



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 02:18 PM GMT

PDB ID : 4B8H
Title : RNA3
Authors : Gao, Y.G.; Feng, S.; Chen, Y.
Deposited on : 2012-08-28
Resolution : 3.70 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>

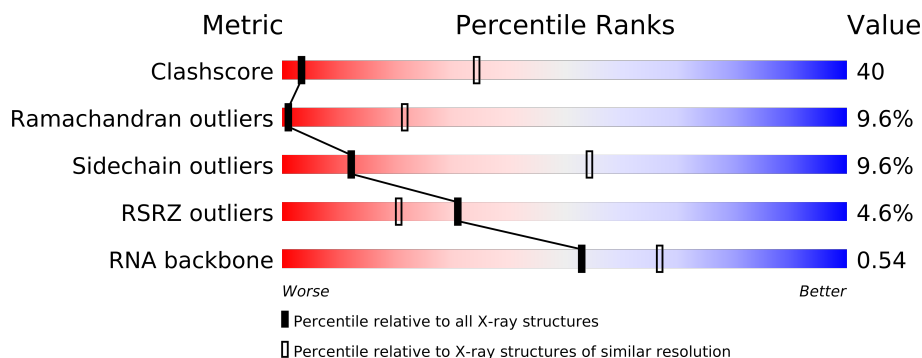
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.70 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	1009 (3.94-3.46)
Ramachandran outliers	78287	1016 (3.98-3.42)
Sidechain outliers	78261	1014 (3.98-3.42)
RSRZ outliers	66119	1099 (4.00-3.40)
RNA backbone	1838	1008 (4.52-2.80)

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.

Mol	Chain	Length	Quality of chain
1	A	1522	
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	76	
23	W	77	
24	X	25	
25	Y	691	

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 60287 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	1504	Total	C	N	O	P	0	0	0
			32329	14390	5992	10444	1503			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	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
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	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
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	S	0	0	0
			1010	639	197	174				

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			795	499	157	138	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	125	Total	C	N	O	S	0	0	1
			988	611	206	169	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

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
			734	459	147	126	2			

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	100	Total	C	N	O	S	0	0	1
			824	528	152	142	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	79	Total	C	N	O	S	0	0	1
			630	403	115	110	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

- Molecule 22 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	76	Total	C	N	O	P	0	0	0
			1619	723	290	531	75			

- Molecule 23 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	W	77	Total	C	N	O	P	0	0	0
			1641	733	297	535	76			

- Molecule 24 is a RNA chain called RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	X	12	Total	C	N	O	P	0	0	0
			257	116	49	80	12			

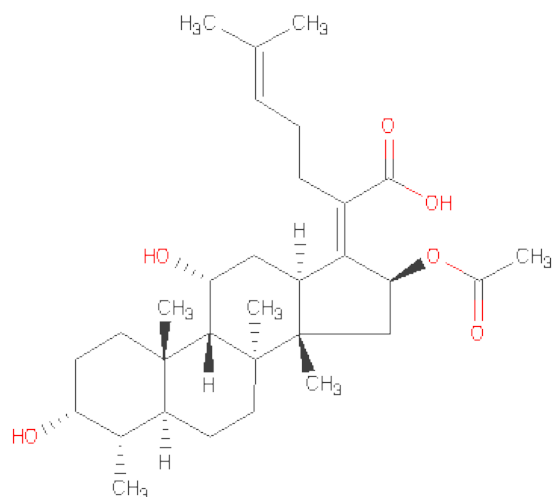
- Molecule 25 is a protein called ELONGATION FACTOR G.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	Y	667	Total	C	N	O	S	0	0	1
			5215	3316	893	988	18			

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

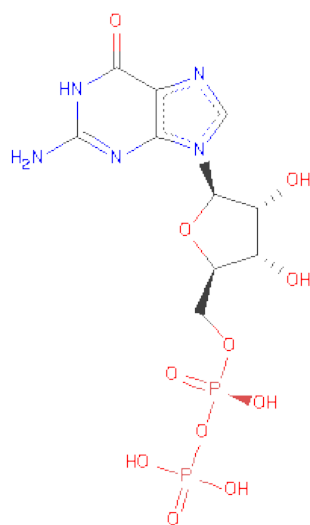
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	W	1	Total	Zn	0	0
			1	1		
26	D	1	Total	Zn	0	0
			1	1		
26	C	1	Total	Zn	0	0
			1	1		
26	N	1	Total	Zn	0	0
			1	1		

- Molecule 27 is FUSIDIC ACID (three-letter code: FUA) (formula: C₃₁H₄₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
27	F	1	Total	C	O	0	0
			37	31	6		

- Molecule 28 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
28	Y	1	Total	C	N	O	P	
			28	10	5	11	2	

