



wwPDB X-ray Structure Validation Summary Report

Mar 31, 2014 – 06:09 PM BST

PDB ID : 2X9R
Title : STRUCTURE OF THE 70S RIBOSOME BOUND TO RELEASE FACTOR 2
AND A SUBSTRATE ANALOG PROVIDES INSIGHTS INTO CATALYSIS
OF PEPTIDE RELEASE
Authors : Jin, H.; Kelley, A.C.; Loakes, D.; Ramakrishnan, V.
Deposited on : 2010-03-24
Resolution : 3.10 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>

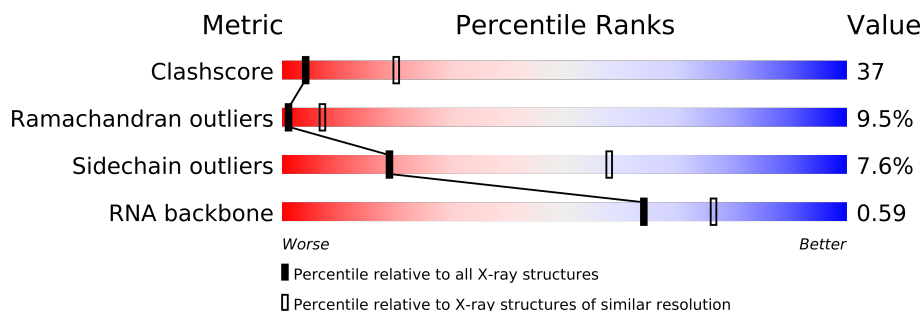
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23004

1 Overall quality at a glance

The reported resolution of this entry is 3.10 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	1078 (3.16-3.04)
Ramachandran outliers	78287	1044 (3.16-3.04)
Sidechain outliers	78261	1044 (3.16-3.04)
RNA backbone	1838	1047 (3.60-2.60)

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	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	
15	O	89	

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Mol	Chain	Length	Quality of chain
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	V	77	
22	W	77	
23	X	8	
24	Y	351	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 58266 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 RRNA.

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
			1011	639	198	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 E-SITE TRNA PHE OR P-SITE TRNA PHE (UNMODIFIED BASES).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	77	Total	C	N	O	P	0	0	0
			1630	732	292	531	75			
22	W	77	Total	C	N	O	P	0	0	0
			1630	732	292	531	75			

- Molecule 23 is a RNA chain called MRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	X	8	Total	C	N	O	P	0	0	0
			165	76	29	53	7			

- Molecule 24 is a protein called PEPTIDE CHAIN RELEASE FACTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	Y	351	Total	C	N	O	S	0	0	0
			2801	1752	506	535	8			

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	Z	548	Total	Mg	0	0
			548	548		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	Z	3	Total	Zn	0	0
			3	3		

- Molecule 27 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	V	1	Total	O	0	0
			1	1		
27	Y	2	Total	O	0	0
			2	2		

