Full wwPDB EM Validation Report ⓘ

May 21, 2024 – 10:09 AM JST

PDB ID	:	8HMZ
EMDB ID	:	EMD-34905
Title	:	Cryo-EM structure of the human post-catalytic TSEN/pre-tRNA complex
Authors	:	Zhang, X.; Yang, F.; Zhan, X.; Shi, Y.
Deposited on	:	2022-12-06
Resolution	:	2.90 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:

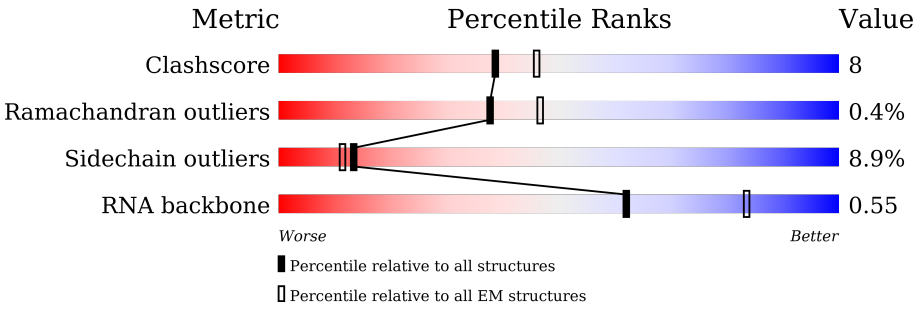
EMDB validation analysis	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	485	45% 16% • 35%
2	B	330	60% 19% • 20%
3	C	546	42% 8% •• 48%
4	D	213	44% 15% 41%
5	5	72	33% 14% 12% • 38%
6	3	42	71% 14% • 12%
7	E	445	78% 8% 15%

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 11542 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	313	Total	C	N	O	S	0	0
			2602	1680	443	466	13		

There are 20 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

- 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
			2062	1301	388	369	4		

There are 20 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

- Molecule 3 is a protein called tRNA-splicing endonuclease subunit Sen54.

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

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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 4 is a protein called Chromosome 1 open reading frame 19, isoform CRA_a.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	126	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 5 is a RNA chain called Pre-tRNA 5' END.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	45	Total	C	N	O	P	0	0
			968	430	174	318	46		

- Molecule 6 is a RNA chain called Pre-tRNA 3' END.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	3	37	Total	C	N	O	P	0	0
			788	353	142	257	36		

- Molecule 7 is a protein called Polyribonucleotide 5'-hydroxyl-kinase Clp1.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

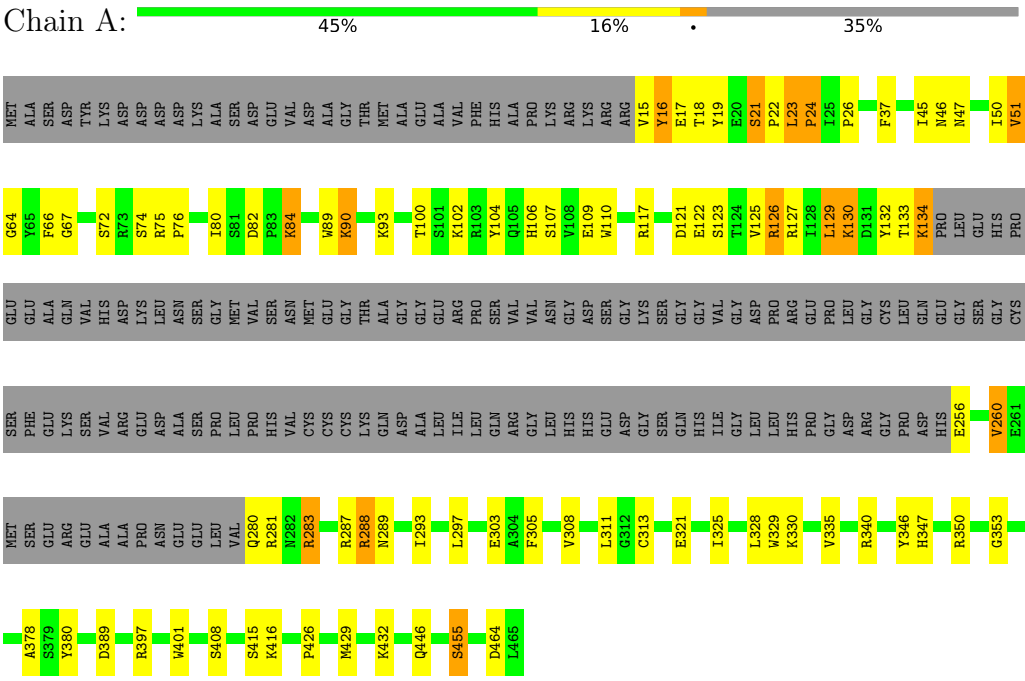
Mol	Chain	Residues	Atoms	AltConf
8	5	3	Total Mg 3 3	0
8	3	3	Total Mg 3 3	0