- Molecule 29 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

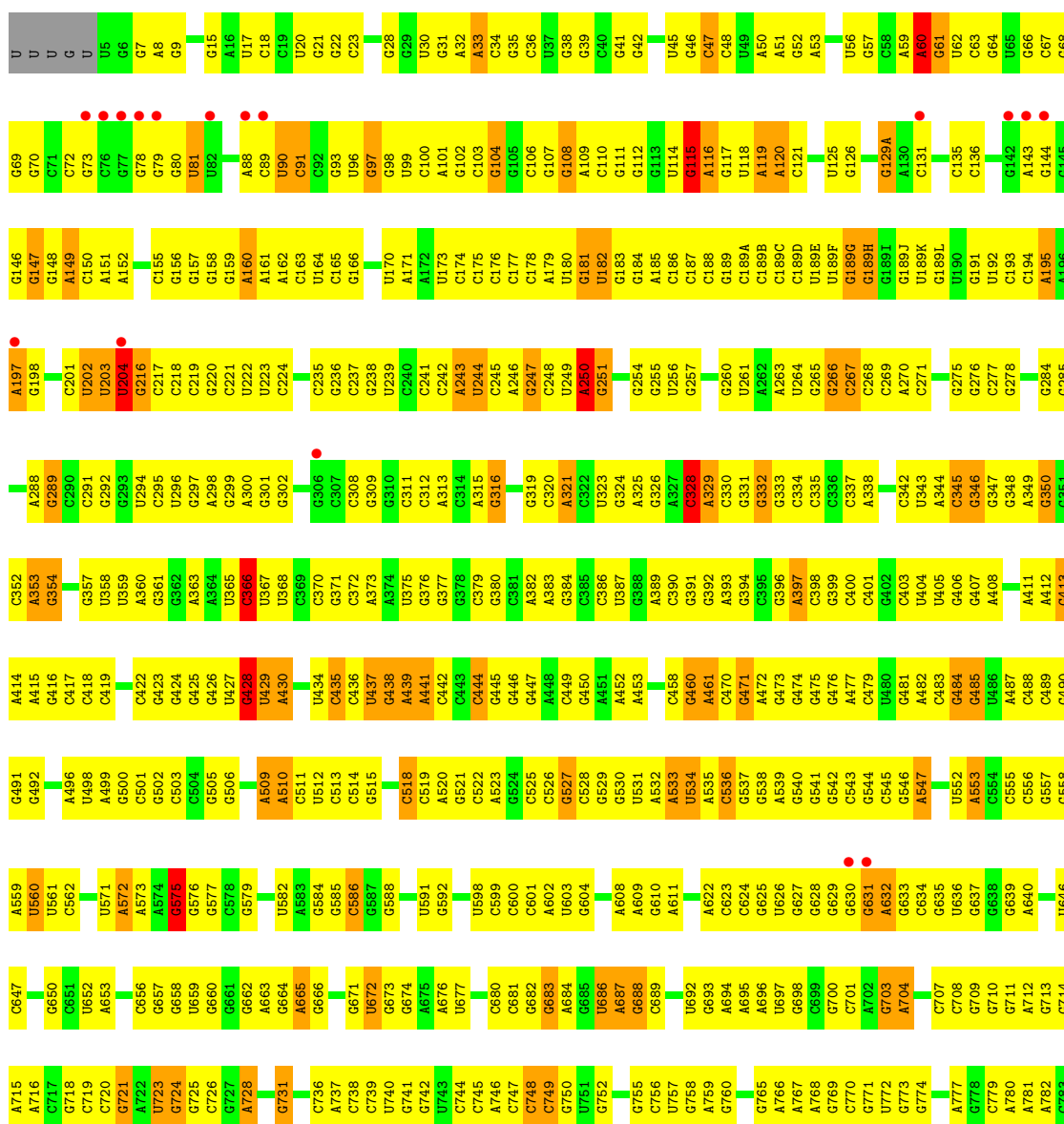
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
29	Y	1	Total 1	Mg 1	0	0

3 Residue-property plots

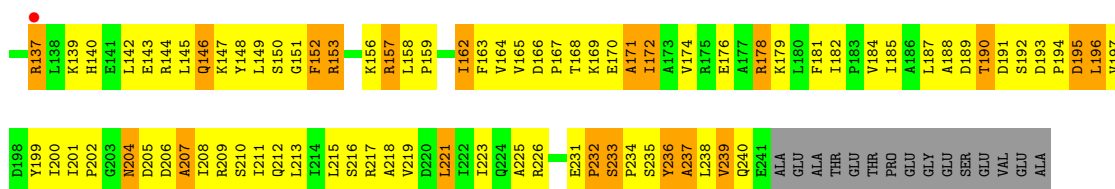
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($RSRZ > 2$). 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

Chain A: 

