



wwPDB X-ray Structure Validation Summary Report

Oct 10, 2014 – 02:28 PM EDT

PDB ID : 4RB7
Title : Crystal structure of the *Thermus thermophilus* 70S ribosome in complex with amicoumacin, mRNA and three deacylated tRNAs in the A, P and E sites
Authors : Polikanov, Y.S.; Osterman, I.A.; Szal, T.; Tashlitsky, V.N.; Serebryakova, M.V.; Kusochev, P.; Bulkley, D.; Malanicheva, I.A.; Efimenko, T.A.; Efremenkova, O.V.; Konevega, A.L.; Shaw, K.J.; Bogdanov, A.A.; Rodnina, M.V.; Dontsova, O.A.; Mankin, A.S.; Steitz, T.A.; Sergiev, P.V.
Deposited on : 2014-09-12
Resolution : 2.40 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>

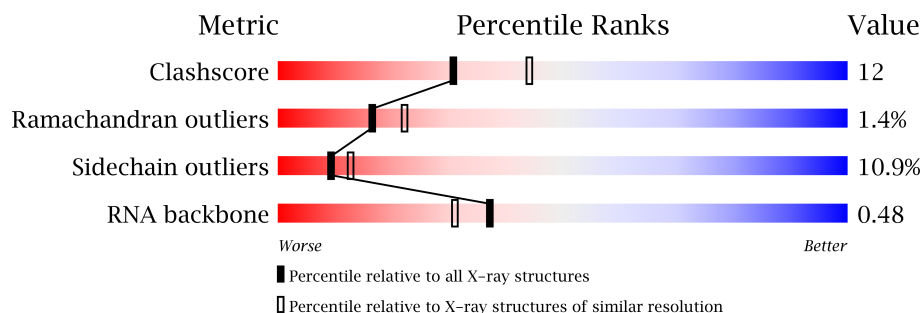
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23828

1 Overall quality at a glance

The reported resolution of this entry is 2.40 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))
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RNA backbone	1838	1029 (3.00-1.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1521	
2	B	256	
3	C	239	
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	132	
13	M	126	
14	N	61	

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Mol	Chain	Length	Quality of chain
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	V	24	
23	W	76	
23	Y	76	
24	X	77	

2 Entry composition

There are 30 unique types of molecules in this entry. The entry contains 56383 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	1503	Total	C	N	O	P	0	0	0
			32312	14381	5990	10438	1503			

- Molecule 2 is a protein called 30S Ribosomal Protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	231	Total	C	N	O	S	0	0	0
			1825	1167	326	327	5			

- Molecule 3 is a protein called 30S Ribosomal Protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	206	Total	C	N	O	S	0	0	0
			1542	968	300	273	1			

- Molecule 4 is a protein called 30S Ribosomal Protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	S	0	0	0
			1674	1050	333	284	7			

- Molecule 5 is a protein called 30S Ribosomal Protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	148	Total	C	N	O	S	0	0	0
			1133	716	214	199	4			

- Molecule 6 is a protein called 30S Ribosomal Protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			816	516	146	151	3			

- Molecule 7 is a protein called 30S Ribosomal Protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1235	769	244	216	6			

- Molecule 8 is a protein called 30S Ribosomal Protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	137	Total	C	N	O	S	0	0	0
			1088	689	206	191	2			

- Molecule 9 is a protein called 30S Ribosomal Protein S9.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	0	0	0
			978	619	190	169			

- Molecule 10 is a protein called 30S Ribosomal Protein S10.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	96	Total	C	N	O	0	0	0
			714	445	138	131			

- Molecule 11 is a protein called 30S Ribosomal Protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	114	Total	C	N	O	S	0	0	0
			833	519	156	155	3			

- Molecule 12 is a protein called 30S Ribosomal Protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	122	Total	C	N	O	S	0	0	0
			930	585	185	159	1			

- Molecule 13 is a protein called 30S Ribosomal Protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	122	Total	C	N	O	S	0	0	0
			950	586	197	165	2			

- Molecule 14 is a protein called 30S Ribosomal Protein S14.

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

- Molecule 15 is a protein called 30S Ribosomal Protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			728	456	144	126	2			

- Molecule 16 is a protein called 30S Ribosomal Protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	82	Total	C	N	O	S	0	0	0
			677	430	133	113	1			

- Molecule 17 is a protein called 30S Ribosomal Protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0	0
			823	528	151	142	2			

- Molecule 18 is a protein called 30S Ribosomal Protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	68	Total	C	N	O	0	0	0
			555	355	108	92			

- Molecule 19 is a protein called 30S Ribosomal Protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	83	Total	C	N	O	S	0	0	0
			646	412	119	113	2			

- Molecule 20 is a protein called 30S Ribosomal Protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	96	Total	C	N	O	S	0	0	0
			727	446	155	124	2			

- Molecule 21 is a protein called 30S Ribosomal Protein THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	23	Total	C	N	O	0	0	0
			199	122	48	29			

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	13	Total	C	N	O	P	0	0	0
			277	125	51	88	13			

- Molecule 23 is a RNA chain called A/P-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	W	72	Total	C	N	O	P	S	0	0	0
			1544	690	278	502	72	2			
23	Y	73	Total	C	N	O	P	S	0	0	0
			1565	698	283	510	73	1			