3 Residue-property plots (i)

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.

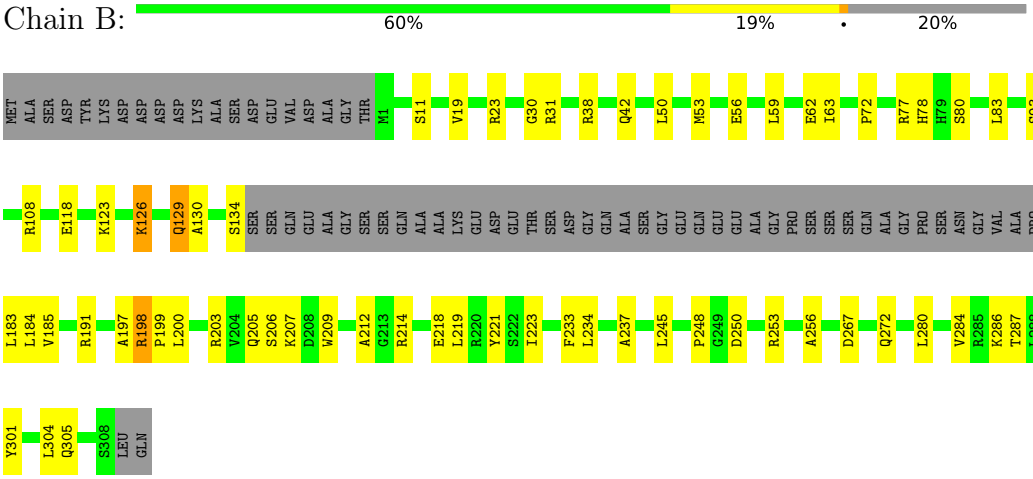
- Molecule 1: tRNA-splicing endonuclease subunit Sen2

Chain A:



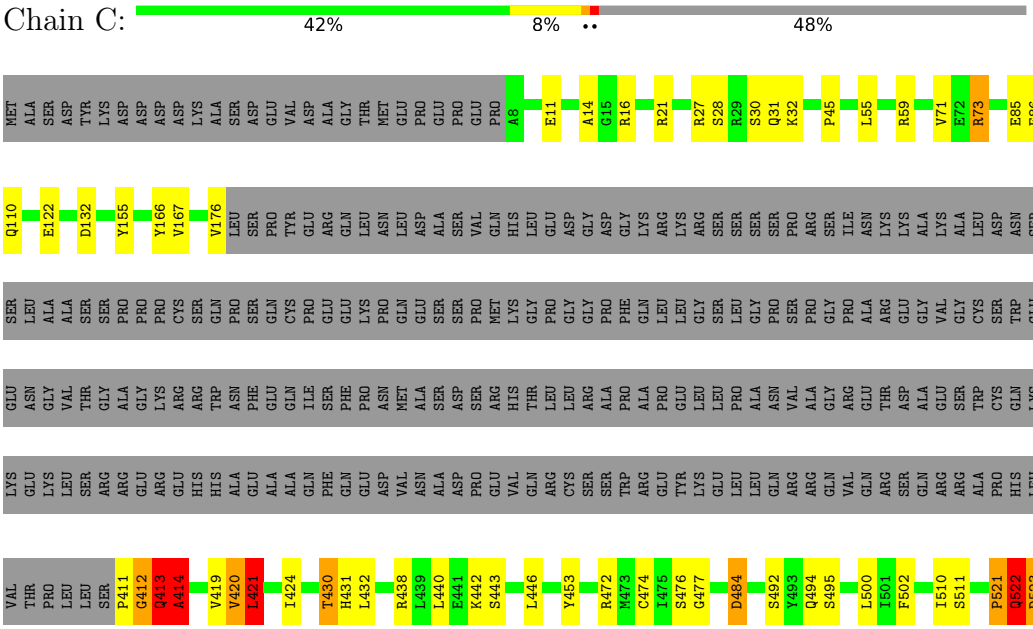
- Molecule 2: tRNA-splicing endonuclease subunit Sen34

