



wwPDB X-ray Structure Validation Summary Report

Feb 26, 2014 – 03:56 PM GMT

PDB ID : 4KD2
Title : 70S RIBOSOME TRANSLOCATION INTERMEDIATE GDPNP-I CONTAINING ELONGATION FACTOR EFG/GDPNP, MRNA, AND TRNA BOUND IN THE pe^*/E STATE. THIS ENTRY CONTAINS THE 50S RIBOSOMAL SUBUNIT B. THE 30S SUBUNIT B CAN BE FOUND IN 4KD0. MOLECULE A IN THE SAME ASYMMETRIC UNIT IS DEPOSITED AS 4KCY (30S) AND 4KCZ (50S).
Authors : Zhou, J.; Lancaster, L.; Donohue, J.P.; Noller, H.F.
Deposited on : 2013-04-24
Resolution : 3.50 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>

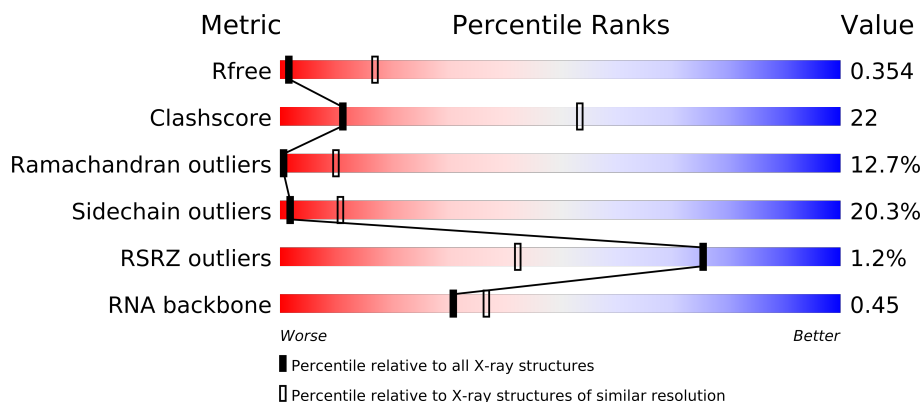
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1243 (3.70-3.30)
Clashscore	79885	1039 (3.66-3.34)
Ramachandran outliers	78287	1000 (3.66-3.34)
Sidechain outliers	78261	1000 (3.66-3.34)
RSRZ outliers	66119	1243 (3.70-3.30)
RNA backbone	1838	1007 (4.22-2.76)

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	C	228	
2	D	275	
3	E	205	
4	F	208	
5	G	181	
6	H	167	
7	J	170	
8	K	140	
9	N	138	
10	O	122	
11	P	146	
12	Q	141	

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Mol	Chain	Length	Quality of chain
13	R	117	
14	S	99	
15	T	138	
16	U	117	
17	V	101	
18	W	113	
19	X	93	
20	Y	107	
21	Z	185	
22	0	84	
23	2	71	
24	3	60	
25	5	59	
26	6	50	
27	7	49	
28	8	64	
29	9	37	
30	f	31	
30	g	31	
31	h	30	
32	1	93	
33	4	35	
34	e	102	
35	A	2879	
36	B	119	

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 95124 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 protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	228	Total	C	N	O	S	0	0	0
			1742	1101	319	319	3			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	20	VAL	ILE	CONFLICT	UNP Q72GV9
C	28	ARG	HIS	CONFLICT	UNP Q72GV9

- Molecule 2 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	275	Total	C	N	O	S	0	0	0
			2145	1353	428	361	3			

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	205	Total	C	N	O	S	0	0	0
			1569	991	300	272	6			

- Molecule 4 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	208	Total	C	N	O	S	0	0	0
			1628	1037	304	284	3			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	2	LYS	-	INSERTION	UNP Q72I05
F	3	GLU	-	INSERTION	UNP Q72I05

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Chain	Residue	Modelled	Actual	Comment	Reference
F	4	VAL	-	INSERTION	UNP Q72I05
F	5	ALA	-	INSERTION	UNP Q72I05
F	6	VAL	-	INSERTION	UNP Q72I05

- Molecule 5 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	5	VAL	LEU	CONFLICT	UNP Q72I16

- Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	167	Total	C	N	O	S	0	0	0
			1274	806	238	229	1			

- Molecule 7 is a protein called 50S RIBOSOMAL PROTEIN L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	J	170	Total	C	N	O	S	0	0	0
			851	510	170	171				

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	K	140	Total	C	N	O	S	0	0	0
			1035	659	183	188	5			

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	N	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	69	ILE	VAL	CONFLICT	UNP Q72I14

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	P	146	Total	C	N	O	S	0	0	0
			1114	692	227	193	2			

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	32	TYR	PHE	CONFLICT	UNP Q72I11

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	R	117	Total	C	N	O		0	0	0
			960	599	202	159				

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	S	99	Total	C	N	O		0	0	0
			775	488	155	132				

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	138	Total	C	N	O	S	0	0	0
			1147	713	235	198	1			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	123	GLN	LYS	CONFLICT	UNP Q72JU9
T	135	ALA	VAL	CONFLICT	UNP Q72JU9

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	U	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	V	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	W	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	X	93	Total	C	N	O	S	0	0	0
			734	477	132	125				

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Y	107	Total	C	N	O	S	0	0	0
			818	524	155	134	5			

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Z	185	Total	C	N	O	S	0	0	0
			1473	939	262	270	2			

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	0	84	Total	C	N	O	S	0	0	0
			662	410	140	111	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	11	ARG	LYS	CONFLICT	UNP Q72HR3

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	2	71	Total	C	N	O	S	0	0	0
			598	370	121	106	1			

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	3	60	Total	C	N	O	S	0	0	0
			477	303	91	82	1			

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
25	5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	29	THR	ILE	CONFLICT	UNP P62652

- Molecule 26 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	6	50	Total	C	N	O	S	0	0	0
			433	270	88	71	4			

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 29 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 30 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
30	f	31	Total	C	N	O	0	0	0
			156	93	31	32			
30	g	31	Total	C	N	O	0	0	0
			156	93	31	32			

- Molecule 31 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
31	h	30	Total	C	N	O	0	0	0
			151	90	30	31			

- Molecule 32 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	1	93	Total	C	N	O	S	0	0	0
			732	460	145	126	1			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	81	LYS	ARG	CONFLICT	UNP Q72G84

- Molecule 33 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
33	4	35	Total	C	N	O	S	0	0	0
			271	174	44	50	3			

- Molecule 34 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
34	e	102	Total	C	N	O	0	0	0
			686	430	119	137			

- Molecule 35 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
35	A	2879	Total	C	N	O	P	0	0	0
			61997	27594	11582	19943	2878			

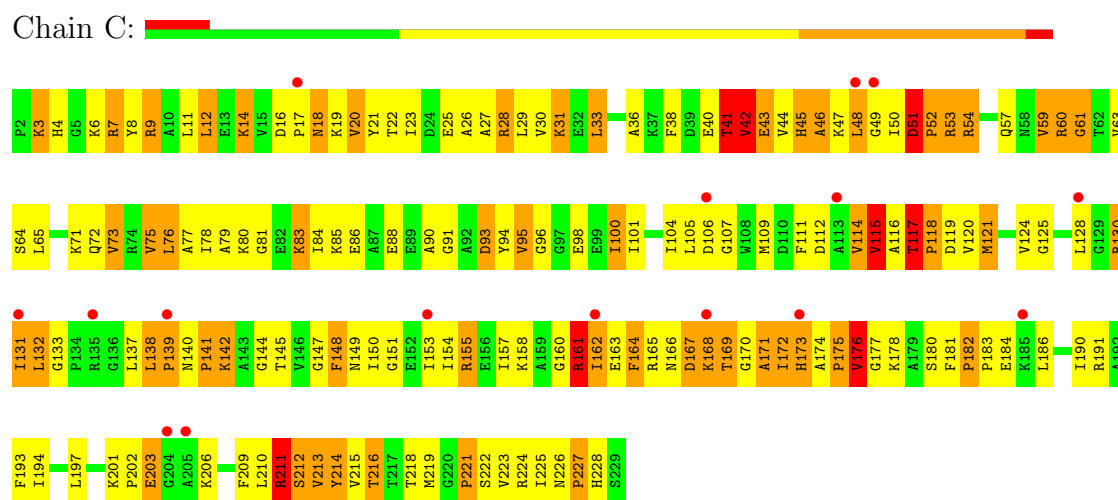
- Molecule 36 is a RNA chain called 5S ribosomal RNA.

