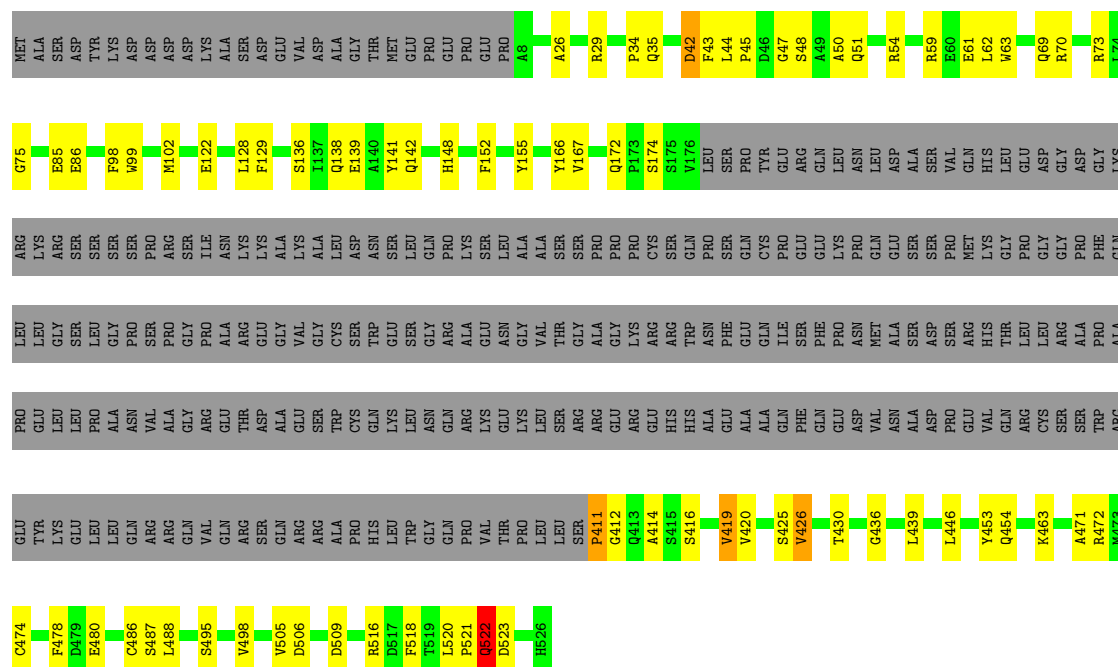
- Molecule 2: tRNA-splicing endonuclease subunit Sen34



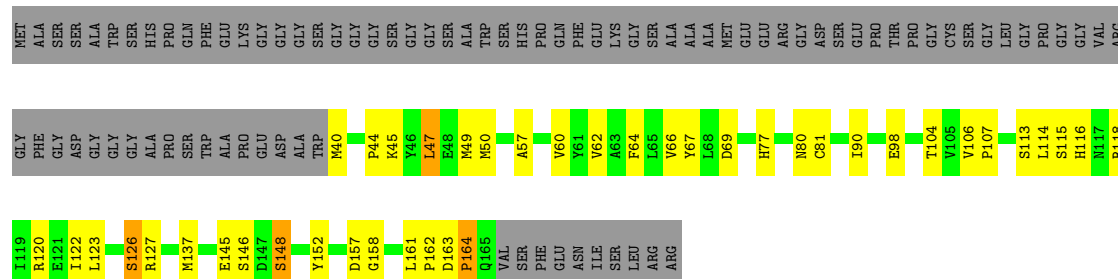
- Molecule 3: Pre-tRNA



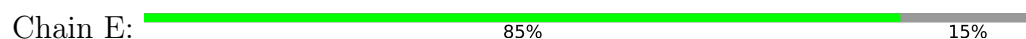
- Molecule 4: tRNA-splicing endonuclease subunit Sen54



- Molecule 5: Chromosome 1 open reading frame 19, isoform CRA a



- Molecule 6: Polyribonucleotide 5'-hydroxyl-kinase Clp1



GLY	THR	GLU	GLU	ASN	LEU	SER	GLU	THR	S382	M422	ASP	LEU	LYS
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	199001	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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 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	0.22	0/2670	0.51	2/3602 (0.1%)
2	B	0.20	0/2102	0.38	0/2848
3	T	0.19	0/2110	0.28	0/3290
4	C	0.28	0/2319	0.46	2/3140 (0.1%)
5	D	0.17	0/1004	0.34	0/1366
6	E	0.62	0/1866	1.11	0/2592
All	All	0.32	0/12071	0.58	4/16838 (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 outliers	#Planarity outliers
4	C	0	1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	411	PRO	CA-N-CD	-8.87	99.59	112.00
1	A	18	THR	CA-CB-OG1	-6.75	99.47	109.60
4	C	426	VAL	N-CA-C	-6.08	107.57	113.53
1	A	18	THR	N-CA-CB	5.01	118.96	110.49