- Molecule 24 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
24	X	76	Total	C	N	O	P	S	0	0	0
			1625	725	294	529	76	1			

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

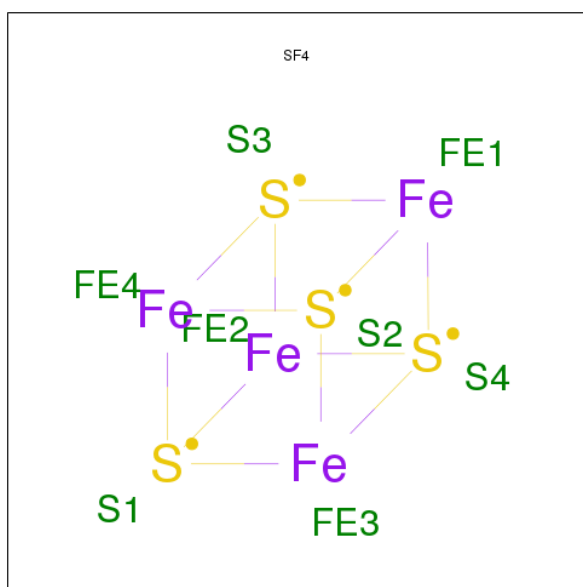
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	P	1	Total	Mg	0	0
			1	1		
25	G	1	Total	Mg	0	0
			1	1		
25	J	2	Total	Mg	0	0
			2	2		
25	Q	2	Total	Mg	0	0
			2	2		
25	D	2	Total	Mg	0	0
			2	2		
25	K	1	Total	Mg	0	0
			1	1		
25	E	1	Total	Mg	0	0
			1	1		
25	V	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	W	4	Total 4	Mg 4	0	0
25	A	201	Total 201	Mg 201	0	0
25	T	1	Total 1	Mg 1	0	0
25	X	6	Total 6	Mg 6	0	0
25	R	1	Total 1	Mg 1	0	0
25	L	2	Total 2	Mg 2	0	0
25	F	2	Total 2	Mg 2	0	0

-
- The chemical structure of UAM (Ureidylated Adenine Monophosphate) is shown. It features a purine base (adenine) linked to a ribose sugar, which is further linked to a phosphate group. The structure is labeled with various atoms and bonds, including NAD, CAT, CBA(S), CBR(S), CAZ(S), CAS, CAW, CAA, CAP, CAY, CAB, CAV, CAX, CAU, OAR, OAH, OAG, OAI, OAF, OAJ, and OAE. The structure is complex, with multiple rings and functional groups, including a phosphate group and a ribose sugar. The labels are color-coded: NAD is blue, CAT is red, CBA(S) is green, CBR(S) is blue, CAZ(S) is green, CAS is red, CAW is green, CAA is red, CAP is green, CAY is red, CAB is green, CAV is red, CAX is green, CAU is red, OAR is green, OAH is red, OAG is green, OAI is red, OAF is green, OAJ is red, and OAE is green.

- Molecule 27 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 28 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
28	N	1	Total	Zn	0	0
			1	1		

- Molecule 29 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	X	1	Total	K	0	0
			1	1		

- Molecule 30 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	A	204	Total	O	0	0
			204	204		
30	D	1	Total	O	0	0
			1	1		
30	G	1	Total	O	0	0
			1	1		
30	I	1	Total	O	0	0
			1	1		