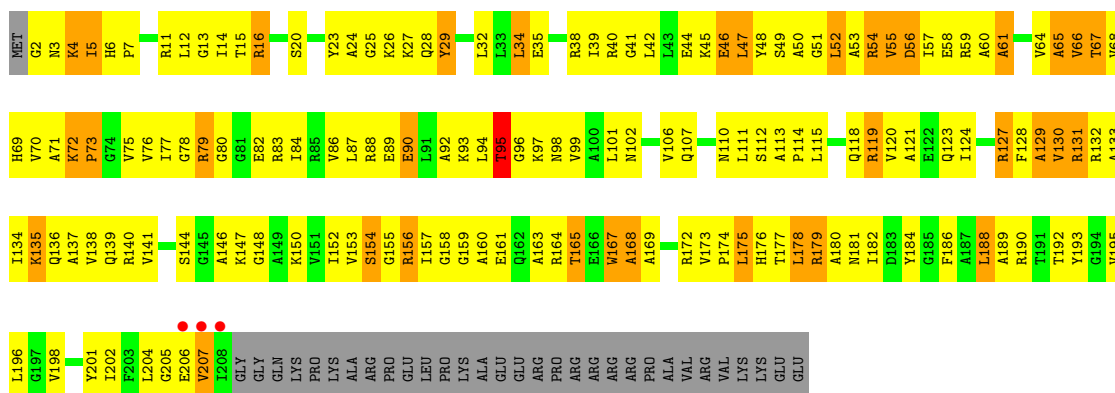






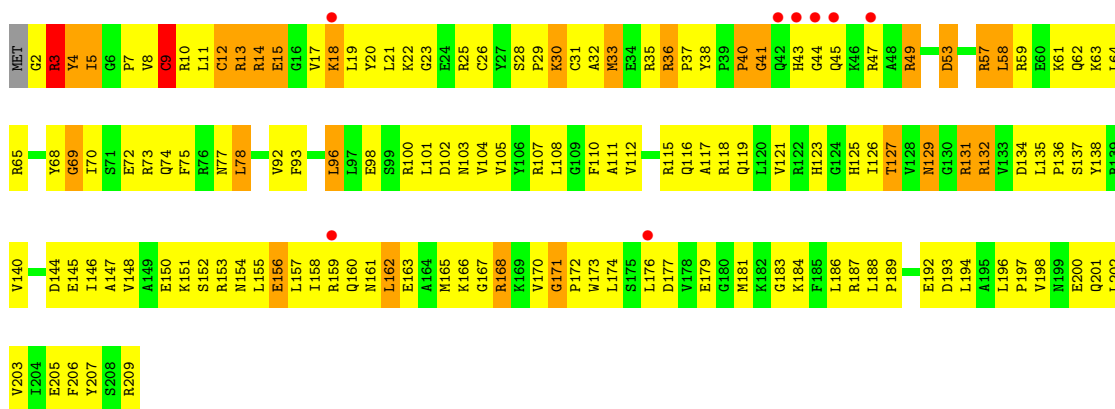
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain C:



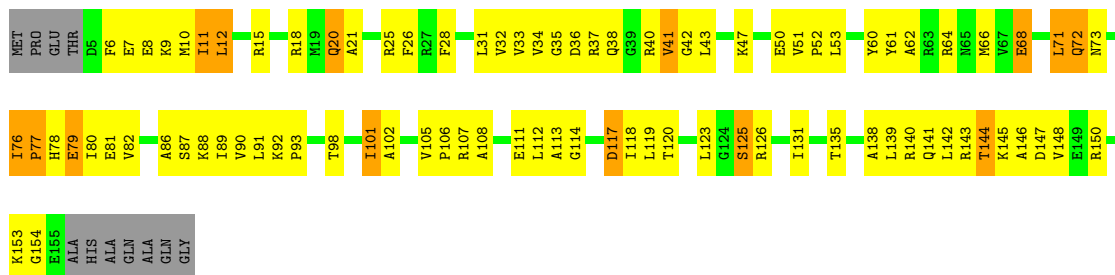
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain D:



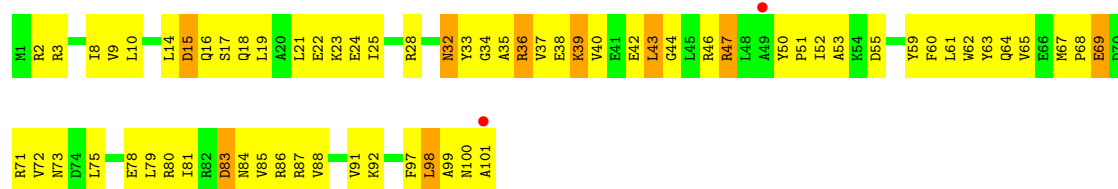
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain E:



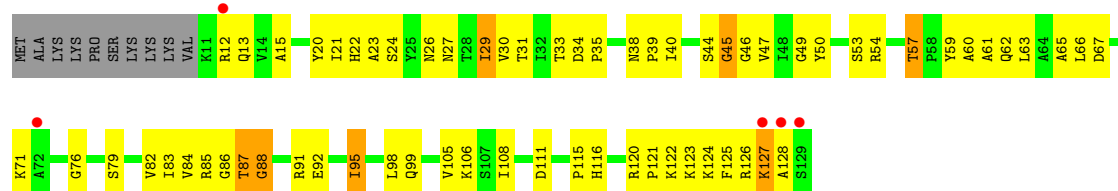
• Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain F: 



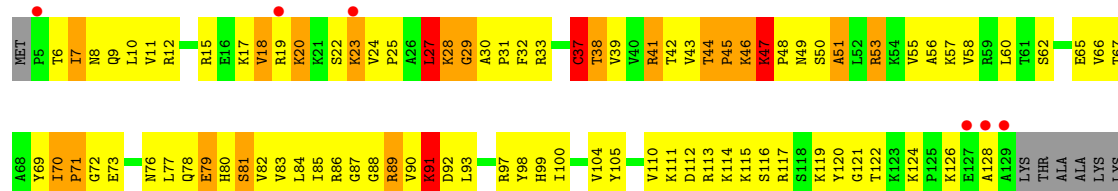
- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K: 