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	C	521	PRO	Peptide

5.2 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 the 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 within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2608	0	2637	59	0
2	B	2057	0	2089	40	0
3	T	1888	0	951	20	0
4	C	2263	0	2234	48	0
5	D	984	0	987	25	0
6	E	1869	0	827	0	0
7	T	6	0	0	0	0
All	All	11675	0	9725	164	0

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 8.

All (164) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:T:19:A:N6	3:T:71:C:H42	1.43	1.14
3:T:19:A:H61	3:T:71:C:N4	1.50	1.07
3:T:19:A:H61	3:T:71:C:H42	0.88	0.86
3:T:19:A:N1	3:T:71:C:N3	2.30	0.80
2:B:248:PRO:HB2	4:C:45:PRO:HG3	1.69	0.73
2:B:23:ARG:NH1	2:B:250:ASP:OD1	2.23	0.72
5:D:45:LYS:O	5:D:49:MET:HG3	1.91	0.69
2:B:181:SER:HB2	4:C:75:GLY:HA3	1.75	0.68
3:T:0:G:H1	3:T:88:G:H22	1.41	0.68
4:C:26:ALA:HB1	4:C:29:ARG:HH21	1.60	0.67
1:A:57:ILE:HG23	1:A:297:LEU:HD12	1.76	0.67
4:C:42:ASP:OD2	4:C:51:GLN:NE2	2.26	0.67
2:B:108:ARG:NH2	3:T:19:A:O2'	2.29	0.66
3:T:16:U:O2'	3:T:19:A:OP1	2.14	0.66
4:C:70:ARG:NH1	4:C:122:GLU:O	2.31	0.64
2:B:237:ALA:HB2	2:B:245:LEU:HG	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:THR:HG22	4:C:69:GLN:HE22	1.63	0.62
1:A:114:LEU:HA	1:A:117:ARG:HB2	1.82	0.62
2:B:303:SER:OG	5:D:158:GLY:O	2.17	0.62
2:B:31:ARG:NH2	4:C:509:ASP:OD1	2.32	0.61
2:B:72:PRO:O	4:C:142:GLN:NE2	2.27	0.61
4:C:122:GLU:OE2	4:C:155:TYR:OH	2.18	0.61
1:A:103:ARG:HH22	1:A:293:ILE:HG12	1.66	0.61
1:A:104:TYR:HA	1:A:107:SER:HB2	1.83	0.60
3:T:36:U:H3	3:T:47:A:H61	1.49	0.60
1:A:362:TYR:HE1	1:A:414:VAL:HG11	1.67	0.59
5:D:77:HIS:ND1	5:D:98:GLU:OE2	2.37	0.58
1:A:15:VAL:HG22	1:A:15:VAL:O	2.03	0.57
2:B:24:GLU:OE1	4:C:63:TRP:NE1	2.35	0.57
2:B:45:ARG:NH1	4:C:34:PRO:O	2.37	0.57
2:B:250:ASP:OD2	4:C:59:ARG:NH2	2.30	0.57
1:A:15:VAL:O	1:A:15:VAL:HG13	2.05	0.57
2:B:206:SER:OG	2:B:207:LYS:N	2.38	0.56
1:A:364:THR:HG21	1:A:381:SER:HB2	1.88	0.56
4:C:167:VAL:HB	4:C:453:TYR:HB2	1.87	0.56
4:C:472:ARG:NH1	4:C:495:SER:O	2.38	0.56
2:B:72:PRO:HG3	2:B:197:ALA:HB2	1.87	0.56
4:C:50:ALA:HB1	4:C:54:ARG:HH12	1.69	0.56
1:A:22:PRO:HA	1:A:30:ASP:OD2	2.07	0.55
2:B:23:ARG:HD2	4:C:63:TRP:HH2	1.71	0.55
4:C:136:SER:HB2	4:C:139:GLU:HG3	1.89	0.55
2:B:268:THR:HG23	5:D:113:SER:HB3	1.87	0.55
1:A:350:ARG:HH12	1:A:355:VAL:HG13	1.71	0.54
2:B:103:GLU:O	2:B:107:THR:HG23	2.06	0.54
4:C:98:PHE:HB2	4:C:102:MET:HE3	1.89	0.54
1:A:365:ASP:OD1	1:A:396:ARG:NH2	2.41	0.53
5:D:40:MET:HB3	5:D:64:PHE:HE1	1.73	0.53
5:D:45:LYS:HG3	5:D:67:TYR:CZ	2.43	0.53
1:A:399:LEU:HD21	1:A:404:LEU:HD21	1.91	0.53
2:B:23:ARG:HD2	4:C:63:TRP:CH2	2.44	0.53
