



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 02:37 AM GMT

PDB ID : 1XMO
Title : Crystal Structure of mnm5U34t6A37-tRNA^{Lys}UUU Complexed with AAG-mRNA in the Decoding Center
Authors : Murphy, F.V.; Ramakrishnan, V.; Malkiewicz, A.; Agris, P.F.
Deposited on : 2004-10-04
Resolution : 3.25 Å (reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

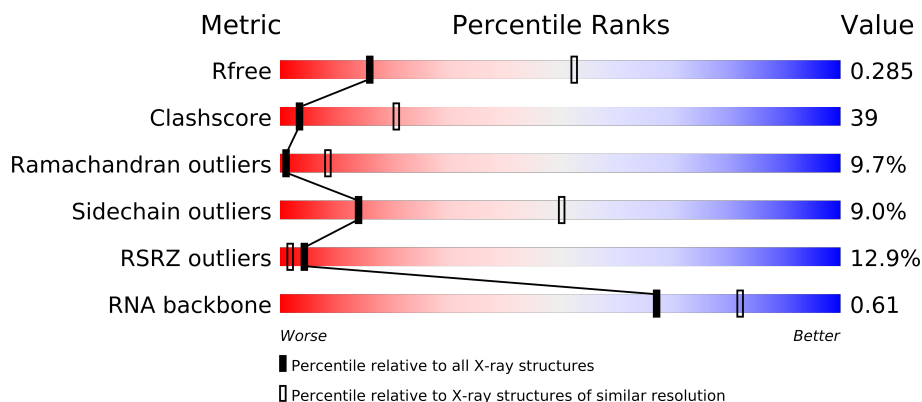
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.25 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.



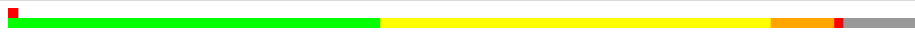
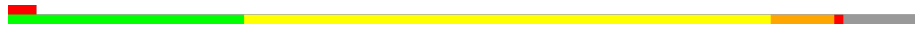


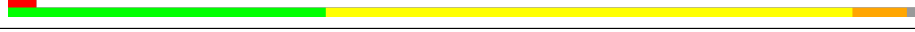

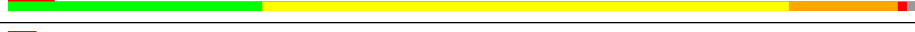


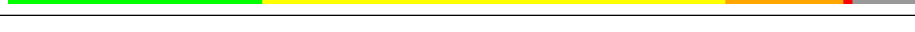

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1085 (3.32-3.20)
Clashscore	79885	1374 (3.32-3.20)
Ramachandran outliers	78287	1348 (3.32-3.20)
Sidechain outliers	78261	1346 (3.32-3.20)
RSRZ outliers	66119	1086 (3.32-3.20)
RNA backbone	1838	1028 (3.82-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1522	
2	W	3	
3	X	11	
4	B	256	
5	C	239	
6	D	209	
7	E	162	
8	F	101	
9	G	156	
10	H	138	
11	I	128	
12	J	105	

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Mol	Chain	Length	Quality of chain
13	K	129	
14	L	135	
15	M	126	
16	N	61	
17	O	89	
18	P	88	
19	Q	105	
20	R	88	
21	S	93	
22	T	106	
23	V	27	

2 Entry composition

There are 26 unique types of molecules in this entry. The entry contains 52063 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1507	Total	C	N	O	P	0	0	0
			32380	14414	5990	10470	1506			

- Molecule 2 is a RNA chain called A-Site Messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	W	3	Total	C	N	O	P	0	0	0
			64	30	15	17	2			

- Molecule 3 is a RNA chain called Anticodon Transfer RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	X	11	Total	C	N	O	P	0	0	0
			239	110	38	81	10			

- Molecule 4 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	234	Total	C	N	O	S	0	0	0
			1900	1213	341	341	5			

- Molecule 5 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	206	Total	C	N	O	S	0	0	0
			1612	1016	314	281	1			

- Molecule 6 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 7 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	150	Total	C	N	O	S	0	0	0
			1146	724	217	201	4			

- Molecule 8 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 9 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 10 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 11 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
11	I	127	Total	C	N	O	0	0	0
			1011	639	198	174			

- Molecule 12 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	J	98	Total	C	N	O	S	0	0	0
			792	498	156	137	1			

- Molecule 13 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 14 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	L	124	Total	C	N	O	S	0	0	0
			970	611	195	163	1			

- Molecule 15 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 16 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 17 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 18 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	P	83	Total	C	N	O	S	0	0	0
			700	443	139	117	1			

- Molecule 19 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 20 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	R	73	Total	C	N	O		0	0	0
			597	380	118	99				

- Molecule 21 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	S	80	Total	C	N	O	S	0	0	0
			647	414	119	112	2			

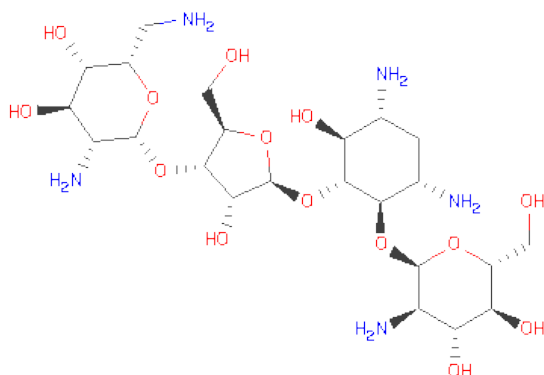
- Molecule 22 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 23 is a protein called 30S ribosomal protein Thx.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
23	V	24	Total	C	N	O	0	0	0
			208	128	50	30			

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula: $\text{C}_{23}\text{H}_{45}\text{N}_5\text{O}_{14}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
24	A	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
25	X	2	Total Mg 2 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	J	1	Total 1	Mg 1	0	0
25	A	104	Total 104	Mg 104	0	0