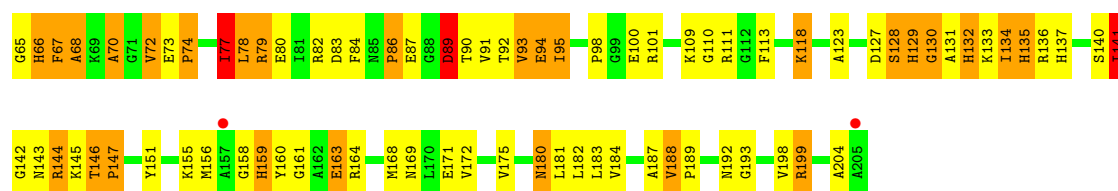
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
36	B	119	Total	C	N	O	P	0	0	0
			2551	1136	471	826	118			

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.

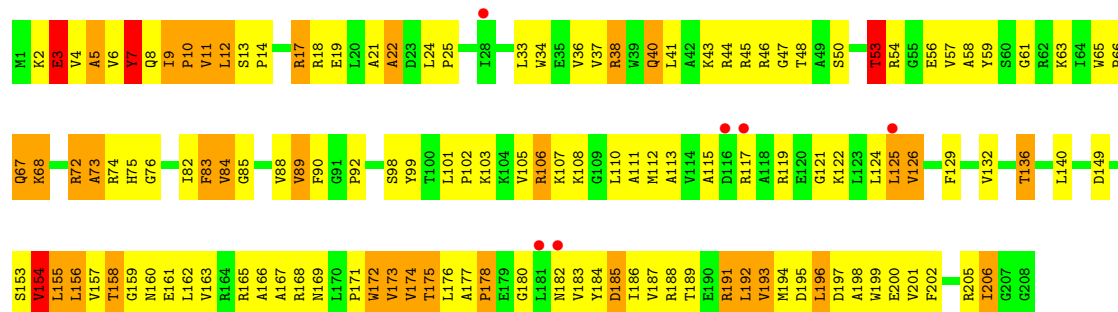
• Molecule 1: 50S ribosomal protein L1





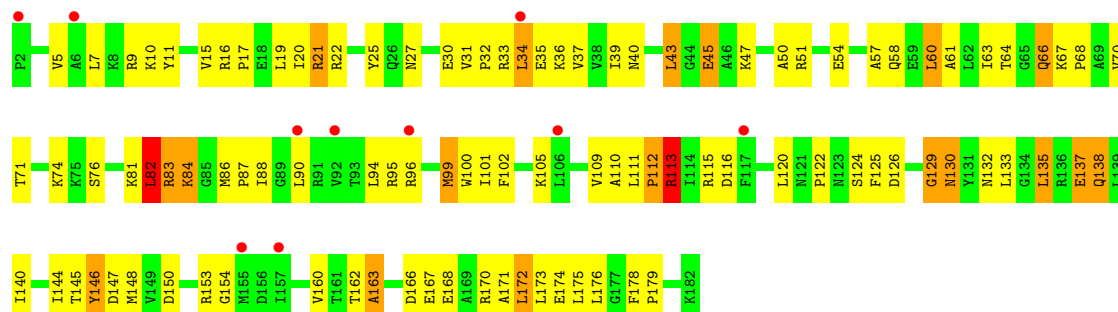
• Molecule 4: 50S ribosomal protein L4

Chain F:



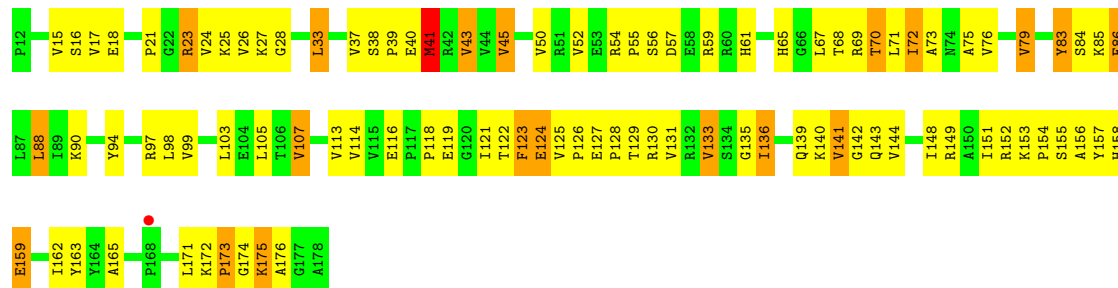
• Molecule 5: 50S ribosomal protein L5

Chain G:



• Molecule 6: 50S ribosomal protein L6

Chain H:

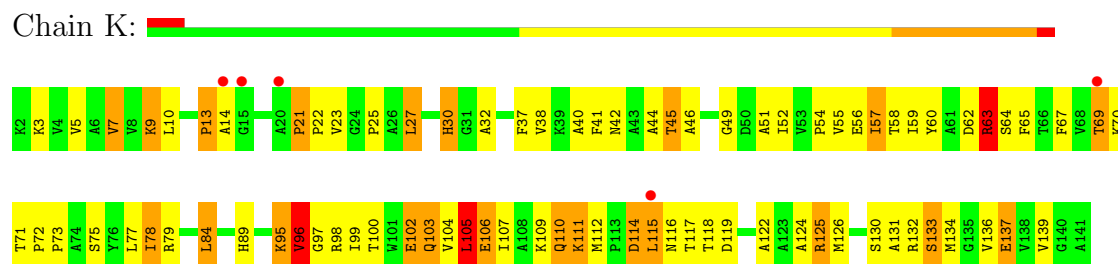


• Molecule 7: 50S RIBOSOMAL PROTEIN L10

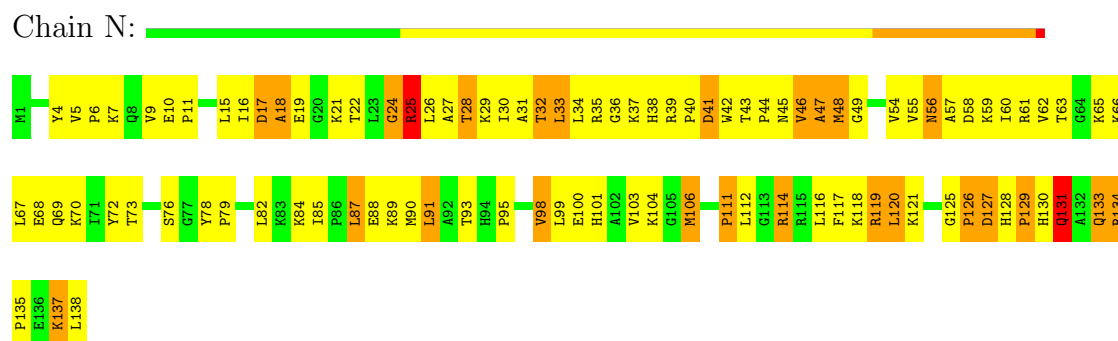
Chain J:



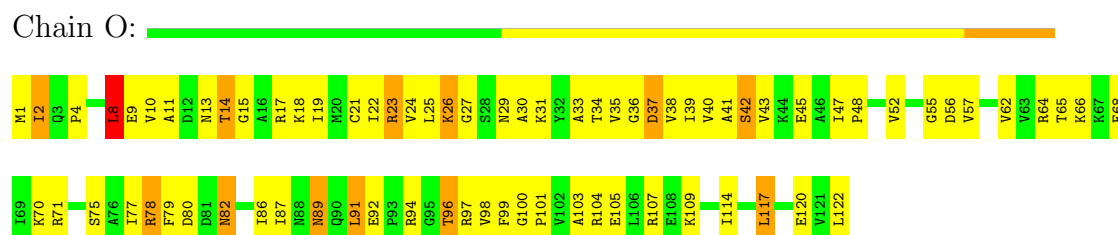
- Molecule 8: 50S ribosomal protein L11



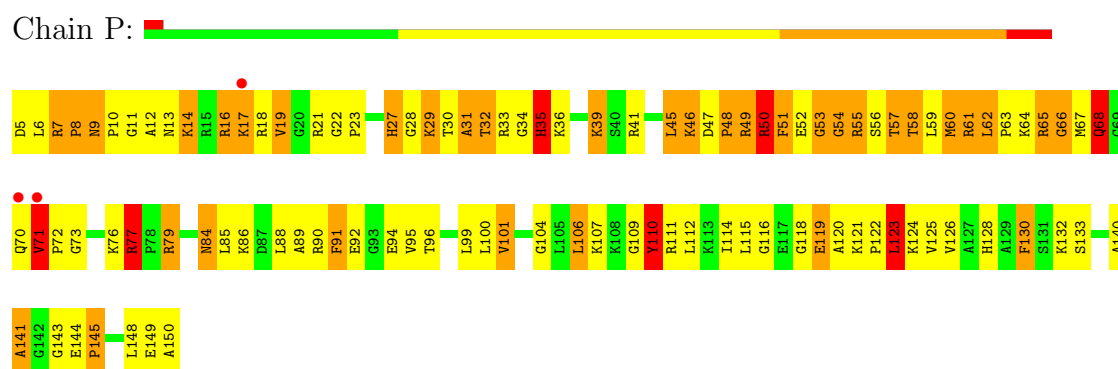
- Molecule 9: 50S ribosomal protein L13



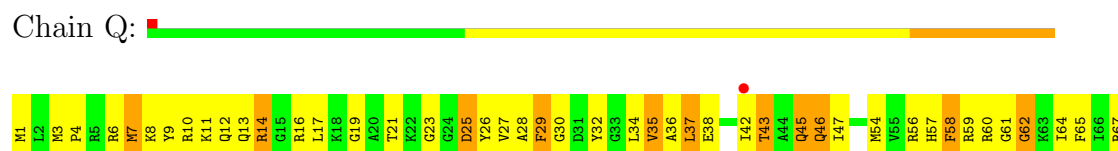
- Molecule 10: 50S ribosomal protein L14