5:D:62:VAL:O	5:D:66:VAL:HG23	2.09	0.53
3:T:19:A:N6	3:T:71:C:N4	2.23	0.52
2:B:28:VAL:HG21	2:B:60:LEU:HD21	1.92	0.52
5:D:81:CYS:SG	5:D:90:ILE:HD11	2.50	0.52
1:A:378:ALA:HB3	1:A:416:LYS:HE2	1.91	0.52
5:D:47:LEU:HA	5:D:50:MET:HE2	1.93	0.51
1:A:261:GLU:HA	1:A:284:LEU:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:42:ASP:N	4:C:42:ASP:OD1	2.43	0.51
2:B:191:ARG:H	4:C:138:GLN:HE21	1.58	0.51
1:A:18:THR:O	1:A:21:SER:OG	2.20	0.51
2:B:223:ILE:HD13	2:B:262:CYS:HB3	1.93	0.51
5:D:104:THR:HG21	5:D:126:SER:HB2	1.93	0.51
5:D:66:VAL:HG21	5:D:107:PRO:HB3	1.93	0.50
4:C:419:VAL:HG12	4:C:420:VAL:H	1.77	0.50
1:A:391:PHE:CE2	4:C:439:LEU:HD11	2.47	0.50
4:C:486:CYS:SG	4:C:487:SER:N	2.85	0.50
1:A:281:ARG:NE	1:A:283:ARG:HB2	2.27	0.49
2:B:301:TYR:O	5:D:120:ARG:NH1	2.45	0.49
2:B:114:GLU:HA	2:B:117:THR:HG22	1.95	0.49
1:A:258:VAL:HG23	1:A:287:ARG:HB3	1.94	0.49
5:D:127:ARG:HD2	5:D:137:MET:HG2	1.95	0.48
1:A:380:TYR:CD1	1:A:417:GLU:HB2	2.49	0.48
3:T:38:G:H4'	3:T:38:G:OP1	2.12	0.48
1:A:53:ASN:O	1:A:57:ILE:HG13	2.14	0.48
2:B:210:PRO:HB2	2:B:214:ARG:NH2	2.29	0.48
2:B:53:MET:HB2	2:B:56:GLU:HG3	1.96	0.48
2:B:223:ILE:HG12	2:B:291:CYS:HB2	1.96	0.48
2:B:264:ALA:HB3	2:B:267:ASP:HB2	1.96	0.48
3:T:32:C:H4'	3:T:33:U:OP2	2.14	0.47
1:A:59:GLN:O	1:A:63:LYS:N	2.34	0.47
1:A:386:LEU:HD11	1:A:425:LYS:HE3	1.95	0.47
1:A:108:VAL:HG13	1:A:129:LEU:HD13	1.95	0.47
4:C:47:GLY:HA3	4:C:51:GLN:HG3	1.96	0.47
4:C:411:PRO:HD2	4:C:412:GLY:N	2.29	0.47
4:C:99:TRP:O	4:C:463:LYS:NZ	2.35	0.47
1:A:424:ILE:O	1:A:443:ILE:HG13	2.14	0.47
5:D:116:HIS:O	5:D:120:ARG:HG2	2.14	0.47
5:D:145:GLU:CD	5:D:146:SER:H	2.22	0.47
5:D:45:LYS:HA	5:D:45:LYS:HD3	1.77	0.46
1:A:47:ASN:HB3	1:A:335:VAL:HG21	1.98	0.46
1:A:444:LYS:HD2	4:C:430:THR:HB	1.98	0.46
1:A:318:TYR:HB2	1:A:323:LEU:HD11	1.98	0.46
1:A:344:MET:HG2	1:A:440:MET:SD	2.56	0.46
1:A:434:MET:HE2	1:A:434:MET:HB3	1.89	0.46
5:D:57:ALA:HA	5:D:60:VAL:HG22	1.99	0.45
1:A:32:GLY:O	1:A:34:LEU:N	2.49	0.45
1:A:68:LYS:NZ	5:D:148:SER:O	2.34	0.45
1:A:348:TYR:CD1	1:A:445:VAL:HG11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:SER:OG	1:A:401:TRP:N	2.50	0.45
4:C:471:ALA:HA	4:C:498:VAL:HG12	1.98	0.45
2:B:191:ARG:H	4:C:138:GLN:NE2	2.15	0.44
2:B:225:ARG:O	2:B:229:GLU:HG3	2.16	0.44
1:A:37:PHE:HB3	4:C:416:SER:HB3	1.98	0.44
1:A:341:THR:HG23	1:A:423:LEU:HD12	2.00	0.44
2:B:214:ARG:O	2:B:218:GLU:HG2	2.17	0.44
4:C:436:GLY:HA2	4:C:439:LEU:HB2	1.99	0.44
4:C:518:PHE:CZ	4:C:520:LEU:HB2	2.53	0.44
2:B:78:HIS:NE2	2:B:81:LEU:HD12	2.32	0.44
2:B:180:ARG:O	2:B:181:SER:HB3	2.17	0.44
3:T:0:G:H1	3:T:88:G:N2	2.13	0.44
4:C:478:PHE:CD2	4:C:506:ASP:HB2	2.52	0.44