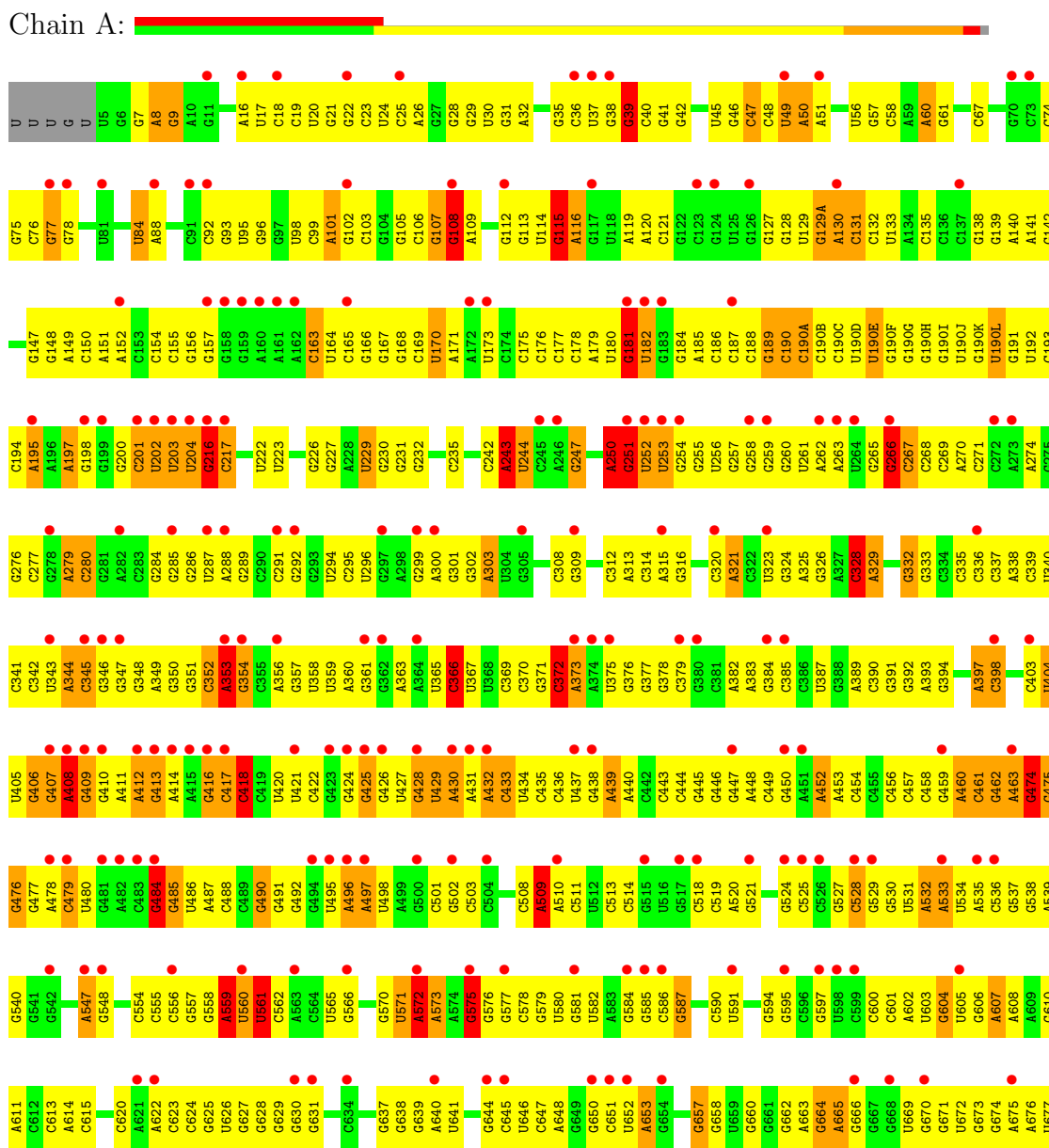
- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

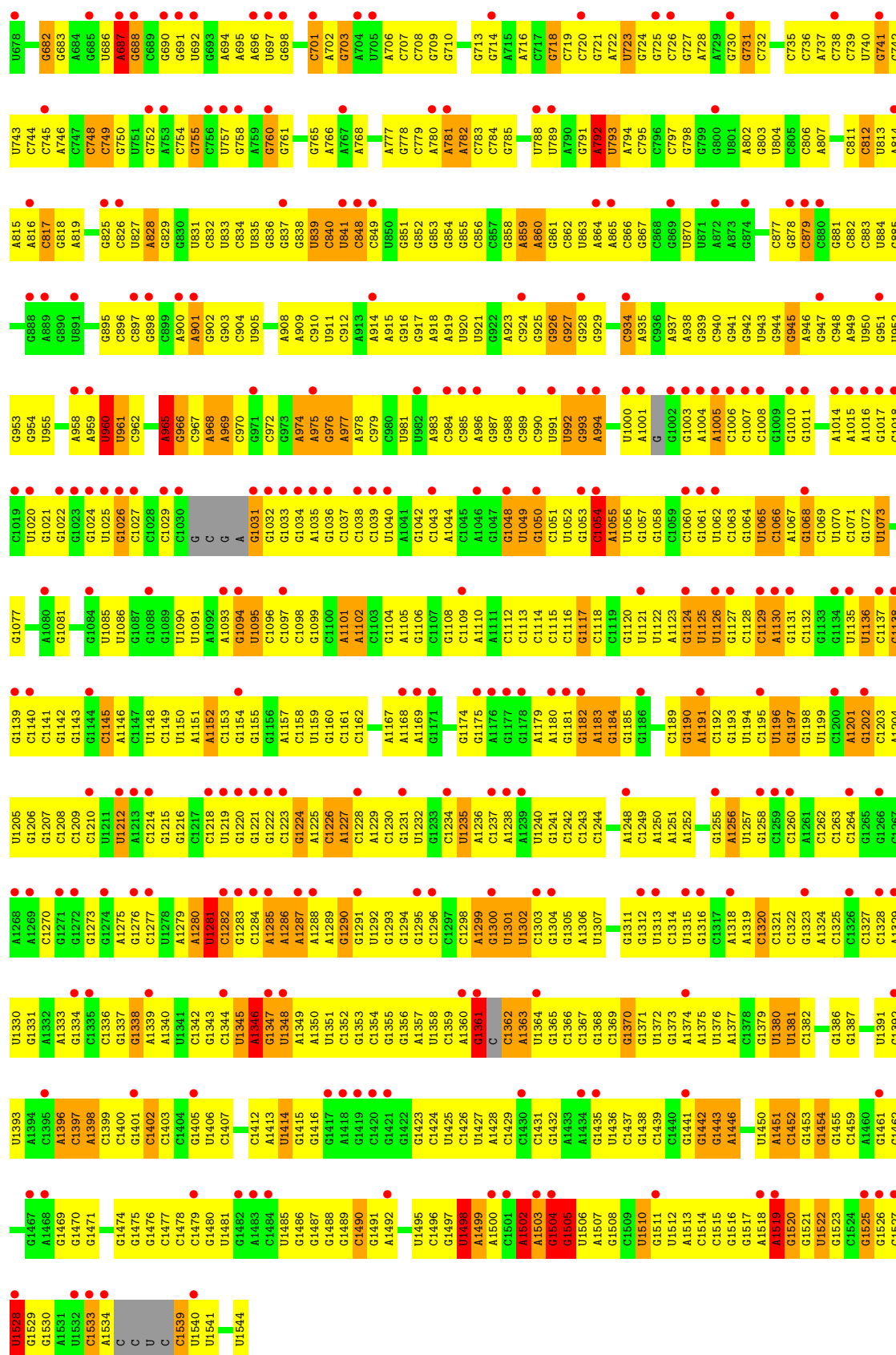
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	D	1	Total 1	Zn 1	0	0
26	N	1	Total 1	Zn 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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: 16S ribosomal RNA