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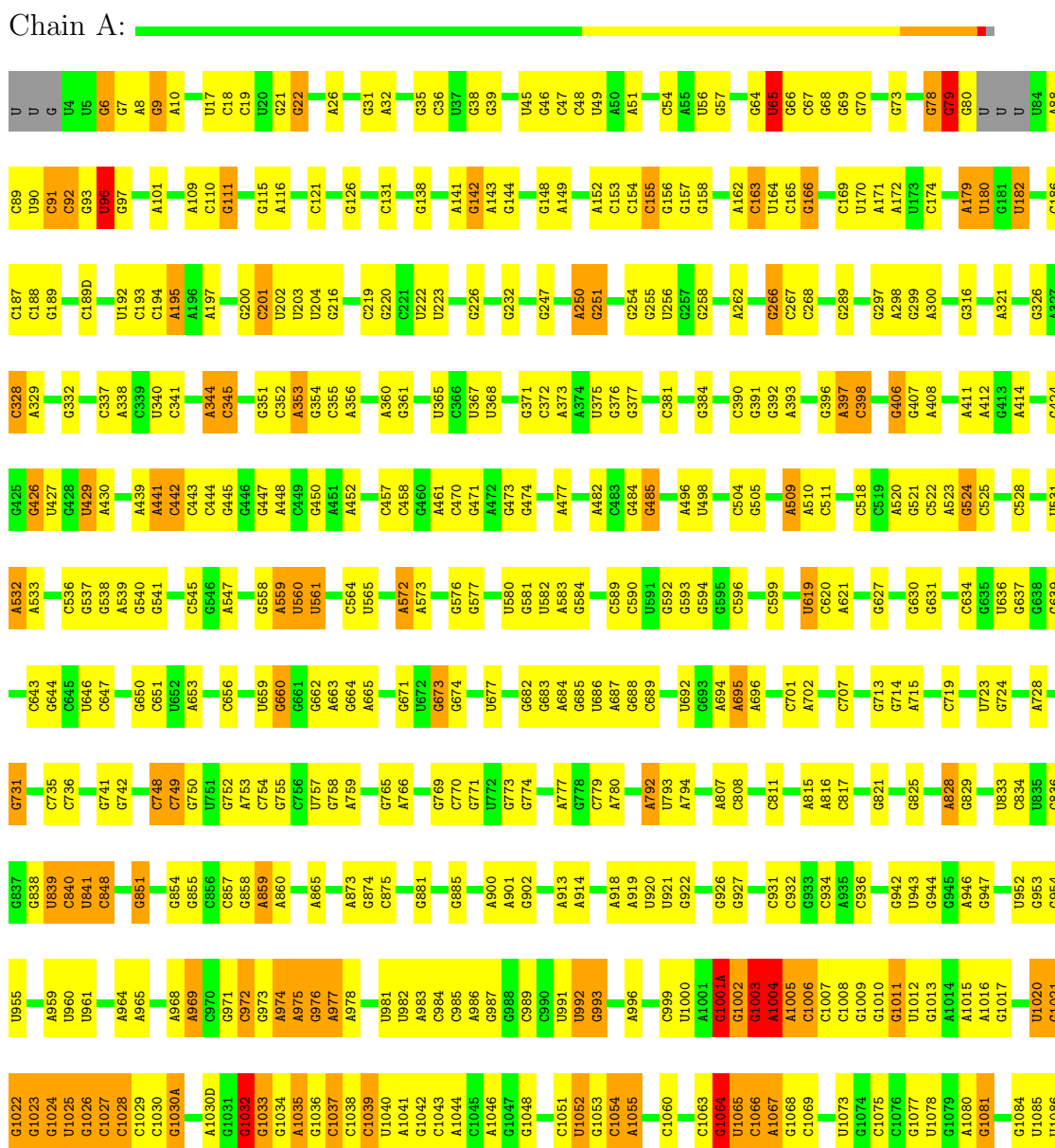
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
30	J	4	Total 4	O 4	0	0
30	L	4	Total 4	O 4	0	0
30	O	1	Total 1	O 1	0	0
30	P	1	Total 1	O 1	0	0
30	R	1	Total 1	O 1	0	0
30	T	1	Total 1	O 1	0	0
30	W	2	Total 2	O 2	0	0
30	X	6	Total 6	O 6	0	0

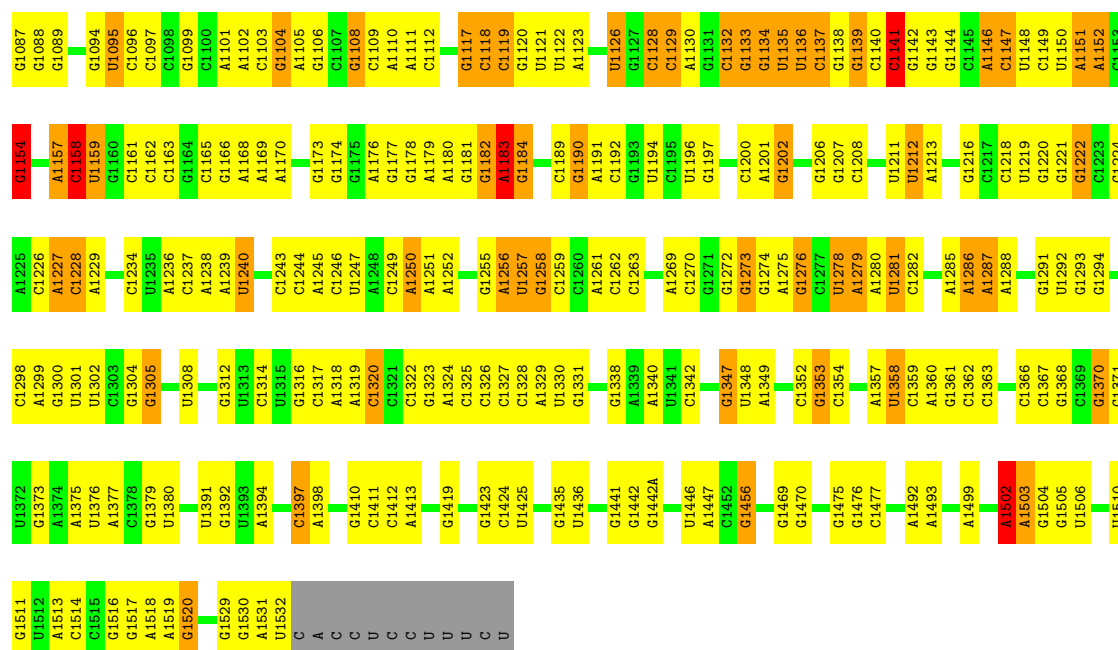
3 Residue-property plots

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 ($RSRZ > 2$). 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.

Note EDS was not executed.