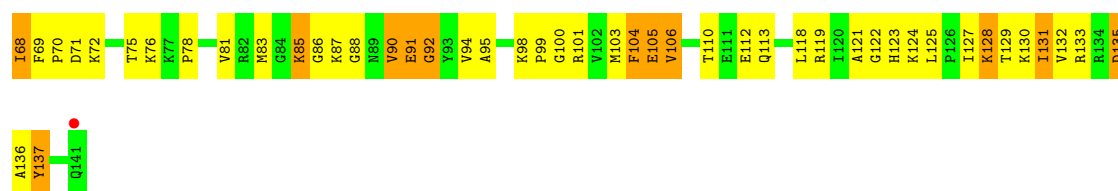


- Molecule 11: 50S ribosomal protein L15



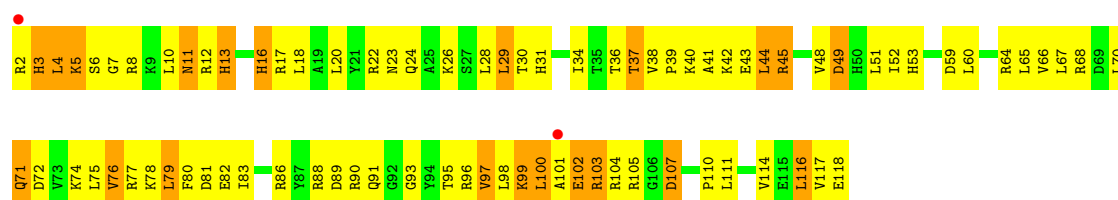
- Molecule 12: 50S ribosomal protein L16





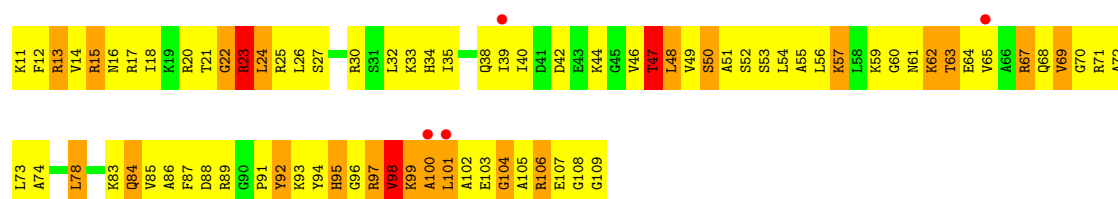
- Molecule 13: 50S ribosomal protein L17

Chain R:



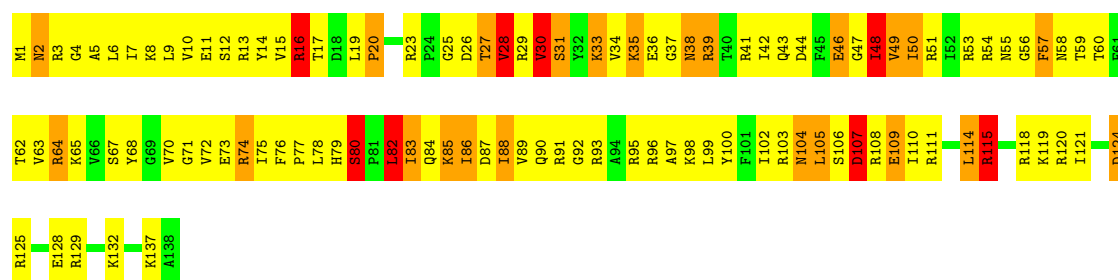
- Molecule 14: 50S ribosomal protein L18

Chain S:



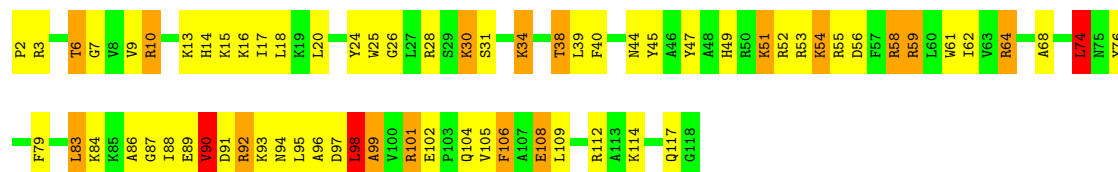
- Molecule 15: 50S ribosomal protein L19

Chain T:



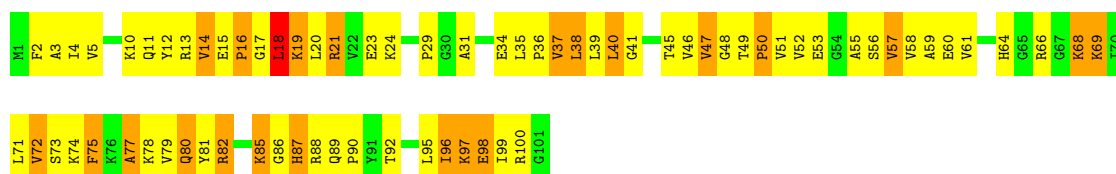
- Molecule 16: 50S ribosomal protein L20

Chain U:



- Molecule 17: 50S ribosomal protein L21

Chain V:



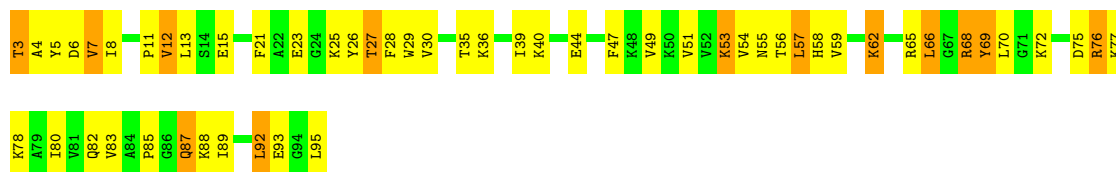
- Molecule 18: 50S ribosomal protein L22

Chain W:



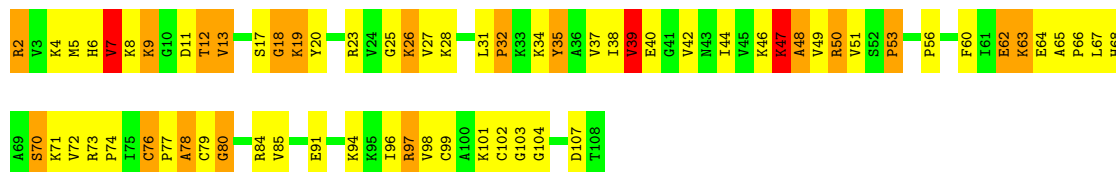
- Molecule 19: 50S ribosomal protein L23

Chain X:



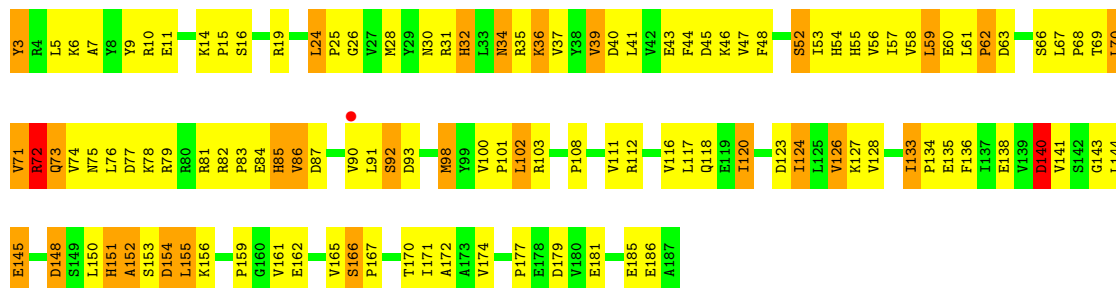
- Molecule 20: 50S ribosomal protein L24