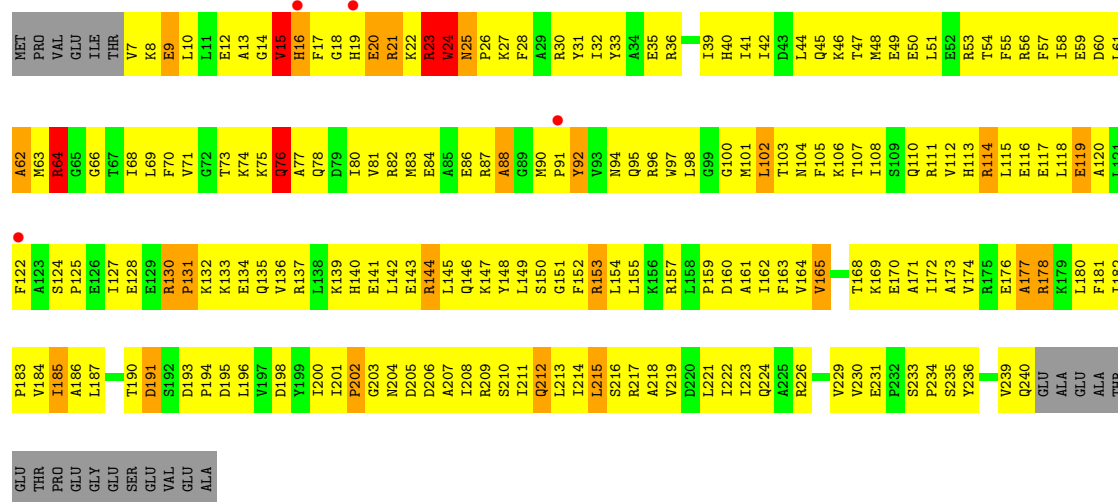


Age Group	Percentage
18-24	35%
25-34	25%
35-44	15%
45-54	10%
55-64	8%
65-74	5%
75-84	3%
85+	2%

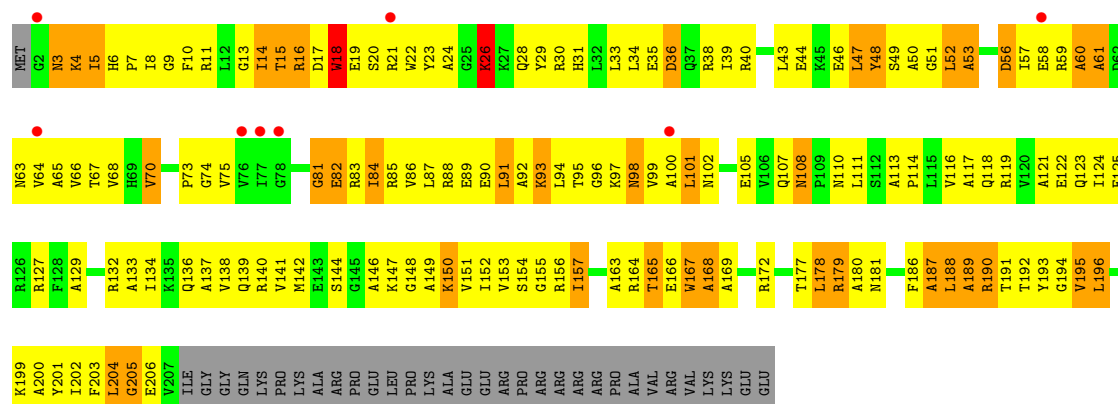
- Molecule 3: Anticodon Transfer RNA

- Molecule 4: 30S ribosomal protein S2

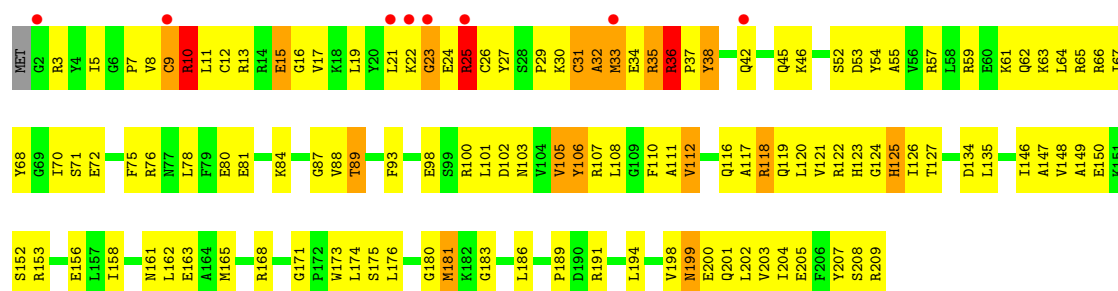
Age Group	Percentage
18-24	~10%
25-34	~35%
35-44	~45%
45-54	~15%
55 and older	~5%