Chain B:



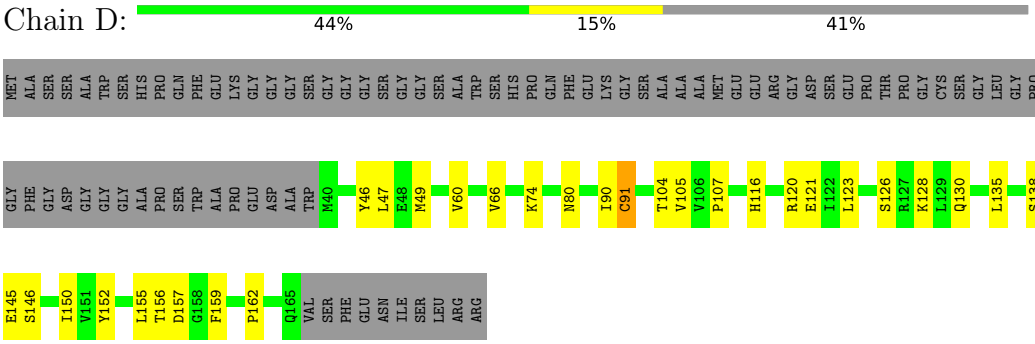
- Molecule 3: tRNA-splicing endonuclease subunit Sen54

Chain C:



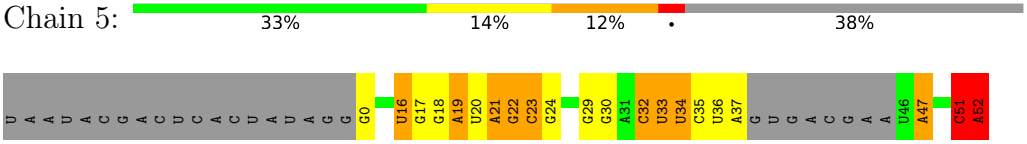
• Molecule 4: Chromosome 1 open reading frame 19, isoform CRA_a

Chain D:



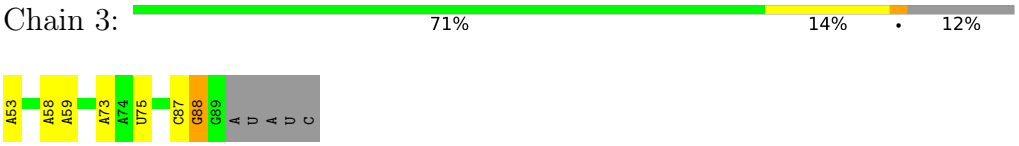
• Molecule 5: Pre-tRNA 5' END

Chain 5:



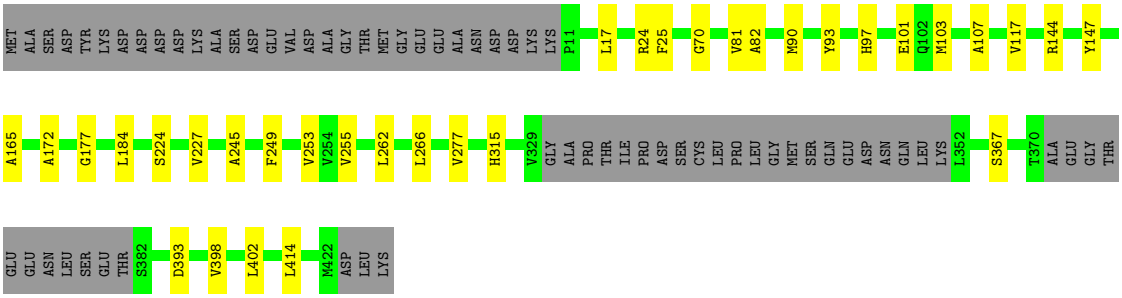
• Molecule 6: Pre-tRNA 3' END

Chain 3:



• Molecule 7: Polyribonucleotide 5'-hydroxyl-kinase Clp1

Chain E:


MET ALA SER ASP TYR LYS ASP ASP ASP LYS ALA SER ASP GLU VAL ASP ALA GLY THR MET GLY GLU GLU ALA ASN ASP ASP LYS LYS
P11 L17 R24 F25 G70 V81 A82 M90 Y93 H97 E101 Q102 M103 A107 V117 R144 Y147
A165 A172 G177 L184 S224 V227 A245 F249 V253 V254 V255 L262 L266 V277 H315 V329
GLY ALA PRO THR ILE PRO ASP SER CYS LEU PRO LEU GLY MET SER GLN GLU ASP ASN GLN LEU LYS
L352 S367 T370
ALA GLU GLY THR
GLU GLU ASN LEU SER GLU THR
S382 D393 V398 L402 L414 M422
ASP LEU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	309195	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 ($e^-/Å^2$)	50.00	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: A23, 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	0.27	0/2665	0.48	0/3596
2	B	0.27	0/2108	0.49	0/2856
3	C	0.36	0/2319	0.68	7/3140 (0.2%)
4	D	0.26	0/1004	0.46	0/1366
5	5	0.59	2/1053 (0.2%)	0.82	1/1638 (0.1%)
6	3	0.32	0/881	0.76	0/1372
7	E	0.26	0/1866	0.51	0/2592
All	All	0.33	2/11896 (0.0%)	0.59	8/16560 (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
3	C	0	4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	5	51	C	P-OP2	-9.36	1.33	1.49
5	5	51	C	P-OP1	-6.88	1.37	1.49