1:A:409:ARG:NH2	3:T:54:U:OP1	2.51	0.43
2:B:59:LEU:O	2:B:63:ILE:HG23	2.18	0.43
3:T:0:G:H22	3:T:88:G:H21	1.65	0.43
3:T:38:G:O6	3:T:46:U:O2	2.35	0.43
1:A:63:LYS:HD3	4:C:414:ALA:O	2.19	0.43
1:A:357:LYS:HB2	1:A:369:TYR:HE2	1.82	0.43
4:C:172:GLN:HG3	4:C:174:SER:H	1.83	0.43
2:B:124:LYS:O	2:B:128:GLU:HG2	2.19	0.43
4:C:128:LEU:HD12	4:C:129:PHE:H	1.83	0.43
1:A:280:GLN:N	1:A:280:GLN:OE1	2.52	0.43
4:C:43:PHE:CD1	4:C:44:LEU:HG	2.54	0.43
5:D:145:GLU:OE2	5:D:146:SER:N	2.44	0.43
1:A:31:HIS:C	1:A:33:PRO:HD3	2.44	0.43
1:A:82:ASP:O	1:A:86:VAL:HG23	2.19	0.43
1:A:326:VAL:HB	1:A:330:LYS:HZ1	1.84	0.43
1:A:97:PRO:O	1:A:259:LEU:HB2	2.18	0.43
1:A:281:ARG:CZ	1:A:283:ARG:HB2	2.48	0.43
2:B:181:SER:HA	4:C:75:GLY:N	2.34	0.43
2:B:239:LYS:NZ	3:T:52:A:OP1	2.52	0.42
3:T:17:G:OP2	4:C:73:ARG:NH2	2.51	0.42
3:T:68:G:H2'	3:T:69:U:H6	1.84	0.42
2:B:226:ASP:OD2	2:B:301:TYR:OH	2.15	0.42
4:C:141:TYR:HE1	4:C:152:PHE:HE2	1.66	0.42
5:D:163:ASP:HB3	5:D:164:PRO:HD3	2.00	0.42
1:A:352:LYS:HB3	4:C:522:GLN:HB3	2.01	0.42
1:A:423:LEU:HB3	1:A:443:ILE:HD11	2.02	0.42
1:A:455:SER:O	4:C:166:TYR:OH	2.32	0.42
1:A:107:SER:HA	1:A:110:TRP:NE1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ARG:O	1:A:107:SER:N	2.50	0.42
2:B:123:LYS:HE3	2:B:123:LYS:HB3	1.86	0.42
4:C:446:LEU:HD12	4:C:446:LEU:HA	1.92	0.42
1:A:31:HIS:CD2	1:A:31:HIS:N	2.87	0.41
1:A:65:TYR:CD2	1:A:372:GLY:HA3	2.55	0.41
4:C:174:SER:O	4:C:174:SER:OG	2.38	0.41
5:D:118:ARG:O	5:D:122:ILE:HG13	2.19	0.41
1:A:297:LEU:HD23	1:A:298:GLN:H	1.85	0.41
5:D:69:ASP:OD1	5:D:152:TYR:OH	2.28	0.41
1:A:292:ARG:HG2	1:A:294:PHE:H	1.85	0.41
3:T:3:C:H2'	3:T:4:U:C6	2.56	0.41
3:T:80:C:H2'	3:T:81:C:H6	1.86	0.41
1:A:284:LEU:O	1:A:284:LEU:HD12	2.21	0.41
4:C:85:GLU:HG2	4:C:86:GLU:OE1	2.21	0.41
1:A:90:LYS:HE2	1:A:90:LYS:HB2	1.90	0.41
4:C:50:ALA:HB1	4:C:54:ARG:NH1	2.36	0.41
1:A:57:ILE:HD11	1:A:296:TYR:HA	2.02	0.41
4:C:43:PHE:HD1	4:C:44:LEU:HG	1.85	0.41
1:A:318:TYR:HB3	1:A:323:LEU:HD21	2.03	0.41
1:A:383:ILE:HD11	1:A:407:LEU:HD13	2.03	0.41
1:A:114:LEU:HD21	5:D:44:PRO:HG3	2.04	0.40
5:D:114:LEU:HD23	5:D:118:ARG:HD3	2.02	0.40
2:B:280:LEU:O	2:B:284:VAL:HG22	2.22	0.40
2:B:193:ARG:HA	2:B:194:PRO:HD3	1.98	0.40
5:D:123:LEU:HD13	5:D:157:ASP:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM 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	308/485 (64%)	280 (91%)	28 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	260/330 (79%)	248 (95%)	12 (5%)	0	100	100
4	C	281/546 (52%)	260 (92%)	20 (7%)	1 (0%)	30	55
5	D	124/213 (58%)	112 (90%)	10 (8%)	2 (2%)	8	22
6	E	373/445 (84%)	369 (99%)	4 (1%)	0	100	100
All	All	1346/2019 (67%)	1269 (94%)	74 (6%)	3 (0%)	45	66