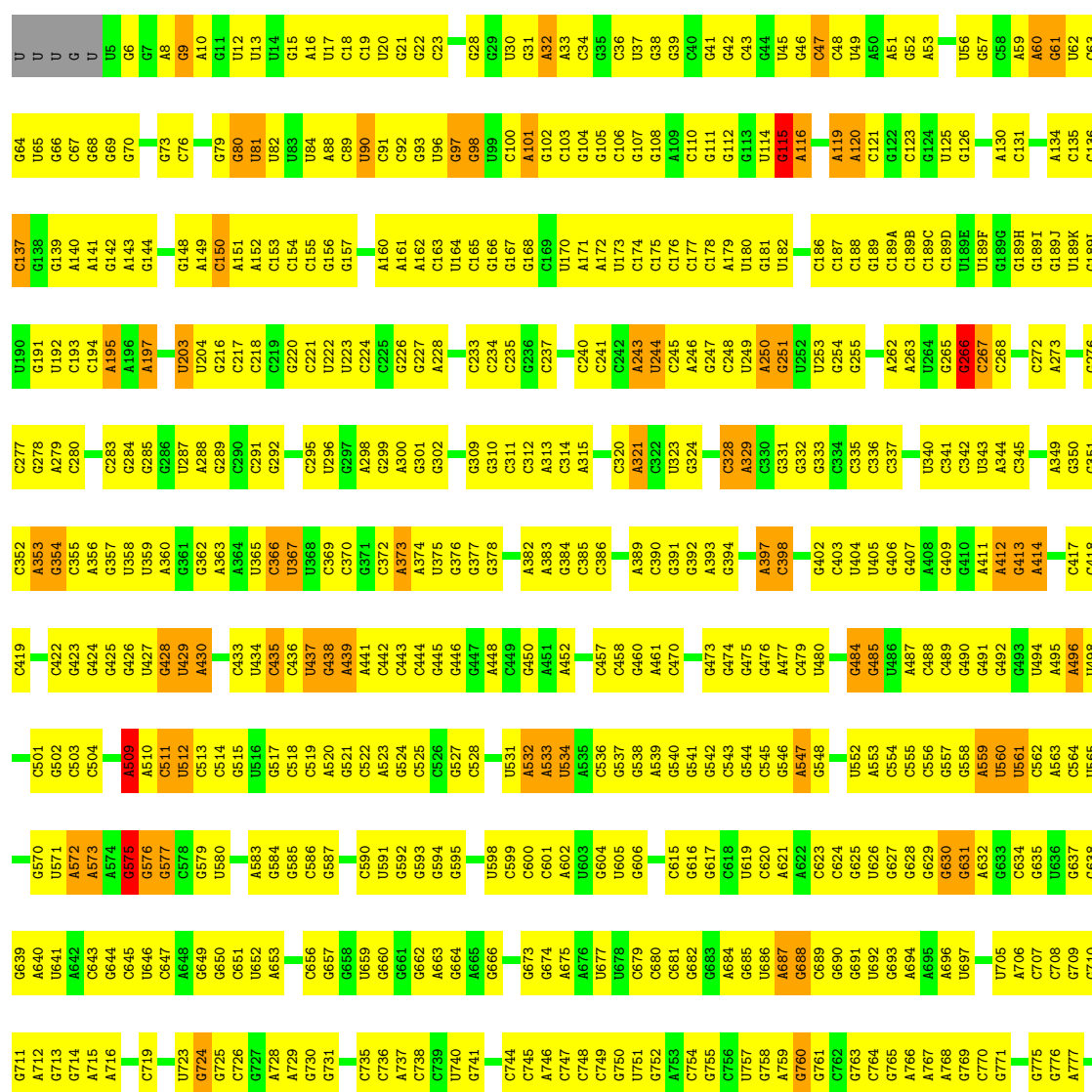
3 Residue-property plots

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 rRNA

Chain A:

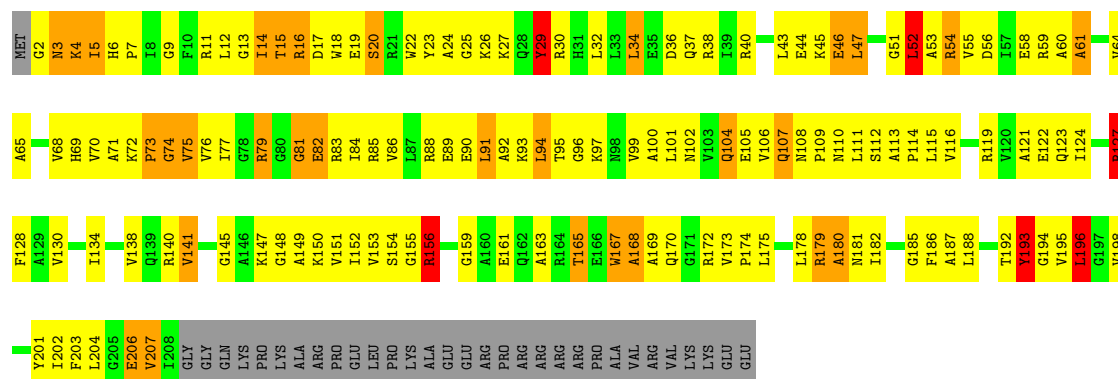


G1145	C1146	G1079	A1015	G954	U870	A781
A1146	G1080	A1016	U1025	U955	G878	A782
C1147	G1081	G1017	G1026	U956	G879	C783
U1148	G1082	C1018	C1027	U957	C880	C784
C1149	U1083	C1019	A965	A958	G881	G785
U1150	G1084	U1020	U960	G882	U793	
A1151	U1085	G1021	U961	C883	C794	
C1152	U1086		C962	G890	C795	
A1153	G1087	U1025	G963	U891	C796	
U1154	G1088	G1026	A964	C797	G798	
C1155	G1089	C1027	A965	A832		
A1156	U1094	C1028	U966	C897	C805	
U1157	U1095	G1030	C967	G898	C806	
C1158	C1096	G1030A	A968			
U1159	C1097	U1030B	A969	G902	A814	
G1160	C1098	G1030C	C970	G906	A815	
C1161	C1099	A1030D	G971	A907	A816	
C1162	C1100	G1031	C972	G908	C817	
C1163	A1101	G1032	G973	A908	G818	
C1164	C1102	G1033	A974	A909	A819	
C1165	C1103	G1034	A975	C910	U820	
G1166	U1104	A1035	G976	U911	C821	
A1167	A1105	G1036	A977	C912		
C1168	U1106	G1037	A978	A913	C826	
U1169	C1107		C979	A914	U827	
C1170	G1108	U1040	C980	U981	A828	
G1171	C1109	A1041	U982	G917	G829	
U1172	C1110	G1042	A983	A918	C830	
C1173	C1111	C1043	C984	A919	U831	
A1174	A1112		C985	U920	C832	
U1175	C1113	G1047	A986	U921	U833	
C1176	G1114	G1048	G987	A923	U834	
U1177	C1115	U1049		G926	U835	
C1178	C1116	G1050	C990	G927	C836	
G1179	U1120	G1053	U991	U839		
U1180	U1121	C1054	U992	C840		
C1181	C1122	A1055	G993	U841		
G1182	A1123	U1056	A994	C848		
A1183	G1124	G1057	U997			
U1184	U1125	U1058	G998	G851		
C1185	C1126	C1059	C999	G852		
U1186	U1127	G1060	U1000	G853		
G1187	C1128	G1061	A1001	G854		
C1188	A1130	U1062	G1001A			
U1189	C1131	C1063	A938	C857		
G1190	G1129	U1064	G1002	G858		
C1191	A1132	U1065	G939	C859		
U1192	C1133	C1066	A1004	A860		
G1193	G1134	U1067	A1005	G861		
C1194	U1135	G1068	C1006	G862		
U1195	U1136	U1069	C1007	C863		
C1196	C1137		U1008	U863		
G1197	C1138	C1071	G1009	G947		
U1198	U1139	U1072	G1010	C948		
C1199	C1140	G1073	G1011	A949		
G1200	U1141	G1074	U1012	G866		
U1201	C1142		G1013	G867		
C1202	U1211		G1014	G868		
G1203	A1212			G951		
A1204	C1213					
U1205	U1214					
C1206	C1215					
G1207	U1216					
U1208	C1217					
C1209	U1218					
A1210	A1219					
U1211	C1220					
C1212	U1221					
G1213	G1222					
A1214	C1223					
U1215	G1224					
C1216	A1225					
G1217	C1226					
A1218	U1227					
U1219	C1228					
C1220	A1229					
G1221	C1230					
U1222	U1231					
A1223	G1232					
C1224	C1233					
G1225	A1234					
U1226	U1235					
A1227	C1236					
C1228	G1237					
A1229	U1238					
G1230	A1239					
U1231	U1240					
C1232	G1241					
A1233	C1242					
G1234	U1243					
U1235	C1244					
C1236	G1245					
A1237	U1246					
U1238	C1247					
G1239	A1248					
C1240	U1249					
U1241	C1250					
C1242	G1251					
G1243	A1252					
U1244	C1253					
A1245	U1254					
C1246	G1255					
U1247	A1256					
G1248	U1257					
A1249	C1258					
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G1253	C1262					
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U1257	A1269					
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C1262	A1274					
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A1265	U1277					
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U1267	A1279					
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A1269	U1281					
C1270	C1282					
U1271	G1283					
C1272	A1284					
G1273	C1285					
A1274	U1286					
U1275	G1287					
C1276	C1288					
G1277	U1289					
U1278	A1290					
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G1281	C1293					
U1282	A1294					
C1283	U1295					
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G1285	G1297					
U1286	C1298					
C1287	U1299					
A1288	C1300					
G1289	U1301					
U1290	C1302					
C1291	G1303					
U1292	A1304					
G1293	C1305					
A1294	U1306					
C1295	G1307					
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A1388	G1406					
C1389	U1407					
U1390	C1408					
G1391	A1409					
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U1393	C1411					
G1394	U1412					
C1395	A1413					
U1396	U1414					
A1397	C1415					
C1398	G1416					
G1399	C1417					
U1400	U1418					
C1401	C1419					
G1402	A1420					
A1403	U1421					
C1404	C1422					