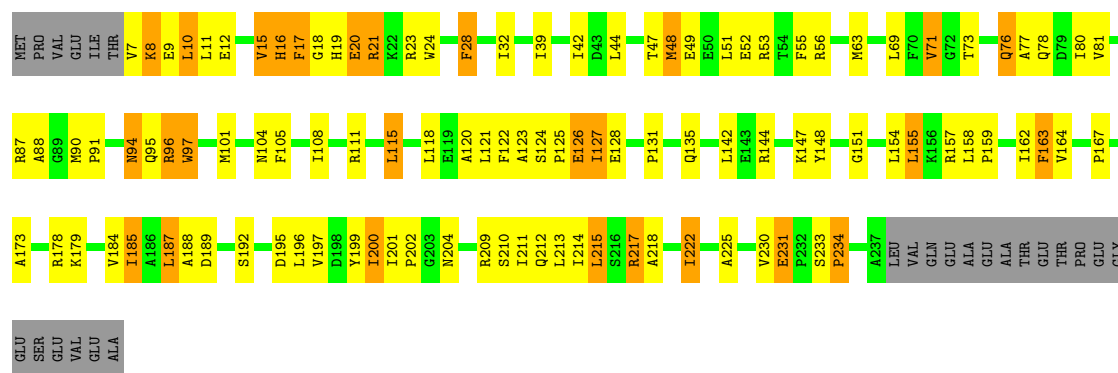
• Molecule 1: 16S Ribosomal RNA





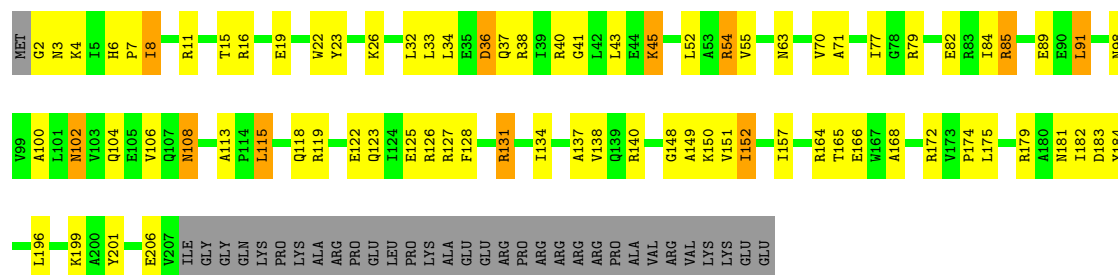
• Molecule 2: 30S Ribosomal Protein S2

Chain B:



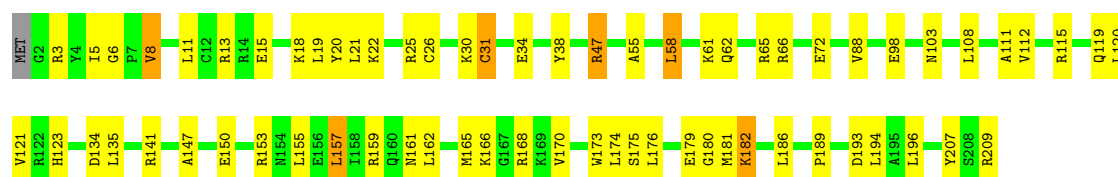
• Molecule 3: 30S Ribosomal Protein S3

Chain C:



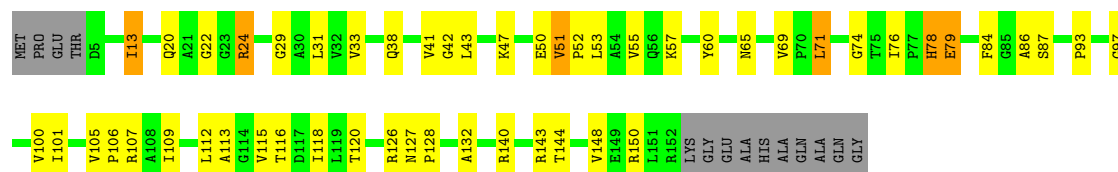
• Molecule 4: 30S Ribosomal Protein S4

Chain D:



- Molecule 5: 30S Ribosomal Protein S5

Chain E:



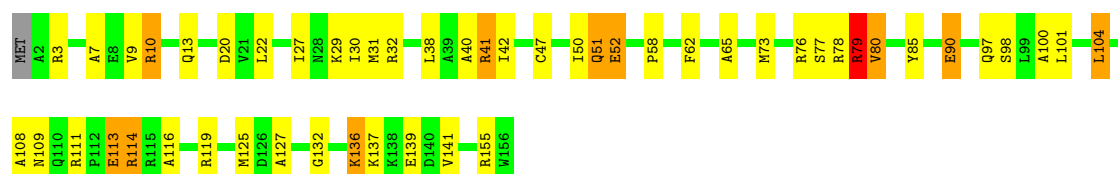
- Molecule 6: 30S Ribosomal Protein S6

Chain F:



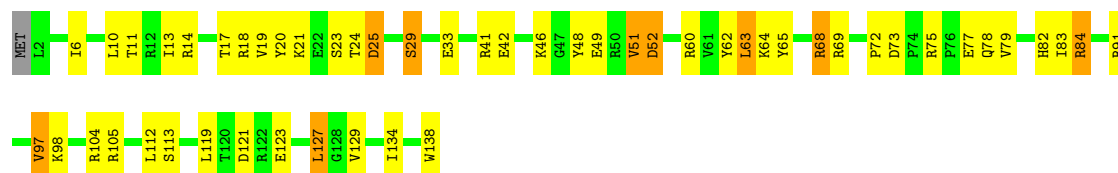
- Molecule 7: 30S Ribosomal Protein S7

Chain G:



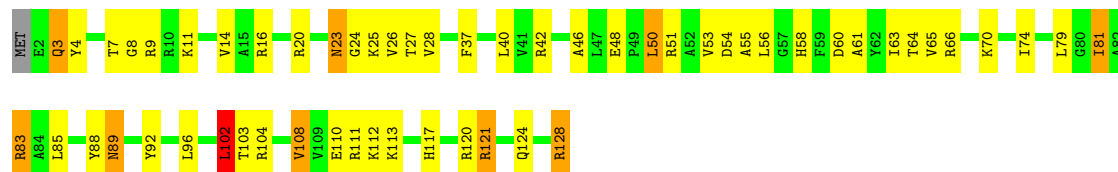
- Molecule 8: 30S Ribosomal Protein S8

Chain H:



- Molecule 9: 30S Ribosomal Protein S9

Chain I:



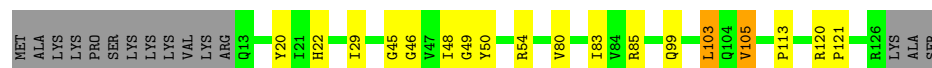
- Molecule 10: 30S Ribosomal Protein S10

Chain J: 



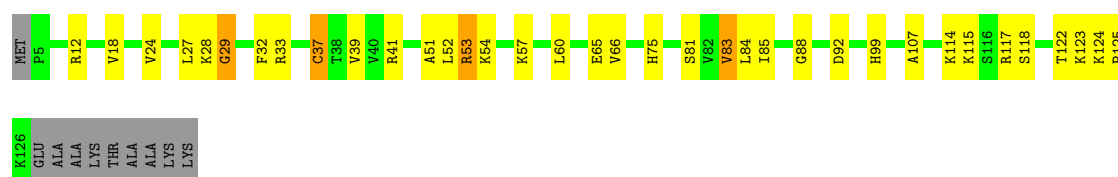
- Molecule 11: 30S Ribosomal Protein S11

Chain K: 



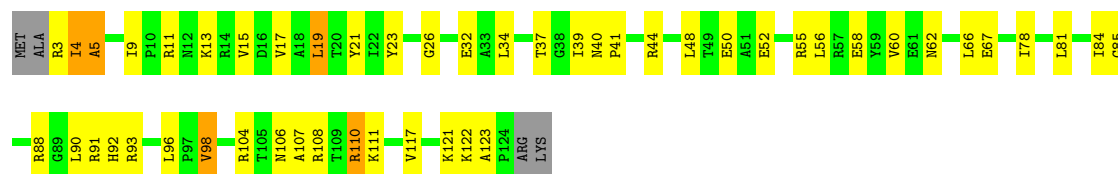
- Molecule 12: 30S Ribosomal Protein S12

Chain L: 



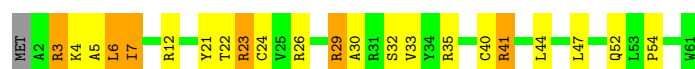
- Molecule 13: 30S Ribosomal Protein S13

Chain M: 



- Molecule 14: 30S Ribosomal Protein S14

Chain N: 



- Molecule 15: 30S Ribosomal Protein S15

Chain O: 



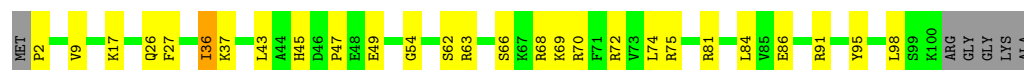
- Molecule 16: 30S Ribosomal Protein S16

Chain P: 



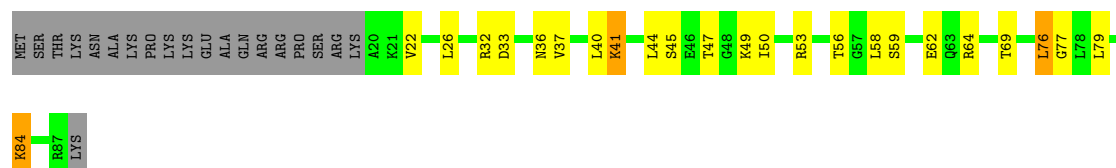
- Molecule 17: 30S Ribosomal Protein S17

Chain Q: 



- Molecule 18: 30S Ribosomal Protein S18

Chain R: 



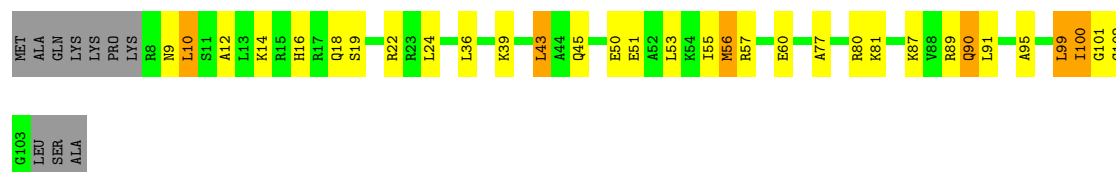
- Molecule 19: 30S Ribosomal Protein S19

Chain S: 



- Molecule 20: 30S Ribosomal Protein S20

Chain T: 