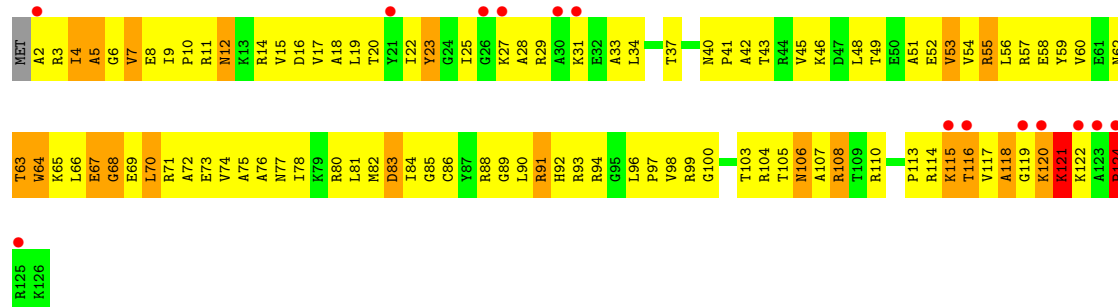
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L: 



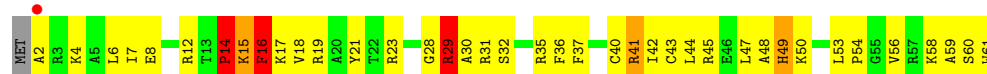
- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M: 



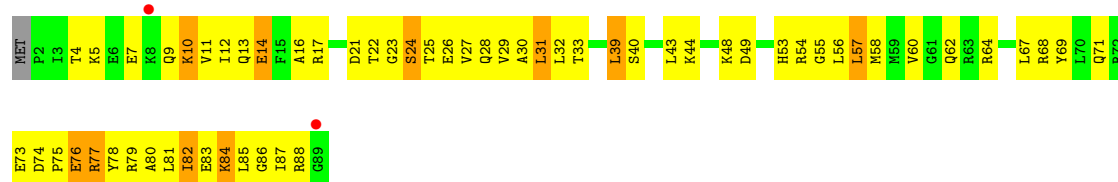
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

Chain N: 



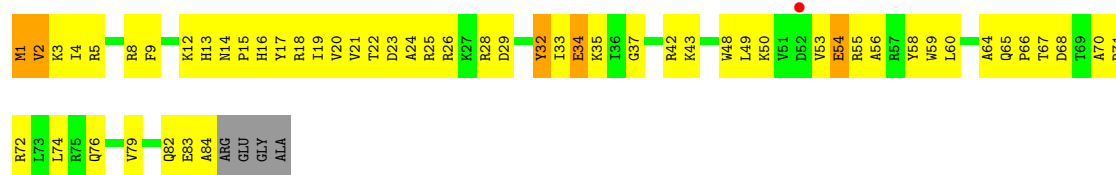
- Molecule 15: 30S RIBOSOMAL PROTEIN S15

Chain O: 



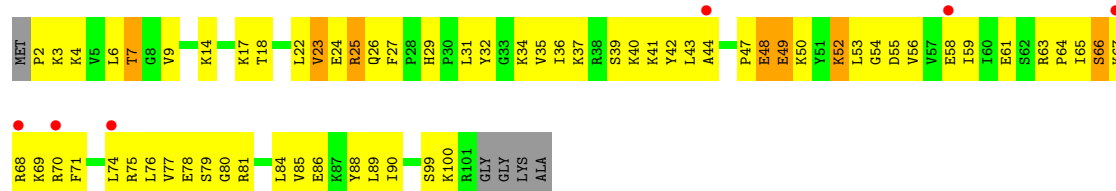
- Molecule 16: 30S RIBOSOMAL PROTEIN S16

Chain P: 



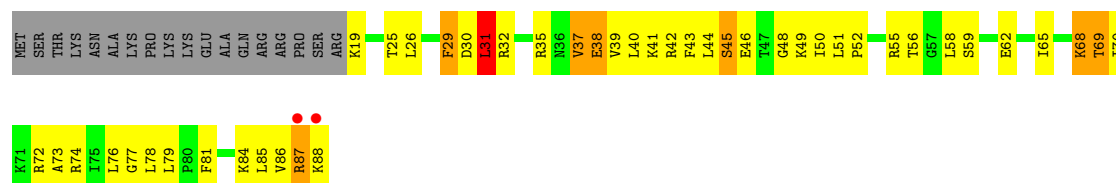
- Molecule 17: 30S RIBOSOMAL PROTEIN S17

Chain Q: 



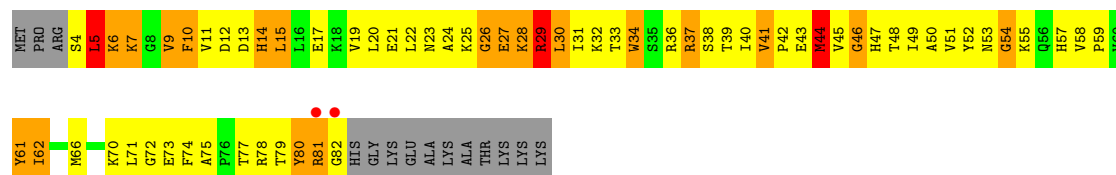
- Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R: 



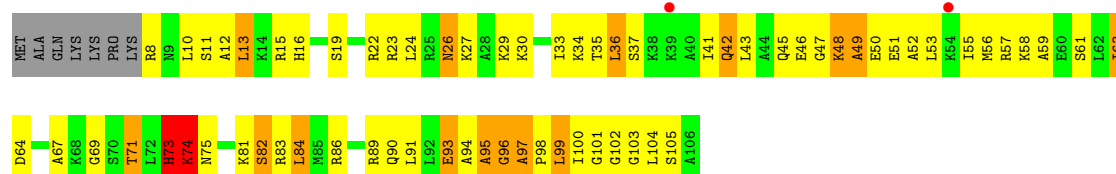
- Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S: 



- Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T: 



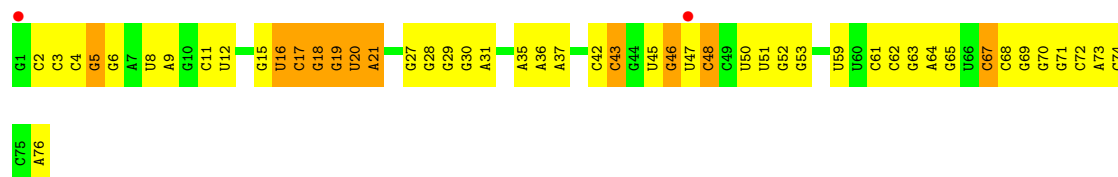
- Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain U: 



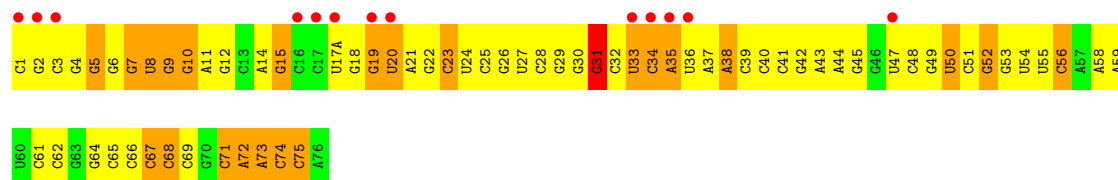
• Molecule 22: MRNA

Chain V:



• Molecule 23: RNA

Chain W:



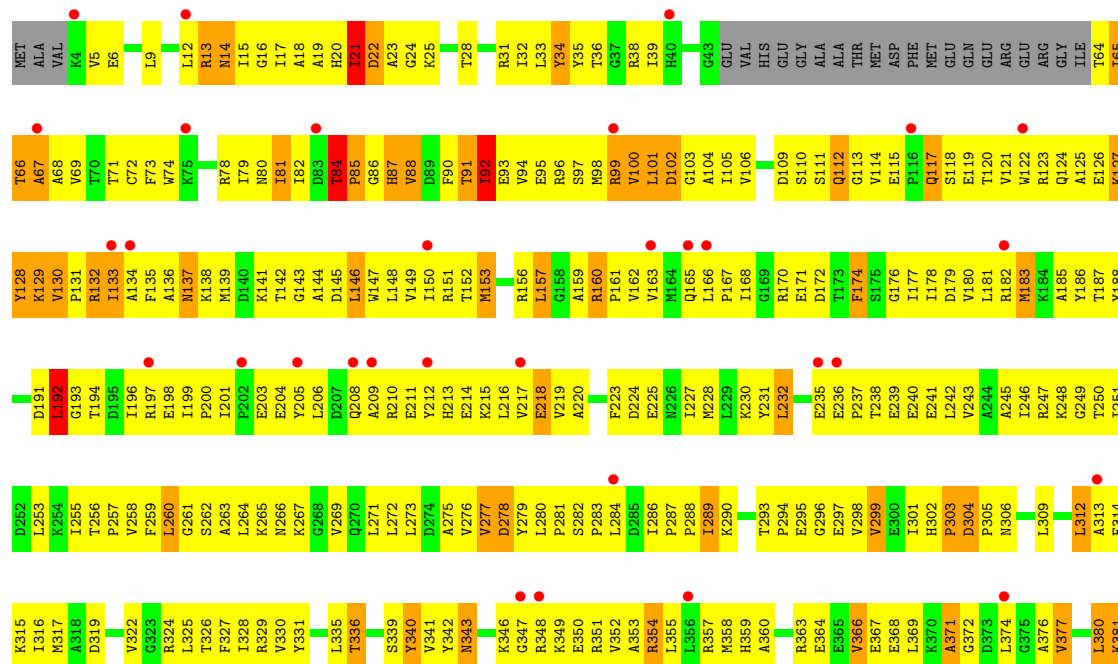
• Molecule 24: RNA

Chain X:



• Molecule 25: ELONGATION FACTOR G

Chain Y:



E643	R644	A645	V647	P648	L649	M652	E579	M580	A581	F582	K583	I584	A585	G586	S587	M588	A589	I590	K591	E592	A593	V594	Q595	K596	G597	D598	P599	V600	I601	L602	E603	F604	I605	M606	R607	V608	E609	V610	T611	T612	P613	E614	E615	Y616	M617	V620	I621	G622	D623	L624	R627	R628	G629	Q630	I631	L632	G633	M634	E635	P636	R637	Q641	V642
E382	T383	T384	T385	G386	D387	T388	L389	V390	G391	E392	D393	A394	P395	R396	V397	L398	L399	E400	S401	I402	E403	V404	P405	E406	P407	V408	I409	D410	V411	A412	I413	E414	P415	K416	T417	K418	A419	D420	Q421	E422	K423	L424	A427	L428	A432	E433	P436	T437	F438	R439	V440	S441	T442	H443	Q448								
E151	I450	I451	S452	G453	M454	C455	E456	L457	H458	L459	E460	I461	I462	L466	K467	R468	E469	F470	K471	A474	R475	V476	P479	Q480	Y483	R484	E485	T486	T487	T488	K489	P490	V491	D492	V493	E494	G495	F496	F497	I498	R499	Q500	T501	G502	G503	R504	G505	Q506	Y507	G508	H509	V510	K511	T512	K513								
V514	E515	P516	L517	P518	R519	G520	S521	V526	N527	A528	I529	V530	G531	G532	V533	I534	P535	K536	E537	Y538	I539	P540	A541	V542	Q543	G544	I546	E547	E548	A549	M550	Q551	S552	G553	P554	L555	I556	G557	F558	P559	V560	I563	K564	V565	T566	L567	Y568	D569	G570	S571	Y572	G573	E574	V575	D576	K577							
E579	M580	A581	F582	K583	I584	A585	G586	S587	M588	A589	I590	K591	E592	A593	V594	Q595	K596	G597	D598	P599	V600	I601	L602	E603	F604	I605	M606	R607	V608	E609	V610	T611	T612	P613	E614	E615	Y616	M617	V620	I621	G622	D623	L624	R627	R628	G629	Q630	I631	L632	G633	M634	E635	P636	R637	Q641	V642							
I643	R644	A645	F646	V647	P648	L649	M652	Y655	A656	G657	D658	L659	R660	S661	K662	T663	Q664	G665	R666	G667	S668	P669	V670	R671	F672	F673	D674	H675	Y676	Q677	E678	V679	P680	K681	Q682	V683	Q684	E685	K686	L687	T688	K689	G690	GLN																			

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	291.36Å 269.43Å 401.95Å 90.00° 91.78° 90.00°	Depositor
Resolution (Å)	49.75 – 3.70 49.75 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.75-3.70) 99.8 (49.75-3.40)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 3.40Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.214 , 0.249 0.427 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	84.2	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 73.1	EDS
Estimated twinning fraction	0.048 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 846438 reflections	Xtriage
F_o, F_c correlation	0.47	EDS
Total number of atoms	60287	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.34% 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: GDP, 5MU, ZN, MG, FUA

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	0.51	0/36190	0.74	16/56486 (0.0%)
2	B	0.41	0/1936	0.68	0/2611
3	C	0.43	0/1637	0.64	0/2207
4	D	0.39	0/1733	0.65	0/2318
5	E	0.50	0/1163	0.68	0/1566
6	F	0.38	0/856	0.64	0/1154
7	G	0.38	0/1276	0.61	0/1709
8	H	0.43	0/1136	0.70	0/1527
9	I	0.40	0/1027	0.66	0/1373
10	J	0.42	0/808	0.69	0/1087
11	K	0.41	0/900	0.69	0/1213
12	L	0.45	0/987	0.70	0/1322
13	M	0.38	0/999	0.67	0/1338
14	N	0.45	0/501	0.67	0/664
15	O	0.39	0/745	0.62	0/992
16	P	0.40	0/717	0.62	0/965
17	Q	0.44	0/837	0.66	0/1119
18	R	0.46	0/579	0.68	0/768
19	S	0.41	0/643	0.68	1/867 (0.1%)
20	T	0.36	0/765	0.65	0/1007
21	U	0.46	0/213	0.62	0/279
22	V	0.46	0/1809	0.69	0/2819
23	W	0.95	2/1810 (0.1%)	0.68	0/2821
24	X	0.69	1/288 (0.3%)	0.85	1/446 (0.2%)
25	Y	0.45	0/5313	0.68	0/7195
All	All	0.50	3/64868 (0.0%)	0.71	18/95853 (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	1	21

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	38	A	O3'-P	37.35	2.06	1.61
24	X	19	A	O3'-P	-9.03	1.50	1.61
23	W	31	G	O3'-P	7.01	1.69	1.61

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1498	U	C2'-C3'-O3'	9.60	130.62	109.50
1	A	115	G	C2'-C3'-O3'	8.27	127.70	109.50
1	A	533	A	C2'-C3'-O3'	7.49	125.97	109.50
1	A	60	A	C2'-C3'-O3'	7.49	125.97	109.50
1	A	328	C	C2'-C3'-O3'	7.21	125.35	109.50

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1498	U	C3'

5 of 21 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	G	Sidechain
1	A	118	U	Sidechain
1	A	189(G)	G	Sidechain
1	A	250	A	Sidechain
1	A	436	C	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	32329	0	16318	1198	0
2	B	1901	0	1951	225	0
3	C	1613	0	1677	191	0
4	D	1703	0	1763	178	0
5	E	1147	0	1207	112	0
6	F	843	0	857	79	0
7	G	1257	0	1296	93	0
8	H	1116	0	1177	88	0
9	I	1010	0	1035	137	0
10	J	795	0	840	159	0
11	K	885	0	904	63	0
12	L	971	0	1057	145	0
13	M	988	0	1059	150	0
14	N	492	0	529	63	0
15	O	734	0	771	71	0
16	P	701	0	720	67	0
17	Q	824	0	891	65	0
18	R	574	0	644	79	0
19	S	630	0	652	102	0
20	T	763	0	861	94	0
21	U	209	0	221	17	0
22	V	1619	0	822	56	0
23	W	1641	0	840	111	0
24	X	257	0	130	50	0
25	Y	5215	0	5287	800	0
26	C	1	0	0	0	0
26	D	1	0	0	0	0
26	N	1	0	0	0	0
26	W	1	0	0	0	0
27	F	37	0	47	26	0
28	Y	28	0	12	10	0
29	Y	1	0	0	0	0
All	All	60287	0	43568	4108	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 40.