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	5	51	C	O4'-C1'-C2'	-9.37	96.43	105.80
3	C	412	GLY	C-N-CA	7.91	141.48	121.70
3	C	414	ALA	O-C-N	6.87	133.69	122.70
3	C	420	VAL	C-N-CA	6.29	137.43	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	419	VAL	C-N-CA	5.99	136.67	121.70
3	C	414	ALA	C-N-CA	5.73	136.03	121.70
3	C	413	GLN	CB-CA-C	-5.66	99.08	110.40
3	C	411	PRO	CA-N-CD	-5.37	103.99	111.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	412	GLY	Mainchain
3	C	414	ALA	Mainchain
3	C	521	PRO	Mainchain
3	C	522	GLN	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in 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	2602	0	2626	54	0
2	B	2062	0	2091	34	0
3	C	2263	0	2234	42	0
4	D	984	0	987	21	0
5	5	968	0	484	17	0
6	3	788	0	400	7	0
7	E	1869	0	827	19	0
8	3	3	0	0	0	0
8	5	3	0	0	0	0
All	All	11542	0	9649	166	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 (166) 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)
7:E:17:LEU:O	7:E:70:GLY:HA2	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:36:U:O2	5:5:47:A:N6	2.10	0.84
1:A:311:LEU:HD21	3:C:414:ALA:HB2	1.61	0.81
1:A:23:LEU:HB2	1:A:26:PRO:HD2	1.67	0.77
7:E:25:PHE:HA	7:E:81:VAL:O	1.85	0.76
2:B:248:PRO:HB2	3:C:45:PRO:HG3	1.68	0.75
7:E:367:SER:O	7:E:414:LEU:HA	1.88	0.74
1:A:346:TYR:OH	1:A:350:ARG:NH1	2.23	0.72
1:A:378:ALA:HB3	1:A:416:LYS:HE2	1.72	0.70
2:B:53:MET:HB2	2:B:56:GLU:HG3	1.75	0.69
2:B:62:GLU:OE1	2:B:221:TYR:OH	2.10	0.69
5:5:52:A23:O1C	6:3:53:A:O5'	2.09	0.69
7:E:315:HIS:O	7:E:402:LEU:HA	1.94	0.68
2:B:237:ALA:HB2	2:B:245:LEU:HG	1.74	0.68
3:C:440:LEU:O	3:C:443:SER:OG	2.12	0.67
5:5:16:U:O2'	5:5:19:A:OP1	2.11	0.67
4:D:49:MET:HG2	4:D:90:ILE:HD11	1.78	0.66
2:B:205:GLN:NE2	2:B:212:ALA:O	2.29	0.65
1:A:16:TYR:O	1:A:18:THR:N	2.30	0.65
7:E:172:ALA:HB1	7:E:177:GLY:HA2	1.79	0.65
4:D:138:SER:HB3	4:D:156:THR:HG23	1.78	0.64
2:B:250:ASP:OD2	3:C:59:ARG:NH2	2.30	0.64
5:5:52:A23:PC	6:3:53:A:O5'	2.56	0.63
7:E:97:HIS:O	7:E:101:GLU:N	2.30	0.63
1:A:260:VAL:HB	1:A:287:ARG:HG3	1.81	0.62
2:B:23:ARG:NH1	2:B:250:ASP:OD1	2.32	0.62
4:D:120:ARG:NH2	4:D:157:ASP:OD1	2.33	0.62
3:C:421:LEU:HD22	3:C:421:LEU:O	1.99	0.61
1:A:389:ASP:HB2	1:A:426:PRO:HA	1.81	0.61
2:B:206:SER:OG	2:B:207:LYS:N	2.34	0.61
1:A:57:ILE:HG12	1:A:297:LEU:HB2	1.82	0.61
2:B:184:LEU:HD21	3:C:27:ARG:HD2	1.82	0.61
3:C:413:GLN:H	3:C:413:GLN:CD	2.04	0.61
3:C:167:VAL:HB	3:C:453:TYR:HB2	1.84	0.60
5:5:52:A23:PC	6:3:53:A:HO5'	2.25	0.60
3:C:472:ARG:NH1	3:C:495:SER:O	2.36	0.58
1:A:358:VAL:HG21	4:D:145:GLU:HG2	1.85	0.58
3:C:73:ARG:NH2	5:5:16:U:O5'	2.37	0.58
1:A:64:GLY:O	1:A:350:ARG:NH2	2.37	0.57
3:C:413:GLN:CD	3:C:413:GLN:N	2.58	0.57
1:A:368:LEU:HD12	1:A:380:TYR:HB2	1.87	0.57
1:A:15:VAL:HB	1:A:24:PRO:HA	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:3:87:C:H2'	6:3:88:G:O4'	2.05	0.57
2:B:256:ALA:HB3	2:B:286:LYS:HE3	1.88	0.56
1:A:21:SER:O	1:A:21:SER:OG	2.20	0.56
2:B:83:LEU:HD11	3:C:132:ASP:HB3	1.88	0.56
7:E:147:TYR:O	7:E:165:ALA:HA	2.06	0.56
2:B:184:LEU:HD22	3:C:71:VAL:HG12	1.89	0.55
7:E:90:MET:O	7:E:93:TYR:CB	2.54	0.55
7:E:24:ARG:O	7:E:82:ALA:HA	2.06	0.55
1:A:47:ASN:HB3	1:A:335:VAL:HG21	1.89	0.55
1:A:106:HIS:HB3	1:A:110:TRP:CH2	2.42	0.55
4:D:116:HIS:O	4:D:120:ARG:HG2	2.07	0.54
3:C:99:TRP:CH2	3:C:110:GLN:HB3	2.42	0.54
2:B:77:ARG:HG3	2:B:78:HIS:CD2	2.42	0.54
2:B:198:ARG:HG3	2:B:199:PRO:HD2	1.89	0.53
3:C:476:SER:OG	3:C:477:GLY:N	2.41	0.53
7:E:117:VAL:HA	7:E:253:VAL:O	2.09	0.53
1:A:129:LEU:O	1:A:133:THR:HG23	2.09	0.53
2:B:130:ALA:O	2:B:134:SER:OG	2.23	0.53
6:3:58:A:H2'	6:3:59:A:C8	2.44	0.53
1:A:256:GLU:O	1:A:289:ASN:ND2	2.42	0.52
4:D:66:VAL:HG21	4:D:107:PRO:HB3	1.91	0.52
3:C:421:LEU:O	3:C:421:LEU:HD13	2.10	0.52
3:C:413:GLN:H	3:C:413:GLN:NE2	2.08	0.51
3:C:122:GLU:OE2	3:C:155:TYR:OH	2.23	0.51
7:E:255:VAL:HA	7:E:277:VAL:O	2.10	0.51
2:B:126:LYS:O	2:B:129:GLN:HG3	2.10	0.51
1:A:106:HIS:HA	1:A:109:GLU:HG2	1.91	0.51
1:A:67:GLY:N	1:A:303:GLU:OE1	2.43	0.51
1:A:107:SER:HA	1:A:110:TRP:NE1	2.26	0.51
4:D:145:GLU:HG3	4:D:146:SER:H	1.76	0.51
3:C:32:LYS:HD3	5:5:23:C:H5'	1.92	0.51
1:A:15:VAL:HG22	1:A:325:ILE:HG23	1.94	0.50
1:A:80:ILE:HG21	1:A:293:ILE:HD13	1.93	0.50
1:A:262:GLU:N	1:A:283:ARG:O	2.45	0.50
5:5:0:G:H1	6:3:88:G:H21	1.58	0.50
1:A:46:ASN:ND2	4:D:46:TYR:OH	2.44	0.50
1:A:311:LEU:HD22	1:A:313:CYS:SG	2.51	0.50
1:A:455:SER:O	3:C:166:TYR:OH	2.29	0.50
3:C:522:GLN:O	3:C:522:GLN:HG3	2.07	0.49