- Molecule 21: 30S Ribosomal Protein THX

Chain U: 



- Molecule 22: mRNA

Chain V: 



- Molecule 23: A/P-site tRNA

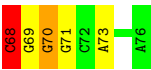
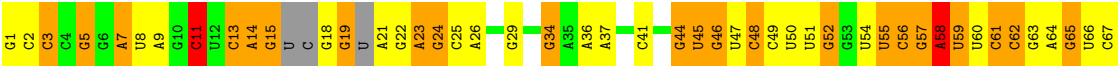
Chain W: 





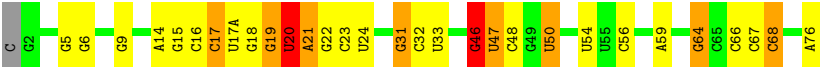
• Molecule 23: A/P-site tRNA

Chain Y: 



• Molecule 24: E-site tRNA

Chain X: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	210.06Å 448.57Å 623.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	256.12 – 2.40	Depositor
% Data completeness (in resolution range)	99.7 (256.12-2.40)	Depositor
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.237 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	56383	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, ZN, MIA, SF4, MG, UAM, 5MC, 4SU, 7MG, K, PSU

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	0.37	1/36170 (0.0%)	0.91	47/56452 (0.1%)
2	B	0.30	0/1860	0.61	1/2518 (0.0%)
3	C	0.30	0/1566	0.56	0/2119
4	D	0.29	0/1704	0.50	0/2284
5	E	0.31	0/1149	0.57	0/1548
6	F	0.30	0/829	0.51	0/1123
7	G	0.27	0/1254	0.53	0/1683
8	H	0.27	0/1108	0.49	0/1494
9	I	0.28	0/997	0.53	1/1343 (0.1%)
10	J	0.29	0/727	0.55	0/988
11	K	0.28	0/848	0.51	0/1149
12	L	0.29	0/946	0.56	1/1274 (0.1%)
13	M	0.28	0/961	0.55	0/1291
14	N	0.30	0/501	0.55	0/664
15	O	0.29	0/739	0.52	0/985
16	P	0.28	0/693	0.50	0/935
17	Q	0.27	0/836	0.48	0/1117
18	R	0.26	0/560	0.49	0/746
19	S	0.31	0/661	0.64	0/893
20	T	0.28	0/729	0.52	0/965
21	U	0.30	0/203	0.51	0/266
22	V	0.40	0/310	0.89	1/480 (0.2%)
23	W	0.51	0/1556	1.23	9/2418 (0.4%)
23	Y	0.56	1/1583 (0.1%)	1.22	12/2459 (0.5%)
24	X	0.49	0/1725	1.13	14/2689 (0.5%)
All	All	0.36	2/60215 (0.0%)	0.85	86/89883 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
7	G	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	1	G	OP3-P	-10.36	1.48	1.61
1	A	1154	G	C6-N1	-5.24	1.35	1.39

The worst 5 of 86 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1154	G	C5-C6-O6	12.79	136.28	128.60
24	X	46	G	C6-N1-C2	-9.19	119.59	125.10
1	A	1004	A	O4'-C1'-N9	8.95	115.36	108.20
1	A	1119	C	C2-N3-C4	8.93	124.36	119.90
1	A	1001(A)	G	N3-C4-N9	8.73	131.24	126.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	G	79	ARG	Peptide

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	32312	0	16307	511	0
2	B	1825	0	1828	83	0
3	C	1542	0	1517	55	0
4	D	1674	0	1714	43	0
5	E	1133	0	1191	38	0
6	F	816	0	808	11	0
7	G	1235	0	1249	32	0
8	H	1088	0	1126	39	0
9	I	978	0	966	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	714	0	672	36	0
11	K	833	0	836	10	0
12	L	930	0	980	23	0
13	M	950	0	988	34	0
14	N	492	0	529	17	0
15	O	728	0	760	23	0
16	P	677	0	686	18	0
17	Q	823	0	891	14	0
18	R	555	0	618	17	0
19	S	646	0	644	29	0
20	T	727	0	796	21	0
21	U	199	0	208	5	0
22	V	277	0	140	6	0
23	W	1544	0	788	38	0
23	Y	1565	0	795	61	0
24	X	1625	0	828	17	0
25	A	201	0	0	0	0
25	D	2	0	0	0	0
25	E	1	0	0	0	0
25	F	2	0	0	0	0
25	G	1	0	0	0	0
25	J	2	0	0	0	0
25	K	1	0	0	0	0
25	L	2	0	0	0	0
25	P	1	0	0	0	0
25	Q	2	0	0	0	0
25	R	1	0	0	0	0
25	T	1	0	0	0	0
25	V	1	0	0	0	0
25	W	4	0	0	0	0
25	X	6	0	0	0	0
26	A	30	0	0	2	0
27	D	8	0	0	0	0
28	N	1	0	0	0	0
29	X	1	0	0	0	0
30	A	204	0	0	12	0
30	D	1	0	0	0	0
30	G	1	0	0	1	0
30	I	1	0	0	0	0
30	J	4	0	0	0	0
30	L	4	0	0	0	0
30	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	P	1	0	0	0	0
30	R	1	0	0	0	0
30	T	1	0	0	0	0
30	W	2	0	0	0	0
30	X	6	0	0	0	0
All	All	56383	0	37865	1086	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 12.