Chain Y:



- Molecule 21: 50S ribosomal protein L25

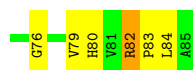
Chain Z:



- Molecule 22: 50S ribosomal protein L27

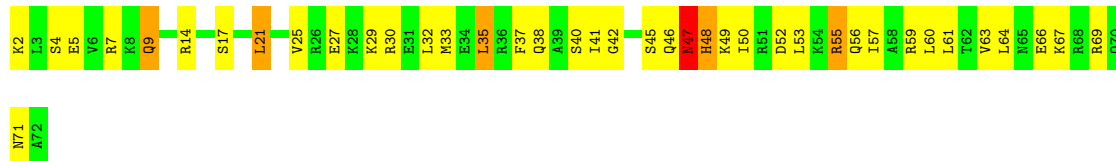
Chain 0:





- Molecule 23: 50S ribosomal protein L29

Chain 2:



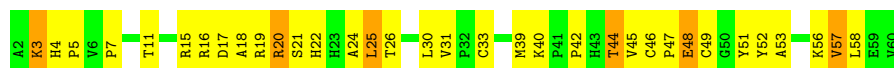
- Molecule 24: 50S ribosomal protein L30

Chain 3:



- Molecule 25: 50S ribosomal protein L32

Chain 5:



- Molecule 26: 50S ribosomal protein L33

Chain 6:



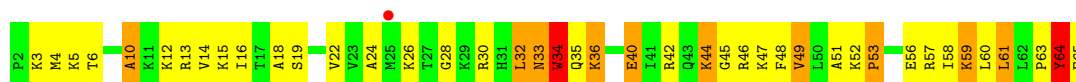
- Molecule 27: 50S ribosomal protein L34

Chain 7:



- Molecule 28: 50S ribosomal protein L35

Chain 8:



- Molecule 29: 50S ribosomal protein L36

Chain 9:



- Molecule 30: 50S ribosomal protein L7/L12

Chain f: 

There are no outlier residues recorded for this chain.

- Molecule 30: 50S ribosomal protein L7/L12

Chain g: 

There are no outlier residues recorded for this chain.

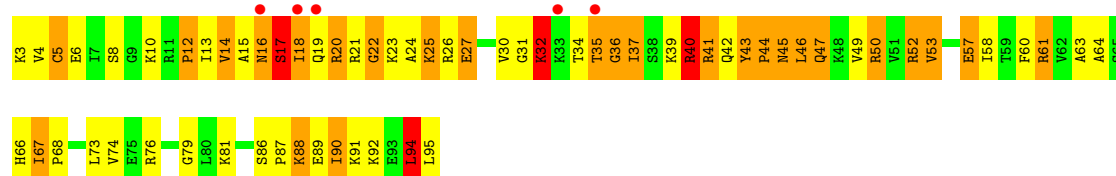
- Molecule 31: 50S ribosomal protein L7/L12

Chain h: 

There are no outlier residues recorded for this chain.

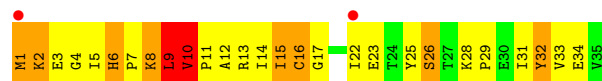
- Molecule 32: 50S ribosomal protein L28

Chain 1: 



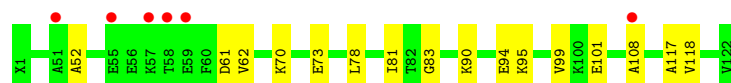
- Molecule 33: 50S ribosomal protein L31

Chain 4: 



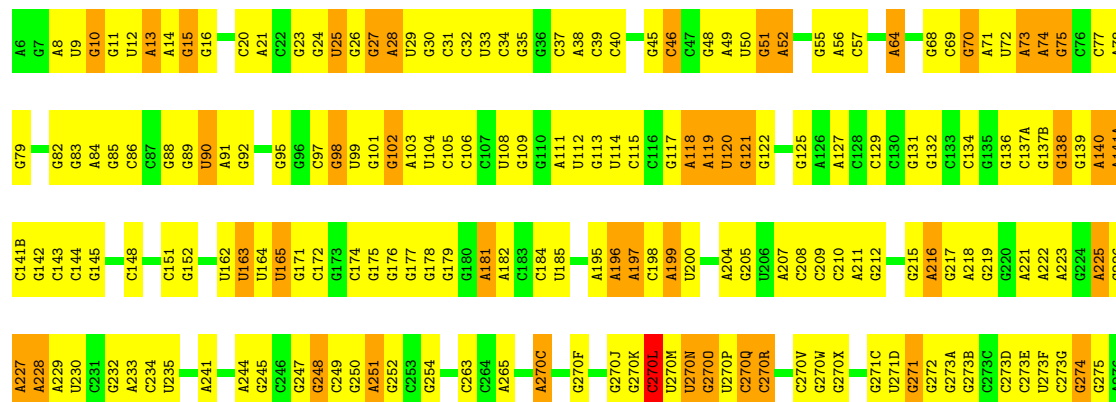
- Molecule 34: 50S ribosomal protein L7/L12

Chain e: 



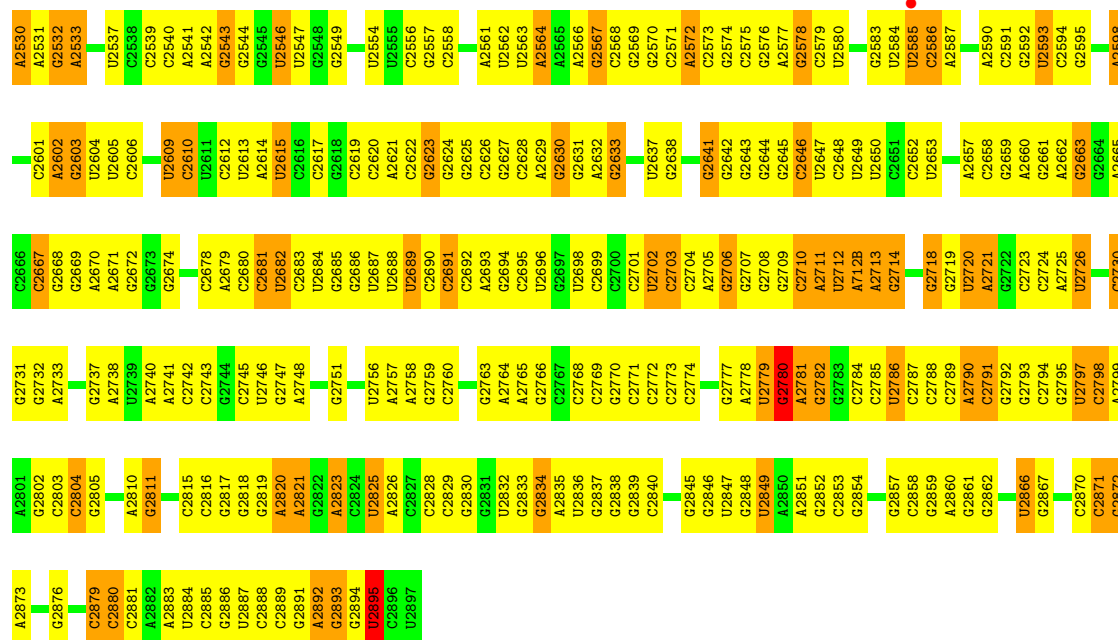
- Molecule 35: 23S ribosomal RNA

Chain A: 