1:A:76:PRO:HG3	1:A:297:LEU:HD13	1.94	0.49
3:C:30:SER:OG	3:C:31:GLN:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:287:THR:HG23	2:B:305:GLN:HG2	1.95	0.49
7:E:245:ALA:O	7:E:249:PHE:N	2.37	0.49
3:C:521:PRO:C	3:C:523:ASP:H	2.17	0.48
4:D:49:MET:HB3	4:D:60:VAL:HG23	1.94	0.48
5:5:51:C:H2'	5:5:51:C:O2	2.13	0.47
1:A:325:ILE:HA	1:A:328:LEU:HB2	1.97	0.47
4:D:135:LEU:HD23	4:D:135:LEU:H	1.78	0.47
1:A:397:ARG:NH1	2:B:272:GLN:OE1	2.47	0.47
1:A:104:TYR:HA	1:A:107:SER:OG	2.14	0.47
6:3:73:A:O2'	6:3:75:U:OP2	2.22	0.47
7:E:144:ARG:H	7:E:224:SER:CB	2.28	0.47
7:E:393:ASP:CB	7:E:398:VAL:O	2.63	0.47
1:A:15:VAL:O	1:A:15:VAL:HG12	2.15	0.46
2:B:123:LYS:O	2:B:126:LYS:HG3	2.15	0.46
1:A:329:TRP:HZ2	1:A:340:ARG:HD3	1.81	0.46
1:A:353:GLY:HA3	3:C:524:VAL:HG23	1.97	0.46
2:B:292:SER:HB3	4:D:116:HIS:ND1	2.31	0.46
5:5:32:C:H4'	5:5:33:U:OP2	2.16	0.46
2:B:304:LEU:HD12	4:D:155:LEU:HG	1.96	0.46
1:A:107:SER:HA	1:A:110:TRP:CD1	2.50	0.46
2:B:191:ARG:O	3:C:14:ALA:HB1	2.15	0.46
3:C:430:THR:HG22	3:C:431:HIS:H	1.81	0.46
7:E:17:LEU:O	7:E:70:GLY:CA	2.58	0.46
5:5:34:U:H2'	5:5:35:C:C6	2.50	0.46
3:C:484:ASP:N	3:C:484:ASP:OD1	2.46	0.45
3:C:446:LEU:HD13	3:C:502:PHE:HE1	1.81	0.45
1:A:66:PHE:CE2	3:C:413:GLN:NE2	2.85	0.45
2:B:219:LEU:O	2:B:223:ILE:HD12	2.17	0.45
1:A:16:TYR:HA	1:A:22:PRO:HA	1.98	0.45
7:E:262:LEU:O	7:E:266:LEU:CB	2.65	0.45
2:B:30:GLY:HA3	2:B:50:LEU:HD21	1.99	0.45
3:C:21:ARG:HH11	3:C:21:ARG:HG2	1.82	0.45
1:A:82:ASP:OD2	1:A:100:THR:HG23	2.17	0.44
2:B:59:LEU:O	2:B:63:ILE:HG23	2.18	0.44
3:C:421:LEU:O	3:C:421:LEU:CG	2.66	0.44
1:A:133:THR:HB	1:A:287:ARG:NH1	2.33	0.44
2:B:72:PRO:HG3	2:B:197:ALA:HB2	2.00	0.44
1:A:305:PHE:HA	1:A:308:VAL:HG12	2.00	0.43
1:A:23:LEU:H	1:A:23:LEU:HD22	1.84	0.43
2:B:180:ARG:HD2	2:B:183:LEU:HD12	1.99	0.43
2:B:253:ARG:HG3	3:C:55:LEU:HD13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:103:MET:O	7:E:107:ALA:N	2.50	0.43
1:A:61:TYR:OH	1:A:74:SER:O	2.16	0.43
3:C:27:ARG:NH1	5:5:16:U:OP1	2.52	0.43
1:A:117:ARG:HH12	4:D:47:LEU:HB2	1.83	0.43
4:D:74:LYS:HE3	4:D:152:TYR:CE2	2.54	0.43
3:C:474:CYS:SG	3:C:500:LEU:HD11	2.59	0.43
1:A:347:HIS:CE1	3:C:424:ILE:HG22	2.54	0.43
2:B:301:TYR:O	4:D:120:ARG:NH1	2.52	0.43
4:D:126:SER:O	4:D:130:GLN:HG2	2.18	0.43
5:5:35:C:H2'	5:5:36:U:C6	2.53	0.43
4:D:91:CYS:SG	4:D:104:THR:HG23	2.58	0.43
1:A:45:ILE:HG22	1:A:50:ILE:HG12	2.01	0.42
5:5:21:A:H5'	5:5:22:G:OP1	2.17	0.42
4:D:105:VAL:HG22	4:D:140:THR:HB	2.00	0.42
3:C:32:LYS:HB2	5:5:23:C:OP1	2.19	0.42
3:C:85:GLU:HG2	3:C:86:GLU:N	2.34	0.42
1:A:16:TYR:CD1	1:A:16:TYR:N	2.87	0.42
4:D:144:VAL:HG13	4:D:150:ILE:HG12	2.01	0.42
4:D:123:LEU:HD13	4:D:157:ASP:HB2	2.00	0.42
1:A:134:LYS:NZ	1:A:288:ARG:HH21	2.17	0.42
2:B:289:LEU:HD21	4:D:159:PHE:CE1	2.55	0.42
2:B:19:VAL:HG13	2:B:50:LEU:HD13	2.01	0.42
3:C:432:LEU:HD12	3:C:432:LEU:HA	1.83	0.41
7:E:147:TYR:HA	7:E:227:VAL:O	2.19	0.41
3:C:28:SER:O	3:C:28:SER:OG	2.35	0.41
5:5:23:C:H2'	5:5:24:G:C8	2.56	0.41
1:A:51:VAL:HG13	1:A:297:LEU:HB3	2.03	0.41
3:C:421:LEU:HD22	3:C:421:LEU:C	2.41	0.41
1:A:121:ASP:O	1:A:125:VAL:HG23	2.21	0.41
3:C:421:LEU:O	3:C:421:LEU:CD2	2.66	0.41
7:E:165:ALA:HB3	7:E:184:LEU:CB	2.51	0.41
1:A:84:LYS:HD2	1:A:84:LYS:O	2.21	0.41
1:A:90:LYS:O	1:A:90:LYS:HG2	2.21	0.41
2:B:214:ARG:O	2:B:218:GLU:HG2	2.20	0.41
1:A:122:GLU:HB3	1:A:126:ARG:CZ	2.51	0.40
5:5:23:C:H2'	5:5:24:G:H8	1.86	0.40
1:A:126:ARG:O	1:A:130:LYS:HB2	2.20	0.40
1:A:129:LEU:O	1:A:133:THR:N	2.52	0.40
2:B:200:LEU:HD21	2:B:209:TRP:HB2	2.04	0.40
2:B:280:LEU:O	2:B:284:VAL:HG22	2.21	0.40
1:A:93:LYS:HA	1:A:93:LYS:HD3	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:521:PRO:C	3:C:523:ASP:N	2.74	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	307/485 (63%)	276 (90%)	29 (9%)	2 (1%)	22 54
2	B	260/330 (79%)	250 (96%)	10 (4%)	0	100 100
3	C	281/546 (52%)	259 (92%)	19 (7%)	3 (1%)	14 42
4	D	124/213 (58%)	118 (95%)	5 (4%)	1 (1%)	19 51
7	E	373/445 (84%)	346 (93%)	27 (7%)	0	100 100
All	All	1345/2019 (67%)	1249 (93%)	90 (7%)	6 (0%)	38 66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
3	C	413	GLN
3	C	421	LEU
3	C	524	VAL
4	D	162	PRO
1	A	24	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all 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	288/428 (67%)	252 (88%)	36 (12%)	4 14
2	B	212/261 (81%)	194 (92%)	18 (8%)	10 31
3	C	242/464 (52%)	224 (93%)	18 (7%)	13 38
4	D	113/171 (66%)	109 (96%)	4 (4%)	36 70
All	All	855/1324 (65%)	779 (91%)	76 (9%)	13 29