GLU
SER
GLU
VAL
GLU
ALA

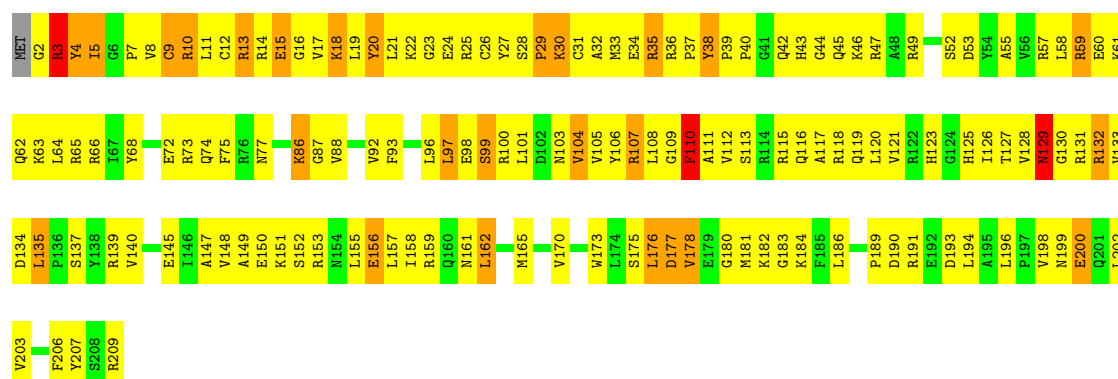
• Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain C:



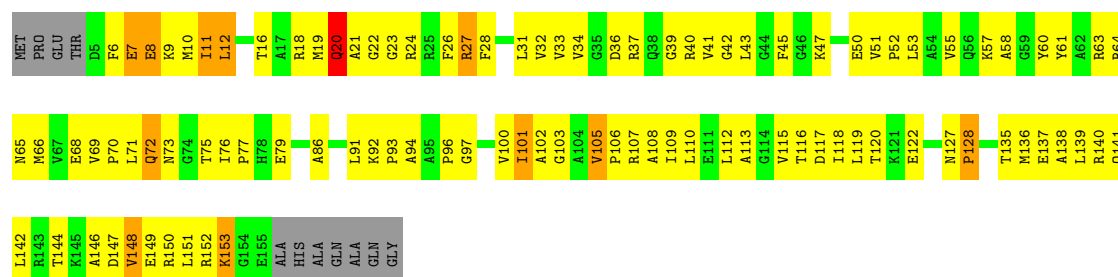
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain D:



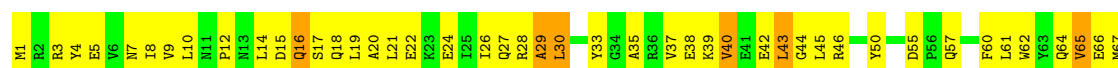
• Molecule 5: 30S RIBOSOMAL PROTEIN S5

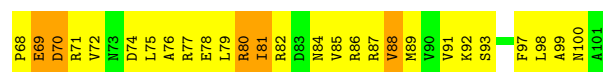
Chain E:



• Molecule 6: 30S RIBOSOMAL PROTEIN S6

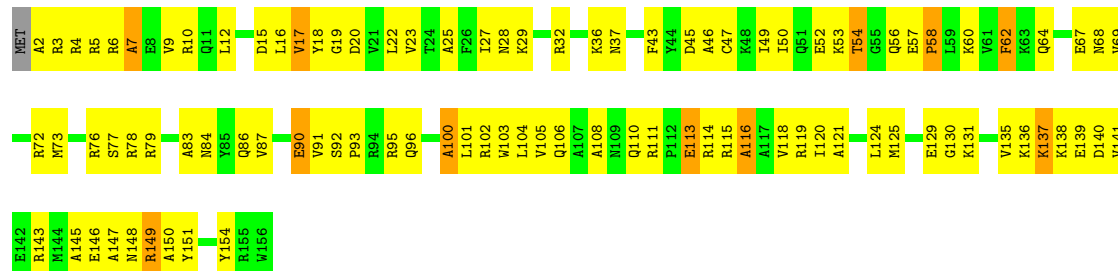
Chain F:





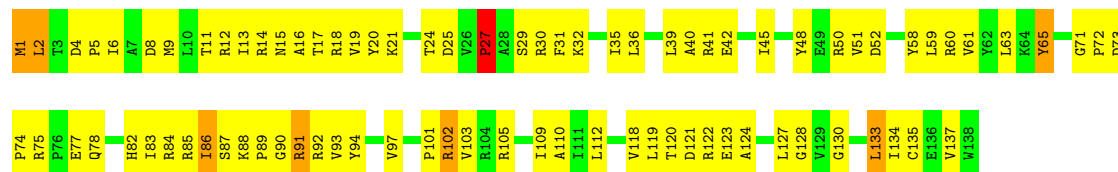
• Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain G:



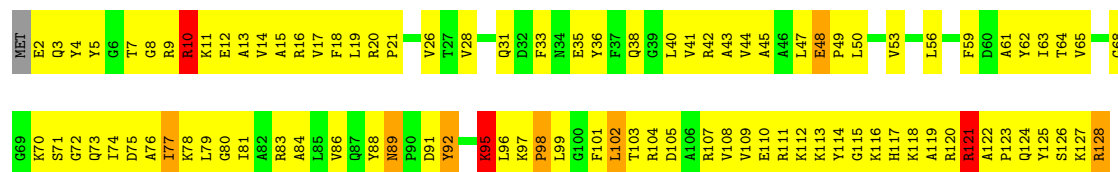
• Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H:



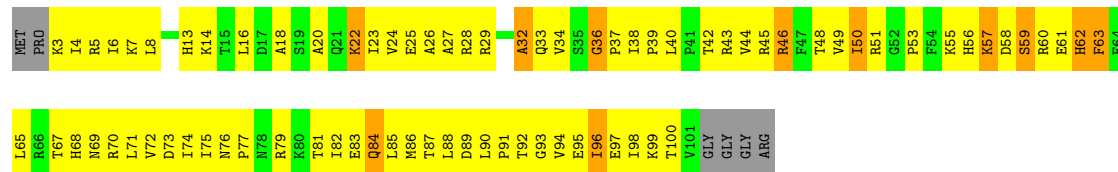
• Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain I:



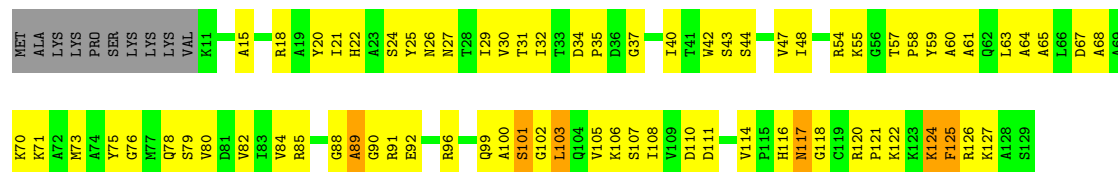
• Molecule 10: 30S RIBOSOMAL PROTEIN S10

Chain J:



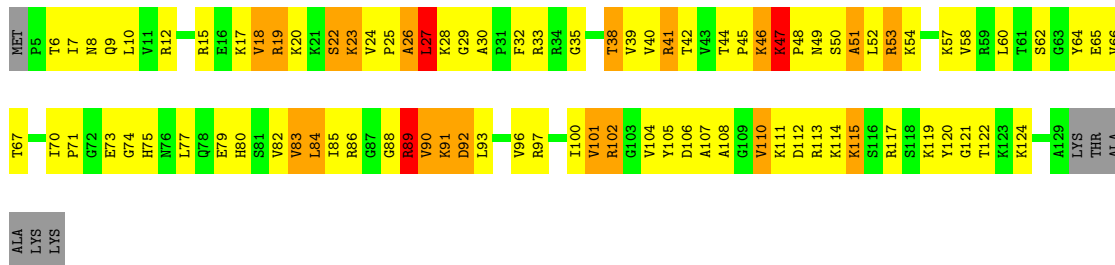
• Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K:



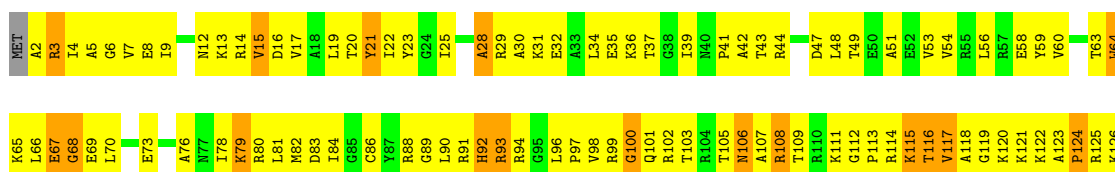
- Molecule 12: 30S RIBOSOMAL PROTEIN S12

Chain L:



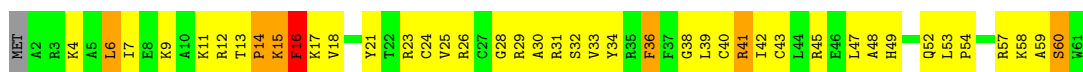
- Molecule 13: 30S RIBOSOMAL PROTEIN S13

Chain M:



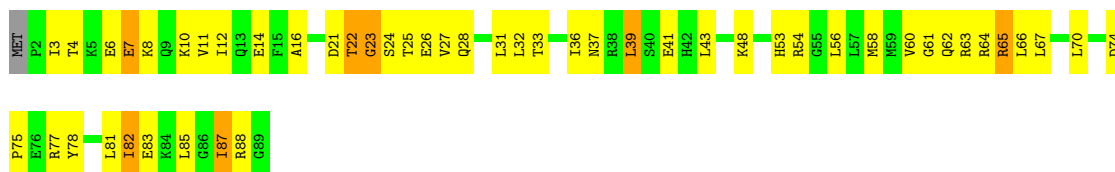
- Molecule 14: 30S RIBOSOMAL PROTEIN S14 TYPE Z

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:





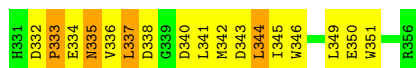
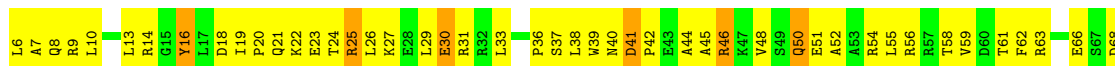
• Molecule 23: MRNA

Chain X:



• Molecule 24: PEPTIDE CHAIN RELEASE FACTOR 2

Chain Y:



4 Data and refinement statistics

EDS was 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	211.42Å 452.50Å 625.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.86 – 3.10	Depositor
% Data completeness (in resolution range)	100.0 (47.86-3.10)	Depositor
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.01Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.223 , 0.264	Depositor
Wilson B-factor (Å ²)	55.0	Xtriage
Anisotropy	0.035	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Outliers	0 of 1179114 reflections	Xtriage
Total number of atoms	58266	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.49% 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: MG, ZN, 8AN, PHA

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	0/36190	0.69	14/56486 (0.0%)
2	B	0.31	0/1936	0.58	0/2611
3	C	0.32	0/1637	0.54	0/2207
4	D	0.33	0/1733	0.63	0/2318
5	E	0.34	0/1163	0.61	0/1566
6	F	0.32	0/856	0.63	0/1154
7	G	0.30	0/1276	0.56	0/1709
8	H	0.32	0/1136	0.61	0/1527
9	I	0.31	0/1027	0.58	0/1372
10	J	0.32	0/808	0.56	0/1087
11	K	0.32	0/900	0.58	0/1213
12	L	0.36	0/987	0.67	0/1322
13	M	0.30	0/994	0.56	0/1322
14	N	0.31	0/501	0.53	0/664
15	O	0.32	0/745	0.57	0/992
16	P	0.36	0/717	0.58	0/965
17	Q	0.33	0/837	0.61	0/1119
18	R	0.33	0/579	0.60	0/768
19	S	0.34	0/643	0.56	0/867
20	T	0.29	0/765	0.58	0/1007
21	U	0.41	0/213	0.49	0/279
22	V	0.38	0/1784	0.70	0/2780
22	W	0.35	0/1784	0.71	0/2780
23	X	0.39	0/184	0.74	0/284
24	Y	0.31	0/2849	0.60	0/3848
All	All	0.35	0/62244	0.66	14/92247 (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	15
22	W	0	1
All	All	1	16