- Molecule 5: 30S ribosomal protein S3

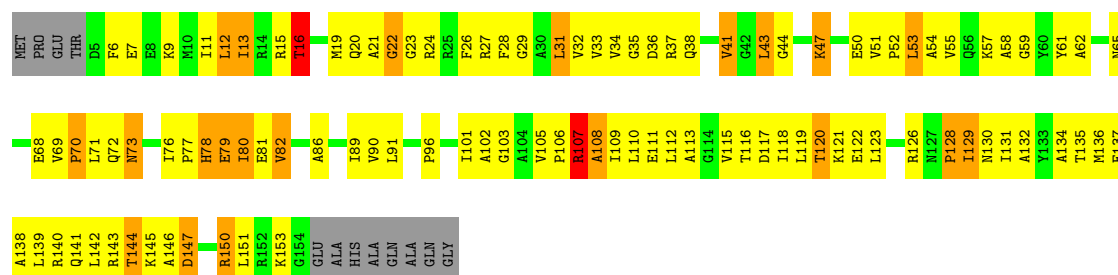


- Molecule 6: 30S ribosomal protein S4



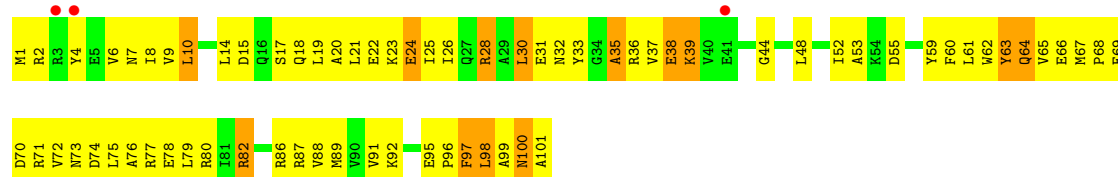
• Molecule 7: 30S ribosomal protein S5

Chain E:



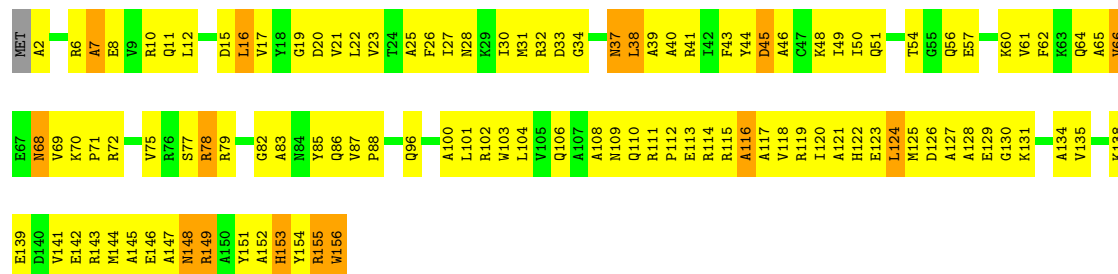
• Molecule 8: 30S ribosomal protein S6

Chain F:



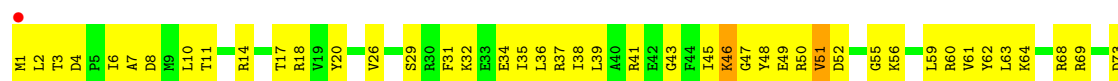
• Molecule 9: 30S ribosomal protein S7

Chain G:



• Molecule 10: 30S ribosomal protein S8

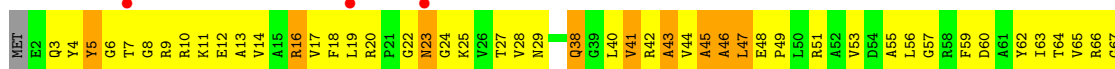
Chain H:





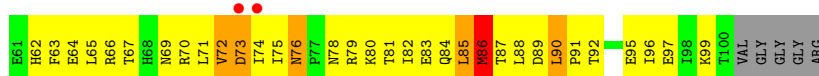
• Molecule 11: 30S ribosomal protein S9

Chain I:



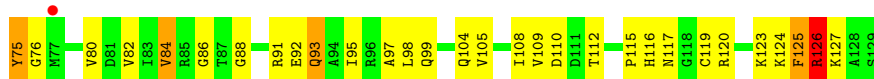
• Molecule 12: 30S ribosomal protein S10

Chain J:



• Molecule 13: 30S ribosomal protein S11

Chain K:



• Molecule 14: 30S ribosomal protein S12

Chain L:



• Molecule 15: 30S ribosomal protein S13

Chain M:





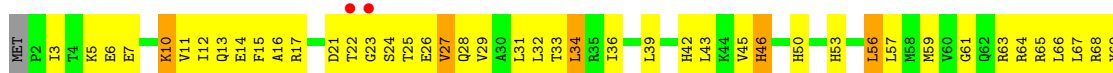
- Molecule 16: 30S ribosomal protein S14

Chain N:



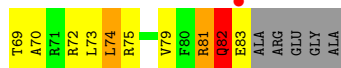
- Molecule 17: 30S ribosomal protein S15

Chain O:



- Molecule 18: 30S ribosomal protein S16

Chain P:



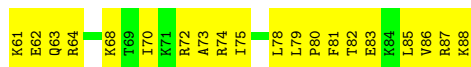
- Molecule 19: 30S ribosomal protein S17

Chain Q:



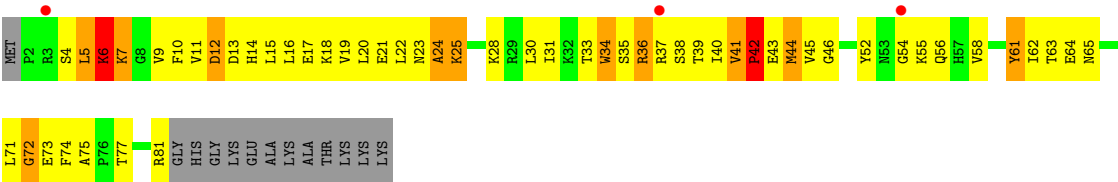
- Molecule 20: 30S ribosomal protein S18

Chain R:

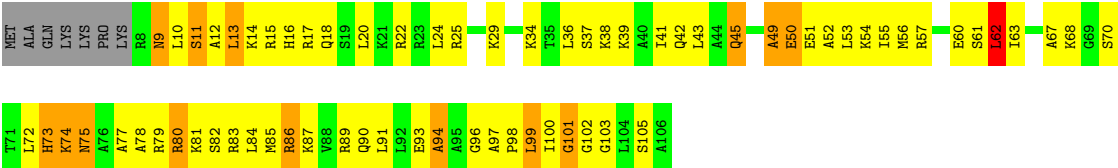


- Molecule 21: 30S ribosomal protein S19

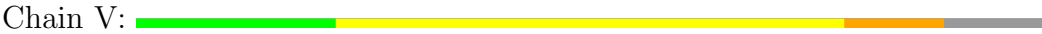
Chain S:



• Molecule 22: 30S ribosomal protein S20



• Molecule 23: 30S ribosomal protein Thx



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	400.81Å 400.81Å 176.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 3.25 200.41 – 3.23	Depositor EDS
% Data completeness (in resolution range)	5.0 (99.00-3.25) 88.5 (200.41-3.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 3.26Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.284 0.231 , 0.285	Depositor DCC
R_{free} test set	10090 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	85.2	Xtriage
Anisotropy	0.267	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 103.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 209982 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	52063	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, T6A, PAR, MNU

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	0.57	2/36244 (0.0%)	0.74	36/56567 (0.1%)
2	W	0.55	0/72	0.95	1/111 (0.9%)
3	X	0.41	0/203	0.78	0/311
4	B	0.34	0/1935	0.65	0/2609
5	C	0.36	0/1636	0.63	0/2205
6	D	0.39	0/1733	0.65	0/2318
7	E	0.44	0/1162	0.74	0/1564
8	F	0.32	0/856	0.59	0/1154
9	G	0.35	0/1276	0.61	0/1709
10	H	0.44	0/1136	0.75	0/1527
11	I	0.35	0/1029	0.63	0/1378
12	J	0.35	0/805	0.69	0/1082
13	K	0.41	0/900	0.68	0/1213
14	L	0.45	0/986	0.77	0/1320
15	M	0.35	0/1008	0.67	0/1347
16	N	0.43	0/501	0.74	0/664
17	O	0.36	0/745	0.63	0/992
18	P	0.47	0/716	0.74	0/963
19	Q	0.47	0/870	0.77	0/1159
20	R	0.35	0/603	0.65	0/799
21	S	0.32	0/661	0.63	0/890
22	T	0.41	0/764	0.77	0/1006
23	V	0.42	0/212	0.72	0/277
All	All	0.52	2/56053 (0.0%)	0.73	37/83165 (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
1	A	4	60
3	X	1	0
All	All	5	60

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1361	G	C3'-O3'	5.22	1.49	1.42
1	A	1361	G	O3'-P	5.14	1.67	1.61

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	G	C2'-C3'-O3'	9.66	130.74	109.50
1	A	115	G	C2'-C3'-O3'	9.52	130.44	109.50
1	A	559	A	C2'-C3'-O3'	9.37	130.12	109.50
1	A	243	A	C2'-C3'-O3'	9.32	130.01	109.50
1	A	1528	U	C2'-C3'-O3'	8.97	129.23	109.50

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	181	G	C3'
1	A	243	A	C3'
1	A	559	A	C3'
1	A	1528	U	C3'
3	X	37	T6A	C14

5 of 60 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	107	G	Sidechain
1	A	108	G	Sidechain
1	A	39	G	Sidechain
1	A	77	G	Sidechain
1	A	84	U	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32380	0	16346	1337	0
2	W	64	0	35	4	0
3	X	239	0	127	7	0
4	B	1900	0	1951	305	0
5	C	1612	0	1677	245	0
6	D	1703	0	1764	150	0
7	E	1146	0	1207	140	0
8	F	843	0	857	102	0
9	G	1257	0	1296	131	0
10	H	1116	0	1177	112	0
11	I	1011	0	1043	153	0
12	J	792	0	835	127	0
13	K	885	0	904	71	0
14	L	970	0	1057	130	0
15	M	997	0	1072	155	0
16	N	492	0	530	67	0
17	O	734	0	771	78	0
18	P	700	0	720	81	0
19	Q	857	0	930	125	0
20	R	597	0	668	100	0
21	S	647	0	673	83	0
22	T	762	0	856	87	0
23	V	208	0	221	19	0
24	A	42	0	45	2	0
25	A	104	0	0	0	0
25	J	1	0	0	0	0
25	X	2	0	0	0	0
26	D	1	0	0	0	0
26	N	1	0	0	1	0
All	All	52063	0	36762	3496	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 39.