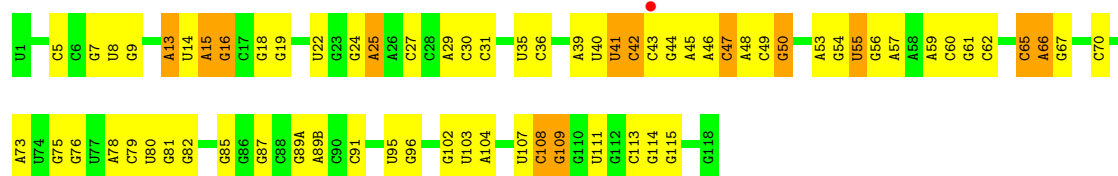
A1349	A1278	A1213	U1142	C1072	A1000	G938	A872	A804	G729	C661	U594	C517	G446	G363D	C277
A1352	G1279	A1214	A114B		A1001	G939	G873	G805	G729	G662	C595	G518	A447	G363E	A278
A1353		G1216	G1144	C1076	G1002	G940	G874	C906	C730	G663		U519	U448	U363F	C279
A1354	A1287			A1077		A941		U807	G731	G664	G600	G520	A449	A363G	C280
G1355	U1288	C1217	A1148	U1078	C1005	G942	A878	G808	G732	G665	C601	C656	C451	C364	G281
G1356	G1149	C1221	G1149	C1079	C1007	G943	A879	G809	G733	G666	G602	U525	G450		
U1291				C1080	C1008	G944	G879	C812	A734		A603	A526	A454	A371	U284
U1292	C1224		C1152	U1081	C1009	A945	G880	U813	G738	A670	G604	C527	A455	G372	C285
C1293	U1225		G1153	U1082	A1009	G946	G881	C910		C671	G605	A528	C456	U373	C286
A1294	A1226		G1154	U1083	A1010	G947	G882	C911	G739	G672	U606	A529	A374	A374	C287
C1295	G1227		G1155	U1084	A1011	G948	G883	C915	U740	C673	U607	G530	A457		C288
G1296			A1155	U1085	C1012	G949	G884	C816	G741	G674	A608	C531	G458	C378	A289
			A1156	A1086	U1013	G950	G885	C917	G742	A675	A609A	A532	U459	G379	C290
			G1157	A1087	U1014	C951	C886	G818	G743	A676	G609B	G533	A460	U380	
			G1158	A1088	U1015	G952	A887	A919		A677		U534	A462	G381	U293
			U1159	A1089	G1016	A953	C888	A820	U747	C678	C611	C535	C462	G382	A294
			G1160	U1090	G1017	G954	C889	A821	G748	C679	G612	A536	G463	U383	C295
			G1161	U1091	C1018	C955	A890	U822	C749	G680	U613	C537	U464	U384	C296
			G1162	U1019	U1019	G956	G892	U823	G768	G681	U614	G539	G465	C385	C297
			G1163	A1020	A1020	A957	C893	U826	U757	G682	G615	G540	A466	G386	G298
			G1164	U1094	A1095	U958	C894	U827	C758		A616	C541	G467	U387	A299
			G1165	A1096	A1096	A959	U895	U828	G761	G685	G617	C542	G468	G388	A300
			G1166	U1097	U1022	A960	A896	A829	U762	G686	G618A		G469	G389	G301
			U1167		G1024	C961	C897	G830	G763	C687	C618B	C546	A470		C302
				U1101	G1025			G831	G764	U688	G619	A547		C392	U303
			G1170	C1102	U1026	C964	A900		G765	U689	G620	A548	G473		G304
			G1171	A1103	A1027	G965	A901	G836	G766	G690	A621	G549	G474	G396	U305
			G1172	C1104	A1028	G966	C902	C937	G767	C691			U475	U306	U306
			G1173	U1105	A1029	G967	C903	C938	U767	C692	A627	G556	G476	G307	
			G1174	U1106	G1030	G968	C904	U839	G768		G628	U557		G400	A401
			G1175	G1107		U969	U905	C840		G695	G629	G558	A479	A402	A310
			G1176	U1108	U1033	C970	G906	A841	G771	G696	G630	G559	A480	U403	
			A1177	U1109		C971	U907	G842		C697	A631	C560	A481	A404	A314
			G1178	C1110	G1036	G972	C908	G843	A774	G698	A632	U562	A482	C404	
			C1179	A1111	G1037	A973	A909		G776	A699	A633	U563	A483	U405	A322
			G1184	G1112	A1045	G974A	A910	C846	A777	G701	C634	G563	C484	G406	G323
			C1185	U1113	A1046	G974B	A911	U847	G778	G702	C635		C485	G407	A324
			G1186	G1114	A1046	G975	C912	G848	G779	U703	G636	A571	G489	G408	G325
			G1187	G1115	A1047	C976	U913		U779	G704	A637	A572	G491	C409	
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			G1190		A1049	G978	C915	G853	A781	A706		C575	G496	G412	A330
				C1119	A1050	G979	A916	G854	A782		A643	U576	G497	C413	C335
			G1193	C1120	G1051	A980	A917	G855	A783	G707		G577	G498	C414	C336
				C1121			A918	G856	G785		A644	A578		A415	
			C1196	G1122	G1055	A983	A919	C856	G786	G710	C645	A579		A422	A340
			G1197	C1123	A1056	A984	G920	C857	U787	G711	A646	G579	A503	A429	
			U1198	G1124	A1057	C985	G921	U858	G788	G712	G647	C580	U504		G355
			C1199	G1125	G1058	C986	U922	G859	A788	G713	G648	C581	A505	G438	A359
			U1200	A1126	G1059	G987	C923	U860	A789	U714	G649	G582	A505	C439	G360
			C1201	A1127	U1060		C924	A861	C790		C650	G583	G506	U441	G361
			C1202		U1061	A990	C925	G862	C791	G717	G651	C584	A507	G442	U362
			G1203	A1132	U1062	C991	G929	A863	G792	A718	U652	G585	A508	C435	
			A1204	U1133	G1063	C992	G930	G864	A793	C719	C653	A586	C509	G346	G363A
			U1205	C1135	C1064	G993	U930	C965	G794	C720	U854	C587	C510	G438	A363B
			G1206	G1136	U1065	C994	G931	A866	A789	C721	A655	U588	G360	G440	
			C1207	G1137	U1066	C995	G932	C867	C796	A722	G656	C589	G512	U441	G361
				G1138	A1067	A996	A933	U868	G799	G723	U857	A590	A513	G442	U362
			A1210	G1139		G997	G934	G869	G799	U724	C658	C591	A514	A443	G363A
			G1211	C1140	A1070	C998	C935	A870	A800	G725	G592	G592	A515	C444	A363B
			G1212	U1141	G1071	U999		U871		G726	G660	G593		C445	G363C