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1504	G	C2'-C3'-O3'	8.26	127.67	109.50
1	A	115	G	C2'-C3'-O3'	7.41	125.81	109.50
1	A	575	G	C2'-C3'-O3'	6.99	124.89	113.70
1	A	366	C	C2'-C3'-O3'	6.93	124.78	113.70
1	A	913	A	C2'-C3'-O3'	6.76	124.52	113.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	1504	G	C3'

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	G	Sidechain
1	A	575	G	Sidechain
1	A	587	G	Sidechain
1	A	760	G	Sidechain
1	A	832	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	16314	1189	0
2	B	1901	0	1951	258	0
3	C	1613	0	1677	199	0
4	D	1703	0	1763	216	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	1147	0	1207	125	0
6	F	843	0	857	88	0
7	G	1257	0	1296	113	0
8	H	1116	0	1177	118	0
9	I	1011	0	1041	126	0
10	J	795	0	840	146	0
11	K	885	0	904	74	0
12	L	971	0	1057	122	0
13	M	988	0	1055	158	0
14	N	492	0	530	66	0
15	O	734	0	771	54	0
16	P	701	0	720	81	0
17	Q	824	0	891	62	0
18	R	574	0	644	59	0
19	S	630	0	651	98	0
20	T	763	0	861	73	0
21	U	209	0	221	24	0
22	V	1630	0	831	72	0
22	W	1630	0	831	89	0
23	X	165	0	87	11	0
24	Y	2801	0	2816	344	0
25	Z	548	0	0	0	0
26	Z	3	0	0	0	0
27	V	1	0	0	0	0
27	Y	2	0	0	1	0
All	All	58266	0	40993	3624	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 37.

The worst 5 of 3624 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
24:Y:302:VAL:O	24:Y:303:ARG:HG3	1.34	1.20
1:A:1442(A):G:H3'	1:A:1442(B):A:H5''	1.19	1.17
22:W:70:G:H2'	22:W:71:G:H5''	1.15	1.14
4:D:86:LYS:HE3	4:D:87:GLY:H	0.99	1.10
4:D:128:VAL:HG12	4:D:129:ASN:H	1.07	1.09

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%)	127 (54%)	71 (30%)	35 (15%)	0	1
3	C	205/239 (86%)	129 (63%)	40 (20%)	36 (18%)	0	0
4	D	206/209 (99%)	139 (68%)	45 (22%)	22 (11%)	1	5
5	E	149/162 (92%)	115 (77%)	23 (15%)	11 (7%)	2	11
6	F	99/101 (98%)	70 (71%)	21 (21%)	8 (8%)	1	10
7	G	153/156 (98%)	117 (76%)	26 (17%)	10 (6%)	2	15
8	H	136/138 (99%)	106 (78%)	23 (17%)	7 (5%)	3	22
9	I	121/128 (94%)	86 (71%)	24 (20%)	11 (9%)	1	8
10	J	97/105 (92%)	70 (72%)	22 (23%)	5 (5%)	3	21
11	K	117/129 (91%)	86 (74%)	27 (23%)	4 (3%)	6	32
12	L	123/132 (93%)	84 (68%)	21 (17%)	18 (15%)	0	2
13	M	113/126 (90%)	71 (63%)	25 (22%)	17 (15%)	0	1
14	N	58/61 (95%)	40 (69%)	13 (22%)	5 (9%)	1	9
15	O	86/89 (97%)	66 (77%)	18 (21%)	2 (2%)	10	45
16	P	82/88 (93%)	58 (71%)	17 (21%)	7 (8%)	1	9
17	Q	98/105 (93%)	76 (78%)	13 (13%)	9 (9%)	1	7
18	R	68/88 (77%)	45 (66%)	16 (24%)	7 (10%)	1	6
19	S	77/93 (83%)	44 (57%)	22 (29%)	11 (14%)	0	2
20	T	97/106 (92%)	63 (65%)	26 (27%)	8 (8%)	1	10
21	U	23/27 (85%)	16 (70%)	5 (22%)	2 (9%)	1	9
24	Y	349/351 (99%)	263 (75%)	65 (19%)	21 (6%)	2	17
All	All	2690/2889 (93%)	1871 (70%)	563 (21%)	256 (10%)	1	7