The worst 5 of 3496 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1489:G:H2'	1:A:1490:C:H5''	1.26	1.10
6:D:36:ARG:H	6:D:37:PRO:HD3	1.13	1.08
5:C:179:ARG:HG2	5:C:180:ALA:H	0.98	1.06

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:C:26:LYS:HD3	5:C:26:LYS:H	1.14	1.06
4:B:132:LYS:HA	4:B:135:GLN:HB3	1.36	1.05

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 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 X-ray entries followed by that with respect to entries of similar resolution. 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	
4	B	232/256 (91%)	129 (56%)	80 (34%)	23 (10%)	1	8
5	C	204/239 (85%)	123 (60%)	48 (24%)	33 (16%)	0	2
6	D	206/209 (99%)	151 (73%)	38 (18%)	17 (8%)	1	12
7	E	148/162 (91%)	120 (81%)	18 (12%)	10 (7%)	2	18
8	F	99/101 (98%)	68 (69%)	24 (24%)	7 (7%)	2	16
9	G	153/156 (98%)	99 (65%)	41 (27%)	13 (8%)	1	11
10	H	136/138 (99%)	106 (78%)	25 (18%)	5 (4%)	5	39
11	I	125/128 (98%)	85 (68%)	27 (22%)	13 (10%)	1	7
12	J	96/105 (91%)	57 (59%)	23 (24%)	16 (17%)	0	1
13	K	117/129 (91%)	85 (73%)	26 (22%)	6 (5%)	3	28
14	L	122/135 (90%)	85 (70%)	24 (20%)	13 (11%)	1	6
15	M	123/126 (98%)	75 (61%)	30 (24%)	18 (15%)	0	2
16	N	58/61 (95%)	34 (59%)	16 (28%)	8 (14%)	0	3
17	O	86/89 (97%)	54 (63%)	28 (33%)	4 (5%)	4	30
18	P	81/88 (92%)	59 (73%)	16 (20%)	6 (7%)	2	15
19	Q	102/105 (97%)	75 (74%)	17 (17%)	10 (10%)	1	8
20	R	71/88 (81%)	50 (70%)	16 (22%)	5 (7%)	2	17
21	S	78/93 (84%)	56 (72%)	14 (18%)	8 (10%)	1	7
22	T	97/106 (92%)	56 (58%)	30 (31%)	11 (11%)	1	5
23	V	22/27 (82%)	18 (82%)	2 (9%)	2 (9%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2356/2541 (93%)	1585 (67%)	543 (23%)	228 (10%)	1 8

5 of 228 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	B	13	ALA
4	B	15	VAL
4	B	16	HIS
4	B	21	ARG
4	B	24	TRP

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 X-ray entries followed by that with respect to entries of similar resolution. 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
4	B	202/220 (92%)	181 (90%)	21 (10%)	10 41
5	C	160/188 (85%)	145 (91%)	15 (9%)	13 47
6	D	180/181 (99%)	164 (91%)	16 (9%)	14 51
7	E	115/123 (94%)	96 (84%)	19 (16%)	3 17
8	F	90/90 (100%)	83 (92%)	7 (8%)	18 60
9	G	126/127 (99%)	115 (91%)	11 (9%)	15 53
10	H	119/119 (100%)	107 (90%)	12 (10%)	11 42
11	I	98/99 (99%)	87 (89%)	11 (11%)	9 38
12	J	87/92 (95%)	85 (98%)	2 (2%)	63 91
13	K	90/99 (91%)	79 (88%)	11 (12%)	7 33
14	L	104/111 (94%)	100 (96%)	4 (4%)	44 85
15	M	100/101 (99%)	88 (88%)	12 (12%)	7 34
16	N	49/50 (98%)	47 (96%)	2 (4%)	41 83
17	O	79/80 (99%)	76 (96%)	3 (4%)	44 85
18	P	72/74 (97%)	66 (92%)	6 (8%)	16 56
19	Q	96/97 (99%)	90 (94%)	6 (6%)	25 70
20	R	64/77 (83%)	59 (92%)	5 (8%)	18 60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	S	71/80 (89%)	63 (89%)	8 (11%)	9	37
22	T	75/82 (92%)	67 (89%)	8 (11%)	10	40
23	V	19/22 (86%)	18 (95%)	1 (5%)	32	76
All	All	1996/2112 (94%)	1816 (91%)	180 (9%)	14	50

5 of 180 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	G	45	ASP
10	H	134	ILE
21	S	34	TRP
9	G	124	LEU
10	H	51	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
8	F	32	ASN
11	I	23	ASN
21	S	23	ASN
8	F	57	GLN
8	F	100	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1506/1522 (98%)	240 (15%)	62 (4%)
2	W	2/3 (66%)	1 (50%)	0
3	X	9/11 (81%)	0	0
All	All	1517/1536 (98%)	241 (15%)	62 (4%)

5 of 241 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G

5 of 62 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	701	C
1	A	965	A
1	A	1498	U
1	A	812	C
1	A	992	U

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

2 non-standard protein/DNA/RNA residues are 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$
3	MNU	X	34	3,2	22,24,25	0.84	1 (4%)	27,34,37	1.40	1 (3%)
3	T6A	X	37	3	32,34,35	1.45	6 (18%)	46,49,52	3.14	12 (26%)

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
3	MNU	X	34	3,2	-	0/9/28/29	0/2/2/2
3	T6A	X	37	3	1/1/9/11	0/24/41/42	0/1/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	X	37	T6A	O14-C14	-4.05	1.34	1.43
3	X	37	T6A	C15-C14	-3.20	1.43	1.51
3	X	34	MNU	P-OP1	2.70	1.49	1.46
3	X	37	T6A	ODA-C13	2.62	1.31	1.22
3	X	37	T6A	ODB-C13	-2.39	1.21	1.30

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	X	37	T6A	O14-C14-C15	12.19	145.26	109.74
3	X	37	T6A	C12-N11-C10	6.81	132.66	121.12
3	X	37	T6A	O14-C14-C12	-6.41	95.20	109.15
3	X	34	MNU	C6-N1-C2	-6.30	120.62	122.41
3	X	37	T6A	C13-C12-N11	6.30	121.79	109.91