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	522	GLN
5	D	162	PRO
5	D	164	PRO

5.3.2 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 EM 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	288/427 (67%)	264 (92%)	24 (8%)	9	22
2	B	211/260 (81%)	196 (93%)	15 (7%)	12	29
4	C	242/464 (52%)	225 (93%)	17 (7%)	12	29
5	D	113/171 (66%)	106 (94%)	7 (6%)	15	34
All	All	854/1322 (65%)	791 (93%)	63 (7%)	14	27

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	25	ILE
1	A	34	LEU
1	A	45	ILE
1	A	58	GLU
1	A	59	GLN
1	A	98	ILE

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Mol	Chain	Res	Type
1	A	99	ILE
1	A	100	THR
1	A	106	HIS
1	A	283	ARG
1	A	307	LEU
1	A	324	THR
1	A	361	LYS
1	A	379	SER
1	A	384	ILE
1	A	389	ASP
1	A	399	LEU
1	A	401	TRP
1	A	433	GLU
1	A	435	GLU
1	A	438	GLU
1	A	446	GLN
1	A	458	GLU
2	B	11	SER
2	B	28	VAL
2	B	42	GLN
2	B	112	LEU
2	B	185	VAL
2	B	204	VAL
2	B	205	GLN
2	B	223	ILE
2	B	235	SER
2	B	239	LYS
2	B	243	ASP
2	B	246	VAL
2	B	268	THR
2	B	274	LEU
2	B	291	CYS
4	C	35	GLN
4	C	42	ASP
4	C	48	SER
4	C	61	GLU
4	C	62	LEU
4	C	148	HIS
4	C	419	VAL
4	C	425	SER
4	C	426	VAL
4	C	454	GLN

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Mol	Chain	Res	Type
4	C	474	CYS
4	C	480	GLU
4	C	488	LEU
4	C	505	VAL
4	C	516	ARG
4	C	522	GLN
4	C	523	ASP
5	D	47	LEU
5	D	80	ASN
5	D	106	VAL
5	D	115	SER
5	D	126	SER
5	D	148	SER
5	D	161	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	47	ASN
1	A	59	GLN
1	A	106	HIS
1	A	280	GLN
1	A	298	GLN
1	A	347	HIS
1	A	390	HIS
1	A	446	GLN
1	A	462	GLN
2	B	89	GLN
2	B	110	GLN
2	B	205	GLN
2	B	272	GLN
2	B	294	GLN
2	B	305	GLN
4	C	35	GLN
4	C	69	GLN
4	C	138	GLN
4	C	160	HIS
5	D	117	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	T	89/114 (78%)	26 (29%)	0

All (26) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	T	13	C
3	T	15	A
3	T	16	U
3	T	19	A
3	T	20	U
3	T	21	A
3	T	22	G
3	T	23	C
3	T	32	C
3	T	33	U
3	T	34	U
3	T	38	G
3	T	39	U
3	T	40	G
3	T	41	A
3	T	42	C
3	T	43	G
3	T	44	A
3	T	45	A
3	T	47	A
3	T	48	G
3	T	51	C
3	T	52	A
3	T	53	A
3	T	57	A
3	T	74	A

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.