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	TYR
1	A	19	TYR
1	A	21	SER
1	A	23	LEU
1	A	37	PHE
1	A	51	VAL
1	A	61	TYR
1	A	72	SER
1	A	75	ARG
1	A	84	LYS
1	A	89	TRP
1	A	90	LYS
1	A	102	LYS
1	A	123	SER
1	A	126	ARG
1	A	127	ARG
1	A	129	LEU
1	A	130	LYS
1	A	132	TYR
1	A	134	LYS
1	A	260	VAL
1	A	280	GLN
1	A	281	ARG
1	A	283	ARG
1	A	288	ARG
1	A	321	GLU
1	A	330	LYS
1	A	375	PHE
1	A	401	TRP
1	A	408	SER

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Mol	Chain	Res	Type
1	A	415	SER
1	A	429	MET
1	A	432	LYS
1	A	446	GLN
1	A	455	SER
1	A	464	ASP
2	B	11	SER
2	B	31	ARG
2	B	38	ARG
2	B	42	GLN
2	B	80	SER
2	B	93	SER
2	B	96	GLU
2	B	100	LEU
2	B	108	ARG
2	B	118	GLU
2	B	126	LYS
2	B	129	GLN
2	B	185	VAL
2	B	198	ARG
2	B	203	ARG
2	B	233	PHE
2	B	234	LEU
2	B	267	ASP
3	C	11	GLU
3	C	16	ARG
3	C	73	ARG
3	C	100	GLN
3	C	176	VAL
3	C	413	GLN
3	C	420	VAL
3	C	421	LEU
3	C	430	THR
3	C	438	ARG
3	C	442	LYS
3	C	484	ASP
3	C	492	SER
3	C	494	GLN
3	C	510	ILE
3	C	511	SER
3	C	522	GLN
3	C	523	ASP