C2467	C2468	A2469	C2470	C2471	C2472	C2473	C2474	C2475	A2476	C2477	A2478	C2479	C2480	G2481	C2482	C2483	C2484	C2485	C2486	G2487	A2488	U2489	G2494	C2495	C2496	C2497	C2498	C2499	U2500	C2501	A2502	C2503	U2504	C2505	U2506	C2507	C2508	C2509	C2510	C2511	C2512	C2513	C2514	C2515	C2516	C2517	A2518	U2519	C2520	U2521	U2522	C2523	C2524	C2525	C2526	C2529																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
G2397	U2398	G2399	G2400	U2401	C2402	C2403	C2404	C2405	A2406	C2407	G2410	A2411	A2412	G2415	C2416	C2417	A2418	U2419	C2420	C2421	A2422	U2423	C2424	A2425	C2426	C2427	C2428	C2429	A2430	U2431	A2432	C2433	A2435	C2436	U2437	U2438	C2439	C2440	C2441	C2442	C2443	G2446	G2447	A2448	U2449	A2450	G2454	U2457	U2458	C2459	C2460	C2461	C2462	C2463	C2464																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
G2325	C2326	A2327	A2328	G2329	G2330	G2331	U2334	A2335	A2336	G2339	G2340	U2344	G2345	A2346	C2347	U2348	G2349	C2350	G2351	C2355	C2356	U2357	C2358	A2361	A2366	A2369	G2370	G2373	C2374	G2375	A2376	A2377	A2378	C2379	C2380	C2381	G2382	C2383	C2384	C2385	C2386	U2387	A2388	C2389	U2390	U2391	C2392	A2393	C2394	C2395	C2396	C2397	C2398																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															
A2176	C2177	C2178	C2179	G2184	C2185	C2186	A2187	C2188	G2189	C2190	C2191	A2192	C2193	C2194	U2195	A2196	A2197	C2198	C2199	C2200	C2201	C2202	C2203	C2204	C2205	C2206	C2207	C2208	C2209	C2210	C2211	C2212	C2213	C2214	C2215	C2216	C2217	C2218	C2219	C2220	C2221	C2222	C2223	C2224	C2225	C2226	C2227	C2228	C2229	C2230	C2231	C2232	C2233	C2234	C2235	C2236	C2237	C2238	C2239	C2240	C2241	C2242	C2243	C2244	C2245	C2246	C2247	C2248	C2249	C2250	C2251	C2252	C2253	C2254	C2255	C2256	C2257	C2258	C2259	C2260	C2261	C2262	C2263	C2264	C2265	C2266	C2267	C2268	C2269	C2270	C2271	C2272	C2273	C2274	C2275	C2276	C2277	C2278	C2279	C2280	C2281	C2282	C2283	C2284	C2285	C2286	C2287	C2288	C2289	C2290	C2291	C2292	C2293	C2294	C2295	C2296	C2297	C2298	C2299	C2300	C2301	C2302	C2303	C2304	C2305	C2306	C2307	C2308	C2309	C2310	C2311	C2312	C2313	C2314	C2315	C2316	C2317	C2318	C2319	C2320	C2321	C2322	C2323	C2324	C2325	C2326	C2327	C2328	C2329	C2330	C2331	C2332	C2333	C2334	C2335	C2336	C2337	C2338	C2339	C2340	C2341	C2342	C2343	C2344	C2345	C2346	C2347	C2348	C2349	C2350	C2351	C2352	C2353	C2354	C2355	C2356	C2357	C2358	C2359	C2360	C2361	C2362	C2363	C2364	C2365	C2366	C2367	C2368	C2369	C2370	C2371	C2372	C2373	C2374	C2375	C2376	C2377	C2378	C2379	C2380	C2381	C2382	C2383	C2384	C2385	C2386	C2387	C2388	C2389	C2390	C2391	C2392	C2393	C2394	C2395	C2396	C2397	C2398	C2399	C2400	C2401	C2402	C2403	C2404	C2405	C2406	C2407	C2408	C2409	C2410	C2411	C2412	C2413	C2414	C2415	C2416	C2417	C2418	C2419	C2420	C2421	C2422	C2423	C2424	C2425	C2426	C2427	C2428	C2429	C2430	C2431	C2432	C2433	C2434	C2435	C2436	C2437	C2438	C2439	C2440	C2441	C2442	C2443	C2444	C2445	C2446	C2447	C2448	C2449	C2450	C2451	C2452	C2453	C2454	C2455	C2456	C2457	C2458	C2459	C2460	C2461	C2462	C2463	C2464	C2465	C2466	C2467	C2468	C2469	C2470	C2471	C2472	C2473	C2474	C2475	C2476	C2477	C2478	C2479	C2480	C2481	C2482	C2483	C2484	C2485	C2486	C2487	C2488	C2489	C2490	C2491	C2492	C2493	C2494	C2495	C2496	C2497	C2498	C2499	C2500	C2501	C2502	C2503	C2504	C2505	C2506	C2507	C2508	C2509	C2510	C2511	C2512	C2513	C2514	C2515	C2516	C2517	C2518	C2519	C2520	C2521	C2522	C2523	C2524	C2525	C2526	C2527	C2528	C2529	C2530	C2531	C2532	C2533	C2534	C2535	C2536	C2537	C2538	C2539	C2540	C2541	C2542	C2543	C2544	C2545	C2546	C2547	C2548	C2549	C2550	C2551	C2552	C2553	C2554	C2555	C2556	C2557	C2558	C2559	C2560	C2561	C2562	C2563	C2564	C2565	C2566	C2567	C2568	C2569	C2570	C2571	C2572	C2573	C2574	C2575	C2576	C2577	C2578	C2579	C2580	C2581	C2582	C2583	C2584	C2585	C2586	C2587	C2588	C2589	C2590	C2591	C2592	C2593	C2594	C2595	C2596	C2597	C2598	C2599	C2600	C2601	C2602	C2603	C2604	C2605	C2606	C2607	C2608	C2609	C2610	C2611	C2612	C2613	C2614	C2615	C2616	C2617	C2618	C2619	C2620	C2621	C2622	C2623	C2624	C2625	C2626	C2627	C2628	C2629	C2630	C2631	C2632	C2633	C2634	C2635	C2636	C2637	C2638	C2639	C2640	C2641	C2642	C2643	C2644	C2645	C2646	C2647	C2648	C2649	C2650	C2651	C2652	C2653	C2654	C2655	C2656	C2657	C2658	C2659	C2660	C2661	C2662	C2663	C2664	C2665	C2666	C2667	C2668	C2669	C2670	C2671	C2672	C2673	C2674	C2675	C2676	C2677	C2678	C2679	C2680	C2681	C2682	C2683	C2684	C2685	C2686	C2687	C2688	C2689	C2690	C2691	C2692	C2693	C2694	C2695	C2696	C2697	C2698	C2699	C2700	C2701	C2702	C2703	C2704	C2705	C2706	C2707	C2708	C2709	C2710	C2711	C2712	C2713	C2714	C2715	C2716	C2717	C2718	C2719	C2720	C2721	C2722	C2723	C2724	C2725	C2726	C2727	C2728	C2729	C2730	C2731	C2732	C2733	C2734	C2735	C2736	C2737	C2738	C2739	C2740	C2741	C2742	C2743	C2744	C2745	C2746	C2747	C2748	C2749	C2750	C2751	C2752	C2753	C2754	C2755	C2756	C2757	C2758	C2759	C2760	C2761	C2762	C2763	C2764	C2765	C2766	C2767	C2768	C2769	C2770	C2771	C2772	C2773	C2774	C2775	C2776	C2777	C2778	C2779	C2780	C2781	C2782	C2783	C2784	C2785	C2786	C2787	C2788	C2789	C2790	C2791	C2792	C2793	C2794	C2795	C2796	C2797	C2798	C2799	C2800	C2801	C2802	C2803	C2804	C2805	C2806	C2807	C2808	C2809	C2810	C2811	C2812	C2813	C2814	C2815	C2816	C2817	C2818	C2819	C2820	C2821	C2822	C2823	C2824	C2825	C2826	C2827	C2828	C2829	C2830	C2831	C2832	C2833	C2834	C2835	C2836	C2837	C2838	C2839	C2840	C2841	C2842	C2843	C2844	C2845	C2846	C2847	C2848	C2849	C2850	C2851	C2852	C2853	C2854	C2855	C2856	C2857	C2858	C2859	C2860	C2861	C2862	C2863	C2864	C2865	C2866	C2867	C2868	C2869	C2870	C2871	C2872	C2873	C2874	C2875	C2876	C2877	C2878	C2879	C2880	C2881	C2882	C2883	C2884	C2885	C2886	C2887	C2888	C2889	C2890	C2891	C2892	C2893	C2894	C2895	C2896	C2897	C2898	C2899	C2900	C2901	C2902	C2903	C2904	C2905	C2906	C2907	C2908	C2909	C2910	C2911	C2912	C2913	C2914	C2915	C2916	C2917	C2918	C2919	C2920	C2921	C2922	C2923	C2924	C2925	C2926	C2927	C2928	C2929	C2930	C2931	C2932	C2933	C2934	C2935	C2936	C2937	C2938	C2939	C2940	C2941	C2942	C2943	C2944	C2945	C2946	C2947	C2948	C2949	C2950	C2951	C2952	C2953	C2954	C2955	C2956	C2957	C2958	C2959	C2960	C2961	C2962	C2963	C2964	C2965	C2966	C2967	C2968	C2969	C2970	C2971	C2972	C2973	C2974	C2975	C2976	C2977	C2978	C2979	C2980	C2981	C2982	C2983	C2984	C2985	C2986	C2987	C2988	C2989	C2990	C2991	C2992	C2993	C2994	C2995	C2996	C2997	C2998	C2999	C3000	C3001	C3002	C3003	C3004	C3005	C3006	C3007	C3008	C3009	C3010	C3011	C3012	C3013	C3014	C3015	C3016	C3017	C3018	C3019	C3020	C3021	C3022	C3023	C3024	C3025	C3026	C3027	C3028	C3029	C3030	C3031	C3032	C3033	C3034	C3035	C3036	C3037	C3038	C3039	C3040	C3041	C3042	C3043	C3044	C3045	C3046	C3047	C3048	C3049	C3050	C3051	C3052	C3053	C3054	C3055	C3056	C3057	C3058	C3059	C3060	C3061	C3062	C3063	C3064	C3065	C3066	C3067	C3068	C3069	C3070	C3071	C3072	C3073	C3074	C3075	C3076	C3077	C3078	C3079	C3080	C3081	C3082	C3083	C3084	C3085	C3086	C3087	C3088	C3089	C3090	C3091	C3092	C3093	C3094	C3095	C3096	C3097	C3098	C3099	C3100	C3101	C3102	C3103	C3104	C3105	C3106	C3107	C3108	C3109	C3110	C3111	C3112	C3113	C3114	C3115	C3116	C3117	C3118	C3119	C3120	C3121	C3122	C3123	C3124	C3125	C3126	C3127	C3128	C3129	C3130	C3131	C3132	C3133	C3134	C3135	C3136	C3137	C3138	C3139	C3140	C3141	C3142	C3143	C3144	C3145	C3146	C3147	C3148	C3149	C3150	C3151	C3152	C3153	C3154	C3155	C3156	C3157	C3158	C3159	C3160	C3161	C3162	C3163	C3164	C3165	C3166	C3167	C3168	C3169	C3170	C3171	C3172	C3173	C3174	C3175	C3176	C3177	C3178	C3179	C3180	C3181	C3182	C3183	C3184	C3185	C3186	C3187	C3188	C3189	C3190	C3191	C3192	C3193	C3194	C3195	C3196	C3197	C3198	C3199	C3200	C3201	C3202	C3203	C3204	C3205	C3206	C3207	C3208	C3209	C3210	C3211	C3212	C3213	C3214	C3215	C3216	C3217	C3218	C3219	C3220	C3221	C3222	C3223	C3224	C3225	C3226	C3227	C3228	C3229	C3230	C3231	C3232	C3233	C3234	C3235	C3236	C3237	C3238	C3239	C3240	C3241	C3242	C3243	C3244	C3245	C3246	C3247	C3248	C3249	C3250	C3251	C3252	C3253	C3254	C3255	C3256	C3257	C3258	C3259	C3260	C3261	C3262	C3263	C3264	C3265	C3266	C3267	C3268	C3269	C3270	C3271	C3272	C3273	C3274	C3275	C3276	C3277	C3278	C3279	C3280	C3281	C3282	C3283	C3284	C3285	C3286	C3287	C3288	C3289	C3290	C3291	C3292	C3293	C3294	C3295	C3296	C3297	C3298	C3299	C3300	C3301	C3302	C3303	C3304	C3305	C3306	C3307	C3308	C3309	C3310	C3311	C3312	C3313	C3314	C3315	C3316	C3317	C3318	C3319	C3320	C3321	C3322	C3323	C3324	C3325	C3326	C3327	C3328	C3329	C3330	C3331	C3332	C3333	C3334	C3335	C3336	C3337	C3338	C3339	C3340	C3341	C3342	C3343	C3344	C3345	C3346	C3347	C3348	C3349	C3350	C3351	C3352	C3353	C3354	C3355	C3356	C3357	C3358	C3359	C3360	C3361	C3362	C3363	C3364	C3365	C3366	C3367	C3368	C3369	C3370	C3371	C3372	C3373	C3374	C3375	C3376	C3377	C3378	C3379	C3380	C3381	C3382	C3383	C33