The worst 5 of 4108 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
23:W:34:C:C3'	23:W:35:A:H5''	1.42	1.47
22:V:36:A:N1	24:X:16:U:O4	1.61	1.32
24:X:11:A:H4'	24:X:12:A:C5'	1.69	1.23
23:W:34:C:C2'	23:W:35:A:H5''	1.71	1.19

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:185:ILE:HG22	2:B:199:TYR:HB2	1.24	1.16

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	233/256 (91%)	148 (64%)	52 (22%)	33 (14%)	0	10
3	C	205/239 (86%)	148 (72%)	31 (15%)	26 (13%)	0	13
4	D	206/209 (99%)	138 (67%)	49 (24%)	19 (9%)	1	24
5	E	149/162 (92%)	118 (79%)	26 (17%)	5 (3%)	6	56
6	F	99/101 (98%)	69 (70%)	26 (26%)	4 (4%)	5	50
7	G	153/156 (98%)	112 (73%)	29 (19%)	12 (8%)	1	29
8	H	136/138 (99%)	105 (77%)	27 (20%)	4 (3%)	7	60
9	I	121/128 (94%)	87 (72%)	25 (21%)	9 (7%)	2	31
10	J	97/105 (92%)	68 (70%)	18 (19%)	11 (11%)	1	16
11	K	117/129 (91%)	85 (73%)	23 (20%)	9 (8%)	1	29
12	L	123/132 (93%)	84 (68%)	19 (15%)	20 (16%)	0	7
13	M	123/126 (98%)	75 (61%)	30 (24%)	18 (15%)	0	10
14	N	58/61 (95%)	42 (72%)	11 (19%)	5 (9%)	1	25
15	O	86/89 (97%)	54 (63%)	25 (29%)	7 (8%)	1	27
16	P	82/88 (93%)	63 (77%)	14 (17%)	5 (6%)	2	37
17	Q	98/105 (93%)	80 (82%)	15 (15%)	3 (3%)	7	59
18	R	68/88 (77%)	48 (71%)	12 (18%)	8 (12%)	1	15
19	S	77/93 (83%)	40 (52%)	19 (25%)	18 (23%)	0	2
20	T	97/106 (92%)	57 (59%)	27 (28%)	13 (13%)	0	12
21	U	23/27 (85%)	13 (56%)	7 (30%)	3 (13%)	0	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Y	663/691 (96%)	482 (73%)	125 (19%)	56 (8%)	1	26
All	All	3014/3229 (93%)	2116 (70%)	610 (20%)	288 (10%)	1	22

5 of 288 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	12	GLU
2	B	13	ALA
2	B	15	VAL
2	B	74	LYS
2	B	75	LYS

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	202/220 (92%)	183 (91%)	19 (9%)	13	55
3	C	160/188 (85%)	139 (87%)	21 (13%)	6	37
4	D	180/181 (99%)	160 (89%)	20 (11%)	9	46
5	E	115/123 (94%)	104 (90%)	11 (10%)	12	54
6	F	90/90 (100%)	83 (92%)	7 (8%)	18	65
7	G	126/127 (99%)	118 (94%)	8 (6%)	25	75
8	H	119/119 (100%)	110 (92%)	9 (8%)	19	67
9	I	98/99 (99%)	91 (93%)	7 (7%)	21	70
10	J	88/92 (96%)	76 (86%)	12 (14%)	5	35
11	K	90/99 (91%)	87 (97%)	3 (3%)	50	89
12	L	104/109 (95%)	93 (89%)	11 (11%)	10	49
13	M	99/101 (98%)	90 (91%)	9 (9%)	14	57
14	N	49/50 (98%)	44 (90%)	5 (10%)	11	51
15	O	79/80 (99%)	73 (92%)	6 (8%)	19	67
16	P	72/74 (97%)	68 (94%)	4 (6%)	30	78
17	Q	94/97 (97%)	88 (94%)	6 (6%)	25	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
18	R	61/77 (79%)	58 (95%)	3 (5%)	35 82
19	S	69/80 (86%)	60 (87%)	9 (13%)	6 37
20	T	76/82 (93%)	67 (88%)	9 (12%)	8 42
21	U	19/22 (86%)	18 (95%)	1 (5%)	32 80
25	Y	563/582 (97%)	498 (88%)	65 (12%)	8 44
All	All	2553/2692 (95%)	2308 (90%)	245 (10%)	12 54

5 of 245 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	70	ARG
14	N	14	PRO
25	Y	492	ASP
11	K	29	ILE
12	L	53	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
9	I	124	GLN
12	L	8	ASN
25	Y	500	GLN
10	J	13	HIS
10	J	78	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1503/1522 (98%)	252 (16%)	34 (2%)
22	V	75/76 (98%)	15 (20%)	1 (1%)
23	W	76/77 (98%)	27 (35%)	1 (1%)
24	X	12/25 (48%)	7 (58%)	2 (16%)
All	All	1666/1700 (98%)	301 (18%)	38 (2%)

5 of 301 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G

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Mol	Chain	Res	Type
1	A	9	G
1	A	31	G
1	A	32	A
1	A	33	A

5 of 38 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	703	G
1	A	992	U
23	W	72	A
1	A	812	C
1	A	1049	U

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

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$
23	5MU	W	54	23	20,22,23	0.87	2 (10%)	25,32,35	1.38	3 (12%)

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	5MU	W	54	23	-	0/6/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	54	5MU	P-OP1	2.19	1.49	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	W	54	5MU	C6-C5	-2.17	1.34	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	W	54	5MU	C6-N1-C2	-4.87	121.02	122.41
23	W	54	5MU	C5-C6-N1	2.40	123.92	121.59
23	W	54	5MU	C5M-C5-C6	2.01	122.87	118.59

There are no chirality outliers.