5 of 256 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	12	GLU

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Mol	Chain	Res	Type
2	B	15	VAL
2	B	19	HIS
2	B	20	GLU
2	B	64	ARG

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%)	185 (92%)	17 (8%)	16	52
3	C	160/188 (85%)	146 (91%)	14 (9%)	14	49
4	D	180/181 (99%)	160 (89%)	20 (11%)	9	33
5	E	115/123 (94%)	110 (96%)	5 (4%)	40	80
6	F	90/90 (100%)	87 (97%)	3 (3%)	50	86
7	G	126/127 (99%)	121 (96%)	5 (4%)	42	82
8	H	119/119 (100%)	115 (97%)	4 (3%)	49	86
9	I	98/99 (99%)	89 (91%)	9 (9%)	13	45
10	J	88/92 (96%)	82 (93%)	6 (7%)	22	62
11	K	90/99 (91%)	86 (96%)	4 (4%)	39	79
12	L	104/109 (95%)	90 (86%)	14 (14%)	6	22
13	M	99/101 (98%)	92 (93%)	7 (7%)	21	61
14	N	49/50 (98%)	45 (92%)	4 (8%)	17	53
15	O	79/80 (99%)	73 (92%)	6 (8%)	19	58
16	P	72/74 (97%)	68 (94%)	4 (6%)	30	70
17	Q	94/97 (97%)	92 (98%)	2 (2%)	66	92
18	R	61/77 (79%)	59 (97%)	2 (3%)	50	86
19	S	69/80 (86%)	60 (87%)	9 (13%)	6	23
20	T	76/82 (93%)	70 (92%)	6 (8%)	18	55
21	U	19/22 (86%)	17 (90%)	2 (10%)	10	35
24	Y	298/298 (100%)	267 (90%)	31 (10%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2288/2408 (95%)	2114 (92%)	174 (8%)	19 58

5 of 174 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	J	46	ARG
12	L	85	ILE
24	Y	209	GLU
10	J	63	PHE
12	L	27	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 79 such sidechains are listed below:

Mol	Chain	Res	Type
7	G	84	ASN
10	J	84	GLN
24	Y	202	HIS
7	G	97	GLN
8	H	15	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1503/1522 (98%)	203 (13%)	32 (2%)
22	V	74/77 (96%)	18 (24%)	0
22	W	74/77 (96%)	17 (22%)	0
23	X	7/8 (87%)	3 (42%)	0
All	All	1658/1684 (98%)	241 (14%)	32 (1%)

5 of 241 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C

5 of 32 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	533	A
1	A	687	A
1	A	1300	G
1	A	575	G
1	A	748	C

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

4 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	$\# Z > 2$
22	8AN	V	76	25,22	24,24,25	0.68	1 (4%)	34,35,38	1.21	3 (8%)
22	PHA	V	77	22	11,11,11	1.60	1 (9%)	13,13,13	0.91	1 (7%)
22	8AN	W	76	22	24,24,25	0.78	1 (4%)	34,35,38	1.10	2 (5%)
22	PHA	W	77	22	11,11,11	1.83	1 (9%)	13,13,13	0.78	1 (7%)

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
22	8AN	V	76	25,22	-	0/9/25/26	0/1/3/3
22	PHA	V	77	22	-	1/5/6/6	0/1/1/1
22	8AN	W	76	22	-	0/9/25/26	0/1/3/3
22	PHA	W	77	22	-	0/5/6/6	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	W	77	PHA	CA-C	5.15	1.55	1.50
22	V	77	PHA	CA-C	4.46	1.54	1.50
22	V	76	8AN	C3'-N3'	-2.12	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	W	76	8AN	C3'-N3'	-2.02	1.44	1.47

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	V	76	8AN	C4'-C3'-N3'	-3.97	105.02	113.46
22	W	76	8AN	C2'-C1'-N9	2.94	120.82	113.27
22	V	76	8AN	C5'-C4'-C3'	2.60	119.63	115.95
22	W	77	PHA	O-C-CA	-2.46	119.62	125.12
22	W	76	8AN	O1P-P-O5'	-2.40	105.84	113.42

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	V	77	PHA	O-C-CA-CB

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 551 ligands modelled in this entry, 551 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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.