• Molecule 36: 5S ribosomal RNA

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	306.01Å 673.49Å 351.98Å 90.00° 92.69° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50 131.34 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.50) 74.9 (131.34-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.49Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.262 , 0.309 0.352 , 0.354	Depositor DCC
R_{free} test set	38207 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	80.5	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 278.0	EDS
Estimated twinning fraction	0.247 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.26$, $\langle L^2 \rangle = 0.11$	Xtriage
Outliers	0 of 765681 reflections	Xtriage
F_o, F_c correlation	0.64	EDS
Total number of atoms	95124	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	C	0.50	1/1774 (0.1%)	0.76	0/2391
2	D	0.38	0/2195	0.67	0/2955
3	E	0.35	0/1602	0.67	1/2160 (0.0%)
4	F	0.41	0/1663	0.79	4/2249 (0.2%)
5	G	0.59	1/1499 (0.1%)	0.67	3/2016 (0.1%)
6	H	0.34	0/1298	0.62	0/1751
8	K	0.34	0/1054	0.56	1/1427 (0.1%)
9	N	0.54	0/1131	0.80	0/1525
10	O	0.36	0/943	0.64	1/1269 (0.1%)
11	P	0.34	0/1131	0.71	0/1504
12	Q	0.36	0/1143	0.60	0/1527
13	R	0.34	0/974	0.62	1/1302 (0.1%)
14	S	0.40	0/783	0.75	0/1041
15	T	0.37	0/1161	0.67	0/1549
16	U	0.42	0/982	0.68	1/1306 (0.1%)
17	V	0.38	0/790	0.71	0/1057
18	W	0.37	0/911	0.65	0/1220
19	X	0.35	0/748	0.60	0/1004
20	Y	0.34	0/831	0.60	0/1108
21	Z	0.32	0/1505	0.59	0/2042
22	0	0.31	0/671	0.56	0/892
23	2	0.34	0/600	0.60	0/793
24	3	0.31	0/482	0.58	0/646
25	5	0.34	0/473	0.60	0/639
26	6	0.35	0/440	0.79	1/586 (0.2%)
27	7	0.48	0/438	0.69	0/575
28	8	0.36	0/525	0.64	0/691
29	9	0.29	0/310	0.55	0/407
32	1	0.54	0/739	0.84	2/981 (0.2%)
33	4	0.45	0/276	0.66	0/372
34	e	0.35	0/538	0.61	0/715
35	A	0.40	1/69437 (0.0%)	0.97	72/108401 (0.1%)
36	B	0.34	0/2853	0.90	1/4451 (0.0%)
All	All	0.40	3/101900 (0.0%)	0.90	88/152552 (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
1	C	0	2
2	D	0	1
4	F	0	2
5	G	0	1
7	J	0	1
14	S	0	2
15	T	0	1
18	W	0	1
32	1	0	3
All	All	0	14

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	112	PRO	CA-C	17.59	1.88	1.52
1	C	46	ALA	CA-CB	6.31	1.65	1.52
35	A	2780	G	N7-C5	-6.19	1.35	1.39

The worst 5 of 88 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	116	ASP	O-C-N	-10.28	106.25	122.70
4	F	193	VAL	N-CA-C	-10.27	83.28	111.00
35	A	645	C	C2-N1-C1'	9.76	129.54	118.80
35	A	645	C	N1-C2-O2	8.29	123.88	118.90
35	A	270(L)	C	N1-C2-O2	7.29	123.28	118.90

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	171	ALA	Peptide
1	C	211	ARG	Peptide
2	D	78	LYS	Peptide
4	F	154	VAL	Peptide
4	F	173	VAL	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	C	1742	0	1798	147	0
2	D	2145	0	2234	164	0
3	E	1569	0	1634	122	0
4	F	1628	0	1680	141	0
5	G	1474	0	1535	82	0
6	H	1274	0	1342	72	0
7	J	851	0	196	25	0
8	K	1035	0	1082	57	0
9	N	1104	0	1180	115	0
10	O	933	0	996	68	0
11	P	1114	0	1187	111	0
12	Q	1122	0	1179	65	0
13	R	960	0	1021	71	0
14	S	775	0	835	76	0
15	T	1147	0	1207	109	0
16	U	964	0	1022	76	0
17	V	779	0	852	62	0
18	W	900	0	964	57	0
19	X	734	0	789	42	0
20	Y	818	0	908	58	0
21	Z	1473	0	1497	81	0
22	0	662	0	688	40	0
23	2	598	0	653	28	0
24	3	477	0	529	25	0
25	5	459	0	477	34	0
26	6	433	0	461	36	0
27	7	430	0	480	32	0
28	8	517	0	582	50	0
29	9	307	0	335	20	0
30	f	156	0	41	0	0
30	g	156	0	39	0	0
31	h	151	0	37	0	0
32	1	732	0	808	75	0
33	4	271	0	284	20	0
34	e	686	0	619	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	A	61997	0	31250	1726	0
36	B	2551	0	1295	70	0
All	All	95124	0	63716	3497	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 22.

The worst 5 of 3497 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:G:112:PRO:C	5:G:112:PRO:CA	1.88	1.41
35:A:2133:G:H21	35:A:2158:A:N6	1.39	1.19
35:A:2133:G:N2	35:A:2158:A:H62	1.42	1.17
35:A:1170:G:H1	35:A:1179:C:N4	1.46	1.12
35:A:281:G:H21	35:A:359:A:N6	1.48	1.11