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Mol	Chain	Res	Type
4	D	80	ASN
4	D	91	CYS
4	D	121	GLU
4	D	128	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	ASN
1	A	120	GLN
1	A	289	ASN
1	A	446	GLN
2	B	89	GLN
2	B	186	GLN
2	B	205	GLN
3	C	69	GLN
3	C	138	GLN
3	C	454	GLN
3	C	522	GLN
4	D	130	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	5	43/72 (59%)	17 (39%)	0
6	3	36/42 (85%)	1 (2%)	0
All	All	79/114 (69%)	18 (22%)	0

All (18) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	5	16	U
5	5	17	G
5	5	18	G
5	5	19	A
5	5	20	U
5	5	21	A
5	5	22	G
5	5	23	C
5	5	29	G

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Mol	Chain	Res	Type
5	5	30	G
5	5	32	C
5	5	33	U
5	5	34	U
5	5	37	A
5	5	47	A
5	5	51	C
5	5	52	A23
6	3	88	G

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	A23	5	52	5	19,28,29	1.41	3 (15%)	19,43,46	1.85	6 (31%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	A23	5	52	5	-	0/3/35/36	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	5	52	A23	O5'-C5'	-2.85	1.37	1.44
5	5	52	A23	C5'-C4'	-2.81	1.42	1.51
5	5	52	A23	C5-C4	2.50	1.47	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	5	52	A23	O2C-PC-O1C	3.52	121.25	109.89
5	5	52	A23	N3-C2-N1	-3.14	123.78	128.68
5	5	52	A23	C5'-C4'-C3'	2.89	123.96	114.40
5	5	52	A23	C4-C5-N7	-2.67	106.62	109.40
5	5	52	A23	O3'-PC-O1C	-2.46	109.25	115.76
5	5	52	A23	O2'-PC-O1C	-2.46	109.26	115.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	5	52	A23	3	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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 (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.