The worst 5 of 1086 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1002:G:H1	1:A:1038:C:N4	1.51	1.08
1:A:1028:C:N3	1:A:1033:G:C6	2.23	1.06
1:A:1029:C:C4	1:A:1032:G:N1	2.32	0.97
23:W:50:U:H3	23:W:64:A:N6	1.63	0.97
1:A:947:G:H1	1:A:1234:C:H42	0.97	0.96

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
2	B	229/256 (90%)	201 (88%)	16 (7%)	12 (5%)	3 1
3	C	204/239 (85%)	188 (92%)	13 (6%)	3 (2%)	15 20
4	D	206/209 (99%)	201 (98%)	5 (2%)	0	100 100
5	E	146/162 (90%)	140 (96%)	5 (3%)	1 (1%)	30 43
6	F	98/101 (97%)	95 (97%)	3 (3%)	0	100 100
7	G	153/156 (98%)	144 (94%)	7 (5%)	2 (1%)	18 24
8	H	135/138 (98%)	129 (96%)	6 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	I	125/128 (98%)	114 (91%)	10 (8%)	1 (1%)	27	39
10	J	94/105 (90%)	84 (89%)	8 (8%)	2 (2%)	11	12
11	K	112/129 (87%)	108 (96%)	2 (2%)	2 (2%)	13	15
12	L	120/132 (91%)	116 (97%)	4 (3%)	0	100	100
13	M	120/126 (95%)	114 (95%)	4 (3%)	2 (2%)	14	17
14	N	58/61 (95%)	56 (97%)	2 (3%)	0	100	100
15	O	86/89 (97%)	83 (96%)	2 (2%)	1 (1%)	19	26
16	P	80/88 (91%)	78 (98%)	1 (1%)	1 (1%)	18	24
17	Q	97/105 (92%)	96 (99%)	1 (1%)	0	100	100
18	R	66/88 (75%)	65 (98%)	1 (2%)	0	100	100
19	S	81/93 (87%)	74 (91%)	6 (7%)	1 (1%)	19	26
20	T	94/106 (89%)	87 (93%)	2 (2%)	5 (5%)	3	1
21	U	21/27 (78%)	19 (90%)	2 (10%)	0	100	100
All	All	2325/2538 (92%)	2192 (94%)	100 (4%)	33 (1%)	16	22

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	10	LEU
2	B	16	HIS
2	B	20	GLU
2	B	21	ARG
2	B	121	LEU

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	
2	B	187/220 (85%)	158 (84%)	29 (16%)	4	4
3	C	140/188 (74%)	125 (89%)	15 (11%)	10	13
4	D	173/181 (96%)	158 (91%)	15 (9%)	15	22
5	E	114/123 (93%)	101 (89%)	13 (11%)	8	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F	85/90 (94%)	77 (91%)	8 (9%)	13	18
7	G	120/127 (94%)	102 (85%)	18 (15%)	4	5
8	H	114/119 (96%)	100 (88%)	14 (12%)	7	8
9	I	89/99 (90%)	74 (83%)	15 (17%)	3	3
10	J	69/92 (75%)	64 (93%)	5 (7%)	21	31
11	K	83/99 (84%)	81 (98%)	2 (2%)	61	81
12	L	97/109 (89%)	92 (95%)	5 (5%)	32	49
13	M	92/101 (91%)	80 (87%)	12 (13%)	6	7
14	N	49/50 (98%)	39 (80%)	10 (20%)	2	2
15	O	78/80 (98%)	68 (87%)	10 (13%)	6	7
16	P	68/74 (92%)	63 (93%)	5 (7%)	20	30
17	Q	94/97 (97%)	88 (94%)	6 (6%)	25	37
18	R	59/77 (77%)	54 (92%)	5 (8%)	15	23
19	S	67/80 (84%)	61 (91%)	6 (9%)	14	20
20	T	70/82 (85%)	63 (90%)	7 (10%)	11	16
21	U	18/22 (82%)	15 (83%)	3 (17%)	3	3
All	All	1866/2110 (88%)	1663 (89%)	203 (11%)	9	13

5 of 203 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	90	GLU
9	I	23	ASN
19	S	5	LEU
7	G	113	GLU
8	H	52	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	28	ASN
8	H	78	GLN
19	S	65	ASN
7	G	51	GLN
7	G	97	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1501/1521 (98%)	306 (20%)	23 (1%)
22	V	12/24 (50%)	1 (8%)	0
23	W	68/76 (89%)	27 (39%)	1 (1%)
23	Y	69/76 (90%)	28 (40%)	3 (4%)
24	X	75/77 (97%)	16 (21%)	1 (1%)
All	All	1725/1774 (97%)	378 (21%)	28 (1%)

5 of 378 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	9	G
1	A	22	G
1	A	31	G
1	A	32	A

5 of 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1064	G
1	A	1128	C
23	Y	14	A
1	A	1065	U
1	A	1067	A