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	
1	C	226/228 (99%)	105 (46%)	75 (33%)	46 (20%)	0	2
2	D	273/275 (99%)	188 (69%)	47 (17%)	38 (14%)	0	8
3	E	203/205 (99%)	133 (66%)	36 (18%)	34 (17%)	0	5
4	F	206/208 (99%)	137 (66%)	47 (23%)	22 (11%)	1	13
5	G	179/181 (99%)	127 (71%)	44 (25%)	8 (4%)	4	40
6	H	165/167 (99%)	118 (72%)	32 (19%)	15 (9%)	1	18
8	K	138/140 (99%)	86 (62%)	33 (24%)	19 (14%)	0	8
9	N	136/138 (99%)	91 (67%)	27 (20%)	18 (13%)	0	9
10	O	120/122 (98%)	95 (79%)	20 (17%)	5 (4%)	4	43
11	P	144/146 (99%)	76 (53%)	35 (24%)	33 (23%)	0	1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	Q	139/141 (99%)	91 (66%)	31 (22%)	17 (12%)	1	11
13	R	115/117 (98%)	91 (79%)	17 (15%)	7 (6%)	2	30
14	S	97/99 (98%)	57 (59%)	25 (26%)	15 (16%)	0	5
15	T	136/138 (99%)	82 (60%)	28 (21%)	26 (19%)	0	3
16	U	115/117 (98%)	80 (70%)	23 (20%)	12 (10%)	1	14
17	V	99/101 (98%)	64 (65%)	22 (22%)	13 (13%)	0	9
18	W	111/113 (98%)	81 (73%)	16 (14%)	14 (13%)	0	10
19	X	91/93 (98%)	70 (77%)	16 (18%)	5 (6%)	3	34
20	Y	105/107 (98%)	50 (48%)	34 (32%)	21 (20%)	0	2
21	Z	183/185 (99%)	121 (66%)	44 (24%)	18 (10%)	1	16
22	0	82/84 (98%)	65 (79%)	13 (16%)	4 (5%)	3	37
23	2	69/71 (97%)	50 (72%)	17 (25%)	2 (3%)	7	54
24	3	58/60 (97%)	44 (76%)	9 (16%)	5 (9%)	1	19
25	5	57/59 (97%)	42 (74%)	11 (19%)	4 (7%)	2	26
26	6	48/50 (96%)	27 (56%)	8 (17%)	13 (27%)	0	1
27	7	47/49 (96%)	34 (72%)	11 (23%)	2 (4%)	4	42
28	8	62/64 (97%)	40 (64%)	11 (18%)	11 (18%)	0	4
29	9	35/37 (95%)	29 (83%)	4 (11%)	2 (6%)	3	33
32	1	91/93 (98%)	59 (65%)	18 (20%)	14 (15%)	0	6
33	4	33/35 (94%)	15 (46%)	9 (27%)	9 (27%)	0	1
34	e	70/102 (69%)	40 (57%)	22 (31%)	8 (11%)	1	12
All	All	3633/3725 (98%)	2388 (66%)	785 (22%)	460 (13%)	0	10

5 of 460 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	17	PRO
1	C	41	THR
1	C	42	VAL
1	C	43	GLU
1	C	52	PRO

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	
1	C	180/180 (100%)	128 (71%)	52 (29%)	0	4
2	D	217/217 (100%)	175 (81%)	42 (19%)	2	12
3	E	165/165 (100%)	136 (82%)	29 (18%)	3	16
4	F	165/165 (100%)	140 (85%)	25 (15%)	4	25
5	G	155/155 (100%)	130 (84%)	25 (16%)	3	22
6	H	136/136 (100%)	117 (86%)	19 (14%)	5	28
8	K	105/105 (100%)	77 (73%)	28 (27%)	1	5
9	N	117/117 (100%)	93 (80%)	24 (20%)	2	10
10	O	100/100 (100%)	86 (86%)	14 (14%)	5	28
11	P	112/112 (100%)	85 (76%)	27 (24%)	1	6
12	Q	111/111 (100%)	84 (76%)	27 (24%)	1	6
13	R	100/100 (100%)	78 (78%)	22 (22%)	1	8
14	S	77/77 (100%)	59 (77%)	18 (23%)	1	7
15	T	120/120 (100%)	93 (78%)	27 (22%)	1	8
16	U	93/93 (100%)	70 (75%)	23 (25%)	1	6
17	V	82/82 (100%)	62 (76%)	20 (24%)	1	6
18	W	92/92 (100%)	76 (83%)	16 (17%)	3	17
19	X	75/75 (100%)	58 (77%)	17 (23%)	1	7
20	Y	88/88 (100%)	73 (83%)	15 (17%)	3	18
21	Z	162/162 (100%)	125 (77%)	37 (23%)	1	7
22	0	66/66 (100%)	56 (85%)	10 (15%)	4	25
23	2	66/66 (100%)	58 (88%)	8 (12%)	7	36
24	3	52/52 (100%)	45 (86%)	7 (14%)	6	30
25	5	51/51 (100%)	41 (80%)	10 (20%)	2	11
26	6	49/49 (100%)	34 (69%)	15 (31%)	0	4
27	7	42/42 (100%)	36 (86%)	6 (14%)	5	28
28	8	54/54 (100%)	44 (82%)	10 (18%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	9	34/34 (100%)	30 (88%)	4 (12%)	8	38
32	1	78/78 (100%)	58 (74%)	20 (26%)	1	5
33	4	31/31 (100%)	21 (68%)	10 (32%)	0	3
34	e	54/54 (100%)	46 (85%)	8 (15%)	4	26
All	All	3029/3029 (100%)	2414 (80%)	615 (20%)	2	11

5 of 615 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	P	84	ASN
14	S	78	LEU
28	8	49	VAL
12	Q	3	MET
13	R	3	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 25 such sidechains are listed below:

Mol	Chain	Res	Type
12	Q	12	GLN
12	Q	123	HIS
22	0	80	HIS
12	Q	89	ASN
13	R	23	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
35	A	2878/2879 (99%)	629 (21%)	17 (0%)
36	B	118/119 (99%)	19 (16%)	3 (2%)
All	All	2996/2998 (99%)	648 (21%)	20 (0%)

5 of 648 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
35	A	10	G
35	A	12	U
35	A	13	A
35	A	15	G
35	A	23	G

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
35	A	1377	G
35	A	1558	A
35	A	2780	G
35	A	1210	A
35	A	1240	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	C	228/228 (100%)	0.34	16 (7%) 16 7	102, 162, 214, 247	0
2	D	275/275 (100%)	-0.12	2 (0%) 84 56	23, 54, 107, 147	0
3	E	205/205 (100%)	0.07	5 (2%) 56 26	12, 60, 120, 175	0
4	F	208/208 (100%)	0.16	6 (2%) 49 23	34, 83, 176, 205	0
5	G	181/181 (100%)	0.32	10 (5%) 24 10	44, 104, 159, 196	0
6	H	167/167 (100%)	-0.18	1 (0%) 86 59	36, 73, 140, 192	0
7	J	0/170	-	-	-	-
8	K	140/140 (100%)	-0.01	5 (3%) 41 18	72, 142, 197, 229	0
9	N	138/138 (100%)	-0.14	0 100 100	61, 89, 110, 118	0
10	O	122/122 (100%)	-0.05	0 100 100	26, 47, 96, 121	0
11	P	146/146 (100%)	-0.09	3 (2%) 60 29	19, 88, 140, 212	0
12	Q	141/141 (100%)	-0.28	2 (1%) 72 38	34, 58, 126, 178	0
13	R	117/117 (100%)	-0.02	2 (1%) 67 34	34, 67, 108, 138	0
14	S	99/99 (100%)	0.24	4 (4%) 36 16	44, 114, 168, 203	0
15	T	138/138 (100%)	-0.44	0 100 100	25, 71, 133, 177	0
16	U	117/117 (100%)	-0.13	0 100 100	29, 54, 89, 222	0
17	V	101/101 (100%)	-0.28	0 100 100	28, 60, 114, 177	0
18	W	113/113 (100%)	-0.16	0 100 100	11, 60, 133, 215	0
19	X	93/93 (100%)	-0.29	0 100 100	16, 66, 134, 180	0
20	Y	107/107 (100%)	-0.23	0 100 100	45, 96, 167, 200	0
21	Z	185/185 (100%)	-0.32	1 (0%) 88 64	48, 82, 136, 193	0
22	0	84/84 (100%)	-0.13	0 100 100	47, 77, 140, 162	0
23	2	71/71 (100%)	-0.31	0 100 100	33, 85, 127, 141	0
24	3	60/60 (100%)	-0.10	1 (1%) 67 34	32, 73, 137, 160	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
25	5	59/59 (100%)	-0.04	0 100 100	29, 75, 130, 161	0
26	6	50/50 (100%)	-0.13	0 100 100	49, 81, 143, 164	0
27	7	49/49 (100%)	0.07	0 100 100	34, 61, 112, 165	0
28	8	64/64 (100%)	-0.00	1 (1%) 68 35	33, 70, 118, 139	0
29	9	37/37 (100%)	-0.06	0 100 100	46, 60, 134, 159	0
30	f	0/31	-	-	-	-
30	g	0/31	-	-	-	-
31	h	0/30	-	-	-	-
32	1	93/93 (100%)	0.11	5 (5%) 25 10	41, 89, 159, 194	0
33	4	35/35 (100%)	0.36	2 (5%) 23 10	73, 136, 168, 196	0
34	e	72/102 (70%)	0.29	6 (8%) 11 6	87, 141, 192, 236	0
35	A	2879/2879 (100%)	-0.27	5 (0%) 93 80	5, 63, 160, 308	0
36	B	119/119 (100%)	-0.33	1 (0%) 83 53	33, 108, 159, 193	0
All	All	6693/6985 (95%)	-0.15	78 (1%) 75 42	5, 73, 168, 308	0

The worst 5 of 78 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
34	e	59	GLU	6.2
34	e	58	THR	5.9
5	G	90	LEU	5.4
3	E	58	ARG	5.1
8	K	115	LEU	5.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.