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	X	37	T6A	C14

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 110 ligands modelled in this entry, 109 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
24	PAR	A	1545	-	45,45,45	1.74	12 (26%)	67,67,67	1.33	6 (8%)

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
24	PAR	A	1545	-	-	0/18/94/94	0/4/4/4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	1545	PAR	C22-C32	4.22	1.55	1.52
24	A	1545	PAR	O54-C14	4.03	1.52	1.41
24	A	1545	PAR	C31-C21	3.40	1.58	1.53
24	A	1545	PAR	O33-C14	2.98	1.49	1.41
24	A	1545	PAR	O51-C11	2.96	1.49	1.41

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	1545	PAR	O52-C13-C23	5.14	116.68	107.50
24	A	1545	PAR	O54-C54-C64	4.49	112.49	106.97
24	A	1545	PAR	O52-C13-O43	-3.78	107.89	111.51
24	A	1545	PAR	C14-O54-C54	3.14	119.83	113.73
24	A	1545	PAR	O33-C14-C24	2.65	113.33	108.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1507/1522 (99%)	1.73	440 (29%) 1 1	30, 65, 160, 200	0
2	W	3/3 (100%)	1.84	1 (33%) 1 1	56, 56, 63, 72	0
3	X	10/11 (90%)	1.72	4 (40%) 1 0	64, 101, 157, 157	0
4	B	234/256 (91%)	0.36	4 (1%) 67 21	37, 100, 173, 200	0
5	C	206/239 (86%)	0.45	8 (3%) 37 8	44, 93, 169, 200	0
6	D	208/209 (99%)	0.39	8 (3%) 38 8	33, 71, 149, 200	0
7	E	150/162 (92%)	0.38	0 100 100	27, 63, 122, 200	0
8	F	101/101 (100%)	0.46	3 (2%) 48 11	48, 103, 154, 174	0
9	G	155/156 (99%)	0.36	0 100 100	41, 81, 152, 200	0
10	H	138/138 (100%)	0.43	1 (0%) 84 40	20, 54, 113, 174	0
11	I	127/128 (99%)	0.47	3 (2%) 56 14	35, 90, 149, 178	0
12	J	98/105 (93%)	0.87	9 (9%) 9 3	44, 117, 186, 200	0
13	K	119/129 (92%)	0.37	1 (0%) 83 37	30, 67, 138, 187	0
14	L	124/135 (91%)	0.58	4 (3%) 45 10	31, 64, 139, 175	0
15	M	125/126 (99%)	0.67	11 (8%) 10 3	44, 85, 169, 200	0
16	N	60/61 (98%)	0.61	2 (3%) 44 10	42, 82, 139, 179	0
17	O	88/89 (98%)	0.44	3 (3%) 43 10	23, 76, 142, 192	0
18	P	83/88 (94%)	0.48	1 (1%) 75 28	27, 52, 96, 173	0
19	Q	104/105 (99%)	0.76	5 (4%) 29 6	22, 61, 146, 200	0
20	R	73/88 (82%)	0.44	3 (4%) 35 8	40, 79, 175, 188	0
21	S	80/93 (86%)	0.50	3 (3%) 38 8	62, 111, 162, 193	0
22	T	99/106 (93%)	0.40	0 100 100	32, 58, 136, 168	0
23	V	24/27 (88%)	0.41	0 100 100	41, 69, 118, 136	0
All	All	3916/4077 (96%)	0.96	514 (13%) 4 2	20, 73, 159, 200	0

The worst 5 of 514 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	202	U	11.3
1	A	1129	C	8.9
1	A	414	A	8.9
15	M	120	LYS	8.0
12	J	31	GLY	7.9