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 7 ligands modelled in this entry, 5 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	$\# Z > 2$
27	FUA	F	1103	-	40,40,40	1.78	8 (20%)	64,64,64	1.46	10 (15%)
28	GDP	Y	1690	29	30,30,30	1.30	5 (16%)	44,47,47	1.78	10 (22%)

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
27	FUA	F	1103	-	-	0/18/92/92	0/0/4/4
28	GDP	Y	1690	29	-	0/16/32/32	0/1/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	F	1103	FUA	C17-C22	4.55	1.39	1.34
27	F	1103	FUA	C23-C22	-4.28	1.39	1.51
27	F	1103	FUA	C29-C22	4.23	1.53	1.47
27	F	1103	FUA	C23-C24	-3.97	1.39	1.53
27	F	1103	FUA	C24-C25	-3.86	1.39	1.50

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	Y	1690	GDP	C6-C5-N7	-5.12	133.45	134.14
28	Y	1690	GDP	PA-O3A-PB	-4.32	119.01	131.68
27	F	1103	FUA	C16-O2-C31	-4.05	110.67	117.13
27	F	1103	FUA	C24-C23-C22	3.85	121.43	111.93
28	Y	1690	GDP	C2-N3-C4	3.67	120.25	115.09

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	1504/1522 (98%)	0.11	33 (2%) 59 37	43, 89, 174, 200	0
2	B	235/256 (91%)	0.10	3 (1%) 74 50	53, 102, 164, 194	0
3	C	207/239 (86%)	0.12	3 (1%) 72 48	45, 93, 143, 190	0
4	D	208/209 (99%)	0.39	8 (3%) 38 25	48, 107, 157, 188	0
5	E	151/162 (93%)	0.06	0 100 100	45, 76, 117, 200	0
6	F	101/101 (100%)	0.27	2 (1%) 62 39	72, 115, 152, 183	0
7	G	155/156 (99%)	0.30	9 (5%) 22 15	63, 108, 150, 193	0
8	H	138/138 (100%)	0.08	0 100 100	45, 79, 117, 147	0
9	I	127/128 (99%)	0.45	7 (5%) 24 16	68, 111, 151, 175	0
10	J	99/105 (94%)	0.71	8 (8%) 12 10	60, 127, 179, 190	0
11	K	119/129 (92%)	0.27	5 (4%) 35 22	48, 89, 126, 181	0
12	L	125/132 (94%)	0.57	6 (4%) 29 19	42, 82, 124, 200	0
13	M	125/126 (99%)	0.47	14 (11%) 6 6	63, 126, 171, 200	0
14	N	60/61 (98%)	0.31	1 (1%) 67 44	58, 91, 127, 146	0
15	O	88/89 (98%)	0.28	2 (2%) 57 36	31, 82, 119, 141	0
16	P	84/88 (95%)	0.37	1 (1%) 75 52	58, 95, 126, 166	0
17	Q	100/105 (95%)	0.38	6 (6%) 21 15	60, 84, 120, 147	0
18	R	70/88 (79%)	0.18	2 (2%) 49 31	60, 95, 142, 167	0
19	S	79/93 (84%)	0.45	2 (2%) 54 34	74, 117, 181, 199	0
20	T	99/106 (93%)	0.34	2 (2%) 62 39	72, 103, 153, 173	0
21	U	25/27 (92%)	1.69	9 (36%) 1 1	77, 115, 145, 164	0
22	V	76/76 (100%)	-0.12	2 (2%) 53 33	67, 107, 165, 200	0
23	W	77/77 (100%)	0.90	13 (16%) 2 3	97, 190, 200, 200	0
24	X	12/25 (48%)	0.80	2 (16%) 2 3	52, 114, 172, 193	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	Y	667/691 (96%)	0.74	75 (11%) 6 6	84, 151, 186, 200	0
All	All	4731/4929 (95%)	0.31	215 (4%) 31 21	31, 103, 178, 200	0

The worst 5 of 215 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
12	L	129	ALA	11.1
12	L	128	ALA	7.2
25	Y	682	GLN	6.3
25	Y	67	ALA	6.2
23	W	16	C	6.2

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
23	5MU	W	54	21/22	0.18	-	200,200,200,200	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
28	GDP	Y	1690	28/28	0.20	-	96,102,109,110	0
26	ZN	C	1000	1/1	0.12	-	123,123,123,123	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
26	ZN	D	1210	1/1	0.12	-	69,69,69,69	0
26	ZN	W	1000	1/1	0.23	-	200,200,200,200	0
26	ZN	N	1062	1/1	0.05	-	86,86,86,86	0
27	FUA	F	1103	37/37	0.38	-	102,104,107,109	0
29	MG	Y	1691	1/1	0.16	-	46,46,46,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.