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

18 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	$\# Z > 2$
23	PSU	W	32	23	19,21,22	1.78	4 (21%)	23,30,33	1.00	2 (8%)
23	MIA	W	37	23	24,27,32	1.96	6 (25%)	35,39,47	2.01	7 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	PSU	W	39	23	19,21,22	1.85	5 (26%)	23,30,33	0.96	1 (4%)
23	7MG	W	46	23	24,26,27	2.00	6 (25%)	34,39,42	2.28	8 (23%)
23	5MU	W	54	23	20,22,23	1.66	4 (20%)	25,32,35	1.78	4 (16%)
23	PSU	W	55	23	19,21,22	1.77	4 (21%)	23,30,33	1.35	2 (8%)
23	4SU	W	8	23	19,21,22	1.80	4 (21%)	23,30,33	2.77	3 (13%)
24	5MC	X	32	24	20,22,23	1.80	4 (20%)	26,32,35	1.48	4 (15%)
24	5MU	X	54	24	20,22,23	1.70	4 (20%)	25,32,35	2.07	4 (16%)
24	PSU	X	55	24	19,21,22	1.78	4 (21%)	23,30,33	0.98	1 (4%)
24	4SU	X	8	24	19,21,22	1.72	4 (21%)	23,30,33	29.03	2 (8%)
23	PSU	Y	32	23	19,21,22	1.78	4 (21%)	23,30,33	0.95	2 (8%)
23	MIA	Y	37	23	20,24,32	1.71	5 (25%)	27,35,47	1.95	5 (18%)
23	PSU	Y	39	23	19,21,22	1.90	4 (21%)	23,30,33	1.51	2 (8%)
23	7MG	Y	46	23	24,26,27	2.05	8 (33%)	34,39,42	2.73	12 (35%)
23	5MU	Y	54	23	20,22,23	1.85	4 (20%)	25,32,35	2.01	5 (20%)
23	PSU	Y	55	23	19,21,22	1.87	6 (31%)	23,30,33	1.03	3 (13%)
23	4SU	Y	8	23	19,21,22	1.85	4 (21%)	23,30,33	7.20	4 (17%)

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
23	PSU	W	32	23	-	0/8/25/26	0/2/2/2
23	MIA	W	37	23	-	0/12/29/34	0/3/3/3
23	PSU	W	39	23	-	0/8/25/26	0/2/2/2
23	7MG	W	46	23	-	0/8/37/38	0/3/3/3
23	5MU	W	54	23	-	0/6/25/26	0/2/2/2
23	PSU	W	55	23	-	0/8/25/26	0/2/2/2
23	4SU	W	8	23	-	0/6/25/26	0/2/2/2
24	5MC	X	32	24	-	0/6/25/26	0/2/2/2
24	5MU	X	54	24	-	0/6/25/26	0/2/2/2
24	PSU	X	55	24	-	0/8/25/26	0/2/2/2
24	4SU	X	8	24	-	0/6/25/26	0/2/2/2
23	PSU	Y	32	23	-	0/8/25/26	0/2/2/2
23	MIA	Y	37	23	-	0/8/25/34	0/3/3/3
23	PSU	Y	39	23	-	0/8/25/26	0/2/2/2
23	7MG	Y	46	23	-	0/8/37/38	0/3/3/3
23	5MU	Y	54	23	-	1/6/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	PSU	Y	55	23	-	0/8/25/26	0/2/2/2
23	4SU	Y	8	23	-	0/6/25/26	0/2/2/2

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	37	MIA	C2-S10	-6.01	1.70	1.75
23	W	46	7MG	C6-C5	5.83	1.48	1.41
24	X	32	5MC	C5-C4	4.88	1.49	1.41
23	Y	8	4SU	P-OP1	4.68	1.52	1.46
23	Y	46	7MG	C6-C5	4.66	1.47	1.41

The worst 5 of 71 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	X	8	4SU	C4-N3-C2	138.99	127.55	121.60
23	Y	8	4SU	C4-N3-C2	-33.30	120.18	121.60
23	W	8	4SU	C4-N3-C2	10.15	122.04	121.60
23	Y	46	7MG	N3-C4-N9	8.80	140.70	126.80
24	X	8	4SU	C2-N1-C1'	7.91	123.17	118.21

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	Y	54	5MU	OP2-P-O5'-C5'

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 232 ligands modelled in this entry, 230 are monoatomic - leaving 2 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	$\# Z > 2$
26	UAM	A	3202	-	31,31,31	1.44	2 (6%)	44,44,44	1.38	7 (15%)
27	SF4	D	501	4	12,12,12	21.81	12 (100%)	0,24,24	0.00	-

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
26	UAM	A	3202	-	-	0/28/40/40	0/2/2/2
27	SF4	D	501	4	-	0/0/48/48	0/6/5/5

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	501	SF4	S4-FE2	-22.39	2.18	2.33
27	D	501	SF4	S3-FE2	-22.18	2.18	2.33
27	D	501	SF4	S4-FE1	-22.15	2.18	2.33
27	D	501	SF4	S3-FE1	-22.09	2.18	2.33
27	D	501	SF4	S1-FE3	-21.99	2.18	2.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	3202	UAM	CAO-CBD-CBC	-4.53	109.27	116.45
26	A	3202	UAM	CBD-OAR-CAU	-3.24	113.71	118.73
26	A	3202	UAM	OAR-CAU-OAG	2.80	121.32	117.68
26	A	3202	UAM	CAP-CBC-CBD	-2.65	108.58	112.59
26	A	3202	UAM	OAH-CAV-CAX	-2.32	116.59	121.11

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.