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	T6A	X	37	32/33	0.35	-	76,80,80,80	0
3	MNU	X	34	23/24	0.28	-	56,96,115,115	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
25	MG	A	1561	1/1	0.28	-	23,23,23,23	1
25	MG	A	471	1/1	0.25	-	23,23,23,23	1
25	MG	A	1614	1/1	0.24	-	23,23,23,23	1
25	MG	A	1607	1/1	0.71	-	23,23,23,23	1
25	MG	A	1583	1/1	0.15	-	23,23,23,23	0
25	MG	A	1551	1/1	0.27	-	23,23,23,23	0
25	MG	A	1585	1/1	0.33	-	23,23,23,23	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	A	1555	1/1	0.27	-	23,23,23,23	0
25	MG	A	1565	1/1	0.28	-	23,23,23,23	0
25	MG	A	1624	1/1	0.20	-	23,23,23,23	1
25	MG	A	1595	1/1	1.51	-	23,23,23,23	1
25	MG	A	1601	1/1	0.72	-	23,23,23,23	1
25	MG	A	1562	1/1	0.70	-	23,23,23,23	1
25	MG	A	1572	1/1	0.15	-	23,23,23,23	0
26	ZN	D	306	1/1	0.32	-	23,23,23,23	1
25	MG	A	1603	1/1	0.29	-	23,23,23,23	1
25	MG	A	1584	1/1	0.15	-	23,23,23,23	0
25	MG	A	1558	1/1	0.19	-	23,23,23,23	0
25	MG	A	1578	1/1	0.19	-	23,23,23,23	0
25	MG	X	502	1/1	0.34	-	23,23,23,23	1
25	MG	A	1605	1/1	0.44	-	23,23,23,23	1
25	MG	A	1573	1/1	0.22	-	23,23,23,23	0
25	MG	A	1576	1/1	0.24	-	23,23,23,23	0
25	MG	A	441	1/1	0.17	-	23,23,23,23	1
25	MG	A	86	1/1	0.24	-	23,23,23,23	1
25	MG	A	473	1/1	0.35	-	23,23,23,23	1
25	MG	A	1596	1/1	1.69	-	23,23,23,23	1
25	MG	A	1571	1/1	0.14	-	23,23,23,23	0
25	MG	A	1547	1/1	0.35	-	23,23,23,23	0
25	MG	A	1626	1/1	0.21	-	23,23,23,23	1
25	MG	A	71	1/1	0.32	-	23,23,23,23	1
25	MG	A	470	1/1	0.38	-	23,23,23,23	1
25	MG	A	1598	1/1	0.36	-	23,23,23,23	0
25	MG	A	1580	1/1	0.33	-	23,23,23,23	1
25	MG	A	1621	1/1	0.38	-	23,23,23,23	1
25	MG	A	1574	1/1	0.21	-	23,23,23,23	0
25	MG	A	210	1/1	0.44	-	23,23,23,23	1
25	MG	A	1609	1/1	0.27	-	23,23,23,23	0
25	MG	A	1589	1/1	0.33	-	23,23,23,23	0
25	MG	A	1563	1/1	0.47	-	23,23,23,23	1
25	MG	A	1625	1/1	0.24	-	23,23,23,23	1
25	MG	A	1550	1/1	0.30	-	23,23,23,23	1
25	MG	A	1579	1/1	0.32	-	23,23,23,23	1
25	MG	A	87	1/1	0.39	-	23,23,23,23	1
25	MG	A	1629	1/1	0.21	-	23,23,23,23	0
25	MG	A	1564	1/1	0.28	-	23,23,23,23	0
25	MG	A	1590	1/1	0.23	-	23,23,23,23	0
25	MG	A	1600	1/1	0.20	-	23,23,23,23	1
25	MG	A	1630	1/1	0.24	-	23,23,23,23	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	A	1597	1/1	0.31	-	23,23,23,23	1
25	MG	A	1606	1/1	0.44	-	23,23,23,23	1
25	MG	A	1552	1/1	0.20	-	23,23,23,23	0
25	MG	A	1570	1/1	0.17	-	23,23,23,23	0
25	MG	A	1618	1/1	0.22	-	23,23,23,23	0
25	MG	A	1616	1/1	0.30	-	23,23,23,23	1
25	MG	A	1615	1/1	0.29	-	23,23,23,23	1
25	MG	A	1593	1/1	0.27	-	23,23,23,23	1
25	MG	A	1577	1/1	0.15	-	23,23,23,23	0
25	MG	A	1612	1/1	0.27	-	23,23,23,23	1
25	MG	A	1623	1/1	0.39	-	23,23,23,23	1
25	MG	A	1549	1/1	0.38	-	23,23,23,23	1
25	MG	A	1627	1/1	0.28	-	23,23,23,23	1
25	MG	A	1560	1/1	0.26	-	23,23,23,23	0
25	MG	A	1556	1/1	0.26	-	23,23,23,23	0
25	MG	A	1599	1/1	0.25	-	23,23,23,23	1
25	MG	A	1569	1/1	0.20	-	23,23,23,23	1
25	MG	A	1613	1/1	0.36	-	23,23,23,23	1
25	MG	A	1608	1/1	0.30	-	23,23,23,23	1
25	MG	A	1566	1/1	0.53	-	23,23,23,23	1
25	MG	A	1602	1/1	0.21	-	23,23,23,23	0
25	MG	A	1635	1/1	0.48	-	23,23,23,23	1
25	MG	X	500	1/1	0.20	-	23,23,23,23	1
25	MG	A	1548	1/1	0.24	-	23,23,23,23	1
25	MG	A	1588	1/1	0.30	-	23,23,23,23	0
25	MG	A	1567	1/1	0.30	-	23,23,23,23	0
25	MG	A	466	1/1	0.41	-	23,23,23,23	1
25	MG	A	1619	1/1	0.23	-	23,23,23,23	1
26	ZN	N	307	1/1	0.21	-	23,23,23,23	1
25	MG	A	1582	1/1	0.10	-	23,23,23,23	0
25	MG	A	1604	1/1	0.38	-	23,23,23,23	1
25	MG	A	1592	1/1	0.23	-	23,23,23,23	0
25	MG	A	1631	1/1	0.13	-	23,23,23,23	1
25	MG	A	1575	1/1	1.07	-	23,23,23,23	1
25	MG	A	1581	1/1	0.45	-	23,23,23,23	1
25	MG	A	1554	1/1	0.30	-	23,23,23,23	1
25	MG	A	211	1/1	0.34	-	23,23,23,23	0
25	MG	A	1594	1/1	0.22	-	23,23,23,23	1
25	MG	A	1553	1/1	0.29	-	23,23,23,23	0
25	MG	A	1617	1/1	0.17	-	23,23,23,23	1
25	MG	A	1586	1/1	0.18	-	23,23,23,23	1
25	MG	A	1611	1/1	0.26	-	23,23,23,23	1

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	A	1557	1/1	0.21	-	23,23,23,23	0
25	MG	A	1559	1/1	0.33	-	23,23,23,23	0
25	MG	A	1587	1/1	0.14	-	23,23,23,23	0
25	MG	A	1622	1/1	0.51	-	23,23,23,23	1
25	MG	A	1628	1/1	0.29	-	23,23,23,23	1
25	MG	A	469	1/1	0.20	-	23,23,23,23	1
24	PAR	A	1545	42/42	0.32	-	25,25,25,25	0
25	MG	A	1610	1/1	0.33	-	23,23,23,23	1
25	MG	A	1568	1/1	0.18	-	23,23,23,23	0
25	MG	A	1546	1/1	0.26	-	23,23,23,23	0
25	MG	A	1634	1/1	0.42	-	23,23,23,23	1
25	MG	A	1633	1/1	0.34	-	23,23,23,23	1
25	MG	A	1620	1/1	0.27	-	23,23,23,23	1
25	MG	A	1632	1/1	0.22	-	23,23,23,23	1
25	MG	A	467	1/1	0.75	-	23,23,23,23	1
25	MG	J	449	1/1	0.23	-	23,23,23,23	1
25	MG	A	214	1/1	0.36	-	23,23,23,23	1
25	MG	A	493	1/1	1.16	-	23,23,23,23	1
25	MG	A	1591	1/1	0.29	-	23,23,23,23	1

6.5 Other polymers ⓘ

There are no such residues in this entry.